



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:26 AM GMT

PDB ID : 2WSE  
Title : Improved Model of Plant Photosystem I  
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.  
Deposited on : 2009-09-05  
Resolution : 3.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

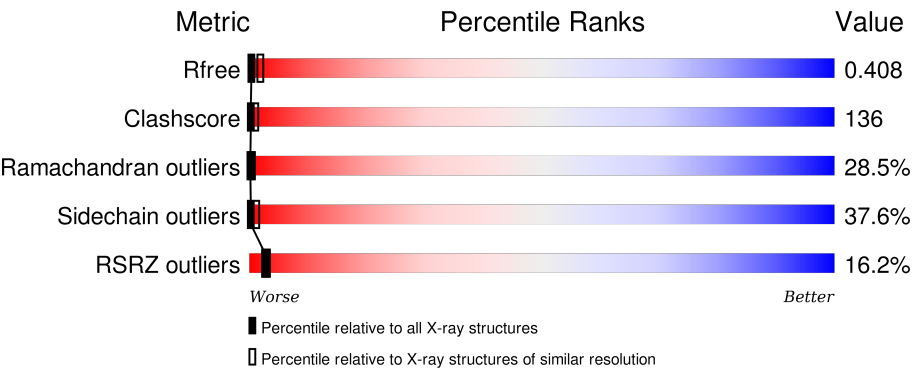
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	241	<div><div>19%</div><div>27%26%12%•32%</div></div>
2	2	269	<div><div>15%</div><div>7%20%25%13%35%</div></div>
3	3	276	<div><div>24%</div><div>17%18%17%6%42%</div></div>
4	4	251	<div><div>12%</div><div>6%18%26%17%34%</div></div>
5	A	758	<div><div>12%</div><div>6%47%34%9%•</div></div>

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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	212	
9	E	143	
10	F	231	
11	G	167	
12	H	144	
13	I	40	
14	J	44	
15	K	131	
16	L	216	
17	N	170	
18	R	53	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	1010	X	-	-	-
19	CLA	1	1014	X	-	X	-
19	CLA	1	1142	X	-	-	-
19	CLA	1	1145	X	-	X	-
19	CLA	1	1146	X	-	-	-
19	CLA	1	1148	X	-	X	-
19	CLA	1	1149	X	-	-	-
19	CLA	1	1187	X	-	-	-
19	CLA	1	1188	X	-	X	-
19	CLA	1	1189	X	-	-	-
19	CLA	1	1190	X	-	-	-
19	CLA	1	1191	X	-	-	-
19	CLA	1	1192	X	-	-	-
19	CLA	1	1193	X	-	-	-
19	CLA	1	1194	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	1195	X	-	-	-
19	CLA	1	1196	X	-	-	-
19	CLA	1	1197	X	-	-	-
19	CLA	1	1198	X	-	-	-
19	CLA	1	1241	X	-	-	-
19	CLA	1	1303	X	-	-	-
19	CLA	1	1307	X	-	-	-
19	CLA	1	1308	X	-	X	-
19	CLA	1	1309	X	-	-	-
19	CLA	1	1505	X	-	-	-
19	CLA	2	1212	X	-	-	-
19	CLA	2	1213	X	-	-	-
19	CLA	2	1214	X	-	-	-
19	CLA	2	1215	X	-	-	-
19	CLA	2	1216	X	-	-	-
19	CLA	2	1217	X	-	-	-
19	CLA	2	1218	X	-	-	-
19	CLA	2	1219	X	-	-	-
19	CLA	2	1220	X	-	-	-
19	CLA	2	1221	X	-	-	X
19	CLA	2	1222	X	-	-	-
19	CLA	2	1223	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	3	1212	X	-	X	-
19	CLA	3	1213	X	-	-	-
19	CLA	3	1214	X	-	-	-
19	CLA	3	1215	X	-	-	-
19	CLA	3	1216	X	-	-	X
19	CLA	3	1217	X	-	-	-
19	CLA	3	1218	X	-	-	-
19	CLA	3	1219	X	-	-	X
19	CLA	3	1220	X	-	-	-
19	CLA	3	1221	X	-	-	-
19	CLA	3	1222	X	-	-	-
19	CLA	3	1223	X	-	-	-
19	CLA	3	1224	X	-	X	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3008	X	-	-	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3015	X	-	-	-
19	CLA	4	1196	X	-	X	-
19	CLA	4	1197	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	1198	X	-	X	-
19	CLA	4	1199	X	-	-	-
19	CLA	4	1200	X	-	-	X
19	CLA	4	1201	X	-	-	-
19	CLA	4	1202	X	-	-	-
19	CLA	4	1203	X	-	-	X
19	CLA	4	1204	X	-	-	-
19	CLA	4	1205	X	-	-	-
19	CLA	4	1206	X	-	-	-
19	CLA	4	1207	X	-	-	-
19	CLA	4	1208	X	-	-	-
19	CLA	4	1209	X	-	-	-
19	CLA	4	1210	X	-	-	-
19	CLA	4	1211	X	-	-	-
19	CLA	4	4007	X	-	-	-
19	CLA	4	4014	X	-	-	-
19	CLA	A	1759	X	-	-	-
19	CLA	A	1760	X	-	X	-
19	CLA	A	1761	X	-	X	-
19	CLA	A	1762	X	-	X	-
19	CLA	A	1763	X	-	X	X
19	CLA	A	1764	X	-	X	-
19	CLA	A	1765	X	-	X	-
19	CLA	A	1766	X	-	-	X
19	CLA	A	1767	X	-	X	X
19	CLA	A	1768	X	-	-	-
19	CLA	A	1769	X	-	-	-
19	CLA	A	1770	X	-	X	X
19	CLA	A	1771	X	-	X	-
19	CLA	A	1772	X	-	X	X
19	CLA	A	1773	X	-	-	-
19	CLA	A	1774	X	-	X	X
19	CLA	A	1775	X	-	-	-
19	CLA	A	1776	X	-	X	X
19	CLA	A	1777	X	-	-	X
19	CLA	A	1778	X	-	-	-
19	CLA	A	1779	X	-	X	-
19	CLA	A	1780	X	-	-	X
19	CLA	A	1781	X	-	X	-
19	CLA	A	1782	X	-	X	-
19	CLA	A	1783	X	-	X	X
19	CLA	A	1784	X	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1785	X	-	-	-
19	CLA	A	1786	X	-	-	X
19	CLA	A	1787	X	-	X	-
19	CLA	A	1788	X	-	X	-
19	CLA	A	1789	X	-	-	-
19	CLA	A	1790	X	-	-	-
19	CLA	A	1791	X	-	-	-
19	CLA	A	1792	X	-	-	-
19	CLA	A	1793	X	-	-	-
19	CLA	A	1794	X	-	-	-
19	CLA	A	1795	X	-	-	-
19	CLA	A	1796	X	-	X	-
19	CLA	A	1797	X	-	X	-
19	CLA	A	1798	X	-	-	-
19	CLA	A	1799	X	-	X	-
19	CLA	A	1800	X	-	-	X
19	CLA	A	1810	X	-	-	-
19	CLA	A	1811	X	-	X	-
19	CLA	A	1812	X	-	X	-
19	CLA	B	1735	X	-	X	-
19	CLA	B	1736	X	-	-	-
19	CLA	B	1737	X	-	-	-
19	CLA	B	1738	X	-	-	-
19	CLA	B	1739	X	-	X	-
19	CLA	B	1740	X	-	X	-
19	CLA	B	1741	X	-	-	-
19	CLA	B	1742	X	-	-	-
19	CLA	B	1743	X	-	-	-
19	CLA	B	1744	X	-	X	-
19	CLA	B	1745	X	-	-	-
19	CLA	B	1746	X	-	-	-
19	CLA	B	1747	X	-	X	X
19	CLA	B	1748	X	-	X	-
19	CLA	B	1749	X	-	-	-
19	CLA	B	1750	X	-	-	-
19	CLA	B	1751	X	-	-	-
19	CLA	B	1752	X	-	X	-
19	CLA	B	1753	X	-	-	-
19	CLA	B	1754	X	-	X	-
19	CLA	B	1755	X	-	X	-
19	CLA	B	1756	X	-	X	-
19	CLA	B	1757	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1758	X	-	X	-
19	CLA	B	1759	X	-	X	-
19	CLA	B	1760	X	-	X	-
19	CLA	B	1761	X	-	-	-
19	CLA	B	1762	X	-	-	-
19	CLA	B	1763	X	-	X	-
19	CLA	B	1764	X	-	-	-
19	CLA	B	1765	X	-	X	-
19	CLA	B	1766	X	-	X	X
19	CLA	B	1767	X	-	-	-
19	CLA	B	1768	X	-	-	-
19	CLA	B	1769	X	-	X	-
19	CLA	B	1770	X	-	X	-
19	CLA	B	1771	X	-	X	X
19	CLA	B	1772	X	-	X	-
19	CLA	B	1773	X	-	-	X
19	CLA	B	1786	X	-	X	-
19	CLA	B	1787	X	-	X	-
19	CLA	B	1788	X	-	X	-
19	CLA	F	1155	X	-	-	-
19	CLA	F	1156	X	-	-	-
19	CLA	F	1157	X	-	-	-
19	CLA	G	1099	X	-	-	-
19	CLA	I	1031	X	-	-	-
19	CLA	J	1043	X	-	X	-
19	CLA	J	1044	X	-	X	-
19	CLA	K	1085	X	-	X	-
19	CLA	L	1166	X	-	-	-
19	CLA	L	1167	X	-	X	-
19	CLA	L	1168	X	-	-	-
19	CLA	R	1054	X	-	-	-
19	CLA	R	1055	X	-	-	-
20	LMU	A	1808	-	-	-	X
20	LMU	A	1809	-	-	-	X
20	LMU	A	7014	X	-	-	-
20	LMU	A	7016	-	-	X	-
20	LMU	A	7021	-	-	X	-
20	LMU	A	7023	-	-	X	-
20	LMU	A	7032	-	-	X	-
20	LMU	A	7037	-	-	X	-
20	LMU	A	7042	-	-	X	-
20	LMU	A	7047	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	LMU	A	7048	-	-	X	-
20	LMU	A	7050	-	-	X	-
20	LMU	B	1783	-	-	X	-
20	LMU	N	1086	-	-	X	-
20	LMU	R	1056	-	-	X	-
21	SUC	2	1225	X	-	X	-
21	SUC	3	1226	X	-	X	-
21	SUC	B	8051	X	-	-	-
21	SUC	B	8052	X	-	X	-
21	SUC	B	8053	X	-	X	-
21	SUC	B	8054	X	-	-	-
21	SUC	B	8055	X	-	X	-
21	SUC	B	8056	X	-	-	-
21	SUC	B	8059	X	-	X	-
21	SUC	B	8060	X	-	-	-
21	SUC	B	8061	X	-	-	-
21	SUC	B	8062	X	-	X	-
21	SUC	F	1158	X	-	-	-
22	BCR	3	1225	-	-	X	-
22	BCR	A	1802	-	-	X	X
22	BCR	A	1803	-	-	X	X
22	BCR	A	1804	-	-	X	-
22	BCR	A	1805	-	-	X	-
22	BCR	A	1806	-	-	X	X
22	BCR	A	1807	-	-	X	X
22	BCR	B	1776	-	-	-	X
22	BCR	B	1778	-	-	X	X
22	BCR	B	1779	-	-	X	X
22	BCR	B	1780	-	-	X	-
22	BCR	B	1781	-	-	X	X
22	BCR	B	1782	-	-	-	X
22	BCR	I	1032	-	-	X	X
22	BCR	L	1169	-	-	X	X
23	PQN	A	1801	X	-	-	X
23	PQN	B	1774	X	-	X	X
24	LMG	B	1784	-	-	X	X
25	SF4	B	1785	-	-	X	-
25	SF4	C	1082	-	-	X	-
25	SF4	C	1083	-	-	X	-



## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36461 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	164	Total	C	N	O	S	0	0	0
			1255	817	206	228	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	CONFLICT	UNP Q9C5R7
1	-1	ARG	LYS	CONFLICT	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1380	902	229	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	INSERTION	UNP Q41038
2	.	-	GLY	DELETION	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	160	Total	C	N	O	S	0	0	0
			1233	811	200	217	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1322	864	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	.	-	ALA	DELETION	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	CONFLICT	UNP P12353
D	-50	PRO	GLN	CONFLICT	UNP P12353
D	-44	ARG	PRO	CONFLICT	UNP P12353
D	-34	GLU	ASP	CONFLICT	UNP P12353
D	-11	LEU	HIS	CONFLICT	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	CONFLICT	UNP P12353
D	12	THR	PRO	CONFLICT	UNP P12353
D	14	ALA	GLY	CONFLICT	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	ILE	LEU	CONFLICT	UNP P36886

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	161	Total	C	N	O	S	0	0	0
			1203	791	193	214	5			

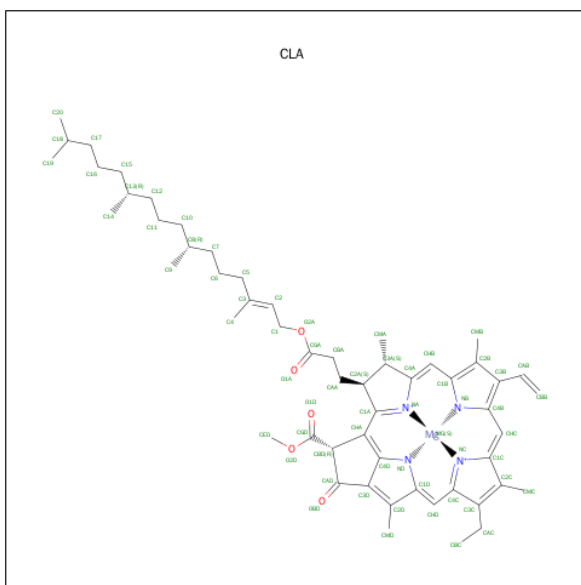
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	1	1	Total 57	C 47	Mg 1	N 4	O 5	0	0
19	1	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	1	1	Total 25	C 20	Mg 1	N 4		0	0
19	1	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
19	1	1	Total 25	C 20	Mg 1	N 4		0	0
19	1	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
19	1	1	Total 25	C 20	Mg 1	N 4		0	0
19	1	1	Total 25	C 20	Mg 1	N 4		0	0
19	2	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	2	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	2	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	2	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	2	1	Total	C	Mg	N	0	0
			36	30	1	4		
19	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	2	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	2	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	3	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			36	30	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			42	34	1	4		
19	3	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			65	55	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	4	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	4	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	4	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	4	1	Total 52	C 42	Mg 1	N 4 O 5	0	0
19	4	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
19	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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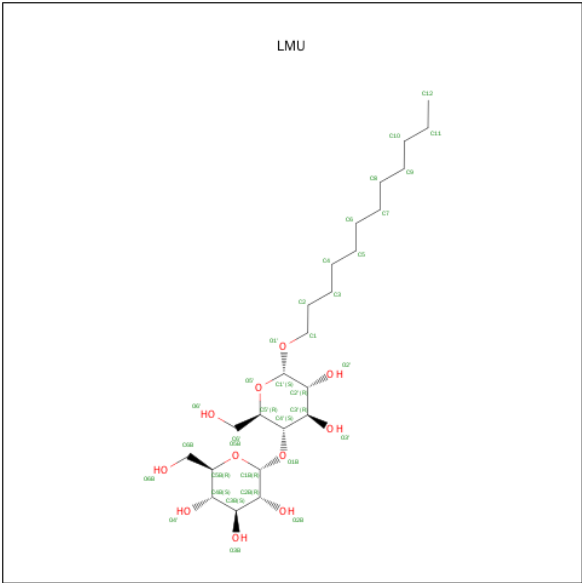
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	1	1	Total	C	Mg	N	0	0
			48	38	1	4		
19	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	1	1	Total	C	Mg	N	0	0
			55	45	1	4		
19	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	3	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	4	1	Total	C	Mg	N	0	0
			52	42	1	4		
19	4	1	Total	C	Mg	N	0	0
			47	37	1	4		

- Molecule 20 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	1	1	Total	C	O	0	0
			35	24	11		
20	1	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	4	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	B	1	Total	C	O	0	0
			35	24	11		
20	K	1	Total	C	O	0	0
			35	24	11		
20	L	1	Total	C	O	0	0
			35	24	11		
20	N	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			34	23	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

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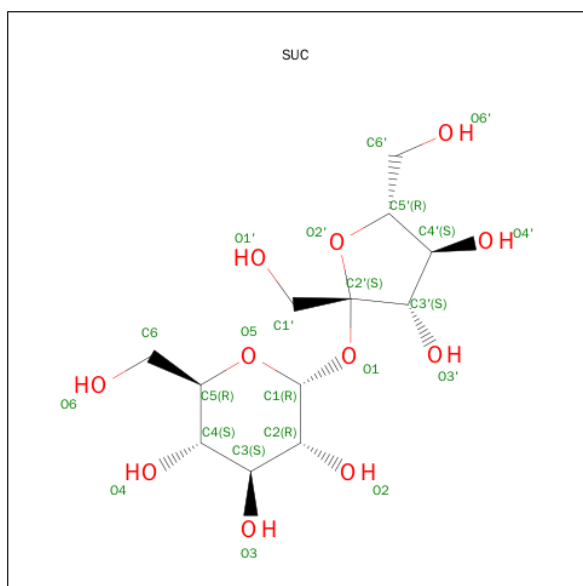
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 21 is SUGAR (SUCROSE) (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			22	12	10		
21	3	1	Total	C	O	0	0
			23	12	11		
21	F	1	Total	C	O	0	0
			23	12	11		

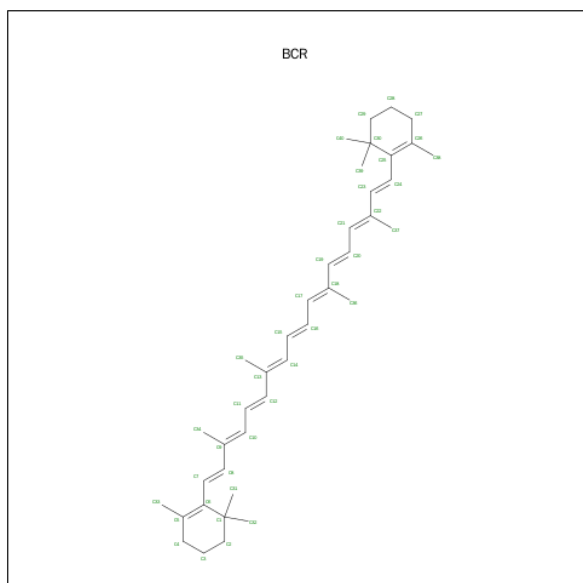
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0
21	B	1	Total C O 23 12 11	0	0

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



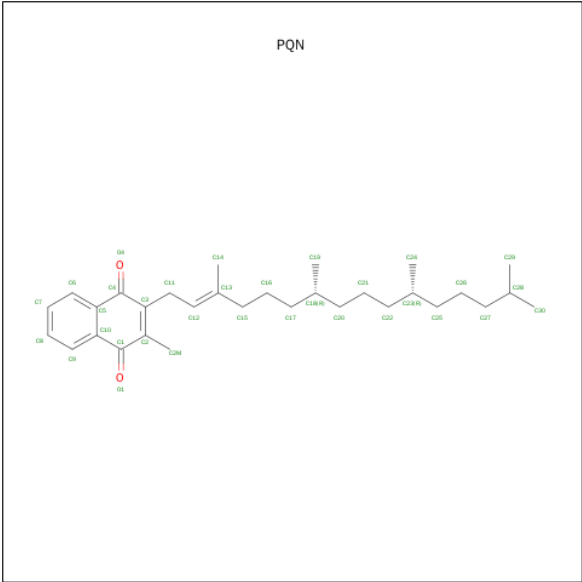
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	3	1	Total C 40 40	0	0

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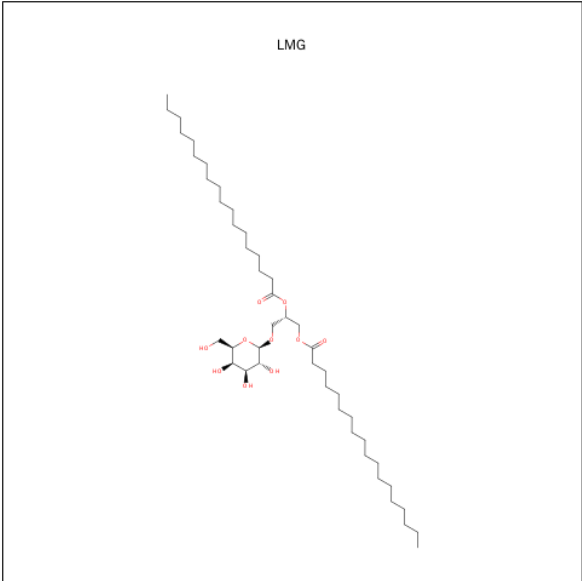
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



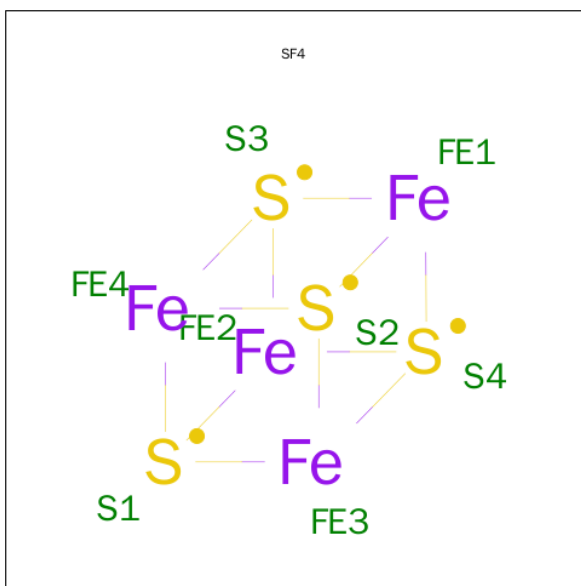
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			33	31	2		
23	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		

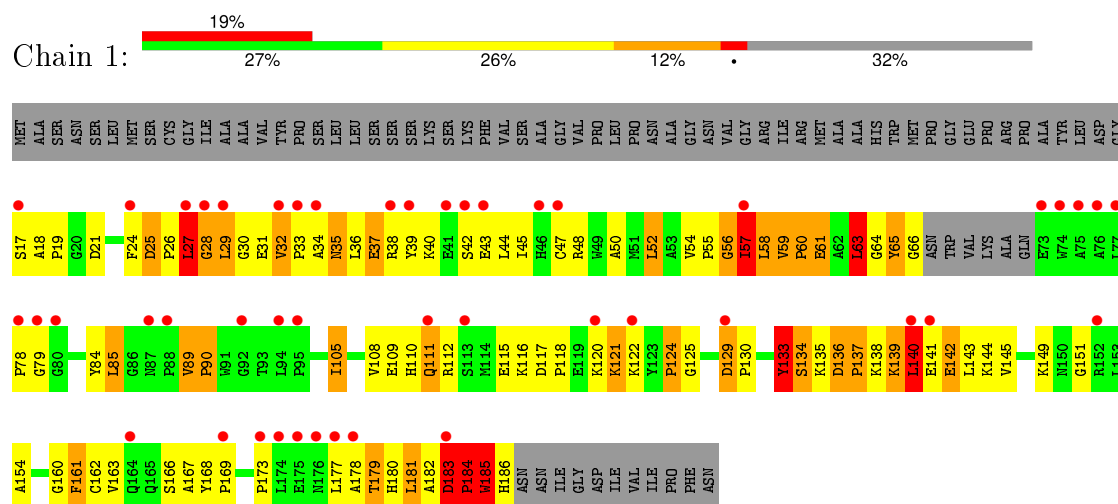
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			23	12	11		

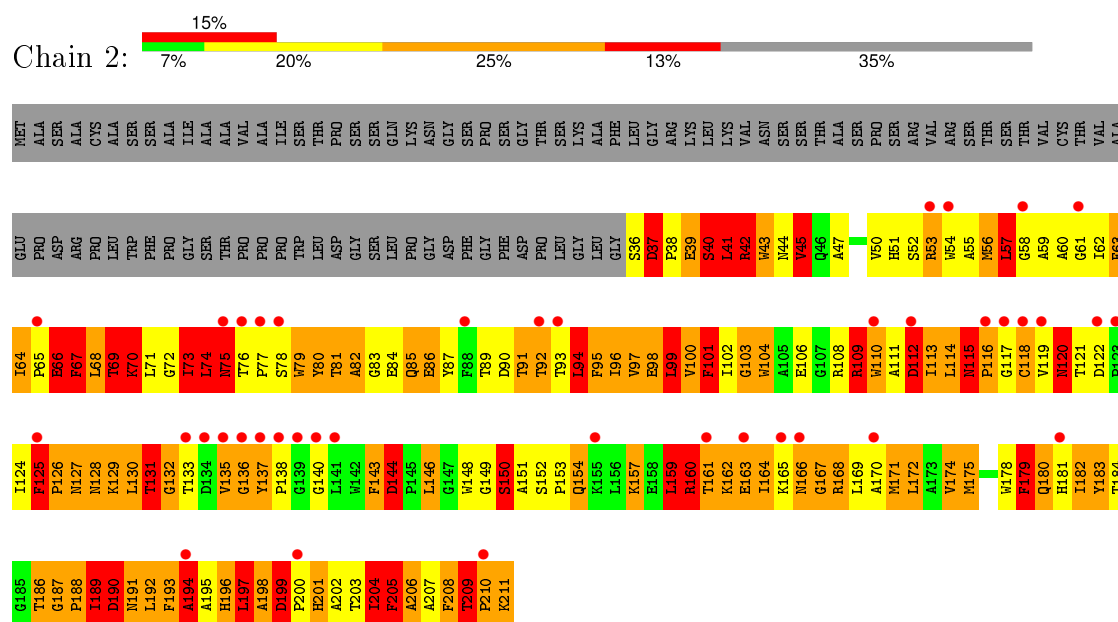
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

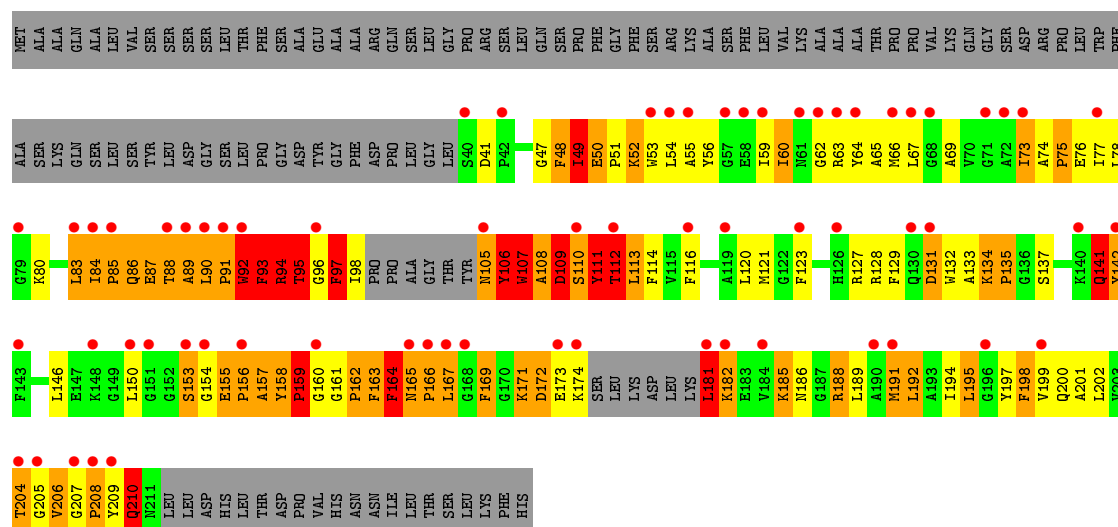
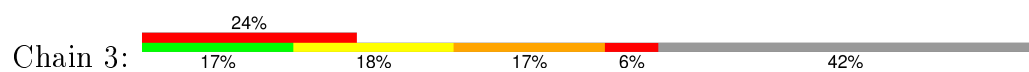
#### • Molecule 1: AT3G54890



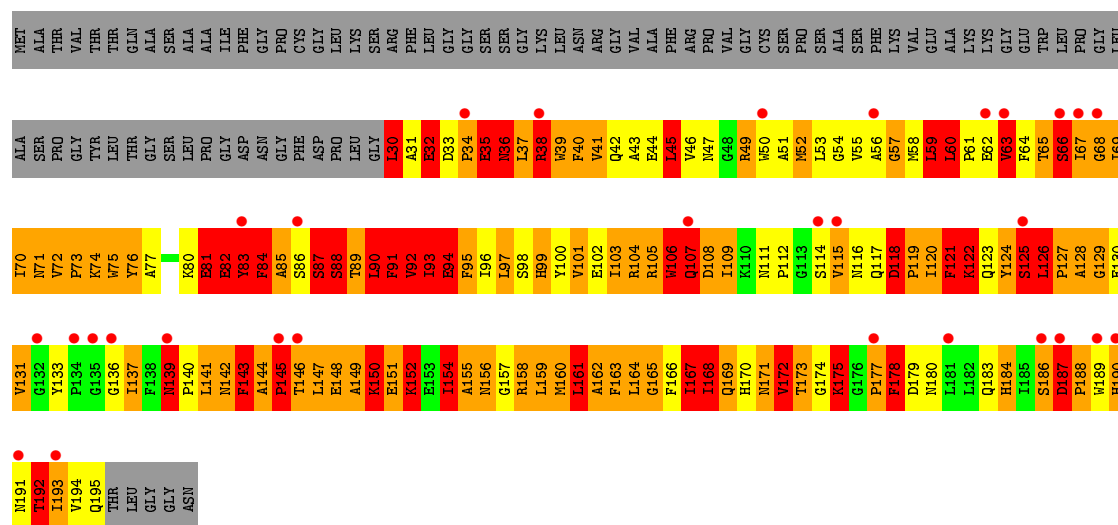
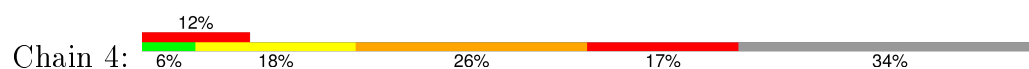
#### • Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I



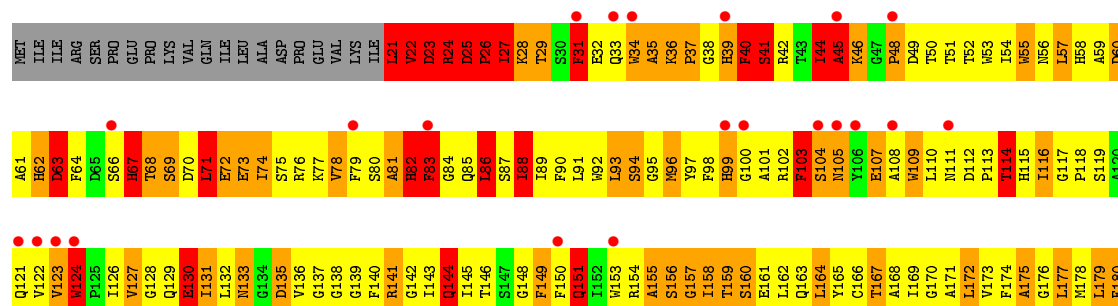
#### • Molecule 3: LHCA3

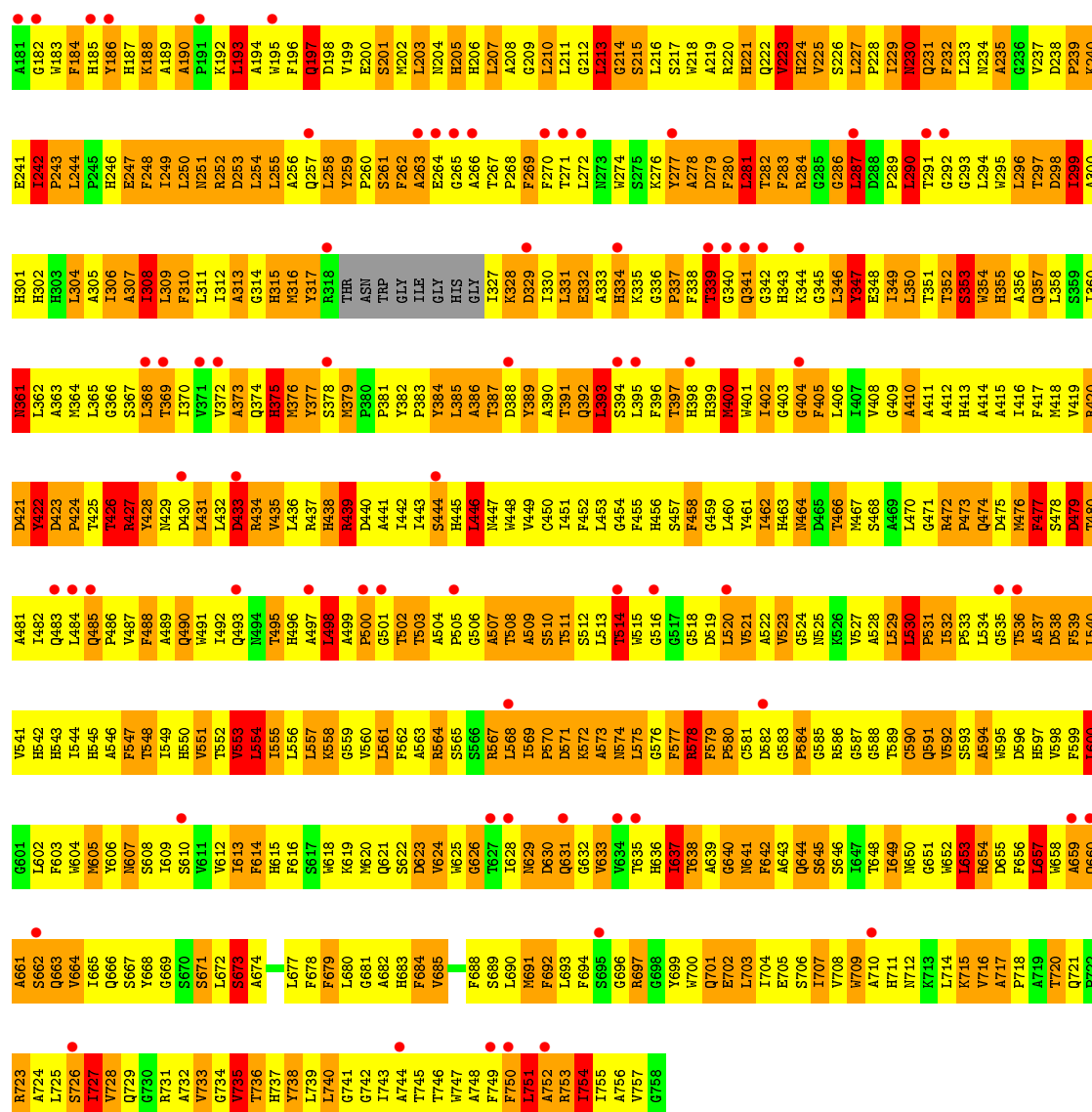


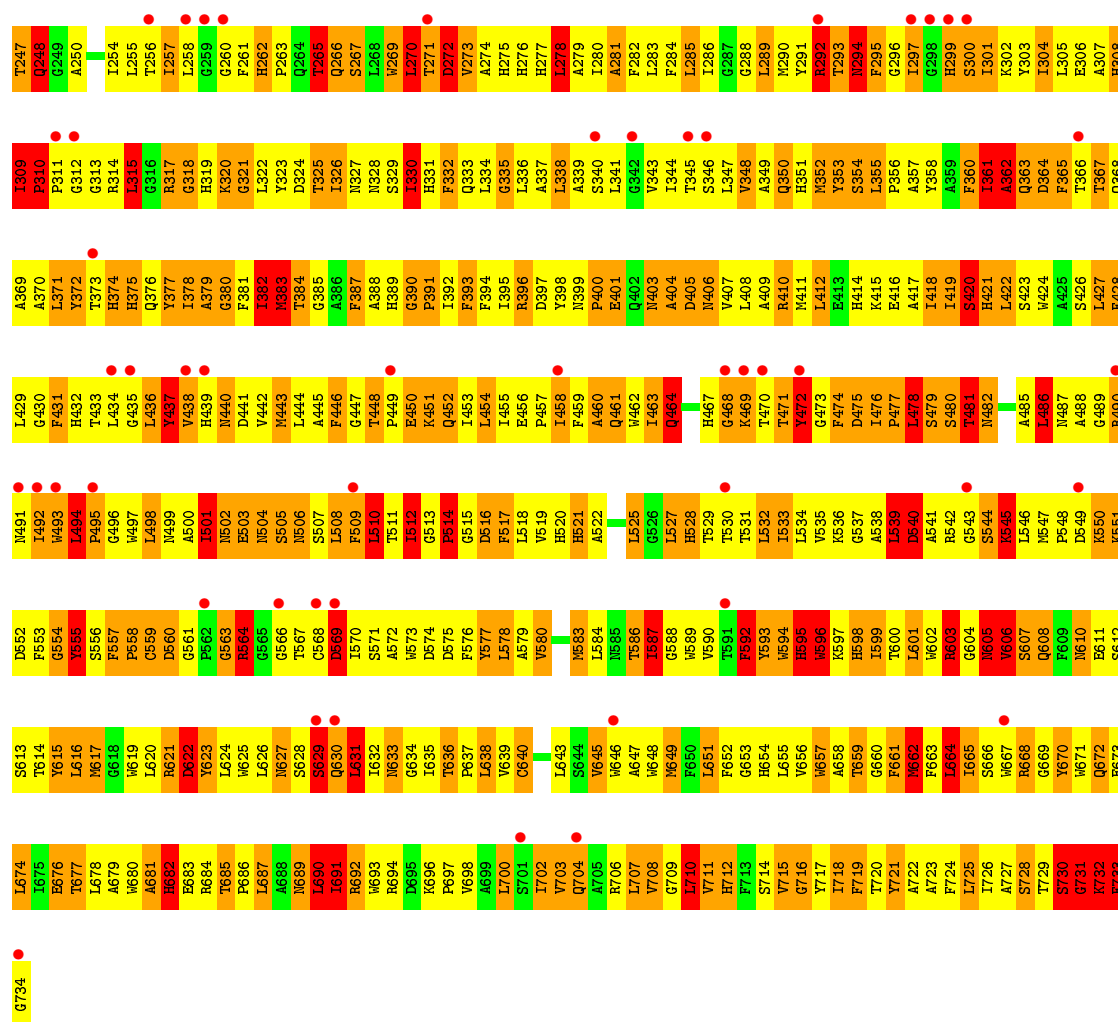
• Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC



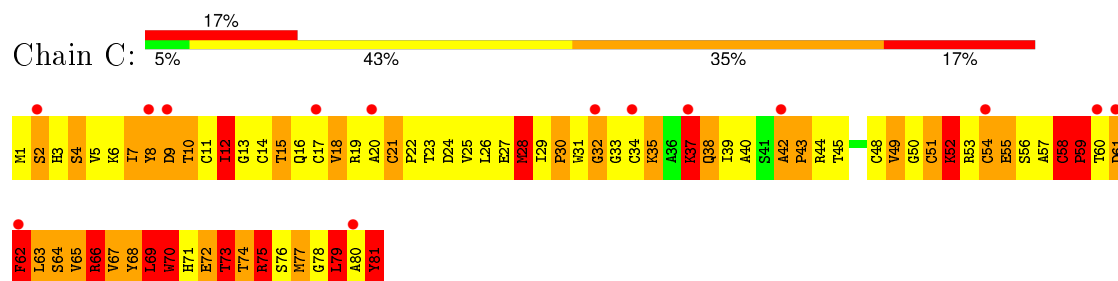
• Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



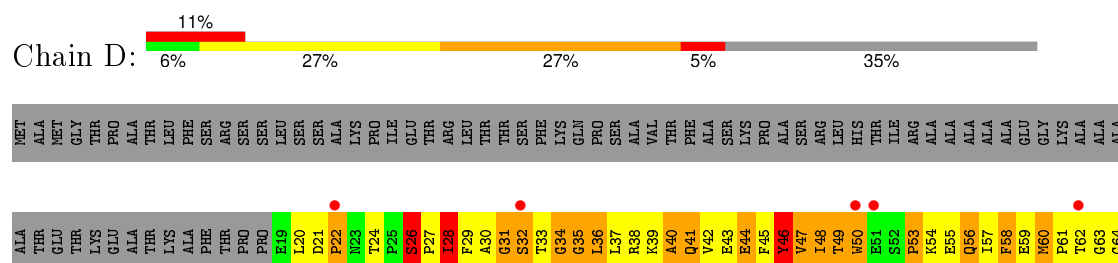




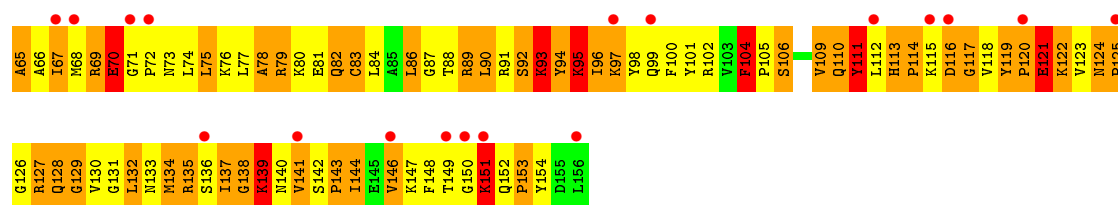
### • Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



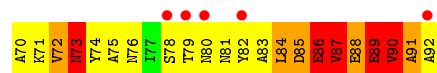
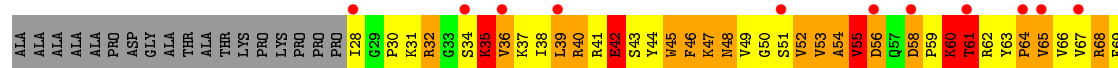
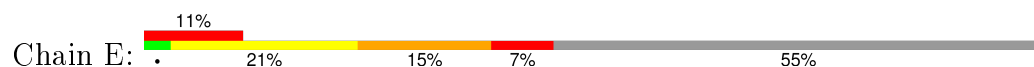
### • Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC



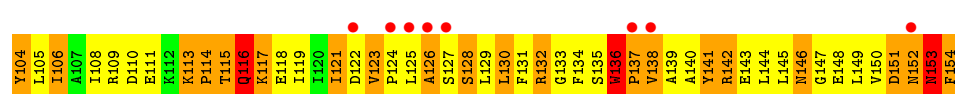
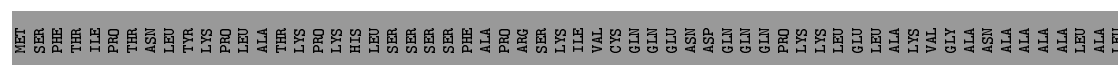




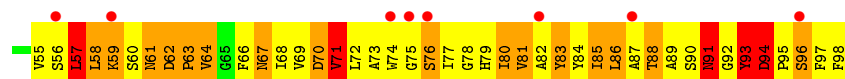
• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC



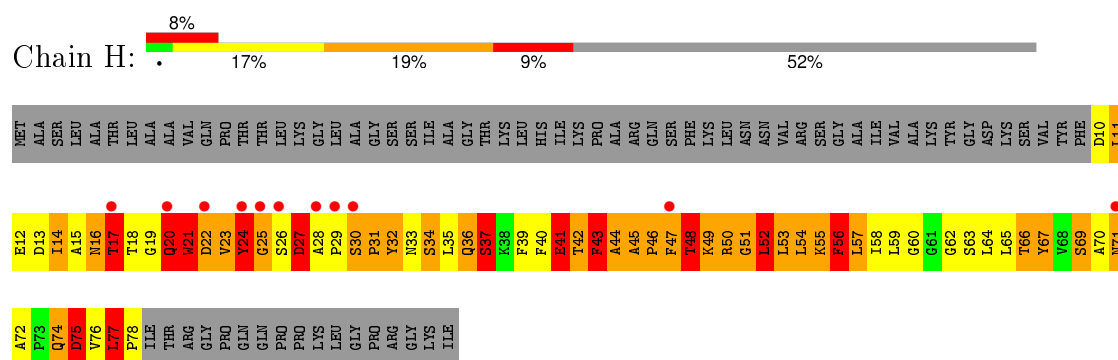
• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC



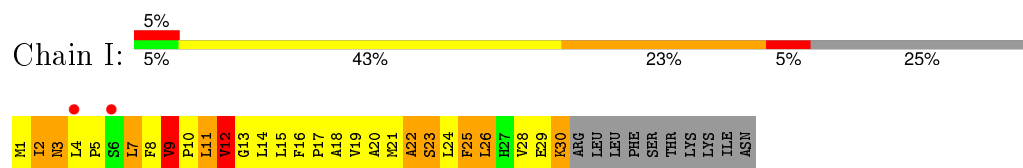
• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC



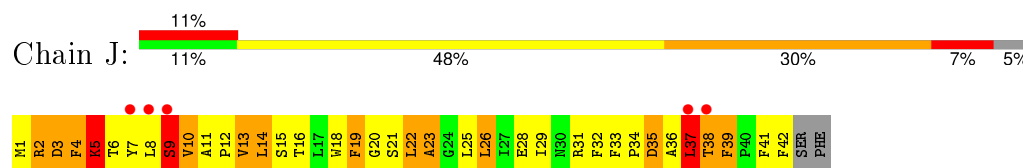
• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC



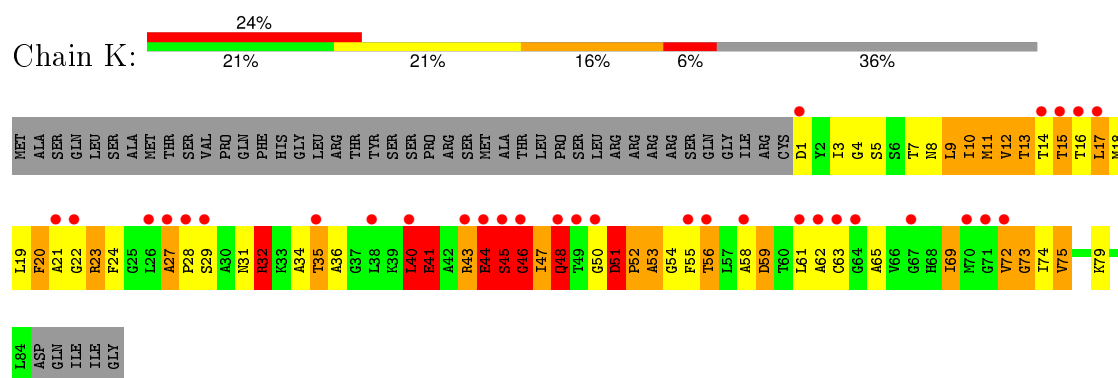
- Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



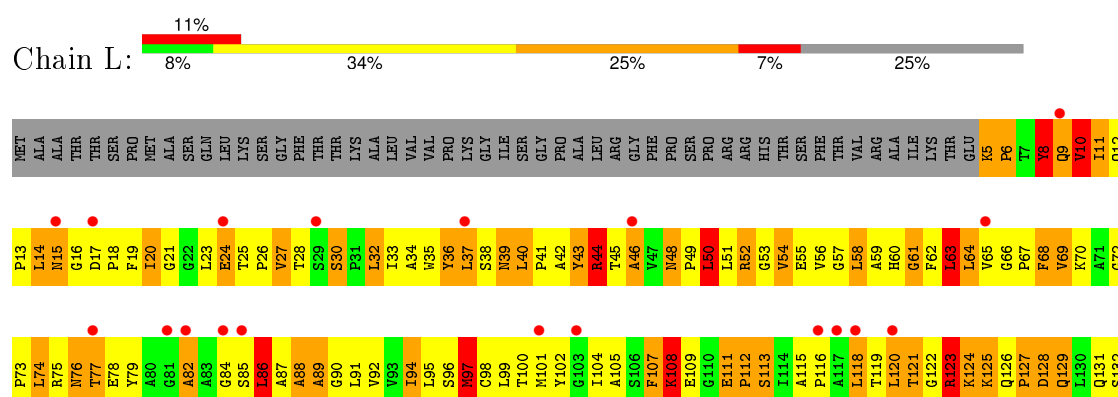
- Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

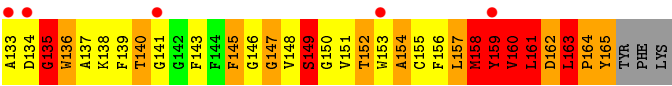


- Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

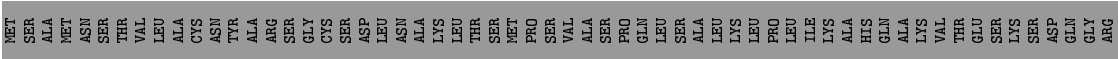
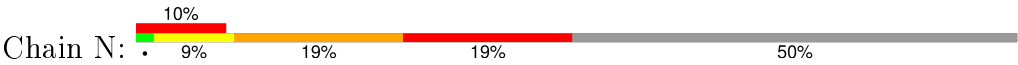


- Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC





• Molecule 17: PHOTOSYSTEM I-N SUBUNIT



• Molecule 18: PHOTOSYSTEM I-N SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.49 39.96 – 3.49	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-3.49) 90.6 (39.96-3.49)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.369 , 0.375 0.392 , 0.408	Depositor DCC
$R_{free}$ test set	1333 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	90.9	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 113.5	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 66880 reflections	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	36461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SUC, SF4, CLA, PQN, LMU, UNL, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.62	0/1294	0.89	5/1762 (0.3%)
2	2	1.05	1/1426 (0.1%)	1.32	15/1950 (0.8%)
3	3	0.88	6/1270 (0.5%)	0.96	4/1714 (0.2%)
4	4	1.27	9/1362 (0.7%)	1.35	17/1855 (0.9%)
5	A	0.89	0/5938	1.06	15/8104 (0.2%)
6	B	0.89	2/6058 (0.0%)	1.03	13/8278 (0.2%)
7	C	1.42	7/632 (1.1%)	1.34	5/856 (0.6%)
8	D	1.00	0/1122	1.06	0/1514
9	E	1.10	0/530	1.17	2/718 (0.3%)
10	F	1.05	1/1250 (0.1%)	1.07	3/1687 (0.2%)
11	G	1.04	0/760	1.27	10/1031 (1.0%)
12	H	1.10	0/543	1.20	2/741 (0.3%)
13	I	0.89	0/235	0.98	0/320
14	J	0.93	0/349	1.09	1/475 (0.2%)
15	K	0.63	0/599	1.16	6/810 (0.7%)
16	L	1.02	0/1238	1.14	6/1691 (0.4%)
17	N	1.28	1/699 (0.1%)	1.32	7/936 (0.7%)
All	All	0.97	27/25305 (0.1%)	1.11	111/34442 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	6
2	2	3	22
3	3	0	19
4	4	0	22
5	A	0	30
6	B	0	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	3
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	3
16	L	0	5
17	N	0	21
18	R	0	17
All	All	4	217

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.89	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
7	C	72	GLU	CD-OE1	-7.90	1.17	1.25
4	4	83	TYR	CE1-CZ	-7.46	1.28	1.38
3	3	93	PHE	CD2-CE2	7.39	1.54	1.39
7	C	72	GLU	CD-OE2	-6.96	1.18	1.25
7	C	58	CYS	CB-SG	6.87	1.94	1.82
6	B	640	CYS	CB-SG	6.82	1.93	1.82
7	C	81	TYR	CE1-CZ	-6.78	1.29	1.38
3	3	93	PHE	CE2-CZ	6.62	1.50	1.37
7	C	72	GLU	CG-CD	-6.60	1.42	1.51
17	N	70	GLU	CB-CG	6.16	1.63	1.52
4	4	88	SER	C-O	5.83	1.34	1.23
4	4	81	GLU	CG-CD	-5.75	1.43	1.51
4	4	83	TYR	CD1-CE1	-5.73	1.30	1.39
4	4	93	ILE	C-O	5.73	1.34	1.23
4	4	39	TRP	CE3-CZ3	-5.62	1.28	1.38
7	C	54	CYS	CB-SG	-5.61	1.72	1.81
2	2	45	VAL	CB-CG2	-5.61	1.41	1.52
7	C	81	TYR	CD2-CE2	-5.58	1.30	1.39
4	4	39	TRP	CB-CG	5.55	1.60	1.50
4	4	94	GLU	CG-CD	5.45	1.60	1.51
3	3	93	PHE	CD1-CE1	5.39	1.50	1.39
4	4	39	TRP	CA-C	-5.34	1.39	1.52
10	F	47	GLU	CG-CD	5.20	1.59	1.51
3	3	92	TRP	CG-CD1	5.12	1.44	1.36
6	B	401	GLU	CG-CD	5.11	1.59	1.51

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	57	ILE	N-CA-C	9.01	135.32	111.00
5	A	93	LEU	CA-CB-CG	8.09	133.90	115.30
6	B	732	LYS	N-CA-C	-8.08	89.19	111.00
16	L	160	VAL	CB-CA-C	-7.79	96.61	111.40
4	4	39	TRP	C-N-CA	-7.68	102.51	121.70
1	1	59	VAL	CB-CA-C	-7.54	97.07	111.40
6	B	486	LEU	CA-CB-CG	7.44	132.41	115.30
1	1	58	LEU	N-CA-C	-7.42	90.97	111.00
16	L	86	LEU	CA-CB-CG	7.38	132.27	115.30
6	B	315	LEU	CA-CB-CG	7.34	132.18	115.30
17	N	33	TYR	N-CA-C	-7.28	91.34	111.00
1	1	57	ILE	CB-CA-C	-7.26	97.07	111.60
11	G	16	LEU	CA-CB-CG	7.11	131.65	115.30
5	A	530	LEU	CA-CB-CG	7.09	131.60	115.30
6	B	710	LEU	N-CA-C	-7.03	92.03	111.00
4	4	39	TRP	CA-CB-CG	6.95	126.90	113.70
4	4	126	LEU	N-CA-C	6.88	129.59	111.00
5	A	540	LEU	CA-CB-CG	6.88	131.11	115.30
2	2	57	LEU	CA-CB-CG	6.79	130.92	115.30
5	A	554	LEU	CA-CB-CG	6.79	130.92	115.30
3	3	181	LEU	C-N-CA	6.71	138.47	121.70
4	4	92	VAL	O-C-N	-6.68	112.01	122.70
10	F	22	LEU	CB-CG-CD1	-6.60	99.78	111.00
15	K	46	GLY	N-CA-C	-6.57	96.68	113.10
2	2	41	LEU	CA-CB-CG	-6.55	100.24	115.30
2	2	74	LEU	N-CA-C	-6.52	93.39	111.00
3	3	93	PHE	N-CA-CB	-6.41	99.07	110.60
2	2	101	PHE	N-CA-CB	6.40	122.13	110.60
2	2	132	GLY	N-CA-C	6.38	129.06	113.10
11	G	43	HIS	N-CA-C	-6.38	93.78	111.00
9	E	90	VAL	N-CA-C	-6.37	93.79	111.00
4	4	66	SER	N-CA-C	6.35	128.14	111.00
4	4	93	ILE	N-CA-C	6.33	128.08	111.00
4	4	161	LEU	CA-CB-CG	6.32	129.84	115.30
5	A	25	ASP	C-N-CD	-6.29	106.75	120.60
7	C	79	LEU	CA-CB-CG	6.28	129.73	115.30
4	4	143	PHE	N-CA-C	6.27	127.94	111.00
6	B	494	LEU	CA-CB-CG	6.26	129.70	115.30
3	3	95	THR	N-CA-C	6.25	127.86	111.00
5	A	271	THR	N-CA-C	-6.25	94.14	111.00
6	B	338	LEU	CA-CB-CG	6.18	129.51	115.30
17	N	24	THR	N-CA-C	-6.14	94.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	91	ASN	N-CA-C	6.09	127.45	111.00
17	N	27	ALA	N-CA-C	-6.07	94.60	111.00
15	K	51	ASP	N-CA-C	6.05	127.33	111.00
16	L	135	GLY	N-CA-C	-6.04	98.01	113.10
4	4	124	TYR	N-CA-C	-6.01	94.77	111.00
11	G	44	PHE	N-CA-C	-6.01	94.78	111.00
4	4	88	SER	N-CA-C	6.00	127.21	111.00
7	C	69	LEU	CA-CB-CG	5.95	128.99	115.30
14	J	35	ASP	N-CA-C	5.94	127.04	111.00
11	G	57	LEU	CA-CB-CG	5.90	128.87	115.30
6	B	194	LEU	CB-CG-CD1	-5.89	100.98	111.00
4	4	108	ASP	CB-CG-OD2	-5.82	113.06	118.30
4	4	60	LEU	CA-CB-CG	5.80	128.65	115.30
2	2	94	LEU	CA-CB-CG	5.78	128.60	115.30
6	B	380	GLY	N-CA-C	-5.78	98.65	113.10
2	2	175	MET	CB-CA-C	5.77	121.94	110.40
11	G	51	ALA	N-CA-C	5.77	126.58	111.00
5	A	350	LEU	CA-CB-CG	-5.77	102.03	115.30
17	N	31	ARG	N-CA-C	-5.77	95.42	111.00
15	K	53	ALA	C-N-CA	-5.68	110.38	122.30
2	2	172	LEU	CA-CB-CG	-5.67	102.25	115.30
7	C	79	LEU	CB-CG-CD2	5.67	120.63	111.00
7	C	75	ARG	NE-CZ-NH2	5.65	123.12	120.30
4	4	30	LEU	CA-CB-CG	-5.64	102.32	115.30
12	H	27	ASP	N-CA-C	-5.62	95.82	111.00
4	4	145	PRO	N-CA-C	-5.62	97.49	112.10
17	N	62	SER	N-CA-C	-5.62	95.83	111.00
6	B	478	LEU	CA-CB-CG	5.59	128.15	115.30
7	C	75	ARG	CA-CB-CG	5.58	125.67	113.40
17	N	74	LYS	N-CA-C	5.54	125.95	111.00
17	N	6	TYR	N-CA-C	-5.46	96.27	111.00
9	E	60	LYS	N-CA-C	5.45	125.71	111.00
5	A	653	LEU	CA-CB-CG	5.44	127.81	115.30
4	4	41	VAL	CB-CA-C	-5.38	101.18	111.40
6	B	104	PHE	N-CA-C	-5.37	96.50	111.00
16	L	163	LEU	C-N-CD	-5.37	108.80	120.60
11	G	14	LEU	CA-CB-CG	-5.35	102.99	115.30
6	B	631	LEU	CA-CB-CG	5.35	127.61	115.30
2	2	56	MET	N-CA-C	5.34	125.41	111.00
4	4	40	PHE	CB-CA-C	5.33	121.06	110.40
10	F	59	TYR	CB-CA-C	-5.29	99.82	110.40
16	L	50	LEU	CA-CB-CG	5.28	127.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	41	LEU	CB-CG-CD2	-5.27	102.04	111.00
15	K	51	ASP	C-N-CD	-5.26	109.03	120.60
2	2	199	ASP	C-N-CD	-5.25	109.05	120.60
5	A	287	LEU	CA-CB-CG	5.24	127.36	115.30
1	1	63	LEU	CA-CB-CG	-5.24	103.26	115.30
15	K	12	VAL	CB-CA-C	-5.23	101.46	111.40
12	H	52	LEU	N-CA-C	5.19	125.00	111.00
6	B	289	LEU	CA-CB-CG	5.19	127.23	115.30
2	2	43	TRP	N-CA-C	-5.16	97.06	111.00
5	A	626	GLY	N-CA-C	-5.16	100.19	113.10
11	G	21	PHE	N-CA-C	5.15	124.90	111.00
2	2	174	VAL	N-CA-C	5.15	124.90	111.00
4	4	154	ILE	CB-CA-C	-5.14	101.32	111.60
5	A	753	ARG	NE-CZ-NH1	-5.13	117.73	120.30
5	A	600	LEU	CA-CB-CG	5.11	127.05	115.30
16	L	158	MET	N-CA-C	-5.07	97.31	111.00
3	3	111	TYR	CA-CB-CG	5.06	123.02	113.40
5	A	573	ALA	N-CA-C	-5.05	97.35	111.00
15	K	22	GLY	C-N-CA	-5.05	109.06	121.70
2	2	125	PHE	N-CA-C	5.05	124.64	111.00
5	A	385	LEU	CA-CB-CG	5.05	126.92	115.30
5	A	214	GLY	N-CA-C	-5.04	100.49	113.10
11	G	20	ARG	N-CA-C	-5.04	97.38	111.00
6	B	68	VAL	N-CA-C	-5.03	97.43	111.00
11	G	16	LEU	N-CA-C	-5.03	97.43	111.00
2	2	67	PHE	CB-CA-C	5.02	120.44	110.40
10	F	136	TRP	CA-CB-CG	5.01	123.21	113.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	67	PHE	CA
2	2	101	PHE	CA
2	2	174	VAL	CA
11	G	21	PHE	CA

All (217) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide
1	1	185	TRP	Peptide
1	1	56	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	1	57	ILE	Peptide
1	1	60	PRO	Peptide
1	1	63	LEU	Peptide
2	2	111	ALA	Peptide
2	2	112	ASP	Peptide
2	2	126	PRO	Peptide
2	2	131	THR	Peptide
2	2	144	ASP	Peptide
2	2	166	ASN	Peptide
2	2	189	ILE	Peptide
2	2	194	ALA	Peptide
2	2	197	LEU	Peptide
2	2	201	HIS	Peptide
2	2	209	THR	Peptide
2	2	37	ASP	Peptide
2	2	39	GLU	Peptide
2	2	40	SER	Peptide
2	2	42	ARG	Peptide
2	2	73	ILE	Peptide
2	2	74	LEU	Peptide
2	2	75	ASN	Peptide
2	2	80	TYR	Peptide
2	2	84	GLU	Peptide
2	2	92	THR	Peptide
2	2	99	LEU	Peptide
3	3	105	ASN	Peptide
3	3	106	TYR	Peptide
3	3	107	TRP	Peptide
3	3	109	ASP	Peptide
3	3	111	TYR	Peptide
3	3	112	THR	Peptide
3	3	155	GLU	Peptide
3	3	159	PRO	Peptide
3	3	169	PHE	Peptide
3	3	172	ASP	Peptide
3	3	181	LEU	Peptide
3	3	49	ILE	Peptide
3	3	87	GLU	Peptide
3	3	89	ALA	Peptide
3	3	91	PRO	Peptide
3	3	92	TRP	Peptide
3	3	93	PHE	Peptide

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Mol	Chain	Res	Type	Group
3	3	94	ARG	Peptide
3	3	95	THR	Peptide
4	4	106	TRP	Peptide
4	4	142	ASN	Peptide
4	4	144	ALA	Peptide
4	4	149	ALA	Peptide
4	4	152	LYS	Peptide
4	4	155	ALA	Peptide
4	4	190	HIS	Peptide
4	4	192	THR	Peptide
4	4	30	LEU	Peptide
4	4	35	GLU	Peptide
4	4	36	ASN	Peptide
4	4	37	LEU	Peptide
4	4	38	ARG	Peptide
4	4	63	VAL	Peptide
4	4	65	THR	Peptide
4	4	68	GLY	Peptide
4	4	81	GLU	Peptide
4	4	83	TYR	Peptide
4	4	87	SER	Peptide
4	4	88	SER	Peptide
4	4	89	THR	Peptide
4	4	90	LEU	Peptide
5	A	103	PHE	Peptide
5	A	117	GLY	Peptide
5	A	123	VAL	Peptide
5	A	151	GLN	Peptide
5	A	197	GLN	Peptide
5	A	199	VAL	Peptide
5	A	201	SER	Peptide
5	A	21	LEU	Peptide
5	A	22	VAL	Peptide
5	A	23	ASP	Peptide
5	A	24	ARG	Peptide
5	A	240	LYS	Peptide
5	A	242	ILE	Peptide
5	A	26	PRO	Peptide
5	A	27	ILE	Peptide
5	A	315	HIS	Peptide
5	A	347	TYR	Peptide
5	A	37	PRO	Peptide

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Mol	Chain	Res	Type	Group
5	A	393	LEU	Peptide
5	A	41	SER	Peptide
5	A	427	ARG	Peptide
5	A	44	ILE	Peptide
5	A	45	ALA	Peptide
5	A	482	ILE	Peptide
5	A	502	THR	Peptide
5	A	55	TRP	Peptide
5	A	551	VAL	Peptide
5	A	573	ALA	Peptide
5	A	67	HIS	Peptide
5	A	81	ALA	Peptide
6	B	104	PHE	Peptide
6	B	126	THR	Peptide
6	B	232	LEU	Peptide
6	B	265	THR	Peptide
6	B	304	ILE	Peptide
6	B	310	PRO	Peptide
6	B	362	ALA	Peptide
6	B	377	TYR	Peptide
6	B	390	GLY	Peptide
6	B	404	ALA	Peptide
6	B	481	THR	Peptide
6	B	510	LEU	Peptide
6	B	563	GLY	Peptide
6	B	595	HIS	Peptide
6	B	622	ASP	Peptide
6	B	728	SER	Peptide
6	B	730	SER	Peptide
6	B	731	GLY	Peptide
6	B	732	LYS	Peptide
6	B	99	PRO	Peptide
7	C	42	ALA	Peptide
7	C	51	CYS	Peptide
7	C	79	LEU	Peptide
8	D	104	PHE	Peptide
8	D	111	TYR	Peptide
8	D	113	HIS	Peptide
8	D	117	GLY	Peptide
8	D	141	VAL	Peptide
8	D	90	LEU	Peptide
9	E	59	PRO	Peptide

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Mol	Chain	Res	Type	Group
9	E	85	ASP	Peptide
9	E	86	GLU	Peptide
9	E	87	VAL	Peptide
9	E	88	GLU	Peptide
9	E	89	GLU	Peptide
10	F	136	TRP	Peptide
10	F	148	GLU	Peptide
10	F	18	GLU	Peptide
10	F	20	GLN	Peptide
10	F	22	LEU	Peptide
10	F	24	LYS	Peptide
10	F	26	GLN	Peptide
10	F	28	SER	Peptide
10	F	31	LEU	Peptide
10	F	41	ALA	Peptide
10	F	51	LYS	Peptide
10	F	56	TYR	Peptide
11	G	15	SER	Peptide
11	G	22	VAL	Peptide
11	G	26	PHE	Peptide
11	G	36	PRO	Peptide
11	G	39	ASN	Peptide
11	G	40	GLY	Peptide
11	G	42	SER	Peptide
11	G	43	HIS	Peptide
11	G	44	PHE	Peptide
11	G	45	GLU	Peptide
11	G	47	GLY	Peptide
11	G	48	ASP	Peptide
11	G	49	THR	Peptide
11	G	50	ARG	Peptide
11	G	90	SER	Peptide
11	G	94	ASP	Peptide
12	H	12	GLU	Peptide
12	H	20	GLN	Peptide
12	H	21	TRP	Peptide
12	H	22	ASP	Peptide
12	H	25	GLY	Peptide
12	H	27	ASP	Peptide
12	H	43	PHE	Peptide
12	H	48	THR	Peptide
12	H	51	GLY	Peptide

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Mol	Chain	Res	Type	Group
15	K	45	SER	Peptide
15	K	46	GLY	Peptide
15	K	50	GLY	Peptide
16	L	157	LEU	Mainchain
16	L	160	VAL	Peptide
16	L	161	LEU	Peptide
16	L	162	ASP	Peptide
16	L	82	ALA	Peptide
17	N	12	THR	Peptide
17	N	15	GLU	Peptide
17	N	17	ASN	Peptide
17	N	23	ALA	Peptide
17	N	26	GLY	Peptide
17	N	28	ASN	Peptide
17	N	29	PHE	Peptide
17	N	30	ALA	Peptide
17	N	32	ALA	Peptide
17	N	43	PRO	Peptide
17	N	44	GLU	Peptide
17	N	46	PHE	Peptide
17	N	52	LEU	Peptide
17	N	53	ALA	Peptide
17	N	54	LYS	Peptide
17	N	56	LYS	Peptide
17	N	67	LEU	Peptide
17	N	7	LEU	Peptide
17	N	70	GLU	Peptide
17	N	73	ASP	Peptide
17	N	75	TYR	Peptide
18	R	27	UNK	Peptide
18	R	28	UNK	Peptide
18	R	30	UNK	Peptide
18	R	31	UNK	Peptide
18	R	32	UNK	Peptide
18	R	33	UNK	Peptide
18	R	34	UNK	Peptide
18	R	36	UNK	Peptide
18	R	37	UNK	Peptide
18	R	40	UNK	Peptide
18	R	42	UNK	Peptide
18	R	46	UNK	Peptide
18	R	47	UNK	Peptide

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Mol	Chain	Res	Type	Group
18	R	48	UNK	Peptide
18	R	50	UNK	Peptide
18	R	51	UNK	Peptide
18	R	52	UNK	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1255	0	1222	206	0
2	2	1380	0	1341	484	0
3	3	1233	0	1199	280	7
4	4	1322	0	1287	741	7
5	A	5745	0	5595	1663	0
6	B	5848	0	5653	1489	8
7	C	619	0	608	234	0
8	D	1095	0	1112	222	0
9	E	520	0	528	154	0
10	F	1221	0	1246	306	1
11	G	740	0	709	304	11
12	H	529	0	514	122	0
13	I	229	0	252	63	0
14	J	338	0	340	78	0
15	K	593	0	618	120	0
16	L	1203	0	1213	369	7
17	N	685	0	670	446	11
18	R	265	0	65	65	0
19	1	1065	0	708	316	1
19	2	557	0	397	100	0
19	3	663	0	432	131	0
19	4	775	0	534	179	0
19	A	2523	0	2349	1000	1
19	B	2420	0	2313	850	0
19	F	130	0	86	31	0
19	G	51	0	40	20	0
19	I	60	0	58	12	0
19	J	122	0	120	59	0
19	K	50	0	36	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	147	0	110	44	0
19	R	115	0	106	22	0
20	1	70	0	92	15	0
20	2	35	0	46	3	1
20	4	35	0	46	4	0
20	A	1468	0	1909	526	6
20	B	35	0	46	28	30
20	K	35	0	45	6	0
20	L	35	0	46	3	0
20	N	35	0	45	36	0
20	R	35	0	46	20	4
21	2	22	0	19	10	0
21	3	23	0	22	14	0
21	B	230	0	219	108	0
21	F	23	0	19	5	0
22	3	40	0	54	19	28
22	A	240	0	321	252	0
22	B	320	0	432	226	0
22	I	40	0	54	46	0
22	L	80	0	105	64	0
23	A	33	0	46	15	0
23	B	33	0	46	32	0
24	B	49	0	71	30	0
25	B	8	0	0	19	0
25	C	16	0	0	8	0
26	B	23	0	0	2	0
All	All	36461	0	35190	9731	62

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 136.

All (9731) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:69:ILE:CD1	4:4:175:LYS:HG2	1.30	1.61
2:2:43:TRP:CH2	2:2:125:PHE:CE1	1.88	1.61
4:4:69:ILE:HD11	4:4:175:LYS:CG	1.24	1.61
2:2:43:TRP:CZ3	2:2:125:PHE:CD1	1.89	1.59
16:L:164:PRO:HD2	16:L:165:TYR:CE2	1.36	1.59
1:1:27:LEU:HD21	6:B:314:ARG:CG	1.25	1.59
19:A:1776:CLA:H92	22:A:1804:BCR:C37	1.16	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:122:LYS:HB2	4:4:143:PHE:CD2	1.31	1.57
20:A:7036:LMU:C2	20:A:7036:LMU:H82	1.34	1.57
20:A:7042:LMU:C7	20:A:7042:LMU:H22	1.34	1.56
2:2:43:TRP:CZ2	2:2:125:PHE:CE1	1.87	1.55
19:B:1743:CLA:HAC2	19:B:1744:CLA:CBB	1.12	1.55
2:2:43:TRP:HH2	2:2:125:PHE:CE2	1.17	1.55
1:1:179:THR:CG2	4:4:87:SER:HB3	1.32	1.55
23:B:1774:PQN:C19	22:B:1781:BCR:H10C	1.34	1.55
16:L:163:LEU:HB3	16:L:164:PRO:CG	1.35	1.55
3:3:132:TRP:CZ3	3:3:155:GLU:HG2	1.37	1.55
19:1:1188:CLA:H8	19:1:1188:CLA:C4	1.35	1.55
2:2:42:ARG:CD	2:2:45:VAL:HG21	1.37	1.54
19:A:1776:CLA:C9	22:A:1804:BCR:H373	1.32	1.53
6:B:25:ILE:HG21	22:L:1169:BCR:C29	1.09	1.53
19:A:1779:CLA:C4C	22:A:1804:BCR:H19C	1.32	1.53
23:B:1774:PQN:H162	22:B:1781:BCR:C33	1.28	1.53
19:B:1743:CLA:CAC	19:B:1744:CLA:CBB	1.84	1.51
19:1:1188:CLA:C8	19:1:1188:CLA:H41	1.35	1.51
17:N:62:SER:HB3	17:N:66:ASP:CB	1.39	1.51
19:1:1148:CLA:HED1	19:1:1148:CLA:C2	1.30	1.51
2:2:43:TRP:CZ2	2:2:125:PHE:CZ	1.95	1.51
11:G:45:GLU:CG	11:G:49:THR:HG23	1.38	1.51
5:A:744:ALA:CB	22:A:1806:BCR:H391	1.41	1.50
20:A:7023:LMU:H91	20:A:7023:LMU:C2	1.41	1.50
2:2:205:PHE:CD1	2:2:206:ALA:N	1.77	1.50
3:3:132:TRP:CZ3	3:3:155:GLU:CG	1.91	1.50
19:1:1014:CLA:C11	19:1:1014:CLA:H43	1.42	1.50
17:N:45:ASN:ND2	17:N:54:LYS:HG2	1.24	1.49
5:A:328:LYS:CE	5:A:332:GLU:HG3	1.40	1.49
4:4:107:GLN:CA	19:4:1196:CLA:HMA3	1.40	1.48
18:R:32:UNK:CB	18:R:33:UNK:CB	1.85	1.48
16:L:164:PRO:HB2	16:L:165:TYR:CB	1.39	1.48
4:4:36:ASN:HB2	4:4:39:TRP:CZ3	1.48	1.48
20:B:1783:LMU:H3'	20:B:1783:LMU:C6B	1.42	1.48
6:B:732:LYS:HG2	6:B:733:PHE:C	1.21	1.48
4:4:69:ILE:HD11	4:4:175:LYS:CB	1.01	1.48
6:B:25:ILE:CG2	22:L:1169:BCR:C29	1.94	1.46
19:1:1014:CLA:HED3	19:1:1014:CLA:C1A	1.45	1.46
3:3:181:LEU:N	3:3:182:LYS:HG3	1.16	1.46
20:A:7048:LMU:H32	20:A:7048:LMU:C5'	1.43	1.46
20:A:7016:LMU:C2	20:A:7016:LMU:H81	1.44	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:308:ILE:CD1	19:A:1772:CLA:H91	1.44	1.46
19:1:1148:CLA:HAA1	19:1:1148:CLA:CGD	1.44	1.46
20:A:7042:LMU:C6'	20:A:7042:LMU:H32	1.42	1.45
4:4:34:PRO:CA	4:4:35:GLU:HB2	1.46	1.45
4:4:69:ILE:CD1	4:4:175:LYS:CB	1.90	1.45
19:4:1198:CLA:HAA2	19:4:1198:CLA:CED	1.45	1.45
19:1:1188:CLA:C2A	19:1:1188:CLA:HED3	1.47	1.45
1:1:112:ARG:HH12	19:1:1195:CLA:CGD	1.24	1.45
20:A:7048:LMU:C2'	20:A:7048:LMU:H22	1.36	1.44
21:B:8052:SUC:C5'	21:B:8052:SUC:H1	1.46	1.44
19:1:1188:CLA:CGA	19:1:1188:CLA:HMA2	1.45	1.44
16:L:164:PRO:HD2	16:L:165:TYR:CZ	1.52	1.43
15:K:44:GLU:CG	15:K:45:SER:N	1.71	1.43
7:C:14:CYS:HA	7:C:17:CYS:SG	1.56	1.43
4:4:40:PHE:HB3	4:4:43:ALA:CB	1.48	1.43
19:A:1796:CLA:H141	22:A:1806:BCR:C2	1.48	1.43
5:A:368:LEU:HD21	19:A:1774:CLA:C9	1.49	1.43
19:J:1043:CLA:HED3	19:J:1043:CLA:C1A	1.47	1.43
2:2:43:TRP:CH2	2:2:125:PHE:CD1	2.03	1.42
11:G:48:ASP:CB	11:G:49:THR:HG22	1.45	1.42
16:L:164:PRO:HG2	16:L:165:TYR:CD1	1.55	1.41
6:B:732:LYS:CG	6:B:733:PHE:C	1.82	1.41
17:N:45:ASN:HD22	17:N:54:LYS:CG	1.28	1.41
2:2:103:GLY:N	19:2:1222:CLA:HBB2	1.33	1.41
19:B:1769:CLA:H152	22:B:1780:BCR:C31	1.51	1.41
20:B:1783:LMU:H112	20:B:1783:LMU:C6	1.48	1.41
11:G:93:TYR:HA	11:G:94:ASP:CB	1.42	1.41
19:A:1771:CLA:HAA1	19:A:1771:CLA:CED	1.47	1.41
4:4:122:LYS:HB3	4:4:143:PHE:CB	1.51	1.40
2:2:43:TRP:CH2	2:2:125:PHE:CE2	1.98	1.40
7:C:54:CYS:HB2	25:C:1082:SF4:S3	1.61	1.40
4:4:194:VAL:HG12	4:4:195:GLN:CB	1.51	1.40
5:A:23:ASP:CG	5:A:24:ARG:HD3	1.42	1.40
17:N:48:GLY:HA2	17:N:49:CYS:SG	1.62	1.39
4:4:149:ALA:HB3	4:4:151:GLU:CG	1.52	1.39
19:1:1142:CLA:CED	19:K:1085:CLA:HMB2	1.49	1.39
19:A:1779:CLA:CHD	22:A:1804:BCR:H19C	1.51	1.39
4:4:40:PHE:CB	4:4:43:ALA:HB2	1.52	1.39
19:1:1148:CLA:H2	19:1:1148:CLA:CED	1.51	1.39
4:4:36:ASN:HB2	4:4:39:TRP:CE3	1.57	1.38
17:N:61:LEU:HD11	17:N:63:ASP:C	1.40	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:163:LEU:CG	16:L:164:PRO:HB3	1.51	1.38
19:J:1044:CLA:C7	19:J:1044:CLA:H41	1.49	1.38
2:2:42:ARG:CG	2:2:45:VAL:HG21	1.48	1.38
4:4:128:ALA:HB2	4:4:143:PHE:CE2	1.56	1.38
6:B:732:LYS:HB3	6:B:733:PHE:CA	1.48	1.38
4:4:93:ILE:HA	4:4:96:ILE:CD1	1.53	1.37
17:N:58:VAL:HB	17:N:59:PRO:CD	1.47	1.37
19:1:1188:CLA:HBA2	19:1:1188:CLA:CED	1.54	1.37
20:N:1086:LMU:C6'	20:N:1086:LMU:H51	1.51	1.37
19:A:1771:CLA:HMC1	19:A:1771:CLA:CBC	1.51	1.37
4:4:37:LEU:C	4:4:39:TRP:HB3	1.39	1.37
17:N:62:SER:HB3	17:N:66:ASP:CG	1.45	1.37
5:A:744:ALA:HB2	22:A:1806:BCR:C39	1.53	1.36
9:E:52:VAL:O	9:E:53:VAL:CG2	1.73	1.36
19:G:1099:CLA:HBC3	19:G:1099:CLA:CHD	1.52	1.36
19:4:1201:CLA:CBA	19:4:1201:CLA:HMA2	1.55	1.36
2:2:43:TRP:CH2	2:2:125:PHE:CD2	2.13	1.36
19:A:1770:CLA:C4B	22:A:1802:BCR:H19C	1.55	1.36
17:N:72:LYS:HB3	17:N:73:ASP:CA	1.48	1.36
17:N:72:LYS:HG3	17:N:74:LYS:CB	1.56	1.35
19:A:1783:CLA:H203	22:A:1807:BCR:C17	1.55	1.35
2:2:42:ARG:HA	2:2:45:VAL:CG2	1.54	1.35
14:J:31:ARG:HH22	19:J:1043:CLA:C4B	1.38	1.35
3:3:194:ILE:CD1	19:3:1214:CLA:HMC2	1.54	1.35
4:4:121:PHE:CE2	4:4:122:LYS:O	1.79	1.35
16:L:164:PRO:HB2	16:L:165:TYR:CA	1.44	1.35
20:A:7033:LMU:H3'	20:A:7033:LMU:C6B	1.55	1.34
16:L:161:LEU:HD12	16:L:162:ASP:CA	1.54	1.34
20:N:1086:LMU:H121	20:N:1086:LMU:C8	1.56	1.34
17:N:61:LEU:HD11	17:N:63:ASP:CA	1.56	1.34
20:A:7037:LMU:C7	20:A:7037:LMU:H32	1.52	1.34
4:4:122:LYS:CB	4:4:143:PHE:CD2	2.07	1.34
17:N:47:THR:HG21	17:N:54:LYS:NZ	1.37	1.34
16:L:164:PRO:HD2	16:L:165:TYR:CD2	1.60	1.34
1:1:27:LEU:CD2	6:B:314:ARG:CG	2.04	1.34
4:4:101:VAL:HG13	4:4:104:ARG:NH2	1.40	1.34
19:A:1797:CLA:HHH	19:A:1797:CLA:CBC	1.55	1.34
21:B:8055:SUC:C6'	21:B:8055:SUC:H1'1	1.55	1.34
20:A:7048:LMU:C3	20:A:7048:LMU:H5'	1.58	1.33
1:1:185:TRP:HB2	1:1:186:HIS:CE1	1.63	1.33
19:3:1224:CLA:HBC3	19:3:1224:CLA:CMC	1.50	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1754:CLA:CBC	19:B:1754:CLA:HMC1	1.59	1.33
20:K:1086:LMU:H81	20:K:1086:LMU:C4	1.47	1.33
19:4:1198:CLA:C20	19:4:1198:CLA:H151	1.58	1.32
13:I:11:LEU:CD1	22:I:1032:BCR:H10C	1.60	1.32
2:2:205:PHE:HD1	2:2:206:ALA:N	1.15	1.32
19:J:1044:CLA:H72	19:J:1044:CLA:C4	1.58	1.32
11:G:6:LEU:HB3	11:G:9:SER:CB	1.59	1.32
9:E:52:VAL:O	9:E:53:VAL:HG23	1.23	1.32
2:2:42:ARG:CA	2:2:45:VAL:HG23	1.58	1.32
4:4:107:GLN:C	19:4:1196:CLA:CMA	1.96	1.32
19:A:1797:CLA:CMA	19:A:1797:CLA:HBA1	1.55	1.32
19:1:1014:CLA:CBC	19:1:1014:CLA:HHD	1.55	1.32
5:A:316:MET:HG2	5:A:317:TYR:CD1	1.62	1.32
19:1:1308:CLA:HBA2	19:1:1308:CLA:CBD	1.58	1.32
10:F:24:LYS:CA	10:F:24:LYS:HE2	1.47	1.32
16:L:163:LEU:HB3	16:L:164:PRO:CB	1.59	1.31
16:L:163:LEU:HD22	16:L:164:PRO:CA	1.58	1.31
16:L:163:LEU:CD1	16:L:164:PRO:HB3	1.60	1.31
20:N:1086:LMU:H52	20:N:1086:LMU:C9	1.44	1.31
19:1:1187:CLA:HBC3	19:1:1187:CLA:CMC	1.46	1.31
4:4:194:VAL:HB	4:4:195:GLN:C	1.50	1.31
4:4:94:GLU:HB3	4:4:95:PHE:CE1	1.64	1.30
20:A:7036:LMU:C7	20:A:7036:LMU:H31	1.45	1.30
17:N:66:ASP:C	17:N:67:LEU:HD12	1.49	1.30
2:2:55:ALA:HB3	2:2:56:MET:CE	1.60	1.30
5:A:316:MET:HB3	5:A:317:TYR:CB	1.62	1.30
20:A:7032:LMU:C2B	20:A:7032:LMU:H31	1.60	1.30
1:1:57:ILE:HD13	1:1:58:LEU:N	1.47	1.30
5:A:567:ARG:NH1	8:D:35:GLY:HA2	1.48	1.29
1:1:112:ARG:NH1	19:1:1195:CLA:CGD	1.91	1.29
4:4:149:ALA:HB3	4:4:151:GLU:CD	1.52	1.29
23:B:1774:PQN:C16	22:B:1781:BCR:C33	2.10	1.29
19:1:1148:CLA:CBC	19:1:1148:CLA:HHD	1.61	1.29
20:B:1783:LMU:H5B	20:B:1783:LMU:C3'	1.63	1.29
19:3:1224:CLA:C10	19:3:1224:CLA:H142	1.62	1.29
19:B:1769:CLA:CBB	19:B:1769:CLA:H93	1.61	1.29
11:G:45:GLU:CG	11:G:49:THR:CG2	2.10	1.29
20:A:7023:LMU:H82	20:A:7023:LMU:C3	1.61	1.29
5:A:24:ARG:C	5:A:26:PRO:HG2	1.53	1.29
19:3:1224:CLA:CED	19:3:1224:CLA:HAA2	1.60	1.29
19:1:1145:CLA:HMC1	19:1:1145:CLA:CBC	1.58	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1803:BCR:C40	22:A:1803:BCR:H23C	1.60	1.28
19:A:1770:CLA:C3B	22:A:1802:BCR:H19C	1.61	1.28
5:A:711:HIS:CD2	19:A:1795:CLA:HBC1	1.67	1.28
3:3:205:GLY:N	5:A:252:ARG:HH22	1.30	1.28
19:1:1148:CLA:HED1	19:1:1148:CLA:C1	1.62	1.28
20:A:7048:LMU:C9	20:A:7048:LMU:H31	1.61	1.28
11:G:6:LEU:CB	11:G:9:SER:HB3	1.60	1.28
2:2:128:ASN:C	2:2:130:LEU:H	1.30	1.28
16:L:163:LEU:HD22	16:L:164:PRO:CB	1.62	1.28
20:A:7023:LMU:C9	20:A:7023:LMU:H21	1.60	1.28
19:4:4014:CLA:HED2	19:4:4014:CLA:C2A	1.61	1.28
19:A:1779:CLA:CBB	22:A:1804:BCR:C35	2.10	1.27
19:3:1224:CLA:CBC	19:3:1224:CLA:HMC1	1.63	1.27
22:3:1225:BCR:C39	22:3:1225:BCR:H23C	1.55	1.27
20:A:7036:LMU:H82	20:A:7036:LMU:C3	1.62	1.27
2:2:118:CYS:O	2:2:119:VAL:HG13	1.18	1.27
6:B:732:LYS:CB	6:B:733:PHE:HA	1.63	1.27
16:L:161:LEU:HD12	16:L:162:ASP:N	1.50	1.27
17:N:65:LEU:HD23	17:N:65:LEU:C	1.53	1.27
20:A:7037:LMU:H72	20:A:7037:LMU:C3	1.55	1.27
3:3:132:TRP:CH2	3:3:155:GLU:CG	2.12	1.27
7:C:17:CYS:HB2	7:C:58:CYS:SG	1.74	1.27
4:4:147:LEU:HD21	4:4:148:GLU:CG	1.63	1.27
4:4:37:LEU:N	4:4:39:TRP:HB2	1.46	1.27
17:N:67:LEU:HB2	17:N:68:GLU:CG	1.65	1.27
12:H:20:GLN:HB3	12:H:22:ASP:CB	1.64	1.27
19:A:1781:CLA:HED1	19:A:1782:CLA:C2D	1.65	1.26
19:4:1201:CLA:HAA2	19:4:1201:CLA:CGD	1.66	1.26
19:4:4014:CLA:H2A	19:4:4014:CLA:CED	1.65	1.26
19:1:1188:CLA:C12	19:1:1188:CLA:H92	1.58	1.26
17:N:45:ASN:ND2	17:N:54:LYS:CB	1.99	1.26
20:A:7023:LMU:C9	20:A:7023:LMU:H41	1.64	1.26
12:H:25:GLY:CA	12:H:27:ASP:H	1.47	1.26
5:A:79:PHE:CE2	5:A:185:HIS:CD2	2.24	1.26
20:A:7020:LMU:H6E	20:A:7020:LMU:C5B	1.64	1.26
4:4:40:PHE:O	4:4:43:ALA:HB3	1.34	1.25
17:N:41:LYS:HB2	17:N:42:PHE:CB	1.66	1.25
17:N:67:LEU:CB	17:N:68:GLU:HG2	1.66	1.25
20:A:7048:LMU:C3'	20:A:7048:LMU:H22	1.64	1.25
20:N:1086:LMU:C1'	20:N:1086:LMU:H32	1.64	1.25
19:A:1776:CLA:CMD	19:A:1778:CLA:HBB2	1.66	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1797:CLA:C12	19:A:1797:CLA:H71	1.47	1.25
19:4:1200:CLA:HBC2	19:4:1200:CLA:CMC	1.59	1.25
17:N:72:LYS:CG	17:N:74:LYS:HG3	1.67	1.25
11:G:93:TYR:CA	11:G:94:ASP:HB2	1.64	1.25
15:K:7:THR:CA	15:K:10:ILE:HD13	1.55	1.25
19:2:1212:CLA:O1A	19:2:1212:CLA:H42	1.37	1.25
19:1:1014:CLA:H43	19:1:1014:CLA:C10	1.67	1.25
20:A:7048:LMU:C3	20:A:7048:LMU:H82	1.66	1.25
4:4:104:ARG:HH11	4:4:105:ARG:CB	1.47	1.24
3:3:74:ALA:HA	19:3:1217:CLA:C3D	1.68	1.24
4:4:94:GLU:HG2	4:4:95:PHE:CD1	1.72	1.24
22:I:1032:BCR:HC8	22:I:1032:BCR:C31	1.61	1.24
20:A:7042:LMU:C6	20:A:7042:LMU:H22	1.58	1.24
5:A:25:ASP:N	5:A:26:PRO:HG2	1.52	1.24
19:1:1187:CLA:CBC	19:1:1187:CLA:HMC1	1.64	1.24
4:4:34:PRO:CB	4:4:35:GLU:HB2	1.67	1.24
22:B:1780:BCR:H321	22:B:1780:BCR:C8	1.55	1.24
4:4:149:ALA:CB	4:4:151:GLU:HG2	1.66	1.24
4:4:39:TRP:C	4:4:40:PHE:HD1	1.38	1.24
1:1:27:LEU:CD2	6:B:314:ARG:HG2	1.60	1.24
3:3:181:LEU:N	3:3:182:LYS:CG	2.01	1.24
20:A:7050:LMU:C10	20:A:7050:LMU:H32	1.67	1.24
20:A:7039:LMU:C6B	20:A:7039:LMU:H3'	1.66	1.24
4:4:121:PHE:O	4:4:122:LYS:HD2	1.36	1.24
19:1:1014:CLA:C8	19:1:1014:CLA:H41	1.66	1.24
19:4:1198:CLA:HED3	19:4:1198:CLA:CAA	1.68	1.23
4:4:192:THR:HG22	4:4:193:ILE:O	1.35	1.23
15:K:11:MET:SD	15:K:12:VAL:HA	1.76	1.23
6:B:732:LYS:CB	6:B:733:PHE:CA	2.14	1.23
20:N:1086:LMU:C5	20:N:1086:LMU:H92	1.67	1.23
12:H:20:GLN:CB	12:H:22:ASP:HB3	1.65	1.23
19:4:4007:CLA:CED	19:4:4007:CLA:H12	1.67	1.23
19:4:1200:CLA:CBC	19:4:1200:CLA:HMC1	1.58	1.23
20:A:7042:LMU:C2	20:A:7042:LMU:H71	1.69	1.23
20:A:7016:LMU:C3	20:A:7016:LMU:H81	1.69	1.23
20:A:7050:LMU:C3	20:A:7050:LMU:H81	1.66	1.23
7:C:62:PHE:CE2	9:E:42:GLU:OE1	1.90	1.23
19:K:1085:CLA:O1A	19:K:1085:CLA:H3A	1.38	1.23
6:B:25:ILE:CG2	22:L:1169:BCR:C28	2.16	1.23
4:4:147:LEU:CD1	4:4:148:GLU:H	1.52	1.23
6:B:25:ILE:CG2	22:L:1169:BCR:H292	1.59	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:1086:LMU:H6E	20:N:1086:LMU:C5	1.68	1.22
20:K:1086:LMU:H42	20:K:1086:LMU:C8	1.67	1.22
19:A:1783:CLA:C20	22:A:1807:BCR:H17C	1.68	1.22
6:B:732:LYS:HG2	6:B:734:GLY:N	0.90	1.22
3:3:74:ALA:HA	19:3:1217:CLA:C2D	1.67	1.22
20:A:7022:LMU:H2'	20:A:7022:LMU:C2	1.65	1.22
7:C:7:ILE:O	7:C:8:TYR:O	1.55	1.22
4:4:68:GLY:O	4:4:71:ASN:HB2	1.34	1.22
20:A:7023:LMU:H2B	20:A:7023:LMU:C6B	1.65	1.22
20:A:7032:LMU:C1B	20:A:7032:LMU:H31	1.68	1.22
19:A:1763:CLA:C1	19:A:1765:CLA:HED3	1.69	1.22
5:A:342:GLY:CA	5:A:430:ASP:HB2	1.69	1.22
4:4:30:LEU:CA	4:4:31:ALA:HB3	1.69	1.22
20:A:7050:LMU:H32	20:A:7050:LMU:C8	1.68	1.22
4:4:144:ALA:HB3	4:4:147:LEU:O	1.38	1.22
4:4:124:TYR:O	4:4:127:PRO:HD2	1.36	1.22
6:B:517:PHE:O	6:B:517:PHE:CD2	1.93	1.22
19:A:1781:CLA:HED1	19:A:1782:CLA:C3D	1.69	1.21
19:A:1781:CLA:HED2	19:A:1782:CLA:CAD	1.70	1.21
5:A:331:LEU:HD11	5:A:346:LEU:CB	1.68	1.21
2:2:43:TRP:CH2	2:2:125:PHE:CG	2.18	1.21
19:1:1148:CLA:CED	19:1:1148:CLA:C2	2.13	1.21
20:A:7050:LMU:C5	20:A:7050:LMU:H92	1.49	1.21
21:B:8056:SUC:H3'	21:B:8056:SUC:O2	1.38	1.21
4:4:170:HIS:O	4:4:171:ASN:O	1.58	1.21
5:A:328:LYS:CG	5:A:332:GLU:HB2	1.70	1.21
16:L:163:LEU:CD2	16:L:164:PRO:HB3	1.71	1.21
20:B:1783:LMU:H61	20:B:1783:LMU:C11	1.69	1.21
20:A:7050:LMU:C3	20:A:7050:LMU:H101	1.69	1.21
19:R:1054:CLA:HED3	19:R:1054:CLA:C1A	1.68	1.21
19:4:1196:CLA:HHD	19:4:1196:CLA:CBC	1.71	1.21
17:N:57:LYS:CG	17:N:58:VAL:H	1.52	1.21
5:A:21:LEU:HD12	5:A:21:LEU:O	1.38	1.21
20:A:7020:LMU:C6'	20:A:7020:LMU:H5B	1.70	1.21
1:1:179:THR:HG21	4:4:87:SER:CB	1.70	1.21
19:A:1779:CLA:CBB	22:A:1804:BCR:H351	1.71	1.21
18:R:41:UNK:CB	18:R:42:UNK:HA	1.68	1.21
19:4:1201:CLA:CMA	19:4:1201:CLA:HBA1	1.55	1.21
5:A:316:MET:HB3	5:A:317:TYR:CG	1.74	1.21
17:N:61:LEU:HD12	17:N:62:SER:C	1.62	1.21
19:1:1014:CLA:HED3	19:1:1014:CLA:C2A	1.69	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:48:PHE:CD2	3:3:49:ILE:HG22	1.74	1.21
4:4:171:ASN:O	4:4:173:THR:N	1.74	1.21
5:A:76:ARG:NH1	5:A:192:LYS:HG2	1.56	1.20
9:E:86:GLU:HG3	9:E:87:VAL:N	1.49	1.20
4:4:122:LYS:CB	4:4:143:PHE:HD2	1.46	1.20
19:A:1771:CLA:HED2	19:A:1771:CLA:CAA	1.69	1.20
4:4:94:GLU:HG2	4:4:95:PHE:CE1	1.75	1.20
17:N:45:ASN:ND2	17:N:54:LYS:HB2	1.53	1.20
19:A:1797:CLA:HMA2	19:A:1797:CLA:CBA	1.66	1.20
6:B:403:ASN:O	6:B:406:ASN:CB	1.89	1.20
19:B:1769:CLA:C15	22:B:1780:BCR:C31	2.18	1.20
20:A:7036:LMU:H22	20:A:7036:LMU:C8	1.72	1.20
17:N:79:SER:HA	17:N:80:ASN:O	1.37	1.20
6:B:120:VAL:HA	6:B:123:TRP:CD1	1.75	1.20
4:4:118:ASP:OD1	4:4:123:GLN:HB2	1.38	1.20
4:4:147:LEU:CG	4:4:148:GLU:H	1.53	1.20
1:1:179:THR:CG2	4:4:87:SER:CB	2.20	1.19
4:4:104:ARG:HD2	19:4:1208:CLA:C2C	1.71	1.19
17:N:70:GLU:OE2	17:N:72:LYS:O	1.58	1.19
20:A:7016:LMU:C9	20:A:7016:LMU:H32	1.72	1.19
4:4:107:GLN:HA	19:4:1196:CLA:CMA	1.70	1.19
11:G:46:ALA:N	11:G:48:ASP:HB3	1.56	1.19
4:4:192:THR:HG22	4:4:193:ILE:C	1.60	1.19
19:4:4007:CLA:HED3	19:4:4007:CLA:C1	1.71	1.19
1:1:63:LEU:HD22	1:1:63:LEU:C	1.50	1.19
18:R:52:UNK:HA	18:R:53:UNK:CB	1.69	1.19
5:A:541:VAL:HG11	5:A:615:HIS:CD2	1.78	1.19
19:B:1756:CLA:HBB1	19:B:1770:CLA:CMB	1.73	1.19
19:1:1196:CLA:CAD	19:1:1196:CLA:HED2	1.66	1.19
19:G:1099:CLA:CBC	19:G:1099:CLA:HHD	1.71	1.19
17:N:48:GLY:CA	17:N:49:CYS:SG	2.30	1.19
19:1:1014:CLA:CGD	19:1:1014:CLA:HBA1	1.71	1.19
20:A:7021:LMU:C1'	20:A:7021:LMU:H31	1.67	1.19
5:A:331:LEU:O	5:A:331:LEU:HD23	1.42	1.18
19:B:1754:CLA:H43	19:B:1754:CLA:C1A	1.72	1.18
6:B:25:ILE:CG2	22:L:1169:BCR:H282	1.72	1.18
21:B:8052:SUC:C4'	21:B:8052:SUC:H1	1.65	1.18
22:3:1225:BCR:C23	22:3:1225:BCR:H393	1.67	1.18
2:2:169:LEU:HD22	19:2:1215:CLA:CAB	1.72	1.18
22:B:1780:BCR:C27	22:B:1780:BCR:H403	1.52	1.18
10:F:24:LYS:HE2	10:F:24:LYS:N	1.56	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:342:GLY:HA3	5:A:430:ASP:CB	1.73	1.18
1:1:25:ASP:H	6:B:314:ARG:NH2	1.40	1.18
20:A:7039:LMU:H6'2	20:A:7039:LMU:C3'	1.74	1.18
4:4:34:PRO:HA	4:4:35:GLU:CB	1.70	1.18
22:A:1806:BCR:C31	19:A:1812:CLA:C14	2.20	1.18
19:B:1754:CLA:C10	19:B:1754:CLA:H151	1.65	1.18
1:1:57:ILE:HD13	1:1:57:ILE:C	1.62	1.18
11:G:45:GLU:HG2	11:G:49:THR:HG23	1.19	1.17
3:3:132:TRP:CZ3	3:3:155:GLU:CD	2.06	1.17
20:A:7050:LMU:C9	20:A:7050:LMU:H32	1.73	1.17
19:B:1756:CLA:CBC	19:B:1756:CLA:HHD	1.74	1.17
19:A:1781:CLA:HED1	19:A:1782:CLA:CMD	1.74	1.17
16:L:163:LEU:CB	16:L:164:PRO:HG3	1.75	1.17
17:N:57:LYS:HG3	17:N:58:VAL:N	1.44	1.17
14:J:31:ARG:NH2	19:J:1043:CLA:C4B	2.06	1.17
4:4:107:GLN:CA	19:4:1196:CLA:CMA	2.21	1.17
19:B:1769:CLA:C9	19:B:1769:CLA:HBB2	1.75	1.17
7:C:1:MET:H2	7:C:3:HIS:N	1.42	1.17
19:A:1779:CLA:C4C	22:A:1804:BCR:C19	2.23	1.17
17:N:72:LYS:CB	17:N:73:ASP:HA	1.73	1.17
19:A:1781:CLA:H72	19:A:1782:CLA:CED	1.73	1.16
4:4:147:LEU:CD2	4:4:148:GLU:HG3	1.75	1.16
4:4:30:LEU:HD12	4:4:30:LEU:O	1.45	1.16
5:A:79:PHE:CE2	5:A:185:HIS:NE2	2.13	1.16
16:L:164:PRO:CG	16:L:165:TYR:CG	2.28	1.16
17:N:41:LYS:CB	17:N:42:PHE:HB3	1.75	1.16
15:K:10:ILE:HA	15:K:13:THR:CG2	1.72	1.16
5:A:702:GLU:OE2	6:B:550:LYS:NZ	1.76	1.16
6:B:25:ILE:HG21	22:L:1169:BCR:C28	1.70	1.16
3:3:132:TRP:HH2	3:3:155:GLU:OE2	0.82	1.16
19:B:1769:CLA:H161	22:B:1780:BCR:H313	1.24	1.16
19:B:1787:CLA:C9	19:B:1788:CLA:H91	1.75	1.16
11:G:46:ALA:N	11:G:49:THR:HG21	1.58	1.16
4:4:194:VAL:CG1	4:4:195:GLN:HB2	1.75	1.16
19:L:1168:CLA:HBC3	19:L:1168:CLA:HHD	1.20	1.16
5:A:81:ALA:CB	19:A:1760:CLA:CMA	2.24	1.16
11:G:33:LYS:CE	11:G:33:LYS:HA	1.66	1.16
3:3:132:TRP:HH2	3:3:155:GLU:CD	1.21	1.16
25:B:1785:SF4:S2	25:B:1785:SF4:S3	2.44	1.16
19:G:1099:CLA:H3A	19:G:1099:CLA:O2A	1.44	1.16
17:N:63:ASP:H	17:N:64:ASP:CB	1.57	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:70:GLU:O	17:N:72:LYS:HD3	1.41	1.16
20:A:7026:LMU:O3B	21:B:8062:SUC:H5'	1.37	1.16
5:A:81:ALA:CB	19:A:1760:CLA:HMA1	1.75	1.15
3:3:110:SER:C	3:3:111:TYR:HD2	1.48	1.15
4:4:36:ASN:OD1	4:4:37:LEU:HA	1.44	1.15
1:1:179:THR:CB	4:4:87:SER:HB3	1.77	1.15
19:1:1241:CLA:HAC2	22:I:1032:BCR:HC31	1.28	1.15
2:2:110:TRP:HD1	2:2:113:ILE:HG21	1.11	1.15
6:B:87:ILE:HA	6:B:115:ASN:HA	1.25	1.15
6:B:672:GLN:HA	6:B:672:GLN:HE21	1.09	1.15
16:L:163:LEU:HD13	16:L:164:PRO:HB3	1.27	1.15
5:A:316:MET:CG	5:A:317:TYR:CD1	2.30	1.15
19:R:1055:CLA:C9	20:R:1056:LMU:O4'	1.94	1.15
20:A:7016:LMU:H21	20:A:7016:LMU:C8	1.75	1.15
20:A:7022:LMU:C2'	20:A:7022:LMU:H21	1.59	1.15
21:B:8062:SUC:H1'2	21:B:8062:SUC:C6'	1.71	1.15
8:D:134:MET:SD	8:D:134:MET:N	2.19	1.15
20:A:7014:LMU:H11	20:A:7014:LMU:H62	1.17	1.15
4:4:94:GLU:CB	4:4:95:PHE:CE1	2.29	1.15
4:4:38:ARG:HG3	4:4:39:TRP:N	1.48	1.15
4:4:174:GLY:O	4:4:175:LYS:HG3	1.47	1.15
5:A:160:SER:O	5:A:163:GLN:HG2	1.44	1.15
4:4:36:ASN:CB	4:4:39:TRP:CE3	2.29	1.15
23:B:1774:PQN:C19	22:B:1781:BCR:C10	2.24	1.15
7:C:1:MET:CB	7:C:4:SER:OG	1.94	1.15
20:N:1086:LMU:O5'	20:N:1086:LMU:H32	1.47	1.15
4:4:36:ASN:C	4:4:39:TRP:HB2	1.66	1.14
16:L:164:PRO:CD	16:L:165:TYR:CE2	2.29	1.14
19:1:1188:CLA:C1A	19:1:1188:CLA:HED3	1.77	1.14
3:3:194:ILE:HD11	19:3:1214:CLA:HMC2	1.26	1.14
11:G:33:LYS:HE3	11:G:33:LYS:HA	1.24	1.14
1:1:185:TRP:CB	1:1:186:HIS:CE1	2.29	1.14
4:4:89:THR:O	4:4:92:VAL:HB	1.48	1.14
19:A:1772:CLA:HMC1	19:A:1772:CLA:HBC3	1.30	1.14
19:A:1781:CLA:HBA2	19:A:1794:CLA:HED1	1.28	1.14
22:A:1803:BCR:H403	22:A:1803:BCR:H23C	1.28	1.14
20:A:7036:LMU:C8	20:A:7036:LMU:H31	1.77	1.14
17:N:72:LYS:HG3	17:N:74:LYS:CG	1.78	1.14
20:B:1783:LMU:C7	20:B:1783:LMU:H112	1.77	1.14
19:3:1224:CLA:HED1	19:3:1224:CLA:HBA1	1.19	1.14
5:A:316:MET:HB3	5:A:317:TYR:CD1	1.82	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:25:GLY:HA3	12:H:27:ASP:N	1.60	1.14
20:A:7004:LMU:H3'	20:A:7004:LMU:H12	1.21	1.14
4:4:99:HIS:CE1	4:4:103:ILE:CD1	2.30	1.14
19:B:1739:CLA:HBB2	19:B:1739:CLA:C9	1.77	1.14
2:2:102:ILE:C	19:2:1222:CLA:HBB2	1.66	1.14
19:A:1781:CLA:C4B	22:A:1805:BCR:H373	1.77	1.14
19:B:1735:CLA:HMD3	22:B:1779:BCR:HC41	1.20	1.14
19:A:1788:CLA:H52	22:B:1781:BCR:H343	1.19	1.14
6:B:493:TRP:O	6:B:495:PRO:HD3	1.48	1.14
16:L:164:PRO:CG	16:L:165:TYR:CD1	2.30	1.14
19:1:1308:CLA:CBA	19:1:1308:CLA:HBD	1.76	1.14
2:2:43:TRP:HH2	2:2:125:PHE:CD2	1.56	1.14
19:A:1779:CLA:CHD	22:A:1804:BCR:C19	2.25	1.14
6:B:22:TRP:NE1	19:B:1771:CLA:HBB1	1.60	1.14
16:L:163:LEU:CD2	16:L:164:PRO:HA	1.76	1.14
3:3:92:TRP:HA	3:3:93:PHE:CD1	1.80	1.14
5:A:76:ARG:CZ	5:A:192:LYS:HG2	1.77	1.13
19:A:1800:CLA:HMA3	16:L:27:VAL:HA	1.17	1.13
5:A:435:VAL:O	5:A:438:HIS:O	1.66	1.13
19:B:1754:CLA:C15	19:B:1754:CLA:H102	1.76	1.13
4:4:74:LYS:N	4:4:75:TRP:HA	1.50	1.13
17:N:61:LEU:C	17:N:61:LEU:HD12	1.65	1.13
19:R:1055:CLA:H92	20:R:1056:LMU:O4'	1.49	1.13
20:A:7010:LMU:O2B	20:A:7010:LMU:H3'	1.47	1.13
19:B:1760:CLA:HMC1	19:B:1760:CLA:CBC	1.77	1.13
25:B:1785:SF4:S2	25:B:1785:SF4:S4	2.46	1.13
2:2:169:LEU:CD2	19:2:1215:CLA:CBB	2.27	1.13
19:B:1743:CLA:CAC	19:B:1744:CLA:HBB2	1.60	1.13
25:B:1785:SF4:S4	25:B:1785:SF4:S1	2.46	1.13
5:A:251:ASN:O	5:A:253:ASP:N	1.80	1.13
20:N:1086:LMU:H121	20:N:1086:LMU:H82	1.26	1.13
5:A:316:MET:CB	5:A:317:TYR:CD1	2.30	1.13
15:K:9:LEU:HD23	15:K:9:LEU:N	1.53	1.13
20:A:7009:LMU:H5B	20:A:7009:LMU:O3'	1.45	1.13
2:2:38:PRO:HB2	2:2:40:SER:OG	1.45	1.13
4:4:94:GLU:CG	4:4:95:PHE:CE1	2.30	1.13
2:2:39:GLU:N	2:2:40:SER:HB2	1.63	1.13
4:4:104:ARG:HH11	4:4:105:ARG:HB2	1.13	1.13
4:4:37:LEU:O	4:4:39:TRP:HB3	1.48	1.13
22:A:1806:BCR:H313	19:A:1812:CLA:C14	1.76	1.13
6:B:596:TRP:CH2	6:B:612:SER:O	2.02	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:14:CYS:CA	7:C:17:CYS:SG	2.36	1.13
21:3:1226:SUC:C1'	21:3:1226:SUC:H6'2	1.69	1.13
19:B:1752:CLA:HBC2	19:B:1752:CLA:HHD	1.13	1.13
3:3:110:SER:O	3:3:111:TYR:HD2	1.31	1.13
21:B:8059:SUC:C1'	21:B:8059:SUC:H6'2	1.75	1.13
21:B:8059:SUC:H1'1	21:B:8059:SUC:H6'2	1.27	1.13
5:A:402:ILE:HG13	19:A:1784:CLA:HBB2	1.29	1.13
16:L:66:GLY:HA3	19:L:1168:CLA:CHC	1.79	1.13
22:B:1780:BCR:C32	22:B:1780:BCR:HC8	1.66	1.12
16:L:164:PRO:CD	16:L:165:TYR:CZ	2.32	1.12
17:N:61:LEU:HD12	17:N:62:SER:N	1.63	1.13
5:A:423:ASP:HB3	5:A:424:PRO:HD3	1.20	1.13
5:A:451:ILE:HD12	19:A:1788:CLA:HED3	1.29	1.12
19:B:1769:CLA:C16	22:B:1780:BCR:H313	1.78	1.12
19:1:1196:CLA:O1D	19:1:1196:CLA:HAA2	1.46	1.12
19:3:1221:CLA:CHA	19:3:3011:CLA:CBC	2.27	1.12
25:B:1785:SF4:S3	25:B:1785:SF4:S4	2.46	1.12
21:B:8060:SUC:O1'	21:B:8060:SUC:H5	1.49	1.12
2:2:40:SER:O	2:2:41:LEU:HD22	1.45	1.12
5:A:590:CYS:SG	25:B:1785:SF4:S4	2.47	1.12
17:N:58:VAL:CB	17:N:59:PRO:HD2	1.77	1.12
19:1:1014:CLA:O2D	19:1:1014:CLA:HBA1	1.47	1.12
15:K:11:MET:SD	15:K:12:VAL:CA	2.36	1.12
15:K:10:ILE:O	15:K:13:THR:HG23	1.50	1.12
21:B:8053:SUC:O2	21:B:8053:SUC:H5'	1.48	1.12
2:2:41:LEU:C	2:2:41:LEU:HD23	1.64	1.12
4:4:122:LYS:CB	4:4:143:PHE:HB2	1.79	1.12
4:4:89:THR:N	4:4:90:LEU:HD22	1.64	1.12
6:B:58:PHE:HB2	6:B:146:SER:HB3	1.27	1.12
17:N:61:LEU:CD1	17:N:63:ASP:HB2	1.79	1.12
17:N:75:TYR:O	17:N:76:LYS:O	1.68	1.12
5:A:316:MET:HG2	5:A:317:TYR:CE1	1.83	1.12
6:B:403:ASN:O	6:B:406:ASN:HB3	0.96	1.12
19:4:1199:CLA:HAA1	19:F:1157:CLA:H42	1.30	1.12
4:4:91:PHE:CD2	19:4:1207:CLA:C3C	2.31	1.12
4:4:107:GLN:C	19:4:1196:CLA:HMA3	1.61	1.12
6:B:131:THR:HB	6:B:134:ASP:HB2	1.16	1.12
22:I:1032:BCR:C4	22:I:1032:BCR:H322	1.59	1.12
20:A:7036:LMU:C8	20:A:7036:LMU:C3	2.28	1.12
20:A:7033:LMU:C3'	20:A:7033:LMU:H6'2	1.78	1.12
3:3:158:TYR:HB3	3:3:159:PRO:HD2	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:168:ARG:O	2:2:172:LEU:HD12	1.50	1.11
22:B:1781:BCR:H382	22:B:1781:BCR:H23C	1.22	1.11
19:1:1145:CLA:HMC1	19:1:1145:CLA:HBC3	1.20	1.11
19:4:1196:CLA:HHD	19:4:1196:CLA:HBC2	1.21	1.11
19:4:1199:CLA:HMC1	19:4:1199:CLA:HBC3	1.11	1.11
4:4:33:ASP:HB3	4:4:34:PRO:HD3	1.32	1.11
19:A:1781:CLA:CED	19:A:1782:CLA:HMD1	1.80	1.11
23:B:1774:PQN:H191	22:B:1781:BCR:C10	1.78	1.11
16:L:164:PRO:CB	16:L:165:TYR:CA	2.28	1.11
19:1:1148:CLA:HBC3	19:1:1148:CLA:HHD	1.18	1.11
15:K:17:LEU:HG	15:K:56:THR:OG1	1.49	1.11
4:4:147:LEU:HD22	4:4:148:GLU:N	1.65	1.11
6:B:608:GLN:HA	6:B:608:GLN:HE21	1.01	1.11
20:B:1783:LMU:H3'	20:B:1783:LMU:C5B	1.80	1.11
21:B:8052:SUC:C1	21:B:8052:SUC:C5'	2.27	1.11
20:A:7030:LMU:H91	20:A:7030:LMU:C5	1.68	1.11
5:A:331:LEU:HD11	5:A:346:LEU:HB3	1.22	1.11
11:G:12:THR:HG22	11:G:72:LEU:HG	1.20	1.11
11:G:45:GLU:C	11:G:49:THR:HG21	1.69	1.11
2:2:44:ASN:ND2	14:J:1:MET:SD	2.22	1.11
19:B:1760:CLA:HMC1	19:B:1760:CLA:HBC2	1.27	1.11
16:L:164:PRO:CD	16:L:165:TYR:CD2	2.33	1.11
19:1:1188:CLA:HED1	19:1:1188:CLA:H2	1.29	1.11
20:A:7023:LMU:H92	20:A:7023:LMU:H41	1.13	1.11
20:A:7048:LMU:C8	20:A:7048:LMU:H31	1.81	1.11
20:A:7016:LMU:H22	20:A:7016:LMU:C6	1.57	1.11
10:F:25:LEU:CD2	10:F:46:MET:HB3	1.80	1.11
20:A:7026:LMU:O4'	21:B:8062:SUC:H3'	1.38	1.11
19:A:1797:CLA:C7	19:A:1797:CLA:H122	1.79	1.11
11:G:43:HIS:CA	11:G:44:PHE:HB3	1.79	1.11
17:N:67:LEU:C	17:N:68:GLU:HG3	1.71	1.11
3:3:52:LYS:O	3:3:56:TYR:CD2	2.03	1.11
20:A:7048:LMU:H52	20:A:7048:LMU:C1	1.72	1.11
20:A:7016:LMU:H22	20:A:7016:LMU:H61	1.25	1.11
10:F:22:LEU:H	10:F:22:LEU:CD1	1.64	1.11
18:R:46:UNK:CB	18:R:47:UNK:CB	2.28	1.11
8:D:113:HIS:NE2	8:D:118:VAL:HG11	1.63	1.11
4:4:128:ALA:CB	4:4:143:PHE:CE2	2.32	1.10
4:4:94:GLU:CG	4:4:95:PHE:CD1	2.34	1.10
19:A:1797:CLA:HHD	19:A:1797:CLA:HBC2	1.27	1.10
22:A:1802:BCR:H402	22:A:1802:BCR:H23C	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:66:ARG:HH21	7:C:66:ARG:HG2	1.16	1.10
4:4:69:ILE:HG22	4:4:70:ILE:H	0.97	1.10
17:N:62:SER:CB	17:N:66:ASP:CB	2.28	1.10
17:N:72:LYS:HG3	17:N:74:LYS:CA	1.79	1.10
19:1:1148:CLA:CGA	19:1:1148:CLA:CED	2.29	1.10
18:R:38:UNK:O	18:R:42:UNK:HA	1.48	1.10
4:4:122:LYS:HB3	4:4:143:PHE:HB2	1.26	1.10
19:A:1770:CLA:HHC	22:A:1802:BCR:H17C	1.31	1.10
2:2:42:ARG:CD	2:2:45:VAL:CG2	2.29	1.10
5:A:308:ILE:CD1	19:A:1772:CLA:C9	2.30	1.10
5:A:208:ALA:HA	5:A:310:PHE:O	1.50	1.10
18:R:34:UNK:CB	18:R:35:UNK:CB	2.29	1.10
20:B:1783:LMU:C5B	20:B:1783:LMU:C3'	2.29	1.10
20:A:7016:LMU:C8	20:A:7016:LMU:H32	1.80	1.10
5:A:331:LEU:HD21	5:A:343:HIS:O	0.94	1.10
6:B:189:ALA:CB	19:B:1759:CLA:H203	1.80	1.10
5:A:98:PHE:CZ	19:A:1763:CLA:HMD3	1.87	1.10
19:A:1771:CLA:HBA1	19:A:1771:CLA:CHA	1.75	1.10
19:1:1014:CLA:HBC3	19:1:1014:CLA:HHD	1.23	1.10
5:A:25:ASP:HB3	5:A:26:PRO:HD2	1.10	1.10
21:B:8062:SUC:H1'2	21:B:8062:SUC:H6'1	1.31	1.10
2:2:211:LYS:HA	2:2:211:LYS:HE2	1.33	1.10
6:B:247:THR:CA	6:B:250:ALA:HB2	1.80	1.10
4:4:93:ILE:HA	4:4:96:ILE:HD12	1.20	1.10
5:A:81:ALA:HB2	19:A:1760:CLA:CMA	1.79	1.10
19:A:1771:CLA:HBC3	19:A:1771:CLA:CMC	1.70	1.10
5:A:581:CYS:HB2	5:A:590:CYS:HA	1.22	1.10
11:G:48:ASP:CB	11:G:49:THR:CG2	2.28	1.10
22:A:1804:BCR:H382	22:A:1804:BCR:H23C	1.19	1.10
6:B:531:THR:HG22	19:B:1756:CLA:HMC2	1.16	1.10
9:E:86:GLU:CG	9:E:87:VAL:H	1.65	1.10
16:L:163:LEU:CB	16:L:164:PRO:CB	2.29	1.10
17:N:72:LYS:HG2	17:N:74:LYS:HG3	1.32	1.10
20:A:7023:LMU:C9	20:A:7023:LMU:C4	2.29	1.10
19:1:1014:CLA:C2A	19:1:1014:CLA:CED	2.29	1.10
20:A:7048:LMU:C3	20:A:7048:LMU:C8	2.30	1.10
20:A:7016:LMU:C2	20:A:7016:LMU:C8	2.30	1.10
10:F:22:LEU:N	10:F:22:LEU:HD12	1.52	1.10
20:A:7030:LMU:C5	20:A:7030:LMU:C9	2.30	1.10
19:A:1797:CLA:H121	19:A:1797:CLA:H71	1.29	1.10
11:G:42:SER:HB2	11:G:45:GLU:CD	1.72	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1770:CLA:HMB2	22:A:1802:BCR:H382	1.34	1.10
17:N:54:LYS:HB3	17:N:57:LYS:HE2	1.19	1.10
20:A:7016:LMU:C3	20:A:7016:LMU:C8	2.29	1.10
5:A:25:ASP:CB	5:A:26:PRO:HD2	1.71	1.10
19:1:1142:CLA:CED	19:K:1085:CLA:CMB	2.30	1.10
19:4:1198:CLA:CAA	19:4:1198:CLA:CED	2.29	1.09
5:A:365:LEU:HD23	19:A:1761:CLA:HED3	1.25	1.09
19:A:1770:CLA:C4B	22:A:1802:BCR:C19	2.28	1.09
4:4:94:GLU:HB3	4:4:95:PHE:CD1	1.86	1.09
6:B:58:PHE:CB	6:B:146:SER:HB3	1.81	1.09
20:A:7023:LMU:C8	20:A:7023:LMU:C4	2.30	1.09
20:B:1783:LMU:C7	20:B:1783:LMU:C11	2.30	1.09
20:A:7048:LMU:C2'	20:A:7048:LMU:C2	2.30	1.09
20:A:7048:LMU:C3	20:A:7048:LMU:H91	1.81	1.09
5:A:25:ASP:HB3	5:A:26:PRO:CD	1.78	1.09
20:A:7033:LMU:C3'	20:A:7033:LMU:C6B	2.30	1.09
20:A:7037:LMU:C1	20:A:7037:LMU:C5	2.29	1.09
5:A:316:MET:HB3	5:A:317:TYR:HB2	1.20	1.09
20:A:7026:LMU:H41	20:A:7026:LMU:C8	1.80	1.09
5:A:335:LYS:HG2	5:A:336:GLY:H	1.12	1.09
4:4:35:GLU:HB3	4:4:36:ASN:HB3	1.32	1.09
19:B:1787:CLA:H93	19:B:1788:CLA:H91	1.13	1.09
19:A:1797:CLA:H122	19:A:1797:CLA:H71	1.18	1.09
9:E:52:VAL:HG12	9:E:53:VAL:H	1.16	1.09
19:B:1741:CLA:H61	12:H:69:SER:HB2	1.10	1.09
19:1:1188:CLA:CGA	19:1:1188:CLA:CMA	2.30	1.09
19:1:1148:CLA:CAA	19:1:1148:CLA:CGD	2.29	1.09
19:1:1014:CLA:C1A	19:1:1014:CLA:CED	2.29	1.09
18:R:41:UNK:CB	18:R:42:UNK:CA	2.29	1.09
20:B:1783:LMU:C6B	20:B:1783:LMU:C3'	2.30	1.09
10:F:47:GLU:HG3	10:F:51:LYS:HE3	1.16	1.09
20:A:7032:LMU:O5B	20:A:7032:LMU:H3'	1.35	1.09
15:K:7:THR:HA	15:K:10:ILE:HD13	1.11	1.09
20:A:7050:LMU:C4	20:A:7050:LMU:H81	1.82	1.09
2:2:42:ARG:CG	2:2:45:VAL:CG2	2.29	1.09
4:4:151:GLU:C	4:4:154:ILE:H	1.56	1.09
5:A:103:PHE:HE1	19:A:1763:CLA:O1D	1.00	1.09
19:A:1781:CLA:CED	19:A:1782:CLA:CAD	2.29	1.09
4:4:95:PHE:CZ	19:4:1210:CLA:NC	1.97	1.09
4:4:94:GLU:CB	4:4:95:PHE:CD1	2.33	1.09
19:A:1760:CLA:H12	19:A:1767:CLA:H61	1.23	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:328:LYS:HG2	5:A:332:GLU:HB2	1.32	1.09
6:B:103:ALA:O	6:B:104:PHE:HB2	1.48	1.09
19:1:1188:CLA:C2A	19:1:1188:CLA:CED	2.30	1.09
19:R:1054:CLA:HED3	19:R:1054:CLA:CHA	1.83	1.09
15:K:20:PHE:HD2	15:K:21:ALA:N	1.50	1.09
19:1:1149:CLA:HBC2	19:1:1149:CLA:HMC1	1.23	1.09
14:J:11:ALA:HB1	14:J:12:PRO:HD2	1.34	1.09
2:2:38:PRO:C	2:2:40:SER:HB2	1.71	1.09
2:2:41:LEU:HG	2:2:42:ARG:N	1.49	1.09
2:2:73:ILE:H	2:2:73:ILE:HD12	1.00	1.09
5:A:588:GLY:CA	6:B:668:ARG:HD3	1.82	1.09
19:1:1241:CLA:CAC	22:I:1032:BCR:HC31	1.81	1.09
16:L:164:PRO:HB2	16:L:165:TYR:CG	1.87	1.09
17:N:72:LYS:CG	17:N:74:LYS:CG	2.31	1.09
17:N:54:LYS:HB3	17:N:57:LYS:CE	1.82	1.09
17:N:72:LYS:CG	17:N:74:LYS:CB	2.31	1.09
20:A:7023:LMU:C8	20:A:7023:LMU:C3	2.30	1.09
19:1:1014:CLA:C11	19:1:1014:CLA:C4	2.29	1.09
19:1:1014:CLA:CHD	19:1:1014:CLA:CBC	2.29	1.09
20:A:7048:LMU:C5	20:A:7048:LMU:C1	2.30	1.09
20:A:7039:LMU:C6B	20:A:7039:LMU:C3'	2.30	1.09
19:1:1196:CLA:CED	19:1:1196:CLA:CAD	2.31	1.09
19:A:1781:CLA:CED	19:A:1782:CLA:CMD	2.30	1.09
22:B:1778:BCR:H23C	22:B:1778:BCR:H382	1.30	1.09
5:A:308:ILE:HD11	19:A:1772:CLA:C9	1.81	1.09
21:B:8052:SUC:H5'	21:B:8052:SUC:H1	1.19	1.09
19:1:1142:CLA:HED1	19:K:1085:CLA:HMB2	1.17	1.09
20:A:7032:LMU:C3	20:A:7032:LMU:C1B	2.30	1.09
20:A:7050:LMU:C9	20:A:7050:LMU:H52	1.81	1.09
5:A:472:ARG:HH12	16:L:74:LEU:HG	1.06	1.08
5:A:328:LYS:CE	5:A:332:GLU:CG	2.30	1.08
16:L:161:LEU:CD1	16:L:162:ASP:CA	2.30	1.08
16:L:163:LEU:CB	16:L:164:PRO:CG	2.29	1.08
18:R:39:UNK:C	18:R:41:UNK:CB	2.30	1.08
8:D:117:GLY:O	8:D:118:VAL:HG23	1.52	1.08
5:A:27:ILE:O	5:A:28:LYS:HG3	1.52	1.08
10:F:102:ARG:HG2	10:F:106:ILE:HD11	1.12	1.08
6:B:282:PHE:HZ	19:B:1747:CLA:C1	1.67	1.08
6:B:119:GLY:HA3	19:B:1759:CLA:HED1	1.11	1.08
19:B:1754:CLA:CMC	19:B:1754:CLA:HBC3	1.65	1.08
19:A:1788:CLA:H161	22:L:1169:BCR:H361	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1014:CLA:C10	19:1:1014:CLA:C4	2.30	1.08
19:J:1044:CLA:C10	19:J:1044:CLA:H152	1.54	1.08
19:3:1224:CLA:CED	19:3:1224:CLA:CAA	2.30	1.08
19:4:4014:CLA:HBC3	19:4:4014:CLA:HMC1	1.21	1.08
19:2:1212:CLA:HMC1	19:2:1212:CLA:CBC	1.82	1.08
4:4:52:MET:HG3	4:4:160:MET:HG3	1.35	1.08
4:4:30:LEU:CA	4:4:31:ALA:CB	2.30	1.08
19:4:1201:CLA:CGA	19:4:1201:CLA:HMA2	1.82	1.08
19:A:1771:CLA:H2A	19:A:1771:CLA:O2D	1.54	1.08
19:B:1743:CLA:CAC	19:B:1744:CLA:HBB1	1.58	1.08
16:L:163:LEU:CD2	16:L:164:PRO:CA	2.29	1.08
20:A:7036:LMU:C7	20:A:7036:LMU:C3	2.29	1.08
19:1:1188:CLA:CED	19:1:1188:CLA:CBA	2.30	1.08
17:N:51:ASP:C	17:N:52:LEU:HD23	1.73	1.08
15:K:11:MET:SD	15:K:11:MET:C	2.30	1.08
3:3:107:TRP:CD1	3:3:108:ALA:N	2.21	1.08
4:4:99:HIS:CE1	4:4:103:ILE:HD12	1.89	1.08
4:4:147:LEU:HD13	4:4:148:GLU:N	1.68	1.08
19:A:1759:CLA:H42	19:A:1796:CLA:H61	1.08	1.08
19:B:1756:CLA:HBC2	19:B:1756:CLA:HHD	1.14	1.08
4:4:119:PRO:HG3	19:4:1208:CLA:C2D	1.82	1.08
16:L:164:PRO:CB	16:L:165:TYR:CB	2.30	1.08
1:1:27:LEU:HD21	6:B:314:ARG:CD	1.83	1.08
20:A:7036:LMU:C8	20:A:7036:LMU:C2	2.30	1.08
20:A:7042:LMU:C3	20:A:7042:LMU:H6D	1.83	1.08
21:B:8055:SUC:O2'	21:B:8055:SUC:H3	1.52	1.08
20:A:7050:LMU:C9	20:A:7050:LMU:C3	2.30	1.08
20:R:1056:LMU:O6B	20:R:1056:LMU:H1B	1.50	1.08
4:4:128:ALA:N	4:4:143:PHE:HZ	1.49	1.07
19:A:1782:CLA:HMC1	19:A:1782:CLA:HBC2	1.31	1.07
2:2:169:LEU:HD23	19:2:1215:CLA:HBB2	1.33	1.07
6:B:302:LYS:O	6:B:303:TYR:HB2	1.50	1.07
22:I:1032:BCR:H313	22:I:1032:BCR:C8	1.74	1.07
20:A:7042:LMU:C3	20:A:7042:LMU:C6'	2.30	1.07
20:N:1086:LMU:O3'	20:N:1086:LMU:H2B	1.54	1.07
3:3:198:PHE:HA	3:3:201:ALA:HB2	1.36	1.07
19:A:1797:CLA:CHD	19:A:1797:CLA:CBC	2.30	1.07
6:B:22:TRP:HE1	19:B:1771:CLA:CBB	1.66	1.07
7:C:54:CYS:CB	25:C:1082:SF4:S3	2.42	1.07
19:A:1780:CLA:OBD	19:A:1780:CLA:H92	1.51	1.07
20:B:1783:LMU:H3'	20:B:1783:LMU:H6'2	1.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:1043:CLA:HED3	19:J:1043:CLA:CHA	1.83	1.07
19:1:1146:CLA:HMC1	19:1:1146:CLA:HBC2	1.35	1.07
10:F:23:LYS:HB2	10:F:24:LYS:HZ1	1.18	1.07
13:I:7:LEU:CD1	22:I:1032:BCR:H333	1.83	1.07
5:A:511:THR:HG23	19:A:1773:CLA:O1A	1.52	1.07
19:B:1754:CLA:H2A	19:B:1754:CLA:O2D	1.52	1.07
6:B:594:TRP:O	6:B:595:HIS:HB3	1.49	1.07
6:B:729:THR:O	6:B:729:THR:HG22	1.53	1.07
11:G:45:GLU:HG3	11:G:49:THR:CG2	1.78	1.07
20:A:7023:LMU:C8	20:A:7023:LMU:H32	1.85	1.07
15:K:10:ILE:C	15:K:13:THR:HG23	1.75	1.07
10:F:42:ILE:HG13	10:F:43:LYS:H	1.14	1.07
5:A:210:LEU:CD1	19:A:1769:CLA:HMB2	1.85	1.07
19:A:1791:CLA:CBC	22:A:1805:BCR:HC31	1.83	1.07
11:G:46:ALA:HA	11:G:48:ASP:OD2	1.54	1.07
4:4:107:GLN:O	19:4:1196:CLA:CMA	1.99	1.07
4:4:75:TRP:CD1	19:4:1205:CLA:HMD3	1.90	1.07
17:N:45:ASN:HD22	17:N:54:LYS:CB	1.64	1.07
20:A:7023:LMU:H32	20:A:7023:LMU:H82	1.13	1.07
2:2:99:LEU:HD22	19:2:1222:CLA:HMC3	1.10	1.07
2:2:169:LEU:CD2	19:2:1215:CLA:CAB	2.32	1.07
2:2:120:ASN:HB3	2:2:121:THR:HB	1.34	1.07
19:A:1782:CLA:HMC1	19:A:1782:CLA:CBC	1.84	1.07
5:A:402:ILE:CG1	19:A:1784:CLA:HBB2	1.85	1.07
17:N:48:GLY:HA3	17:N:49:CYS:O	1.53	1.07
19:J:1044:CLA:C8	19:J:1044:CLA:H41	1.84	1.07
19:J:1044:CLA:C10	19:J:1044:CLA:C15	2.28	1.07
4:4:194:VAL:CG1	4:4:195:GLN:CB	2.28	1.07
20:A:7032:LMU:H12	20:A:7032:LMU:O2'	1.45	1.07
20:A:7050:LMU:H101	20:A:7050:LMU:H31	1.34	1.07
20:A:7050:LMU:C3	20:A:7050:LMU:C8	2.30	1.07
20:A:7050:LMU:C4	20:A:7050:LMU:C8	2.30	1.07
20:A:7021:LMU:C3	20:A:7021:LMU:H1'	1.81	1.07
4:4:123:GLN:O	4:4:143:PHE:CD1	2.07	1.06
23:B:1774:PQN:C16	22:B:1781:BCR:H333	1.79	1.06
6:B:58:PHE:HB2	6:B:146:SER:CB	1.83	1.06
9:E:87:VAL:O	9:E:87:VAL:HG12	1.54	1.06
16:L:64:LEU:HB3	16:L:68:PHE:HE1	1.17	1.06
4:4:36:ASN:CG	4:4:39:TRP:CD2	2.28	1.06
19:A:1776:CLA:HMD3	19:A:1778:CLA:HBB2	1.12	1.06
22:A:1806:BCR:C31	19:A:1812:CLA:H142	1.84	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1737:CLA:O1A	19:B:1737:CLA:H62	1.54	1.06
6:B:310:PRO:HG3	19:B:1754:CLA:HMA1	1.12	1.06
3:3:93:PHE:N	3:3:93:PHE:CD2	2.22	1.06
17:N:52:LEU:N	17:N:52:LEU:HD23	1.65	1.06
20:A:7023:LMU:O3B	20:A:7023:LMU:H6'1	1.46	1.06
20:A:7039:LMU:H3'	20:A:7039:LMU:H6'2	1.08	1.06
20:A:7026:LMU:C5	20:A:7026:LMU:H12	1.82	1.06
2:2:91:THR:O	2:2:94:LEU:HB3	1.55	1.06
19:A:1781:CLA:CBC	19:A:1781:CLA:HHD	1.85	1.06
4:4:36:ASN:CG	4:4:39:TRP:CE2	2.29	1.06
19:L:1168:CLA:HHD	19:L:1168:CLA:CBC	1.83	1.06
20:A:7042:LMU:H5'	20:A:7042:LMU:O2B	1.54	1.06
20:A:7020:LMU:C6'	20:A:7020:LMU:C5B	2.29	1.06
10:F:5:LEU:HG	10:F:6:THR:N	1.66	1.06
6:B:25:ILE:HG23	22:L:1169:BCR:H282	1.37	1.06
11:G:28:ARG:HG2	11:G:28:ARG:HH21	1.20	1.06
5:A:368:LEU:CD2	19:A:1774:CLA:C9	2.32	1.06
19:B:1762:CLA:HBC2	19:B:1762:CLA:HHD	1.35	1.06
6:B:202:SER:O	6:B:245:GLY:HA2	1.52	1.06
19:1:1148:CLA:CHD	19:1:1148:CLA:CBC	2.32	1.06
20:B:1783:LMU:C11	20:B:1783:LMU:C6	2.30	1.06
20:A:7037:LMU:C12	20:A:7051:LMU:C3	2.34	1.06
19:3:1224:CLA:H101	19:3:1224:CLA:H142	1.07	1.06
19:4:4007:CLA:CED	19:4:4007:CLA:C1	2.29	1.06
4:4:147:LEU:CD2	4:4:148:GLU:CG	2.30	1.06
4:4:122:LYS:HB3	4:4:143:PHE:CG	1.90	1.06
19:A:1779:CLA:CAB	22:A:1804:BCR:H351	1.85	1.06
19:A:1812:CLA:HMD3	6:B:578:LEU:HD23	1.09	1.06
13:I:11:LEU:HD12	22:I:1032:BCR:C10	1.83	1.06
13:I:7:LEU:HD12	22:I:1032:BCR:C33	1.86	1.06
16:L:164:PRO:CB	16:L:165:TYR:CG	2.37	1.06
16:L:164:PRO:C	16:L:165:TYR:CD2	2.29	1.06
20:A:7016:LMU:C2	20:A:7016:LMU:C6	2.29	1.06
21:B:8052:SUC:C1	21:B:8052:SUC:H5'	1.83	1.06
19:1:1145:CLA:H2	19:1:1145:CLA:HMA2	1.30	1.06
19:3:3011:CLA:H12	19:3:3011:CLA:HMA2	1.28	1.06
20:A:7030:LMU:H91	20:A:7030:LMU:H51	1.34	1.06
19:4:1211:CLA:HBD	19:4:1211:CLA:HBA1	1.37	1.06
19:B:1743:CLA:C3C	19:B:1744:CLA:HBB1	1.84	1.06
19:B:1756:CLA:HBB1	19:B:1770:CLA:HMB3	1.35	1.06
19:A:1800:CLA:CMA	16:L:27:VAL:HA	1.84	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1791:CLA:HMA2	19:A:1797:CLA:HBB1	1.37	1.06
5:A:605:MET:HA	5:A:608:SER:OG	1.56	1.06
5:A:249:ILE:HG12	5:A:250:LEU:N	1.67	1.06
17:N:58:VAL:CB	17:N:59:PRO:CD	2.30	1.06
17:N:65:LEU:HD23	17:N:65:LEU:O	1.53	1.06
5:A:267:THR:O	5:A:269:PHE:HD2	1.39	1.06
14:J:2:ARG:HH12	14:J:8:LEU:HD13	1.21	1.05
19:4:1198:CLA:H202	19:4:1198:CLA:H151	1.25	1.05
19:4:1198:CLA:H151	19:4:1198:CLA:H203	1.33	1.05
17:N:45:ASN:HD22	17:N:57:LYS:NZ	1.52	1.05
17:N:46:PHE:O	17:N:47:THR:HG23	1.54	1.05
19:1:1014:CLA:HBC2	19:1:1014:CLA:HHD	1.33	1.05
20:A:7048:LMU:H31	20:A:7048:LMU:H91	1.07	1.05
10:F:24:LYS:CA	10:F:24:LYS:CE	2.34	1.05
20:A:7050:LMU:H32	20:A:7050:LMU:H81	1.25	1.05
7:C:44:ARG:HH21	8:D:127:ARG:HB3	1.19	1.05
9:E:72:VAL:O	9:E:73:ASN:HB3	1.55	1.05
4:4:93:ILE:CA	4:4:96:ILE:HD12	1.87	1.05
5:A:454:GLY:H	5:A:457:SER:HB3	1.16	1.05
6:B:560:ASP:OD1	6:B:561:GLY:N	1.89	1.05
7:C:1:MET:HG2	7:C:4:SER:HB3	1.36	1.05
11:G:43:HIS:O	11:G:45:GLU:HB2	1.56	1.05
19:A:1770:CLA:CHC	22:A:1802:BCR:C19	2.35	1.05
22:A:1806:BCR:HC8	22:A:1806:BCR:C31	1.85	1.05
6:B:663:PHE:O	6:B:664:LEU:HB2	1.50	1.05
16:L:161:LEU:C	16:L:161:LEU:HD12	1.58	1.05
2:2:203:THR:O	2:2:204:ILE:HG23	1.54	1.05
4:4:193:ILE:HG22	4:4:194:VAL:H	1.13	1.05
21:B:8055:SUC:C1'	21:B:8055:SUC:H6'2	1.85	1.05
19:3:1224:CLA:HED2	19:3:1224:CLA:HAA2	1.09	1.05
12:H:25:GLY:HA3	12:H:27:ASP:H	1.00	1.05
15:K:11:MET:SD	15:K:12:VAL:N	2.29	1.05
6:B:474:PHE:HE2	6:B:476:ILE:HG13	1.19	1.05
19:1:1241:CLA:C4C	22:I:1032:BCR:HC22	1.85	1.05
5:A:116:ILE:HG23	5:A:137:GLY:HA3	1.39	1.05
5:A:370:ILE:HG22	5:A:400:MET:HA	1.38	1.05
11:G:42:SER:OG	11:G:45:GLU:HB2	1.56	1.05
11:G:46:ALA:H	11:G:48:ASP:CB	1.69	1.05
19:4:1198:CLA:C15	19:4:1198:CLA:C20	2.28	1.05
4:4:39:TRP:C	4:4:40:PHE:CD1	2.29	1.05
5:A:51:THR:HG21	19:A:1795:CLA:HBB2	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1754:CLA:H43	19:B:1754:CLA:HAA1	1.38	1.05
1:1:27:LEU:CD2	6:B:314:ARG:HG3	1.85	1.05
1:1:39:TYR:HB3	19:1:1195:CLA:OBD	1.54	1.05
20:A:7037:LMU:C1	20:A:7037:LMU:H51	1.87	1.05
20:A:7004:LMU:H1B	20:A:7004:LMU:O6B	1.51	1.05
4:4:117:GLN:O	4:4:122:LYS:O	1.72	1.05
19:A:1781:CLA:H72	19:A:1782:CLA:HED2	1.30	1.05
22:A:1803:BCR:H23C	22:A:1803:BCR:H402	1.38	1.05
5:A:365:LEU:HD23	19:A:1761:CLA:CED	1.85	1.05
19:B:1756:CLA:CED	19:B:1757:CLA:HMD1	1.87	1.05
11:G:68:ILE:CG2	11:G:72:LEU:HD13	1.86	1.05
19:4:1198:CLA:O1D	19:4:1198:CLA:H2A	1.56	1.05
5:A:197:GLN:HA	5:A:197:GLN:HE21	0.91	1.05
19:J:1044:CLA:C15	19:J:1044:CLA:H102	1.85	1.05
20:A:7043:LMU:O2'	20:A:7043:LMU:H12	1.57	1.05
5:A:425:THR:HG21	8:D:59:GLU:OE2	1.54	1.05
19:A:1781:CLA:HBC2	19:A:1781:CLA:HHD	1.07	1.05
19:B:1762:CLA:CBC	19:B:1762:CLA:HHD	1.87	1.05
22:B:1781:BCR:H17C	19:B:1787:CLA:H101	1.39	1.05
10:F:130:LEU:HG	10:F:131:PHE:H	1.13	1.05
19:1:1188:CLA:CED	19:1:1188:CLA:H2	1.87	1.05
20:N:1086:LMU:H121	20:N:1086:LMU:H81	1.37	1.05
4:4:193:ILE:HG22	4:4:195:GLN:O	1.57	1.05
19:1:1196:CLA:OBD	19:1:1196:CLA:HED2	1.56	1.05
5:A:27:ILE:HG23	5:A:27:ILE:O	1.55	1.05
4:4:30:LEU:HA	4:4:31:ALA:CB	1.87	1.04
23:B:1774:PQN:H192	22:B:1781:BCR:H10C	1.35	1.04
7:C:1:MET:HB3	7:C:4:SER:OG	1.54	1.04
13:I:11:LEU:HG	22:I:1032:BCR:C7	1.86	1.04
5:A:599:PHE:CE2	5:A:735:VAL:HG21	1.92	1.04
2:2:205:PHE:C	2:2:205:PHE:CD1	2.29	1.04
10:F:23:LYS:O	10:F:26:GLN:HB2	1.57	1.04
12:H:25:GLY:HA3	12:H:27:ASP:CB	1.86	1.04
15:K:10:ILE:HD12	15:K:10:ILE:H	1.19	1.04
6:B:65:LEU:HD22	6:B:124:TRP:HE3	1.20	1.04
11:G:12:THR:CG2	11:G:72:LEU:HG	1.85	1.04
4:4:122:LYS:CB	4:4:143:PHE:CB	2.33	1.04
6:B:340:SER:HA	19:B:1757:CLA:H51	1.37	1.04
6:B:11:GLY:HA3	7:C:71:HIS:HD2	1.18	1.04
22:I:1032:BCR:HC42	22:I:1032:BCR:H322	1.09	1.04
16:L:164:PRO:HB2	16:L:165:TYR:HA	1.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7036:LMU:H71	20:A:7036:LMU:C3	1.83	1.04
20:A:7016:LMU:H6'	20:A:7016:LMU:H51	1.19	1.04
10:F:151:ASP:O	10:F:154:PHE:HB3	1.56	1.04
2:2:41:LEU:CG	2:2:42:ARG:N	2.14	1.04
5:A:281:LEU:HD12	19:A:1772:CLA:HED2	1.37	1.04
9:E:85:ASP:O	9:E:86:GLU:HB3	1.52	1.04
16:L:165:TYR:N	16:L:165:TYR:HD2	1.54	1.04
19:1:1188:CLA:C2	19:1:1188:CLA:HED1	1.86	1.04
20:N:1086:LMU:C1'	20:N:1086:LMU:C3	2.30	1.04
17:N:61:LEU:HD11	17:N:63:ASP:N	1.73	1.04
20:A:7032:LMU:H2B	20:A:7032:LMU:H31	1.34	1.04
5:A:269:PHE:CE1	15:K:14:THR:HG21	1.91	1.04
21:3:1226:SUC:H6'2	21:3:1226:SUC:H1'1	1.06	1.04
5:A:29:THR:O	5:A:29:THR:HG23	1.57	1.04
19:1:1241:CLA:CAC	22:I:1032:BCR:C3	2.36	1.04
19:A:1776:CLA:HMD3	19:A:1778:CLA:CBB	1.86	1.04
5:A:394:SER:HB2	19:A:1783:CLA:HMA1	1.38	1.04
19:B:1739:CLA:H92	19:B:1739:CLA:CBB	1.86	1.04
19:B:1769:CLA:H152	22:B:1780:BCR:H312	1.08	1.04
23:B:1774:PQN:C16	22:B:1781:BCR:H331	1.86	1.04
8:D:78:ALA:HB3	8:D:82:GLN:HE22	1.16	1.04
19:1:1014:CLA:CGD	19:1:1014:CLA:CBA	2.35	1.04
10:F:24:LYS:HE2	10:F:24:LYS:HA	1.40	1.04
3:3:110:SER:O	3:3:111:TYR:CD2	2.10	1.04
1:1:179:THR:HG21	4:4:87:SER:HB3	1.18	1.04
19:A:1770:CLA:HMB2	22:A:1802:BCR:C38	1.87	1.04
6:B:310:PRO:HG2	6:B:311:PRO:HD2	1.38	1.04
2:2:43:TRP:CE3	2:2:125:PHE:CD1	2.46	1.04
19:A:1797:CLA:HHD	19:A:1797:CLA:HBC3	1.29	1.04
16:L:164:PRO:C	16:L:165:TYR:HD2	1.58	1.04
20:A:7042:LMU:C7	20:A:7042:LMU:C2	2.30	1.04
19:1:1308:CLA:HMC1	19:1:1308:CLA:HBC2	1.39	1.04
4:4:34:PRO:CA	4:4:35:GLU:CB	2.28	1.03
19:A:1763:CLA:C1	19:A:1763:CLA:CAA	2.34	1.03
19:A:1796:CLA:C14	22:A:1806:BCR:C2	2.36	1.03
5:A:401:TRP:CD1	19:A:1783:CLA:HHC	1.93	1.03
19:G:1099:CLA:CBC	19:G:1099:CLA:CHD	2.30	1.03
4:4:69:ILE:HD11	4:4:175:LYS:HB2	1.09	1.03
20:A:7048:LMU:C8	20:A:7048:LMU:C4	2.30	1.03
19:3:1224:CLA:C10	19:3:1224:CLA:C14	2.33	1.03
4:4:98:SER:O	4:4:102:GLU:HG3	1.55	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:708:VAL:O	6:B:712:HIS:HB2	1.56	1.03
16:L:163:LEU:HD13	16:L:164:PRO:CB	1.86	1.03
19:1:1188:CLA:HED1	19:1:1188:CLA:CBA	1.85	1.03
19:1:1014:CLA:C8	19:1:1014:CLA:C4	2.35	1.03
21:B:8055:SUC:O6	21:B:8055:SUC:H1	1.58	1.03
19:3:1224:CLA:HBA1	19:3:1224:CLA:CED	1.88	1.03
19:3:1224:CLA:CBC	19:3:1224:CLA:CMC	2.30	1.03
12:H:20:GLN:HB3	12:H:22:ASP:HB3	1.04	1.03
19:4:4007:CLA:CED	19:4:4007:CLA:CGA	2.36	1.03
22:B:1780:BCR:C27	22:B:1780:BCR:C40	2.30	1.03
2:2:118:CYS:O	2:2:119:VAL:CG1	2.06	1.03
2:2:54:TRP:CZ2	2:2:109:ARG:HD2	1.93	1.03
4:4:95:PHE:CZ	19:4:1210:CLA:C1C	2.34	1.03
19:B:1743:CLA:C3C	19:B:1744:CLA:CBB	2.36	1.03
11:G:68:ILE:HG23	11:G:72:LEU:HD13	1.34	1.03
19:4:1199:CLA:CBC	19:4:1199:CLA:HMC1	1.88	1.03
4:4:158:ARG:HA	4:4:161:LEU:HD12	1.39	1.03
19:A:1797:CLA:C12	19:A:1797:CLA:C7	2.31	1.03
22:A:1802:BCR:H311	22:A:1802:BCR:HC8	1.05	1.03
5:A:707:ILE:HG22	5:A:711:HIS:NE2	1.74	1.03
6:B:419:ILE:O	6:B:420:SER:OG	1.77	1.03
4:4:72:VAL:HG13	4:4:72:VAL:O	1.56	1.03
3:3:205:GLY:H	5:A:252:ARG:NH2	1.55	1.03
19:J:1044:CLA:C15	19:J:1044:CLA:H91	1.89	1.03
19:1:1145:CLA:OBD	19:1:1145:CLA:HED3	1.59	1.03
1:1:63:LEU:HD13	1:1:63:LEU:O	1.57	1.03
9:E:51:SER:HB3	9:E:68:ARG:CZ	1.89	1.03
11:G:44:PHE:N	11:G:45:GLU:HB2	1.71	1.03
19:1:1241:CLA:C3C	22:I:1032:BCR:C2	2.36	1.03
2:2:128:ASN:C	2:2:130:LEU:N	2.04	1.03
22:B:1780:BCR:H403	22:B:1780:BCR:H271	1.04	1.03
20:N:1086:LMU:C6'	20:N:1086:LMU:C5	2.30	1.03
4:4:194:VAL:CB	4:4:195:GLN:C	2.26	1.03
10:F:24:LYS:O	10:F:27:ALA:HB2	1.59	1.03
19:R:1055:CLA:HBA2	19:R:1055:CLA:HBD	1.39	1.03
4:4:149:ALA:CB	4:4:151:GLU:CG	2.30	1.02
6:B:382:ILE:HG22	6:B:383:MET:H	1.24	1.02
11:G:47:GLY:H	11:G:48:ASP:CB	1.72	1.02
11:G:48:ASP:HB3	11:G:49:THR:CG2	1.88	1.02
4:4:117:GLN:O	4:4:121:PHE:CE2	2.12	1.02
19:A:1771:CLA:CED	19:A:1771:CLA:CAA	2.29	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:163:LEU:CG	16:L:164:PRO:CB	2.36	1.02
19:1:1188:CLA:C12	19:1:1188:CLA:C9	2.30	1.02
19:1:1188:CLA:HBA2	19:1:1188:CLA:HED1	1.07	1.02
17:N:72:LYS:HB3	17:N:73:ASP:C	1.79	1.02
9:E:45:TRP:CH2	9:E:78:SER:OG	2.11	1.02
19:B:1735:CLA:CMD	22:B:1779:BCR:HC41	1.89	1.02
19:A:1811:CLA:HMB3	19:B:1786:CLA:H18	1.42	1.02
2:2:42:ARG:HB3	2:2:43:TRP:HA	1.37	1.02
19:A:1759:CLA:H42	19:A:1796:CLA:C6	1.89	1.02
5:A:382:TYR:OH	19:A:1784:CLA:H42	1.58	1.02
5:A:355:HIS:ND1	5:A:416:ILE:HG21	1.75	1.02
16:L:88:ALA:C	16:L:90:GLY:H	1.55	1.02
10:F:23:LYS:C	10:F:24:LYS:HE2	1.78	1.02
19:1:1145:CLA:CMA	19:1:1145:CLA:H61	1.90	1.02
1:1:63:LEU:HD22	1:1:63:LEU:O	1.55	1.02
16:L:108:LYS:O	16:L:132:SER:HB2	1.58	1.02
3:3:84:ILE:H	19:3:1212:CLA:C4	1.72	1.02
5:A:281:LEU:CD1	19:A:1772:CLA:HED2	1.88	1.02
5:A:390:ALA:HB2	5:A:754:ILE:HB	1.41	1.02
11:G:45:GLU:HG3	11:G:49:THR:HG23	1.08	1.02
4:4:34:PRO:HB3	4:4:35:GLU:HB2	1.40	1.02
4:4:69:ILE:CD1	4:4:175:LYS:HB3	1.84	1.02
4:4:69:ILE:HD11	4:4:175:LYS:HB3	1.39	1.02
22:A:1806:BCR:C31	19:A:1812:CLA:H143	1.86	1.02
25:B:1785:SF4:S3	25:B:1785:SF4:S1	2.58	1.02
19:A:1769:CLA:HBA1	19:A:1780:CLA:H41	1.40	1.02
4:4:74:LYS:H	4:4:75:TRP:CA	1.72	1.02
20:A:7042:LMU:H1B	20:A:7042:LMU:O3'	1.57	1.02
17:N:76:LYS:HG3	17:N:77:CYS:H	1.22	1.02
19:J:1044:CLA:C8	19:J:1044:CLA:H152	1.88	1.02
19:1:1142:CLA:HED2	19:K:1085:CLA:CMB	1.90	1.02
15:K:1:ASP:HA	15:K:5:SER:HB3	1.40	1.02
19:4:4007:CLA:HBC2	19:4:4007:CLA:HHD	1.36	1.02
22:B:1781:BCR:H19C	19:B:1787:CLA:H151	1.40	1.02
16:L:122:GLY:C	16:L:124:LYS:H	1.61	1.02
19:2:1213:CLA:HHD	19:2:1213:CLA:HBC2	1.41	1.02
4:4:37:LEU:C	4:4:39:TRP:CB	2.27	1.02
6:B:558:PRO:HG2	6:B:703:VAL:HB	1.38	1.02
17:N:61:LEU:CD1	17:N:63:ASP:CB	2.37	1.02
20:N:1086:LMU:C12	20:N:1086:LMU:C8	2.30	1.02
19:1:1014:CLA:C7	19:1:1014:CLA:C4	2.29	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1014:CLA:H8	19:1:1014:CLA:H41	1.40	1.02
19:R:1055:CLA:HBA2	19:R:1055:CLA:CBD	1.90	1.02
19:3:1221:CLA:CHA	19:3:3011:CLA:HBC2	1.90	1.02
2:2:169:LEU:CD2	19:2:1215:CLA:HBB2	1.90	1.01
19:B:1769:CLA:H152	22:B:1780:BCR:H313	1.42	1.01
11:G:43:HIS:HA	11:G:44:PHE:CB	1.89	1.01
2:2:44:ASN:HD21	14:J:1:MET:HB2	1.24	1.01
19:A:1762:CLA:H43	19:A:1785:CLA:H11	1.41	1.01
19:A:1763:CLA:C1	19:A:1765:CLA:CED	2.38	1.01
19:A:1796:CLA:C14	22:A:1806:BCR:HC22	1.90	1.01
5:A:239:PRO:HA	5:A:242:ILE:CD1	1.90	1.01
2:2:182:ILE:O	2:2:204:ILE:O	1.78	1.01
19:1:1014:CLA:H112	19:1:1014:CLA:H43	1.40	1.01
19:3:1221:CLA:CHA	19:3:3011:CLA:HBC1	1.87	1.01
20:1:1200:LMU:H1'	20:1:1200:LMU:O6'	1.54	1.01
2:2:41:LEU:HG	2:2:42:ARG:H	1.10	1.01
5:A:368:LEU:CD2	19:A:1774:CLA:H92	1.87	1.01
19:B:1744:CLA:HBC3	19:B:1744:CLA:HMC1	1.39	1.01
1:1:185:TRP:HA	1:1:185:TRP:CE3	1.93	1.01
5:A:412:ALA:HB2	5:A:598:VAL:HG11	1.42	1.01
19:B:1756:CLA:HED1	19:B:1757:CLA:HMD1	1.42	1.01
17:N:45:ASN:ND2	17:N:53:ALA:O	1.92	1.01
4:4:192:THR:CG2	4:4:193:ILE:C	2.29	1.01
20:A:7021:LMU:H22	20:A:7021:LMU:H62	1.06	1.01
19:3:1221:CLA:C2A	19:3:3011:CLA:HAC2	1.89	1.01
17:N:18:ASP:CB	17:N:22:LEU:HG	1.90	1.01
2:2:103:GLY:N	19:2:1222:CLA:CBB	2.22	1.01
19:A:1791:CLA:CMA	19:A:1797:CLA:HBB1	1.90	1.01
5:A:328:LYS:HE2	5:A:332:GLU:HG3	1.39	1.01
19:B:1754:CLA:H42	19:B:1754:CLA:C4A	1.90	1.01
7:C:1:MET:HB3	7:C:4:SER:HG	1.25	1.01
4:4:149:ALA:HB3	4:4:151:GLU:HG2	1.23	1.01
4:4:36:ASN:ND2	4:4:39:TRP:CE2	2.29	1.01
6:B:361:ILE:HG23	6:B:368:GLN:OE1	1.61	1.01
11:G:43:HIS:C	11:G:45:GLU:HB2	1.80	1.01
5:A:249:ILE:HG12	5:A:250:LEU:H	0.90	1.01
17:N:54:LYS:CG	17:N:57:LYS:HZ3	1.73	1.01
21:B:8052:SUC:O4'	21:B:8052:SUC:H1	1.59	1.01
19:2:1212:CLA:CGA	19:2:1212:CLA:H42	1.90	1.01
20:A:7004:LMU:H11	20:A:7004:LMU:O2'	1.55	1.01
19:A:1781:CLA:C7	19:A:1782:CLA:CED	2.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1768:CLA:HMC1	19:B:1768:CLA:HBC3	1.43	1.01
11:G:12:THR:HG22	11:G:72:LEU:CG	1.88	1.01
7:C:8:TYR:O	7:C:60:THR:HA	1.59	1.01
4:4:75:TRP:CE3	4:4:76:TYR:N	2.28	1.01
6:B:247:THR:HA	6:B:250:ALA:HB2	1.05	1.01
2:2:43:TRP:CZ3	2:2:125:PHE:CD2	2.41	1.01
4:4:154:ILE:HG13	4:4:155:ALA:H	1.21	1.01
22:A:1807:BCR:H23C	22:A:1807:BCR:H393	1.03	1.01
19:B:1787:CLA:H93	19:B:1788:CLA:C9	1.91	1.01
11:G:48:ASP:HB3	11:G:49:THR:HG22	1.43	1.01
17:N:42:PHE:CD1	17:N:43:PRO:N	2.29	1.01
2:2:203:THR:O	2:2:204:ILE:HG12	1.60	1.01
20:A:7033:LMU:H3'	20:A:7033:LMU:H6'2	1.05	1.01
20:A:7050:LMU:C10	20:A:7050:LMU:C3	2.30	1.01
17:N:1:GLY:O	17:N:2:VAL:HG13	1.58	1.01
2:2:110:TRP:HA	2:2:113:ILE:HG23	1.42	1.00
4:4:149:ALA:HB3	4:4:151:GLU:OE1	1.58	1.00
5:A:368:LEU:HD21	19:A:1774:CLA:H93	1.40	1.00
16:L:163:LEU:HB3	16:L:164:PRO:HG3	1.06	1.00
20:A:7023:LMU:H6'2	20:A:7023:LMU:C2B	1.87	1.00
3:3:181:LEU:N	3:3:182:LYS:HE2	1.74	1.00
3:3:64:TYR:HB3	19:3:1222:CLA:C4	1.90	1.00
20:A:7050:LMU:C9	20:A:7050:LMU:C5	2.29	1.00
15:K:17:LEU:O	15:K:17:LEU:HD23	1.59	1.00
9:E:83:ALA:O	9:E:86:GLU:HG2	1.60	1.00
19:A:1781:CLA:HBC2	19:A:1781:CLA:CHD	1.91	1.00
19:A:1788:CLA:H161	22:L:1169:BCR:C36	1.91	1.00
4:4:71:ASN:C	4:4:73:PRO:HD3	1.81	1.00
16:L:164:PRO:HD2	16:L:165:TYR:CE1	1.95	1.00
17:N:62:SER:HB3	17:N:66:ASP:HB3	1.39	1.00
3:3:48:PHE:HD2	3:3:49:ILE:HG22	0.85	1.00
10:F:23:LYS:C	10:F:24:LYS:CE	2.29	1.00
20:A:7013:LMU:O6B	20:A:7013:LMU:H1B	1.56	1.00
2:2:96:ILE:HG13	2:2:97:VAL:H	1.26	1.00
22:A:1806:BCR:H311	22:A:1806:BCR:C8	1.83	1.00
19:B:1740:CLA:H41	22:B:1782:BCR:C23	1.90	1.00
22:A:1802:BCR:HC8	22:A:1802:BCR:C31	1.89	1.00
19:B:1754:CLA:C4A	19:B:1754:CLA:C4	2.30	1.00
9:E:39:LEU:H	9:E:40:ARG:NH1	1.58	1.00
16:L:160:VAL:O	16:L:160:VAL:HG13	1.61	1.00
4:4:192:THR:HG21	4:4:195:GLN:N	1.76	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1142:CLA:HMD1	19:K:1085:CLA:NA	1.75	1.00
10:F:22:LEU:O	10:F:25:LEU:HB2	1.57	1.00
20:1:1200:LMU:C2'	20:1:1200:LMU:H6D	1.82	1.00
17:N:18:ASP:HB2	17:N:22:LEU:HG	1.40	1.00
12:H:58:ILE:HD11	16:L:97:MET:SD	2.00	1.00
5:A:81:ALA:HB1	19:A:1760:CLA:HMA1	1.40	1.00
17:N:62:SER:CB	17:N:66:ASP:CG	2.28	1.00
17:N:70:GLU:C	17:N:72:LYS:H	1.65	1.00
17:N:72:LYS:HB3	17:N:74:LYS:N	1.77	1.00
22:A:1806:BCR:H313	19:A:1812:CLA:H142	1.42	1.00
6:B:530:THR:HG21	19:B:1756:CLA:HAC1	1.40	1.00
17:N:61:LEU:CD1	17:N:63:ASP:C	2.30	1.00
16:L:82:ALA:CB	16:L:86:LEU:HD13	1.92	1.00
1:1:179:THR:HG23	4:4:87:SER:HB3	1.44	1.00
5:A:23:ASP:OD2	5:A:24:ARG:HG2	1.62	1.00
10:F:26:GLN:HA	10:F:26:GLN:OE1	1.61	1.00
15:K:7:THR:HA	15:K:10:ILE:CD1	1.91	1.00
19:A:1774:CLA:H121	19:A:1774:CLA:HBB2	1.41	1.00
5:A:217:SER:HA	22:A:1802:BCR:H351	1.43	1.00
5:A:365:LEU:CD2	19:A:1761:CLA:HED3	1.92	1.00
5:A:368:LEU:HD21	19:A:1774:CLA:H92	1.43	1.00
20:A:7021:LMU:H22	20:A:7021:LMU:C6	1.92	1.00
20:A:7026:LMU:H41	20:A:7026:LMU:H82	1.41	1.00
10:F:102:ARG:CG	10:F:106:ILE:HD11	1.91	1.00
4:4:36:ASN:ND2	4:4:39:TRP:CZ2	2.29	0.99
19:A:1782:CLA:HBA1	19:A:1782:CLA:O1D	1.62	0.99
1:1:39:TYR:CB	19:1:1195:CLA:OBD	2.07	0.99
19:J:1043:CLA:HHD	19:J:1043:CLA:HBC3	1.41	0.99
4:4:107:GLN:O	19:4:1196:CLA:HMA1	1.59	0.99
22:A:1806:BCR:H311	22:A:1806:BCR:HC8	1.00	0.99
16:L:37:LEU:O	16:L:42:ALA:HB3	1.62	0.99
20:N:1086:LMU:H32	20:N:1086:LMU:H1'	1.40	0.99
17:N:55:GLN:O	17:N:56:LYS:HG3	1.60	0.99
3:3:74:ALA:HB3	3:3:75:PRO:HD3	1.45	0.99
17:N:32:ALA:HB1	17:N:35:VAL:HG22	1.44	0.99
19:A:1791:CLA:C3A	19:A:1797:CLA:HBB1	1.91	0.99
6:B:560:ASP:HB2	7:C:66:ARG:NE	1.76	0.99
11:G:48:ASP:HB2	11:G:49:THR:CG2	1.89	0.99
11:G:46:ALA:H	11:G:49:THR:CG2	1.73	0.99
4:4:118:ASP:HA	4:4:123:GLN:N	1.78	0.99
17:N:66:ASP:C	17:N:67:LEU:CD1	2.29	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:1043:CLA:CHA	19:J:1043:CLA:CED	2.40	0.99
20:A:7014:LMU:H11	20:A:7014:LMU:C6	1.90	0.99
5:A:304:LEU:HD22	19:A:1772:CLA:HBB2	1.44	0.99
5:A:370:ILE:HG23	5:A:403:GLY:HA3	1.43	0.99
5:A:451:ILE:CD1	19:A:1788:CLA:CED	2.40	0.99
16:L:164:PRO:HG2	16:L:165:TYR:CG	1.93	0.99
17:N:47:THR:OG1	17:N:54:LYS:HD3	1.61	0.99
20:A:7021:LMU:H31	20:A:7021:LMU:H1'	0.99	0.99
2:2:39:GLU:CA	2:2:40:SER:HB2	1.92	0.99
3:3:84:ILE:HB	19:3:1212:CLA:CGA	1.92	0.99
4:4:128:ALA:HB2	4:4:143:PHE:CZ	1.98	0.99
6:B:608:GLN:HA	6:B:608:GLN:NE2	1.78	0.99
20:B:1783:LMU:O3'	20:B:1783:LMU:H5B	1.63	0.99
4:4:102:GLU:OE2	19:4:1209:CLA:CHC	2.10	0.99
4:4:91:PHE:CG	19:4:1207:CLA:C3C	2.45	0.99
5:A:328:LYS:HE3	5:A:332:GLU:CG	1.91	0.99
5:A:672:LEU:O	5:A:674:ALA:N	1.95	0.99
21:B:8054:SUC:H1'1	21:B:8054:SUC:C2	1.92	0.99
20:A:7037:LMU:O2B	20:A:7037:LMU:H5B	1.63	0.99
20:A:7021:LMU:H41	20:A:7021:LMU:C6'	1.92	0.99
7:C:39:ILE:HG12	7:C:40:ALA:H	1.26	0.99
12:H:44:ALA:CB	16:L:145:PHE:HD1	1.75	0.99
2:2:128:ASN:O	2:2:130:LEU:N	1.95	0.99
4:4:128:ALA:CB	4:4:143:PHE:HE2	1.74	0.99
19:A:1811:CLA:H11	6:B:616:LEU:HG	1.45	0.99
19:1:1142:CLA:HED2	19:K:1085:CLA:HMB2	1.41	0.99
19:R:1055:CLA:HBA2	19:R:1055:CLA:CGD	1.92	0.99
4:4:118:ASP:HA	4:4:122:LYS:C	1.81	0.99
5:A:170:GLY:O	5:A:173:VAL:HG22	1.62	0.99
19:B:1769:CLA:C15	22:B:1780:BCR:H313	1.88	0.99
19:3:1224:CLA:CED	19:3:1224:CLA:CBA	2.41	0.99
19:4:1206:CLA:H192	19:4:1206:CLA:H152	1.43	0.99
2:2:42:ARG:HD3	2:2:45:VAL:HG21	1.43	0.98
5:A:355:HIS:CE1	5:A:416:ILE:HG21	1.98	0.98
6:B:269:TRP:HB2	6:B:497:TRP:HH2	1.23	0.98
22:I:1032:BCR:C8	22:I:1032:BCR:C31	2.28	0.98
1:1:89:VAL:O	11:G:77:ILE:CD1	2.11	0.98
2:2:128:ASN:O	2:2:130:LEU:HD13	1.63	0.98
5:A:381:PRO:HB2	19:A:1774:CLA:HAA2	1.45	0.98
19:A:1763:CLA:HMB1	22:A:1807:BCR:HC7	1.44	0.98
5:A:204:ASN:O	5:A:205:HIS:HB2	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:114:THR:OG1	5:A:525:ASN:HB2	1.63	0.98
11:G:45:GLU:CA	11:G:49:THR:HG21	1.91	0.98
19:1:1146:CLA:HMA2	19:1:1146:CLA:O1A	1.63	0.98
10:F:22:LEU:H	10:F:22:LEU:HD12	0.83	0.98
4:4:36:ASN:CB	4:4:39:TRP:CZ3	2.43	0.98
4:4:94:GLU:HB3	4:4:95:PHE:HE1	1.18	0.98
16:L:164:PRO:CB	16:L:165:TYR:HA	1.88	0.98
19:4:1201:CLA:HAA2	19:4:1201:CLA:O1D	1.62	0.98
4:4:34:PRO:HA	4:4:35:GLU:HB2	1.22	0.98
5:A:442:ILE:HG23	19:A:1786:CLA:HMC3	1.43	0.98
19:A:1770:CLA:CHC	22:A:1802:BCR:H19C	1.92	0.98
4:4:128:ALA:HB2	4:4:143:PHE:HE2	1.26	0.98
4:4:30:LEU:HA	4:4:31:ALA:HB3	0.98	0.98
5:A:451:ILE:CD1	19:A:1788:CLA:HED3	1.93	0.98
19:B:1737:CLA:O1A	19:B:1737:CLA:H2	1.19	0.98
21:B:8055:SUC:C1'	21:B:8055:SUC:C6'	2.30	0.98
5:A:316:MET:CB	5:A:317:TYR:HB2	1.91	0.98
9:E:68:ARG:C	9:E:68:ARG:HE	1.66	0.98
4:4:37:LEU:CA	4:4:39:TRP:CB	2.41	0.98
5:A:197:GLN:NE2	5:A:197:GLN:HA	1.71	0.98
19:B:1769:CLA:H93	19:B:1769:CLA:HBB2	0.99	0.98
11:G:42:SER:HB2	11:G:45:GLU:OE1	1.64	0.98
11:G:42:SER:CB	11:G:45:GLU:CD	2.30	0.98
16:L:161:LEU:CD1	16:L:162:ASP:C	2.31	0.98
17:N:51:ASP:C	17:N:52:LEU:CD2	2.32	0.98
18:R:52:UNK:CA	18:R:53:UNK:CB	2.36	0.98
2:2:196:HIS:CE1	21:2:1225:SUC:O3	2.15	0.98
19:A:1796:CLA:H141	22:A:1806:BCR:HC21	1.44	0.98
11:G:44:PHE:HD2	11:G:44:PHE:O	1.46	0.98
17:N:63:ASP:CA	17:N:64:ASP:C	2.30	0.98
5:A:23:ASP:CG	5:A:24:ARG:CD	2.30	0.98
20:A:7009:LMU:H3'	20:A:7009:LMU:O5B	1.61	0.98
5:A:246:HIS:O	5:A:248:PHE:HD2	1.45	0.98
19:B:1747:CLA:HHD	19:B:1747:CLA:HBC2	1.44	0.98
6:B:421:HIS:NE2	19:B:1762:CLA:ND	2.11	0.98
22:B:1781:BCR:H19C	19:B:1787:CLA:H112	1.42	0.98
8:D:44:GLU:HB2	8:D:46:TYR:HE2	1.25	0.98
17:N:45:ASN:ND2	17:N:57:LYS:HZ1	1.61	0.98
15:K:17:LEU:C	15:K:17:LEU:CD2	2.30	0.98
4:4:147:LEU:HD13	4:4:148:GLU:H	1.18	0.98
19:A:1791:CLA:HBC2	22:A:1805:BCR:HC31	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1737:CLA:O1A	19:B:1737:CLA:C2	2.11	0.98
19:B:1788:CLA:H43	19:B:1788:CLA:HHB	1.45	0.98
19:1:1188:CLA:O1A	19:1:1188:CLA:HMA2	1.63	0.98
22:A:1807:BCR:H23C	22:A:1807:BCR:C39	1.90	0.98
19:A:1812:CLA:HMD3	6:B:578:LEU:CD2	1.94	0.98
5:A:210:LEU:HD13	19:A:1769:CLA:HMB2	1.45	0.98
5:A:302:HIS:O	5:A:306:ILE:HG12	1.64	0.98
19:B:1759:CLA:H142	22:B:1777:BCR:H10C	1.43	0.98
6:B:493:TRP:CH2	19:B:1766:CLA:HMA2	1.98	0.98
17:N:61:LEU:CD1	17:N:62:SER:C	2.32	0.98
4:4:194:VAL:HG12	4:4:195:GLN:CA	1.94	0.98
10:F:5:LEU:HG	10:F:6:THR:H	0.84	0.98
3:3:173:GLU:HG2	3:3:174:LYS:H	1.29	0.98
2:2:55:ALA:CB	2:2:56:MET:HE2	1.94	0.97
4:4:104:ARG:HH11	4:4:105:ARG:HB3	1.24	0.97
20:A:7016:LMU:C2	20:A:7016:LMU:H61	1.91	0.97
3:3:87:GLU:C	22:3:1225:BCR:C38	2.33	0.97
6:B:247:THR:HA	6:B:250:ALA:CB	1.93	0.97
10:F:5:LEU:CG	10:F:6:THR:H	1.74	0.97
6:B:122:GLN:O	6:B:126:THR:OG1	1.81	0.97
13:I:26:LEU:HA	13:I:29:GLU:O	1.63	0.97
20:A:7042:LMU:H2B	20:A:7042:LMU:H3'	1.44	0.97
17:N:61:LEU:CD1	17:N:63:ASP:CA	2.42	0.97
19:1:1145:CLA:HBC2	19:1:1145:CLA:HMC1	1.40	0.97
16:L:82:ALA:HB2	16:L:86:LEU:CD1	1.93	0.97
2:2:54:TRP:CZ2	2:2:109:ARG:CD	2.47	0.97
4:4:58:MET:O	4:4:61:PRO:HD2	1.63	0.97
2:2:99:LEU:CD2	19:2:1222:CLA:HMC3	1.94	0.97
22:A:1803:BCR:C40	22:A:1803:BCR:C23	2.36	0.97
5:A:40:PHE:HE1	5:A:53:TRP:CD1	1.82	0.97
5:A:87:SER:HB2	5:A:178:MET:O	1.63	0.97
19:J:1043:CLA:C1A	19:J:1043:CLA:CED	2.42	0.97
5:A:21:LEU:N	5:A:22:VAL:HB	1.80	0.97
10:F:24:LYS:CE	10:F:24:LYS:N	2.26	0.97
2:2:55:ALA:HB3	2:2:56:MET:HE2	0.98	0.97
19:A:1781:CLA:CED	19:A:1782:CLA:C3D	2.42	0.97
6:B:292:ARG:NE	6:B:292:ARG:HA	1.79	0.97
6:B:588:GLY:O	6:B:592:PHE:HB2	1.62	0.97
20:A:7023:LMU:H6'2	20:A:7023:LMU:H2B	0.98	0.97
5:A:21:LEU:N	5:A:22:VAL:HG12	1.80	0.97
7:C:44:ARG:NH2	8:D:127:ARG:HB3	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:174:ARG:HB2	19:B:1744:CLA:HBC2	1.41	0.97
22:B:1781:BCR:C19	19:B:1787:CLA:H151	1.94	0.97
6:B:295:PHE:H	6:B:295:PHE:HD2	1.07	0.97
6:B:461:GLN:O	6:B:464:GLN:HG2	1.65	0.97
17:N:79:SER:HA	17:N:80:ASN:C	1.83	0.97
25:B:1785:SF4:S2	25:B:1785:SF4:S1	2.62	0.97
6:B:269:TRP:HB2	6:B:497:TRP:CH2	2.00	0.97
21:F:1158:SUC:O2	21:F:1158:SUC:H5	1.62	0.97
17:N:65:LEU:C	17:N:65:LEU:CD2	2.30	0.97
17:N:70:GLU:O	17:N:72:LYS:CD	2.12	0.97
5:A:79:PHE:HE2	5:A:185:HIS:CD2	1.80	0.97
6:B:608:GLN:CA	6:B:608:GLN:HE21	1.78	0.97
16:L:160:VAL:O	16:L:160:VAL:HG22	1.60	0.97
20:N:1086:LMU:C12	20:N:1086:LMU:H81	1.82	0.97
20:N:1086:LMU:C3	20:N:1086:LMU:H1'	1.91	0.97
17:N:72:LYS:HB3	17:N:73:ASP:HA	0.98	0.97
19:B:1748:CLA:H52	19:B:1757:CLA:HMB1	1.45	0.97
6:B:87:ILE:CA	6:B:115:ASN:HA	1.93	0.97
4:4:100:TYR:HA	4:4:103:ILE:HD11	1.47	0.97
4:4:33:ASP:HB3	4:4:34:PRO:CD	1.95	0.97
11:G:94:ASP:N	11:G:95:PRO:HD3	1.80	0.97
19:1:1187:CLA:CBC	19:1:1187:CLA:CMC	2.29	0.97
20:A:7032:LMU:C3	20:A:7032:LMU:C2B	2.42	0.97
19:A:1799:CLA:HMD3	22:B:1781:BCR:HC31	1.44	0.96
5:A:79:PHE:CZ	5:A:185:HIS:NE2	2.32	0.96
17:N:63:ASP:HA	17:N:64:ASP:O	1.65	0.96
2:2:42:ARG:HD2	2:2:45:VAL:HG21	1.43	0.96
4:4:122:LYS:CB	4:4:143:PHE:CG	2.46	0.96
19:B:1769:CLA:C16	22:B:1780:BCR:C31	2.40	0.96
19:1:1148:CLA:CHD	19:1:1148:CLA:HBC3	1.91	0.96
20:A:7023:LMU:C4	20:A:7023:LMU:H82	1.74	0.96
20:A:7037:LMU:H51	20:A:7037:LMU:H12	1.45	0.96
4:4:40:PHE:CG	4:4:43:ALA:HB2	2.00	0.96
11:G:60:SER:HA	11:G:63:PRO:HD2	1.48	0.96
17:N:57:LYS:N	17:N:60:PHE:O	1.87	0.96
1:1:63:LEU:CD2	1:1:63:LEU:C	2.30	0.96
2:2:66:GLU:O	2:2:69:THR:N	1.97	0.96
4:4:147:LEU:CD2	4:4:148:GLU:N	2.28	0.96
4:4:40:PHE:HB3	4:4:43:ALA:HB2	0.98	0.96
19:A:1763:CLA:C4A	19:A:1763:CLA:HBA1	1.93	0.96
6:B:390:GLY:O	22:B:1778:BCR:HC42	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:586:THR:O	6:B:588:GLY:N	1.99	0.96
16:L:164:PRO:CD	16:L:165:TYR:CE1	2.48	0.96
4:4:30:LEU:N	4:4:31:ALA:HB2	1.79	0.96
5:A:114:THR:HG22	5:A:115:HIS:CE1	1.98	0.96
5:A:345:GLY:O	5:A:347:TYR:N	1.96	0.96
22:B:1778:BCR:H23C	22:B:1778:BCR:C38	1.92	0.96
4:4:69:ILE:HG22	4:4:70:ILE:N	1.79	0.96
19:1:1014:CLA:H111	19:1:1014:CLA:H43	1.47	0.96
19:1:1187:CLA:HMA2	19:1:1187:CLA:HBA1	1.46	0.96
2:2:38:PRO:C	2:2:40:SER:CB	2.34	0.96
2:2:39:GLU:N	2:2:40:SER:CB	2.28	0.96
4:4:107:GLN:HA	19:4:1196:CLA:HMA3	0.98	0.96
11:G:44:PHE:N	11:G:45:GLU:CB	2.29	0.96
19:A:1781:CLA:CHC	22:A:1805:BCR:H373	1.95	0.96
19:A:1783:CLA:C20	22:A:1807:BCR:C17	2.35	0.96
6:B:50:HIS:HD2	19:B:1737:CLA:HAA2	1.28	0.96
7:C:62:PHE:HE2	9:E:42:GLU:OE1	1.46	0.96
19:G:1099:CLA:H2A	19:G:1099:CLA:O1D	1.66	0.96
11:G:47:GLY:N	11:G:48:ASP:CB	2.29	0.96
1:1:25:ASP:N	6:B:314:ARG:HH22	1.62	0.96
12:H:20:GLN:CB	12:H:22:ASP:CB	2.34	0.96
10:F:61:LEU:HD23	10:F:69:PRO:HB2	1.46	0.96
2:2:110:TRP:O	2:2:113:ILE:HG12	1.65	0.96
19:A:1794:CLA:HMC1	19:A:1794:CLA:HBC3	1.48	0.96
6:B:732:LYS:CG	6:B:734:GLY:CA	2.43	0.96
10:F:100:VAL:HA	10:F:103:SER:OG	1.64	0.96
16:L:161:LEU:CD1	16:L:161:LEU:C	2.30	0.96
17:N:62:SER:CB	17:N:66:ASP:HB3	1.93	0.96
9:E:56:ASP:HB2	9:E:64:PRO:HB3	1.46	0.96
5:A:452:PHE:CE1	19:A:1793:CLA:HBB2	2.01	0.96
5:A:98:PHE:HZ	19:A:1763:CLA:HMD3	1.31	0.96
19:B:1735:CLA:H191	10:F:104:TYR:HB3	1.46	0.96
19:B:1735:CLA:HED3	19:B:1735:CLA:H2A	1.48	0.96
19:B:1769:CLA:C15	22:B:1780:BCR:H312	1.92	0.96
7:C:52:LYS:HG3	7:C:52:LYS:O	1.66	0.96
7:C:63:LEU:HG	7:C:64:SER:N	1.77	0.96
9:E:52:VAL:O	9:E:53:VAL:HG22	1.63	0.96
17:N:54:LYS:CB	17:N:57:LYS:NZ	2.28	0.96
19:2:1217:CLA:CED	19:2:1217:CLA:CAD	2.44	0.96
2:2:129:LYS:O	2:2:132:GLY:N	1.99	0.96
5:A:328:LYS:HE3	5:A:332:GLU:HG3	0.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:62:SER:HB3	17:N:66:ASP:CA	1.96	0.96
1:1:59:VAL:HG12	1:1:60:PRO:O	1.65	0.96
19:4:4007:CLA:O1A	19:4:4007:CLA:HED1	1.64	0.96
19:4:1198:CLA:C15	19:4:1198:CLA:H203	1.94	0.95
4:4:122:LYS:CG	4:4:143:PHE:HB2	1.95	0.95
4:4:91:PHE:CD2	4:4:92:VAL:N	2.34	0.95
19:B:1756:CLA:HBC2	19:B:1756:CLA:CHD	1.95	0.95
6:B:715:VAL:HG23	6:B:719:PHE:CD2	2.01	0.95
17:N:67:LEU:N	17:N:67:LEU:HD12	1.79	0.95
2:2:203:THR:C	2:2:204:ILE:CG1	2.32	0.95
3:3:74:ALA:HA	19:3:1217:CLA:C4D	1.96	0.95
20:1:1200:LMU:H6D	20:1:1200:LMU:O3'	1.65	0.95
22:A:1802:BCR:H311	22:A:1802:BCR:C8	1.96	0.95
5:A:331:LEU:HD21	5:A:343:HIS:C	1.85	0.95
19:B:1787:CLA:HBB2	19:B:1788:CLA:C1B	1.96	0.95
11:G:94:ASP:N	11:G:95:PRO:CD	2.29	0.95
20:R:1056:LMU:O6'	20:R:1056:LMU:H1'	1.64	0.95
19:A:1812:CLA:CMD	6:B:578:LEU:HD23	1.96	0.95
11:G:43:HIS:HA	11:G:44:PHE:HB3	0.97	0.95
17:N:54:LYS:CG	17:N:57:LYS:NZ	2.29	0.95
1:1:185:TRP:CB	1:1:186:HIS:ND1	2.30	0.95
19:A:1764:CLA:CHC	19:A:1765:CLA:HMD2	1.96	0.95
20:A:7026:LMU:O4'	21:B:8062:SUC:C3'	1.97	0.95
20:A:7009:LMU:C3'	20:A:7009:LMU:H5B	1.96	0.95
19:4:1211:CLA:HBC3	19:4:1211:CLA:HHD	1.46	0.95
20:A:7027:LMU:O2'	20:A:7027:LMU:H12	1.65	0.95
4:4:74:LYS:H	4:4:75:TRP:HA	1.07	0.95
16:L:161:LEU:HD12	16:L:162:ASP:HA	1.43	0.95
20:A:7042:LMU:H32	20:A:7042:LMU:H6D	0.97	0.95
17:N:66:ASP:O	17:N:67:LEU:HG	1.67	0.95
4:4:192:THR:CG2	4:4:195:GLN:N	2.29	0.95
1:1:63:LEU:N	1:1:63:LEU:CD1	2.30	0.95
5:A:335:LYS:HG2	5:A:336:GLY:N	1.82	0.95
19:A:1783:CLA:H43	19:A:1783:CLA:HBA1	1.49	0.95
5:A:246:HIS:O	5:A:248:PHE:N	2.00	0.95
5:A:588:GLY:HA3	6:B:668:ARG:HD3	1.44	0.95
7:C:1:MET:HG2	7:C:4:SER:CB	1.96	0.95
13:I:12:VAL:O	13:I:17:PRO:HD3	1.64	0.95
20:N:1086:LMU:C5	20:N:1086:LMU:C9	2.30	0.95
19:1:1148:CLA:HAA1	19:1:1148:CLA:O2D	1.65	0.95
5:A:21:LEU:N	5:A:22:VAL:CB	2.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7032:LMU:C3	20:A:7032:LMU:H2B	1.96	0.95
4:4:93:ILE:CA	4:4:96:ILE:CD1	2.41	0.95
5:A:103:PHE:HE1	19:A:1763:CLA:CGD	1.77	0.95
5:A:328:LYS:HE2	5:A:332:GLU:CG	1.94	0.95
6:B:127:ILE:HD13	6:B:198:ALA:HB2	1.49	0.95
6:B:119:GLY:CA	19:B:1759:CLA:HED1	1.97	0.95
6:B:11:GLY:HA3	7:C:71:HIS:CD2	2.01	0.95
17:N:52:LEU:N	17:N:52:LEU:CD2	2.29	0.95
19:2:1212:CLA:HMC1	19:2:1212:CLA:HBC3	1.49	0.95
1:1:64:GLY:O	1:1:65:TYR:HB2	1.66	0.95
3:3:110:SER:C	3:3:111:TYR:CD2	2.40	0.95
19:F:1157:CLA:OBD	19:F:1157:CLA:HED2	1.66	0.95
17:N:72:LYS:CB	17:N:73:ASP:CA	2.30	0.95
1:1:144:LYS:NZ	19:1:1187:CLA:OBD	1.99	0.95
19:1:1145:CLA:O1A	19:1:1145:CLA:HMA2	1.65	0.95
15:K:24:PHE:CD1	15:K:52:PRO:HG2	2.01	0.95
9:E:68:ARG:HH21	9:E:69:PHE:HA	1.30	0.95
19:2:1217:CLA:CBA	19:2:1217:CLA:CGD	2.43	0.95
5:A:331:LEU:CD1	5:A:346:LEU:HB3	1.95	0.95
5:A:547:PHE:O	5:A:551:VAL:HG13	1.64	0.95
11:G:46:ALA:H	11:G:48:ASP:HB3	1.17	0.95
3:3:194:ILE:HG13	19:3:1214:CLA:CMC	1.97	0.95
20:A:7037:LMU:C12	20:A:7051:LMU:C4	2.40	0.95
2:2:37:ASP:OD2	3:3:41:ASP:CG	2.05	0.95
4:4:30:LEU:N	4:4:31:ALA:CB	2.30	0.95
16:L:161:LEU:CD1	16:L:162:ASP:N	2.29	0.95
16:L:164:PRO:HB2	16:L:165:TYR:HB3	1.48	0.95
17:N:56:LYS:O	17:N:60:PHE:HD1	1.50	0.95
17:N:72:LYS:CB	17:N:74:LYS:N	2.29	0.95
18:R:40:UNK:N	18:R:41:UNK:CB	2.30	0.95
19:4:4007:CLA:HED1	19:4:4007:CLA:H12	1.47	0.95
21:B:8062:SUC:O2	21:B:8062:SUC:H5	1.64	0.95
1:1:185:TRP:HB3	1:1:186:HIS:CG	2.02	0.94
2:2:110:TRP:CD1	2:2:113:ILE:HG21	2.01	0.94
5:A:81:ALA:HB1	19:A:1760:CLA:CMA	1.92	0.94
19:A:1771:CLA:HAA1	19:A:1771:CLA:HED2	0.95	0.94
19:B:1769:CLA:HBC1	10:F:83:PHE:CZ	2.01	0.94
19:B:1772:CLA:HBC2	19:B:1772:CLA:HMC1	1.47	0.94
17:N:67:LEU:C	17:N:68:GLU:CG	2.32	0.94
15:K:44:GLU:HG3	15:K:45:SER:N	0.75	0.94
15:K:10:ILE:N	15:K:10:ILE:HD12	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:101:VAL:CG1	4:4:104:ARG:NH2	2.28	0.94
4:4:147:LEU:HD22	4:4:148:GLU:CA	1.97	0.94
19:B:1752:CLA:HBC2	19:B:1752:CLA:CHD	1.95	0.94
11:G:13:GLY:HA2	11:G:16:LEU:HG	1.48	0.94
11:G:28:ARG:HG2	11:G:29:GLU:N	1.80	0.94
17:N:51:ASP:O	17:N:52:LEU:HD22	1.66	0.94
17:N:61:LEU:CD1	17:N:62:SER:N	2.29	0.94
20:A:7048:LMU:C3'	20:A:7048:LMU:C2	2.45	0.94
5:A:25:ASP:N	5:A:26:PRO:CG	2.30	0.94
10:F:23:LYS:CB	10:F:24:LYS:NZ	2.30	0.94
1:1:57:ILE:CD1	1:1:58:LEU:N	2.30	0.94
21:B:8059:SUC:O6	21:B:8059:SUC:H1	1.67	0.94
19:3:3011:CLA:H122	19:3:3011:CLA:H172	1.49	0.94
4:4:38:ARG:CG	4:4:39:TRP:N	2.30	0.94
19:A:1781:CLA:HED3	19:A:1782:CLA:HMD1	1.46	0.94
5:A:599:PHE:CE2	5:A:731:ARG:HB3	2.03	0.94
7:C:73:THR:OG1	7:C:76:SER:HB3	1.67	0.94
19:1:1241:CLA:HAC1	22:I:1032:BCR:C3	1.98	0.94
22:I:1032:BCR:C32	22:I:1032:BCR:C4	2.38	0.94
19:J:1043:CLA:O1A	19:J:1043:CLA:H143	1.67	0.94
5:A:162:LEU:O	5:A:165:TYR:HB3	1.66	0.94
19:A:1781:CLA:H2	19:A:1782:CLA:HED3	1.50	0.94
6:B:124:TRP:NE1	6:B:129:LEU:HD22	1.83	0.94
6:B:612:SER:HA	6:B:615:TYR:HE1	1.30	0.94
19:1:1148:CLA:HBC2	19:1:1148:CLA:HHD	1.47	0.94
20:A:7048:LMU:H12	20:A:7048:LMU:H52	1.46	0.94
20:A:7048:LMU:H82	20:A:7048:LMU:C2	1.96	0.94
3:3:194:ILE:CG1	19:3:1214:CLA:HMC2	1.97	0.94
2:2:41:LEU:CD2	2:2:41:LEU:N	2.29	0.94
4:4:147:LEU:CD2	4:4:148:GLU:H	1.81	0.94
4:4:32:GLU:O	4:4:33:ASP:OD1	1.83	0.94
4:4:37:LEU:N	4:4:39:TRP:CB	2.30	0.94
20:A:7048:LMU:C9	20:A:7048:LMU:C3	2.40	0.94
12:H:44:ALA:HB2	16:L:145:PHE:CD1	2.01	0.94
2:2:43:TRP:CE2	2:2:125:PHE:CE1	2.56	0.94
5:A:340:GLY:O	5:A:343:HIS:HB2	1.68	0.94
5:A:462:ILE:HD11	19:B:1787:CLA:H51	1.47	0.94
19:B:1756:CLA:CBB	19:B:1770:CLA:HMB3	1.97	0.94
18:R:34:UNK:N	18:R:36:UNK:CB	2.30	0.94
3:3:181:LEU:N	3:3:181:LEU:CD1	2.30	0.94
2:2:167:GLY:O	2:2:170:ALA:N	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1759:CLA:C4	19:A:1796:CLA:H61	1.97	0.94
5:A:361:ASN:HD21	19:A:1761:CLA:CED	1.79	0.94
6:B:266:GLN:O	6:B:267:SER:HB3	1.66	0.94
7:C:1:MET:H1	7:C:4:SER:N	1.66	0.94
11:G:46:ALA:CA	11:G:48:ASP:CG	2.36	0.94
19:1:1014:CLA:H112	19:1:1014:CLA:C4	1.94	0.94
4:4:96:ILE:O	4:4:99:HIS:HB3	1.66	0.94
5:A:114:THR:HG22	5:A:115:HIS:ND1	1.82	0.94
5:A:626:GLY:HA3	5:A:636:HIS:HA	1.49	0.94
19:B:1756:CLA:HED1	19:B:1757:CLA:CMD	1.97	0.94
19:3:1212:CLA:HMC3	19:A:1770:CLA:HBA2	1.47	0.94
5:A:358:LEU:HD11	5:A:413:HIS:CG	2.02	0.94
8:D:39:LYS:HD2	8:D:42:VAL:CG1	1.98	0.94
16:L:163:LEU:HD22	16:L:164:PRO:HA	1.36	0.94
3:3:181:LEU:N	3:3:182:LYS:CE	2.30	0.94
20:A:7037:LMU:C12	20:A:7051:LMU:H32	1.97	0.94
19:4:4014:CLA:CBC	19:4:4014:CLA:HMC1	1.97	0.94
20:A:7021:LMU:H41	20:A:7021:LMU:O6'	1.67	0.94
16:L:82:ALA:HB2	16:L:86:LEU:HD13	0.97	0.94
2:2:98:GLU:HG3	2:2:99:LEU:CD1	1.97	0.94
4:4:165:GLY:O	4:4:169:GLN:HG2	1.67	0.94
4:4:34:PRO:HA	4:4:35:GLU:CG	1.96	0.94
4:4:34:PRO:HG3	4:4:35:GLU:OE1	1.67	0.94
6:B:422:LEU:HD13	6:B:535:VAL:HG11	1.47	0.94
11:G:46:ALA:N	11:G:48:ASP:CB	2.30	0.94
16:L:164:PRO:HD2	16:L:165:TYR:CG	2.02	0.94
17:N:72:LYS:NZ	17:N:74:LYS:HG2	1.82	0.94
20:A:7023:LMU:C9	20:A:7023:LMU:C2	2.30	0.94
2:2:203:THR:C	2:2:204:ILE:HG12	1.87	0.94
5:A:21:LEU:N	5:A:22:VAL:CG1	2.30	0.94
3:3:74:ALA:CA	19:3:1217:CLA:C2D	2.46	0.94
4:4:100:TYR:HA	4:4:103:ILE:CD1	1.98	0.94
19:A:1764:CLA:H142	22:A:1807:BCR:C14	1.98	0.94
6:B:556:SER:C	6:B:558:PRO:HD2	1.88	0.94
20:A:7048:LMU:C3	20:A:7048:LMU:C5'	2.30	0.94
5:A:316:MET:CB	5:A:317:TYR:HD1	1.76	0.94
15:K:9:LEU:CD2	15:K:9:LEU:N	2.30	0.94
2:2:50:VAL:O	2:2:54:TRP:HD1	1.51	0.93
4:4:147:LEU:CG	4:4:148:GLU:N	2.29	0.93
17:N:47:THR:HG21	17:N:54:LYS:HZ3	0.88	0.93
2:2:203:THR:CG2	2:2:204:ILE:N	2.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1014:CLA:CHD	19:1:1014:CLA:HBC3	1.96	0.93
19:4:1201:CLA:HBA1	19:4:1201:CLA:HMA2	0.95	0.93
20:A:7033:LMU:C5B	20:A:7033:LMU:H3'	1.98	0.93
19:R:1055:CLA:HBA2	19:R:1055:CLA:O1D	1.65	0.93
5:A:100:GLY:HA3	5:A:153:TRP:CH2	2.03	0.93
6:B:22:TRP:HE1	19:B:1771:CLA:HBB1	0.79	0.93
16:L:163:LEU:CB	16:L:164:PRO:HB3	1.96	0.93
17:N:61:LEU:CD1	17:N:63:ASP:N	2.30	0.93
17:N:63:ASP:H	17:N:64:ASP:HB3	1.32	0.93
11:G:93:TYR:CA	11:G:94:ASP:CB	2.30	0.93
5:A:23:ASP:OD1	5:A:24:ARG:HD3	1.66	0.93
6:B:517:PHE:O	6:B:517:PHE:HD2	1.36	0.93
4:4:36:ASN:O	4:4:39:TRP:HB2	1.68	0.93
19:A:1776:CLA:C9	22:A:1804:BCR:C37	2.11	0.93
22:A:1804:BCR:H23C	22:A:1804:BCR:C38	1.98	0.93
22:B:1780:BCR:C32	22:B:1780:BCR:C8	2.30	0.93
19:1:1014:CLA:C7	19:1:1014:CLA:H41	1.83	0.93
19:J:1044:CLA:H72	19:J:1044:CLA:H41	0.95	0.93
6:B:732:LYS:HG2	6:B:734:GLY:H	1.24	0.93
16:L:164:PRO:CD	16:L:165:TYR:CG	2.51	0.93
20:A:7016:LMU:H51	20:A:7016:LMU:O6'	1.66	0.93
1:1:57:ILE:HD13	1:1:58:LEU:H	1.25	0.93
21:3:1226:SUC:C1'	21:3:1226:SUC:C6'	2.39	0.93
21:B:8059:SUC:C6'	21:B:8059:SUC:H1'1	1.99	0.93
10:F:42:ILE:HG13	10:F:43:LYS:N	1.80	0.93
4:4:93:ILE:HA	4:4:96:ILE:HD11	1.48	0.93
19:A:1770:CLA:HHC	22:A:1802:BCR:C17	1.97	0.93
19:A:1810:CLA:HAA1	19:B:1786:CLA:HBB2	1.49	0.93
19:B:1787:CLA:C9	19:B:1788:CLA:C9	2.46	0.93
7:C:5:VAL:C	7:C:65:VAL:HG22	1.87	0.93
20:A:7041:LMU:O2'	20:A:7041:LMU:H5'	1.66	0.93
19:1:1142:CLA:CMD	19:K:1085:CLA:NA	2.30	0.93
16:L:118:LEU:HD12	16:L:119:THR:H	1.30	0.93
2:2:169:LEU:HD23	19:2:1215:CLA:CBB	1.92	0.93
3:3:84:ILE:H	19:3:1212:CLA:H43	1.32	0.93
19:A:1779:CLA:C1D	22:A:1804:BCR:H19C	1.99	0.93
5:A:328:LYS:HG2	5:A:332:GLU:CB	1.99	0.93
19:1:1148:CLA:HAA1	19:1:1148:CLA:O1D	1.69	0.93
3:3:84:ILE:HB	19:3:1212:CLA:O1A	0.76	0.93
4:4:147:LEU:CD1	4:4:148:GLU:N	2.30	0.93
19:A:1791:CLA:H3A	19:A:1797:CLA:CBB	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:331:LEU:HD11	5:A:346:LEU:HB2	1.49	0.93
20:A:7006:LMU:O2'	20:A:7006:LMU:H22	1.69	0.93
9:E:61:THR:HG22	9:E:62:ARG:H	1.34	0.93
19:1:1014:CLA:H71	19:1:1014:CLA:C4	1.99	0.93
20:A:7048:LMU:H3'	20:A:7048:LMU:C2	1.99	0.93
19:4:1196:CLA:CB	19:4:1196:CLA:CHD	2.42	0.93
22:A:1803:BCR:C23	22:A:1803:BCR:H402	1.96	0.93
11:G:46:ALA:N	11:G:49:THR:CG2	2.30	0.93
2:2:44:ASN:ND2	14:J:1:MET:HB2	1.83	0.93
19:J:1044:CLA:OBD	19:J:1044:CLA:HED3	1.67	0.93
8:D:124:ASN:HB3	8:D:125:PRO:HD3	1.51	0.93
20:A:7005:LMU:H11	20:A:7005:LMU:O2'	1.68	0.93
19:A:1783:CLA:C7	22:A:1806:BCR:C37	2.47	0.93
5:A:73:GLU:O	5:A:76:ARG:N	2.02	0.93
19:B:1753:CLA:HBC2	19:B:1754:CLA:HBA1	1.51	0.93
11:G:68:ILE:O	11:G:72:LEU:HB3	1.68	0.93
20:A:7032:LMU:O1'	20:A:7032:LMU:H1B	1.68	0.93
4:4:104:ARG:NH1	4:4:105:ARG:CB	2.29	0.93
6:B:353:TYR:CG	6:B:594:TRP:HZ3	1.86	0.93
1:1:89:VAL:O	11:G:77:ILE:HD13	1.68	0.93
2:2:116:PRO:O	2:2:131:THR:HB	1.67	0.92
5:A:239:PRO:HA	5:A:242:ILE:HD11	1.49	0.92
6:B:279:ALA:O	19:B:1747:CLA:HMB3	1.67	0.92
6:B:525:LEU:HD22	6:B:525:LEU:O	1.69	0.92
2:2:61:GLY:O	2:2:65:PRO:HG2	1.69	0.92
2:2:70:LYS:HG3	2:2:73:ILE:HG13	1.50	0.92
2:2:73:ILE:HD12	2:2:73:ILE:N	1.83	0.92
4:4:71:ASN:O	4:4:73:PRO:HD3	1.69	0.92
19:A:1796:CLA:H141	22:A:1806:BCR:HC22	0.94	0.92
22:A:1802:BCR:H402	22:A:1802:BCR:C23	1.94	0.92
22:A:1807:BCR:C23	22:A:1807:BCR:H393	1.93	0.92
6:B:648:TRP:CZ3	22:B:1781:BCR:H392	2.03	0.92
4:4:74:LYS:N	4:4:75:TRP:CA	2.29	0.92
11:G:93:TYR:HA	11:G:94:ASP:CG	1.89	0.92
21:B:8055:SUC:H1'1	21:B:8055:SUC:H6'2	0.93	0.92
3:3:87:GLU:O	22:3:1225:BCR:H381	1.69	0.92
3:3:84:ILE:H	19:3:1212:CLA:C3	1.82	0.92
1:1:179:THR:OG1	4:4:87:SER:CB	2.17	0.92
6:B:142:LEU:CD2	22:B:1777:BCR:H333	2.00	0.92
20:A:7036:LMU:H71	20:A:7036:LMU:H31	0.94	0.92
5:A:478:SER:HB3	5:A:644:GLN:OE1	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:42:ARG:HG3	2:2:45:VAL:HG21	1.46	0.92
19:A:1788:CLA:C16	22:L:1169:BCR:C36	2.47	0.92
11:G:47:GLY:H	11:G:48:ASP:CA	1.82	0.92
11:G:45:GLU:HG2	11:G:49:THR:CG2	1.86	0.92
2:2:127:ASN:HD21	14:J:7:TYR:HA	1.33	0.92
5:A:24:ARG:O	5:A:26:PRO:HG2	1.68	0.92
10:F:40:LEU:HA	10:F:42:ILE:HG12	1.50	0.92
19:A:1781:CLA:O1A	19:A:1781:CLA:H2	1.68	0.92
5:A:472:ARG:HE	5:A:474:GLN:HG3	1.31	0.92
6:B:596:TRP:HH2	6:B:612:SER:O	1.48	0.92
7:C:1:MET:CG	7:C:4:SER:OG	2.16	0.92
11:G:40:GLY:O	11:G:41:MET:SD	2.28	0.92
11:G:7:VAL:CG2	11:G:8:ILE:H	1.83	0.92
4:4:194:VAL:HG12	4:4:195:GLN:HB2	0.94	0.92
15:K:9:LEU:HD23	15:K:9:LEU:H	1.25	0.92
2:2:43:TRP:HZ2	2:2:125:PHE:CZ	1.84	0.92
4:4:166:PHE:O	4:4:169:GLN:HB2	1.69	0.92
7:C:79:LEU:HD22	7:C:81:TYR:O	1.70	0.92
19:R:1054:CLA:CHA	19:R:1054:CLA:CED	2.47	0.92
4:4:101:VAL:HG13	4:4:104:ARG:HH21	1.11	0.92
19:A:1783:CLA:H203	22:A:1807:BCR:H17C	0.92	0.92
22:A:1806:BCR:H313	19:A:1812:CLA:H143	1.48	0.92
22:B:1780:BCR:H271	22:B:1780:BCR:C40	1.95	0.92
22:B:1781:BCR:C38	22:B:1781:BCR:H23C	1.98	0.92
2:2:162:LYS:NZ	19:2:1215:CLA:OBD	2.02	0.92
4:4:88:SER:O	4:4:90:LEU:HA	1.70	0.92
6:B:351:HIS:HB3	19:B:1748:CLA:HED1	1.49	0.92
21:B:8054:SUC:O2	21:B:8054:SUC:H1'1	1.70	0.92
8:D:102:ARG:NH1	8:D:104:PHE:CE1	2.38	0.92
10:F:23:LYS:C	10:F:24:LYS:HZ3	1.73	0.92
20:A:7009:LMU:C5B	20:A:7009:LMU:C3'	2.47	0.92
4:4:60:LEU:HG	4:4:61:PRO:HD3	1.49	0.92
6:B:369:ALA:O	6:B:725:LEU:HD11	1.70	0.92
19:4:1196:CLA:HBC2	19:4:1196:CLA:CHD	1.99	0.92
19:A:1771:CLA:CMC	19:A:1771:CLA:CBC	2.30	0.92
3:3:93:PHE:H	3:3:95:THR:H	1.10	0.92
17:N:61:LEU:HD11	17:N:63:ASP:CB	1.98	0.92
17:N:72:LYS:NZ	17:N:74:LYS:CG	2.33	0.92
8:D:111:TYR:HD2	8:D:114:PRO:HB3	1.33	0.92
1:1:163:VAL:HA	1:1:166:SER:HB3	1.51	0.92
19:A:1779:CLA:NC	22:A:1804:BCR:H19C	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:602:TRP:O	6:B:604:GLY:N	2.01	0.91
11:G:46:ALA:C	11:G:48:ASP:CG	2.29	0.91
1:1:39:TYR:CG	19:1:1195:CLA:OBD	2.22	0.91
2:2:40:SER:C	2:2:41:LEU:HD22	1.89	0.91
4:4:117:GLN:O	4:4:121:PHE:HE2	1.49	0.91
19:A:1788:CLA:H52	22:B:1781:BCR:C34	2.00	0.91
19:K:1085:CLA:CGA	19:K:1085:CLA:H3A	2.00	0.91
19:1:1145:CLA:CMC	19:1:1145:CLA:HBC3	2.00	0.91
20:A:7022:LMU:C2'	20:A:7022:LMU:C2	2.31	0.91
2:2:54:TRP:CE2	2:2:109:ARG:HD2	2.04	0.91
5:A:411:ALA:HB2	22:A:1805:BCR:H392	1.52	0.91
6:B:382:ILE:CG2	6:B:383:MET:H	1.83	0.91
16:L:123:ARG:HA	16:L:123:ARG:CZ	2.00	0.91
19:1:1014:CLA:CAA	19:1:1014:CLA:CGD	2.49	0.91
20:A:7020:LMU:H6E	20:A:7020:LMU:H5B	1.30	0.91
20:A:7021:LMU:C2	20:A:7021:LMU:H62	1.97	0.91
5:A:259:TYR:HB3	5:A:260:PRO:HD2	1.51	0.91
3:3:83:LEU:HA	19:3:1212:CLA:H43	1.50	0.91
6:B:65:LEU:HD22	6:B:124:TRP:CE3	2.05	0.91
20:A:7042:LMU:H22	20:A:7042:LMU:H71	0.93	0.91
17:N:72:LYS:CG	17:N:74:LYS:HB2	2.00	0.91
2:2:203:THR:HG22	2:2:204:ILE:N	1.84	0.91
8:D:30:ALA:O	16:L:18:PRO:HB2	1.71	0.91
1:1:37:GLU:HA	1:1:40:LYS:HB2	1.49	0.91
6:B:172:GLU:O	6:B:176:ASN:HB2	1.70	0.91
23:B:1774:PQN:H191	22:B:1781:BCR:H10C	0.91	0.91
7:C:5:VAL:HB	7:C:65:VAL:HA	1.52	0.91
11:G:45:GLU:CB	11:G:49:THR:HG21	1.99	0.91
20:A:7048:LMU:H22	20:A:7048:LMU:O2'	1.68	0.91
19:3:1222:CLA:O1D	19:3:1222:CLA:H2A	1.71	0.91
4:4:143:PHE:HB2	4:4:150:LYS:HE2	1.52	0.91
19:A:1779:CLA:C1D	22:A:1804:BCR:C19	2.47	0.91
5:A:248:PHE:HD2	5:A:248:PHE:H	1.11	0.91
6:B:142:LEU:HD22	22:B:1777:BCR:H333	1.52	0.91
17:N:47:THR:CG2	17:N:54:LYS:HZ3	1.81	0.91
20:A:7016:LMU:H21	20:A:7016:LMU:H81	0.93	0.91
20:A:7009:LMU:H3'	20:A:7009:LMU:C5B	2.00	0.91
6:B:561:GLY:HA3	7:C:52:LYS:HG2	1.51	0.91
7:C:78:GLY:O	7:C:81:TYR:HE1	1.53	0.91
16:L:30:SER:OG	16:L:32:LEU:HB2	1.67	0.91
16:L:95:LEU:HD13	22:L:1169:BCR:C31	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:59:VAL:HG13	1:1:60:PRO:HD2	1.53	0.91
12:H:25:GLY:HA2	12:H:27:ASP:OD2	1.69	0.91
5:A:648:THR:HG23	5:A:651:GLY:H	1.34	0.91
6:B:442:VAL:HG21	19:B:1764:CLA:HAC2	1.51	0.91
2:2:41:LEU:O	2:2:42:ARG:CD	2.19	0.91
4:4:91:PHE:C	4:4:91:PHE:CD2	2.39	0.91
6:B:492:ILE:H	6:B:492:ILE:HD13	1.36	0.91
17:N:54:LYS:CB	17:N:57:LYS:HZ1	1.83	0.91
17:N:72:LYS:CG	17:N:74:LYS:N	2.33	0.91
19:1:1145:CLA:H2	19:1:1145:CLA:O1A	1.68	0.91
20:A:7038:LMU:C6	20:A:7038:LMU:H101	1.99	0.91
19:A:1771:CLA:H42	19:A:1771:CLA:CAA	1.99	0.91
5:A:301:HIS:CD2	19:A:1772:CLA:O1D	2.23	0.91
19:B:1740:CLA:HBB2	19:B:1787:CLA:H13	1.53	0.91
19:L:1168:CLA:CGD	19:L:1168:CLA:HAA1	1.99	0.91
3:3:205:GLY:N	5:A:252:ARG:NH2	2.14	0.91
22:3:1225:BCR:C8	22:3:1225:BCR:H311	1.99	0.91
3:3:87:GLU:C	22:3:1225:BCR:H381	1.91	0.91
6:B:120:VAL:HA	6:B:123:TRP:NE1	1.85	0.91
4:4:93:ILE:C	4:4:96:ILE:HD12	1.92	0.90
19:B:1756:CLA:CBC	19:B:1756:CLA:CHD	2.45	0.90
21:3:1226:SUC:H5	21:3:1226:SUC:O2'	1.71	0.90
6:B:5:ILE:HB	6:B:6:PRO:HD2	1.51	0.90
5:A:328:LYS:HG3	5:A:332:GLU:HB2	1.50	0.90
11:G:46:ALA:H	11:G:49:THR:HG21	1.32	0.90
19:1:1145:CLA:H3A	19:1:1145:CLA:CGA	2.00	0.90
20:A:7050:LMU:H81	20:A:7050:LMU:H41	1.51	0.90
5:A:304:LEU:HD22	19:A:1772:CLA:CBB	2.01	0.90
5:A:453:LEU:HB3	5:A:547:PHE:HB2	1.53	0.90
5:A:659:ALA:O	5:A:662:SER:OG	1.87	0.90
6:B:672:GLN:HE21	6:B:672:GLN:CA	1.84	0.90
17:N:47:THR:CG2	17:N:54:LYS:NZ	2.32	0.90
20:A:7048:LMU:H3'	20:A:7048:LMU:H22	1.51	0.90
15:K:52:PRO:O	15:K:56:THR:HG22	1.71	0.90
6:B:282:PHE:CZ	19:B:1747:CLA:C1	2.53	0.90
6:B:362:ALA:HB2	6:B:368:GLN:HG2	1.53	0.90
6:B:382:ILE:O	6:B:384:THR:N	2.05	0.90
13:I:12:VAL:HG21	19:I:1031:CLA:O1A	1.71	0.90
16:L:64:LEU:HB3	16:L:68:PHE:CE1	2.07	0.90
1:1:24:PHE:CD2	6:B:314:ARG:NH2	2.39	0.90
20:A:7026:LMU:H4O1	21:B:8062:SUC:H3'	1.32	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:89:VAL:HB	1:1:90:PRO:HD3	1.52	0.90
4:4:121:PHE:O	4:4:122:LYS:CD	2.19	0.90
19:A:1765:CLA:CBB	19:B:1764:CLA:HMD2	2.01	0.90
19:B:1741:CLA:O2A	19:B:1741:CLA:HMA2	1.71	0.90
6:B:167:TRP:HB2	11:G:41:MET:HE2	1.49	0.90
11:G:42:SER:HB2	11:G:45:GLU:OE2	1.70	0.90
18:R:33:UNK:C	18:R:36:UNK:CB	2.50	0.90
3:3:181:LEU:HD12	3:3:181:LEU:N	1.85	0.90
2:2:41:LEU:N	2:2:41:LEU:HD23	1.85	0.90
2:2:73:ILE:O	2:2:74:LEU:HD23	1.72	0.90
19:A:1781:CLA:C7	19:A:1782:CLA:HED1	2.00	0.90
19:A:1781:CLA:C6	19:A:1782:CLA:HED1	2.02	0.90
6:B:50:HIS:CD2	19:B:1737:CLA:HAA2	2.06	0.90
6:B:732:LYS:CB	6:B:733:PHE:C	2.39	0.90
3:3:64:TYR:HB3	19:3:1222:CLA:H42	1.50	0.90
1:1:63:LEU:N	1:1:63:LEU:HD13	1.84	0.90
8:D:48:ILE:HB	8:D:100:PHE:HB3	1.52	0.90
2:2:196:HIS:O	2:2:197:LEU:HB2	1.70	0.90
4:4:36:ASN:O	4:4:39:TRP:CE3	2.25	0.90
6:B:119:GLY:HA3	19:B:1759:CLA:CED	2.00	0.90
19:B:1766:CLA:HMB1	22:B:1778:BCR:H292	1.53	0.90
19:B:1787:CLA:HBB2	19:B:1788:CLA:CHB	2.00	0.90
6:B:666:SER:HB3	6:B:671:TRP:HE1	1.36	0.90
11:G:48:ASP:HB2	11:G:49:THR:HG22	0.92	0.90
16:L:66:GLY:HA3	19:L:1168:CLA:HHC	1.52	0.90
19:1:1192:CLA:HHD	19:1:1192:CLA:CBC	2.01	0.90
19:1:1145:CLA:HAA2	19:1:1145:CLA:O1D	1.69	0.90
15:K:20:PHE:C	15:K:20:PHE:CD2	2.43	0.90
15:K:74:ILE:HG22	15:K:75:VAL:HG22	1.54	0.90
2:2:43:TRP:CZ3	2:2:125:PHE:CB	2.55	0.90
19:B:1754:CLA:C2	19:B:1754:CLA:H71	1.99	0.90
6:B:697:PRO:O	7:C:79:LEU:CD1	2.19	0.90
13:I:8:PHE:HB2	19:I:1031:CLA:OBD	1.72	0.90
4:4:69:ILE:CG2	4:4:70:ILE:H	1.84	0.90
17:N:40:CYS:SG	17:N:40:CYS:O	2.29	0.90
17:N:63:ASP:HA	17:N:64:ASP:C	1.91	0.90
4:4:124:TYR:O	4:4:127:PRO:CD	2.20	0.90
4:4:39:TRP:CG	4:4:40:PHE:N	2.27	0.90
19:A:1780:CLA:HMD2	19:A:1780:CLA:H142	1.52	0.90
19:B:1738:CLA:H2A	19:B:1738:CLA:O1D	1.72	0.90
19:B:1769:CLA:H161	22:B:1780:BCR:C31	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:75:TRP:HE3	4:4:76:TYR:H	1.18	0.90
20:A:7048:LMU:H31	20:A:7048:LMU:H82	1.45	0.90
1:1:57:ILE:CD1	1:1:58:LEU:H	1.85	0.90
6:B:5:ILE:HB	6:B:6:PRO:CD	2.01	0.90
2:2:42:ARG:HG3	2:2:45:VAL:CB	2.02	0.90
19:A:1781:CLA:C6	19:A:1782:CLA:CED	2.50	0.90
25:B:1785:SF4:FE1	25:B:1785:SF4:S4	1.64	0.90
6:B:551:LYS:NZ	8:D:140:ASN:O	2.05	0.90
2:2:64:ILE:O	2:2:68:LEU:HB2	1.71	0.89
20:A:7036:LMU:H22	20:A:7036:LMU:H82	0.91	0.89
20:B:1783:LMU:H61	20:B:1783:LMU:H112	0.91	0.89
15:K:20:PHE:CD2	15:K:21:ALA:N	2.41	0.89
19:2:1217:CLA:CGD	19:2:1217:CLA:HBA1	2.01	0.89
6:B:504:ASN:H	6:B:504:ASN:HD22	1.14	0.89
1:1:179:THR:OG1	4:4:87:SER:HB3	1.71	0.89
3:3:84:ILE:N	19:3:1212:CLA:H43	1.88	0.89
5:A:545:HIS:ND1	19:A:1792:CLA:HBB2	1.87	0.89
22:A:1806:BCR:H393	22:A:1806:BCR:H23C	1.52	0.89
5:A:470:LEU:CD1	6:B:95:HIS:HB3	2.02	0.89
6:B:621:ARG:O	6:B:625:TRP:HB3	1.71	0.89
4:4:193:ILE:HG22	4:4:194:VAL:N	1.87	0.89
19:2:1212:CLA:C4	19:2:1212:CLA:CGA	2.50	0.89
4:4:52:MET:CE	4:4:156:ASN:HB2	2.02	0.89
5:A:472:ARG:NH1	16:L:74:LEU:HG	1.87	0.89
3:3:92:TRP:CZ2	5:A:250:LEU:HD12	2.08	0.89
21:B:8059:SUC:H3	21:B:8059:SUC:O2'	1.72	0.89
2:2:55:ALA:CB	2:2:56:MET:CE	2.48	0.89
6:B:693:TRP:HD1	19:B:1771:CLA:C2D	1.86	0.89
6:B:635:ILE:O	6:B:636:THR:O	1.91	0.89
8:D:102:ARG:HE	8:D:110:GLN:HB2	1.38	0.89
5:A:567:ARG:HH11	8:D:35:GLY:HA2	1.37	0.89
10:F:93:ILE:O	10:F:96:TRP:HD1	1.55	0.89
20:A:7039:LMU:O6B	20:A:7039:LMU:H4'	1.73	0.89
2:2:98:GLU:CG	2:2:99:LEU:CD1	2.51	0.89
4:4:121:PHE:O	4:4:122:LYS:HB2	1.73	0.89
19:A:1760:CLA:HBB2	19:A:1762:CLA:C3D	2.02	0.89
6:B:87:ILE:HA	6:B:115:ASN:CA	2.03	0.89
19:B:1744:CLA:H41	19:B:1749:CLA:CBC	2.03	0.89
6:B:574:ASP:HA	6:B:577:TYR:HB3	1.52	0.89
3:3:205:GLY:H	5:A:252:ARG:HH22	0.92	0.89
20:A:7050:LMU:O3B	20:A:7050:LMU:H6'1	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:94:LEU:O	2:2:98:GLU:HB3	1.71	0.89
19:A:1763:CLA:CAB	22:A:1807:BCR:C33	2.50	0.89
5:A:578:ARG:CZ	5:A:578:ARG:HB2	2.02	0.89
5:A:714:LEU:HD13	22:B:1780:BCR:C39	2.01	0.89
19:B:1756:CLA:H52	19:B:1770:CLA:CAD	2.03	0.89
17:N:45:ASN:HB2	17:N:57:LYS:HZ2	1.35	0.89
19:2:1217:CLA:HED3	19:2:1217:CLA:OBD	1.71	0.89
2:2:164:ILE:O	2:2:167:GLY:HA3	1.72	0.89
2:2:41:LEU:O	2:2:42:ARG:CB	2.21	0.89
5:A:368:LEU:HD11	19:A:1782:CLA:H61	1.51	0.89
5:A:711:HIS:NE2	19:A:1795:CLA:CAC	2.35	0.89
19:B:1744:CLA:H41	19:B:1749:CLA:HBC3	1.54	0.89
6:B:91:ILE:HG21	19:B:1740:CLA:HMD1	1.54	0.89
16:L:164:PRO:CD	16:L:165:TYR:CD1	2.56	0.89
19:1:1142:CLA:HED1	19:K:1085:CLA:CMB	1.96	0.89
19:3:1224:CLA:C14	19:3:1224:CLA:H102	2.03	0.89
1:1:63:LEU:HD23	1:1:64:GLY:C	1.93	0.89
2:2:43:TRP:HZ3	2:2:125:PHE:CB	1.86	0.89
4:4:95:PHE:HZ	19:4:1210:CLA:NC	1.63	0.89
4:4:122:LYS:HB3	4:4:143:PHE:HB3	1.55	0.89
19:A:1779:CLA:CBB	22:A:1804:BCR:H353	2.02	0.89
19:A:1797:CLA:H91	15:K:61:LEU:HD13	1.54	0.89
19:A:1763:CLA:CMB	22:A:1807:BCR:HC7	2.01	0.89
19:3:1224:CLA:HED1	19:3:1224:CLA:CBA	2.00	0.89
3:3:74:ALA:HA	19:3:1217:CLA:C1D	2.02	0.89
21:B:8059:SUC:O2	21:B:8059:SUC:H1'2	1.70	0.89
9:E:68:ARG:O	9:E:68:ARG:NE	2.05	0.89
4:4:40:PHE:CB	4:4:43:ALA:CB	2.29	0.89
5:A:131:ILE:O	5:A:671:SER:HA	1.73	0.89
5:A:327:ILE:O	5:A:328:LYS:O	1.90	0.89
5:A:355:HIS:ND1	5:A:416:ILE:CG2	2.35	0.89
6:B:25:ILE:CG2	22:L:1169:BCR:H291	2.01	0.89
6:B:292:ARG:O	6:B:293:THR:OG1	1.91	0.89
19:J:1044:CLA:C16	19:J:1044:CLA:H91	2.03	0.89
5:A:25:ASP:CB	5:A:26:PRO:CD	2.46	0.89
20:A:7032:LMU:C5B	20:A:7032:LMU:H3'	2.03	0.89
5:A:81:ALA:HB2	19:A:1760:CLA:HMA2	1.55	0.88
6:B:393:PHE:HD2	6:B:397:ASP:OD1	1.55	0.88
6:B:91:ILE:HD12	6:B:104:PHE:HE2	1.37	0.88
19:4:1198:CLA:C2A	19:4:1198:CLA:CGD	2.51	0.88
4:4:90:LEU:H	4:4:91:PHE:HB3	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:99:HIS:HE1	4:4:103:ILE:HD12	1.35	0.88
19:A:1779:CLA:CAB	22:A:1804:BCR:C35	2.48	0.88
20:A:7040:LMU:O3'	20:A:7040:LMU:H1B	1.65	0.88
19:A:1781:CLA:HMB3	22:A:1805:BCR:C18	2.03	0.88
19:4:1205:CLA:C10	19:4:1205:CLA:H41	2.02	0.88
19:A:1781:CLA:C7	19:A:1782:CLA:HED2	2.01	0.88
19:B:1747:CLA:HHD	19:B:1747:CLA:CBC	2.02	0.88
3:3:98:ILE:HB	17:N:61:LEU:HB2	1.55	0.88
19:J:1043:CLA:H2	19:J:1043:CLA:C16	2.04	0.88
2:2:99:LEU:HD22	19:2:1222:CLA:CMC	2.01	0.88
19:A:1797:CLA:O1A	19:A:1797:CLA:HED1	1.74	0.88
19:B:1739:CLA:H92	19:B:1739:CLA:HBB2	0.90	0.88
19:2:1217:CLA:HBD	19:2:1217:CLA:HBA1	1.55	0.88
2:2:165:LYS:O	2:2:168:ARG:N	2.05	0.88
4:4:104:ARG:NH1	4:4:105:ARG:HB3	1.88	0.88
19:4:1198:CLA:C15	19:4:1198:CLA:H202	1.99	0.88
5:A:711:HIS:CD2	19:A:1795:CLA:CBC	2.56	0.88
22:B:1778:BCR:H321	22:B:1778:BCR:HC8	1.56	0.88
7:C:14:CYS:HA	7:C:17:CYS:HG	1.01	0.88
5:A:27:ILE:HD12	5:A:27:ILE:O	1.72	0.88
17:N:32:ALA:CB	17:N:35:VAL:HG22	2.04	0.88
1:1:185:TRP:CA	1:1:186:HIS:ND1	2.37	0.88
19:A:1783:CLA:H171	22:A:1807:BCR:H15C	1.54	0.88
5:A:711:HIS:CE1	19:A:1795:CLA:HAC1	2.08	0.88
19:B:1741:CLA:H61	12:H:69:SER:CB	2.01	0.88
19:B:1741:CLA:HBB2	13:I:13:GLY:O	1.74	0.88
19:B:1754:CLA:C7	19:B:1754:CLA:C2	2.50	0.88
1:1:27:LEU:HD21	6:B:314:ARG:HG2	0.90	0.88
17:N:67:LEU:HB2	17:N:68:GLU:HG2	0.91	0.88
5:A:267:THR:O	5:A:269:PHE:CD2	2.25	0.88
6:B:70:TRP:CD1	6:B:71:GLN:OE1	2.27	0.88
19:A:1781:CLA:C5	19:A:1782:CLA:HED1	2.03	0.88
5:A:581:CYS:CB	5:A:590:CYS:HA	2.04	0.88
25:B:1785:SF4:S2	25:B:1785:SF4:FE4	1.64	0.88
6:B:230:TRP:CH2	11:G:11:SER:HB2	2.09	0.88
16:L:56:VAL:HG13	19:L:1167:CLA:CED	2.04	0.88
20:A:7030:LMU:C9	20:A:7030:LMU:H52	2.01	0.88
6:B:531:THR:O	6:B:535:VAL:HG12	1.74	0.88
15:K:10:ILE:CA	15:K:13:THR:HG23	2.04	0.88
8:D:113:HIS:H	8:D:114:PRO:HD2	1.38	0.88
19:1:1193:CLA:HBC3	19:1:1193:CLA:HMC1	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:103:GLY:CA	19:2:1222:CLA:HBB2	2.03	0.88
19:A:1797:CLA:CHD	19:A:1797:CLA:HBC2	2.00	0.88
5:A:207:LEU:HA	5:A:211:LEU:HG	1.54	0.88
5:A:358:LEU:HD11	5:A:413:HIS:CB	2.03	0.88
6:B:275:HIS:O	6:B:279:ALA:N	2.05	0.88
6:B:732:LYS:HG2	6:B:733:PHE:CA	2.04	0.88
13:I:11:LEU:CD1	22:I:1032:BCR:C10	2.45	0.88
17:N:48:GLY:HA2	17:N:49:CYS:HG	1.05	0.88
20:A:7032:LMU:H31	20:A:7032:LMU:O5B	1.72	0.88
1:1:184:PRO:C	1:1:185:TRP:HE3	1.77	0.87
4:4:95:PHE:HD1	4:4:95:PHE:N	1.72	0.87
19:A:1761:CLA:H151	22:A:1802:BCR:H393	1.55	0.87
19:A:1771:CLA:HAA1	19:A:1771:CLA:HED1	1.52	0.87
19:A:1787:CLA:HBB1	19:A:1793:CLA:H192	1.55	0.87
19:A:1797:CLA:O2D	19:A:1797:CLA:HAA1	1.74	0.87
20:A:7023:LMU:C9	20:A:7023:LMU:C3	2.49	0.87
18:R:39:UNK:HA	18:R:42:UNK:CB	2.04	0.87
5:A:24:ARG:O	5:A:26:PRO:HB2	1.74	0.87
12:H:25:GLY:HA3	12:H:27:ASP:CA	2.03	0.87
3:3:112:THR:OG1	3:3:113:LEU:N	2.04	0.87
16:L:115:ALA:H	16:L:116:PRO:HD2	1.36	0.87
19:A:1791:CLA:C3A	19:A:1797:CLA:CBB	2.52	0.87
5:A:425:THR:HG1	5:A:428:TYR:HE1	0.93	0.87
17:N:32:ALA:HB1	17:N:35:VAL:CG2	2.05	0.87
5:A:356:ALA:HB2	5:A:417:PHE:HD2	1.39	0.87
6:B:527:LEU:HD12	19:B:1756:CLA:C1D	2.03	0.87
6:B:732:LYS:CG	6:B:733:PHE:CA	2.49	0.87
17:N:72:LYS:HG3	17:N:74:LYS:N	1.87	0.87
15:K:10:ILE:CD1	15:K:10:ILE:H	1.87	0.87
2:2:168:ARG:NH2	2:2:171:MET:HB2	1.88	0.87
4:4:106:TRP:C	4:4:108:ASP:H	1.78	0.87
4:4:38:ARG:HG3	4:4:39:TRP:CA	2.05	0.87
5:A:370:ILE:CG2	5:A:400:MET:HA	2.04	0.87
6:B:732:LYS:HG2	6:B:734:GLY:CA	2.04	0.87
7:C:1:MET:N	7:C:3:HIS:C	2.27	0.87
19:1:1188:CLA:O2D	19:1:1188:CLA:HBA2	1.72	0.87
17:N:48:GLY:CA	17:N:49:CYS:CB	2.50	0.87
19:1:1308:CLA:HMA3	19:J:1044:CLA:HED2	1.54	0.87
19:1:1145:CLA:CGA	19:1:1145:CLA:C3A	2.51	0.87
6:B:137:THR:HA	6:B:140:ILE:HG13	1.55	0.87
2:2:42:ARG:CA	2:2:45:VAL:CG2	2.30	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:331:LEU:C	5:A:331:LEU:HD23	1.94	0.87
25:B:1785:SF4:FE4	25:B:1785:SF4:S3	1.66	0.87
6:B:310:PRO:CG	6:B:311:PRO:HD2	2.04	0.87
24:B:1784:LMG:O3	7:C:70:TRP:CZ2	2.26	0.87
21:B:8052:SUC:C1	21:B:8052:SUC:C4'	2.51	0.87
5:A:349:ILE:HG23	5:A:352:THR:O	1.73	0.87
4:4:37:LEU:O	4:4:39:TRP:CD1	2.27	0.87
5:A:361:ASN:HD21	19:A:1761:CLA:HED3	1.39	0.87
5:A:151:GLN:NE2	5:A:384:TYR:O	2.07	0.87
4:4:75:TRP:CG	19:4:1205:CLA:HMD3	2.09	0.87
5:A:249:ILE:CG1	5:A:250:LEU:H	1.83	0.87
19:4:1201:CLA:CAA	19:4:1201:CLA:CGD	2.51	0.87
10:F:23:LYS:HB2	10:F:24:LYS:NZ	1.89	0.87
10:F:24:LYS:CA	10:F:26:GLN:H	1.87	0.87
8:D:113:HIS:NE2	8:D:118:VAL:CG1	2.37	0.87
19:A:1761:CLA:H42	22:A:1803:BCR:H313	1.56	0.87
19:A:1772:CLA:HBA2	19:A:1772:CLA:H2	1.54	0.87
19:A:1776:CLA:C3C	19:A:1782:CLA:H172	2.03	0.87
19:A:1797:CLA:CHD	19:A:1797:CLA:HBC3	2.01	0.87
5:A:217:SER:CA	22:A:1802:BCR:H351	2.03	0.87
6:B:189:ALA:HB2	19:B:1759:CLA:H203	1.54	0.87
7:C:1:MET:CG	7:C:4:SER:CB	2.53	0.87
9:E:42:GLU:HG2	9:E:43:SER:N	1.90	0.87
12:H:21:TRP:H	12:H:22:ASP:HA	1.38	0.87
22:A:1806:BCR:C31	22:A:1806:BCR:C8	2.46	0.87
5:A:309:LEU:HD21	19:A:1776:CLA:CMC	2.05	0.87
19:A:1788:CLA:C16	22:L:1169:BCR:H361	2.05	0.87
20:A:7048:LMU:C8	20:A:7048:LMU:H41	1.94	0.87
19:R:1055:CLA:H91	20:R:1056:LMU:O4'	1.72	0.87
12:H:44:ALA:CB	16:L:145:PHE:CD1	2.58	0.87
6:B:110:LEU:HD12	6:B:111:GLY:H	1.40	0.87
17:N:4:GLU:O	17:N:4:GLU:HG3	1.72	0.87
6:B:317:ARG:NH1	6:B:405:ASP:O	2.08	0.87
4:4:106:TRP:HD1	19:4:1196:CLA:O1D	1.53	0.87
4:4:36:ASN:OD1	4:4:39:TRP:CG	2.27	0.87
6:B:427:LEU:HD23	6:B:431:PHE:CZ	2.10	0.87
13:I:11:LEU:HD12	22:I:1032:BCR:H10C	0.87	0.87
20:A:7048:LMU:C3	20:A:7048:LMU:H3'	2.04	0.87
20:I:1200:LMU:C6'	20:I:1200:LMU:C2'	2.47	0.87
4:4:169:GLN:NE2	4:4:169:GLN:HA	1.87	0.86
5:A:661:ALA:O	5:A:664:VAL:HG22	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1756:CLA:CBB	19:B:1770:CLA:HHB	2.05	0.86
6:B:86:PRO:O	6:B:87:ILE:HG13	1.73	0.86
13:I:24:LEU:C	13:I:26:LEU:H	1.78	0.86
2:2:178:TRP:C	2:2:182:ILE:HG13	1.95	0.86
15:K:10:ILE:CA	15:K:13:THR:CG2	2.53	0.86
20:A:7050:LMU:C8	20:A:7050:LMU:H41	2.02	0.86
6:B:474:PHE:CE2	6:B:476:ILE:HG13	2.10	0.86
6:B:216:LEU:HD21	6:B:221:GLY:HA2	1.57	0.86
4:4:100:TYR:HA	4:4:103:ILE:CG1	2.05	0.86
22:A:1805:BCR:C33	22:A:1805:BCR:HC8	2.05	0.86
5:A:194:ALA:O	5:A:198:ASP:N	2.07	0.86
5:A:393:LEU:HG	5:A:394:SER:H	1.40	0.86
16:L:95:LEU:HD13	22:L:1169:BCR:H312	1.54	0.86
19:1:1188:CLA:HMA2	19:1:1188:CLA:O2A	1.74	0.86
17:N:61:LEU:HD11	17:N:63:ASP:O	1.76	0.86
17:N:63:ASP:H	17:N:64:ASP:CA	1.88	0.86
19:2:1212:CLA:HBC2	19:2:1212:CLA:HMC1	1.54	0.86
19:A:1763:CLA:C2B	22:A:1807:BCR:C33	2.53	0.86
5:A:606:TYR:O	5:A:610:SER:HB2	1.76	0.86
20:A:7041:LMU:O6'	20:A:7041:LMU:H1B	1.75	0.86
19:1:1148:CLA:CGA	19:1:1148:CLA:HED1	1.98	0.86
2:2:168:ARG:HH21	2:2:171:MET:HB2	1.36	0.86
4:4:121:PHE:CD2	4:4:122:LYS:O	2.27	0.86
6:B:203:ARG:HG2	6:B:204:GLY:N	1.89	0.86
6:B:469:LYS:HG2	6:B:471:THR:OG1	1.76	0.86
11:G:68:ILE:O	11:G:72:LEU:CB	2.22	0.86
20:A:7042:LMU:C2	20:A:7042:LMU:H61	2.00	0.86
15:K:44:GLU:HG3	15:K:45:SER:CA	2.05	0.86
7:C:14:CYS:SG	7:C:18:VAL:O	2.32	0.86
4:4:84:PHE:O	4:4:85:ALA:HB3	1.75	0.86
5:A:452:PHE:HE1	19:A:1793:CLA:CBB	1.87	0.86
17:N:58:VAL:HG23	17:N:60:PHE:CE1	2.11	0.86
19:1:1145:CLA:H2	19:1:1145:CLA:CMA	2.06	0.86
17:N:5:GLU:OE1	17:N:6:TYR:CG	2.29	0.86
1:1:185:TRP:C	1:1:186:HIS:CG	2.44	0.86
2:2:171:MET:SD	2:2:171:MET:C	2.54	0.86
4:4:169:GLN:NE2	19:4:1199:CLA:HHD	1.91	0.86
4:4:122:LYS:HG2	4:4:143:PHE:HB2	1.55	0.86
4:4:149:ALA:HB1	4:4:151:GLU:HG2	1.55	0.86
4:4:152:LYS:HD3	4:4:154:ILE:HD11	1.55	0.86
5:A:195:TRP:CZ2	19:A:1766:CLA:HMA1	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:132:TRP:HZ3	3:3:155:GLU:HG2	1.07	0.86
2:2:174:VAL:O	2:2:178:TRP:CD1	2.29	0.86
2:2:178:TRP:O	2:2:182:ILE:HG13	1.75	0.86
10:F:20:GLN:C	10:F:20:GLN:NE2	2.29	0.86
2:2:188:PRO:O	2:2:190:ASP:N	2.09	0.86
4:4:36:ASN:O	4:4:39:TRP:CB	2.23	0.86
5:A:356:ALA:HB2	5:A:417:PHE:CD2	2.09	0.86
19:B:1748:CLA:CAD	19:B:1757:CLA:HBB2	2.06	0.86
19:A:1788:CLA:C5	22:B:1781:BCR:H343	2.05	0.86
16:L:163:LEU:CD2	16:L:164:PRO:CB	2.30	0.86
1:1:24:PHE:HD2	6:B:314:ARG:NH2	1.71	0.86
17:N:45:ASN:ND2	17:N:57:LYS:NZ	2.20	0.86
17:N:70:GLU:HB3	17:N:72:LYS:N	1.88	0.86
3:3:63:ARG:HH22	3:3:189:LEU:HD23	1.40	0.86
17:N:5:GLU:OE1	17:N:6:TYR:CD1	2.29	0.86
4:4:99:HIS:ND1	4:4:103:ILE:CD1	2.38	0.86
19:A:1771:CLA:H42	19:A:1771:CLA:HAA2	1.57	0.86
19:A:1799:CLA:CMD	22:B:1781:BCR:HC31	2.05	0.86
5:A:197:GLN:HE21	5:A:197:GLN:CA	1.84	0.86
5:A:599:PHE:CE2	5:A:735:VAL:CG2	2.59	0.86
5:A:723:ARG:HH11	5:A:723:ARG:CG	1.88	0.86
19:1:1148:CLA:H2	19:1:1148:CLA:HED3	1.58	0.86
2:2:73:ILE:H	2:2:73:ILE:CD1	1.79	0.86
4:4:52:MET:HE3	4:4:156:ASN:HB2	1.57	0.86
19:A:1790:CLA:CBC	19:A:1790:CLA:HMC1	2.06	0.86
6:B:438:VAL:CG2	19:B:1764:CLA:HMC1	2.05	0.86
19:B:1769:CLA:H121	22:B:1780:BCR:H312	1.57	0.86
10:F:153:ASN:HD22	10:F:153:ASN:C	1.79	0.86
7:C:59:PRO:O	25:C:1083:SF4:S2	2.33	0.86
4:4:118:ASP:CG	4:4:123:GLN:HB2	1.96	0.85
19:B:1769:CLA:C20	22:B:1780:BCR:HC41	2.04	0.85
6:B:348:VAL:HA	19:B:1749:CLA:H42	1.58	0.85
17:N:63:ASP:N	17:N:64:ASP:CB	2.38	0.85
19:1:1014:CLA:O1D	19:1:1014:CLA:HBA1	1.74	0.85
10:F:20:GLN:CD	10:F:21:ALA:H	1.77	0.85
2:2:211:LYS:HG2	3:3:113:LEU:HD11	1.57	0.85
1:1:185:TRP:C	1:1:186:HIS:ND1	2.29	0.85
4:4:128:ALA:N	4:4:143:PHE:CZ	2.40	0.85
4:4:36:ASN:OD1	4:4:39:TRP:CD2	2.29	0.85
6:B:438:VAL:HG22	19:B:1764:CLA:CMC	2.05	0.85
7:C:63:LEU:HG	7:C:64:SER:H	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:23:LYS:C	10:F:24:LYS:NZ	2.28	0.85
5:A:269:PHE:HE1	15:K:14:THR:HG21	1.38	0.85
19:2:1217:CLA:CGD	19:2:1217:CLA:HBA2	2.06	0.85
4:4:107:GLN:C	19:4:1196:CLA:HMA2	1.93	0.85
4:4:124:TYR:CB	4:4:143:PHE:HD1	1.89	0.85
4:4:38:ARG:HG3	4:4:39:TRP:H	1.38	0.85
19:A:1783:CLA:H72	22:A:1806:BCR:H371	1.57	0.85
19:B:1739:CLA:H142	19:B:1739:CLA:H102	1.58	0.85
23:B:1774:PQN:H162	22:B:1781:BCR:H333	0.87	0.85
19:A:1799:CLA:H201	16:L:64:LEU:HD21	1.57	0.85
17:N:61:LEU:CG	17:N:62:SER:N	2.33	0.85
12:H:45:ALA:O	12:H:48:THR:N	2.08	0.85
2:2:59:ALA:HB1	2:2:172:LEU:HD22	1.59	0.85
19:4:1199:CLA:HAA1	19:F:1157:CLA:C4	2.05	0.85
4:4:124:TYR:HB3	4:4:143:PHE:CD1	2.12	0.85
4:4:36:ASN:O	4:4:39:TRP:HE3	1.60	0.85
19:A:1763:CLA:C1	19:A:1763:CLA:HAA1	2.04	0.85
19:A:1767:CLA:HMC1	19:A:1767:CLA:HBC3	1.58	0.85
19:A:1781:CLA:H52	19:A:1782:CLA:HED1	1.56	0.85
6:B:167:TRP:CZ2	19:B:1744:CLA:HAC1	2.12	0.85
7:C:74:THR:OG1	7:C:80:ALA:HB2	1.75	0.85
22:B:1779:BCR:H371	10:F:93:ILE:HG21	1.58	0.85
4:4:69:ILE:HD12	4:4:175:LYS:HG2	0.86	0.85
3:3:132:TRP:CH2	3:3:155:GLU:HG3	2.08	0.85
5:A:316:MET:CB	5:A:317:TYR:CB	2.49	0.85
13:I:1:MET:O	13:I:2:ILE:HG22	1.75	0.85
4:4:30:LEU:HD13	20:4:1212:LMU:H121	1.57	0.85
5:A:402:ILE:CD1	19:A:1784:CLA:HBB2	2.05	0.85
19:B:1758:CLA:O1D	19:B:1759:CLA:HMA1	1.76	0.85
6:B:594:TRP:O	6:B:595:HIS:CB	2.24	0.85
9:E:35:LYS:NZ	9:E:89:GLU:OE2	2.08	0.85
20:A:7033:LMU:O2'	20:A:7033:LMU:H6'2	1.76	0.85
10:F:23:LYS:CB	10:F:24:LYS:HZ1	1.89	0.85
12:H:21:TRP:H	12:H:22:ASP:CA	1.88	0.85
17:N:5:GLU:OE1	17:N:6:TYR:CD2	2.30	0.85
4:4:106:TRP:CD1	19:4:1196:CLA:O1D	2.30	0.85
4:4:154:ILE:HG13	4:4:155:ALA:N	1.92	0.85
19:B:1762:CLA:HMA2	19:B:1762:CLA:H12	1.55	0.85
6:B:571:SER:OG	6:B:574:ASP:OD1	1.95	0.85
6:B:661:PHE:HB2	19:B:1788:CLA:CMC	2.05	0.85
9:E:39:LEU:N	9:E:40:ARG:NH1	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7037:LMU:H6E	20:A:7037:LMU:O3'	1.76	0.85
5:A:349:ILE:HG22	5:A:349:ILE:O	1.74	0.85
1:1:184:PRO:O	1:1:185:TRP:CE3	2.29	0.85
2:2:41:LEU:O	2:2:42:ARG:HB2	1.76	0.85
19:A:1791:CLA:HBC1	22:A:1805:BCR:HC31	1.58	0.85
9:E:58:ASP:OD2	9:E:60:LYS:HG2	1.75	0.85
16:L:56:VAL:HA	19:L:1167:CLA:HED2	1.56	0.85
20:A:7023:LMU:O6'	20:A:7023:LMU:H1'	1.75	0.85
3:3:181:LEU:CD1	3:3:182:LYS:HE2	2.06	0.85
20:A:7020:LMU:H5B	20:A:7020:LMU:O6'	1.76	0.85
3:3:80:LYS:HD3	3:3:105:ASN:HB2	1.59	0.85
19:A:1776:CLA:H92	22:A:1804:BCR:H371	1.51	0.85
5:A:53:TRP:HA	5:A:56:ASN:HB2	1.59	0.85
6:B:388:ALA:C	6:B:391:PRO:HD2	1.95	0.85
6:B:353:TYR:CG	6:B:594:TRP:CZ3	2.64	0.85
16:L:56:VAL:HA	19:L:1167:CLA:CED	2.06	0.85
17:N:42:PHE:H	17:N:43:PRO:CD	1.88	0.85
10:F:20:GLN:CD	10:F:21:ALA:N	2.29	0.85
25:B:1785:SF4:S2	25:B:1785:SF4:FE3	1.67	0.85
6:B:432:HIS:HE1	19:B:1763:CLA:NB	1.73	0.85
5:A:567:ARG:HH12	8:D:35:GLY:HA2	1.37	0.85
10:F:130:LEU:HG	10:F:131:PHE:N	1.92	0.85
19:L:1168:CLA:HBC3	19:L:1168:CLA:CHD	2.05	0.85
4:4:69:ILE:HD12	4:4:175:LYS:CG	1.74	0.85
2:2:116:PRO:HB2	2:2:136:GLY:HA2	1.59	0.85
4:4:90:LEU:N	4:4:91:PHE:HB3	1.91	0.85
4:4:93:ILE:HG22	4:4:94:GLU:N	1.91	0.85
5:A:308:ILE:HD11	19:A:1772:CLA:H91	0.85	0.85
19:A:1796:CLA:C14	22:A:1806:BCR:HC21	2.01	0.85
5:A:581:CYS:HB2	5:A:590:CYS:CA	2.05	0.85
19:B:1754:CLA:CMC	19:B:1754:CLA:CBC	2.31	0.85
10:F:96:TRP:HZ3	10:F:134:PHE:HB2	1.42	0.85
1:1:24:PHE:HB3	6:B:314:ARG:HH21	1.41	0.85
15:K:51:ASP:OD1	15:K:55:PHE:CG	2.30	0.85
17:N:5:GLU:OE2	17:N:5:GLU:HA	1.74	0.85
5:A:368:LEU:CD1	19:A:1782:CLA:H61	2.06	0.84
19:A:1788:CLA:O1A	19:A:1799:CLA:H11	1.76	0.84
5:A:207:LEU:HD21	5:A:314:GLY:HA2	1.59	0.84
5:A:58:HIS:HE1	19:A:1759:CLA:ND	1.75	0.84
20:A:7042:LMU:C6	20:A:7042:LMU:C2	2.29	0.84
19:1:1014:CLA:CHD	19:1:1014:CLA:HBC2	2.02	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:194:VAL:N	4:4:195:GLN:C	2.30	0.84
9:E:60:LYS:HG3	9:E:61:THR:H	1.40	0.84
22:L:1169:BCR:H271	22:L:1169:BCR:H403	1.59	0.84
16:L:63:LEU:HD22	16:L:64:LEU:H	1.40	0.84
4:4:75:TRP:CD1	19:4:1205:CLA:CMD	2.60	0.84
20:K:1086:LMU:H42	20:K:1086:LMU:H81	0.85	0.84
4:4:91:PHE:HD2	4:4:91:PHE:C	1.79	0.84
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.57	0.84
19:B:1754:CLA:HMD2	19:B:1755:CLA:CBB	2.06	0.84
6:B:464:GLN:CD	6:B:469:LYS:HD3	1.96	0.84
16:L:124:LYS:NZ	16:L:124:LYS:HB2	1.91	0.84
16:L:163:LEU:HD23	16:L:164:PRO:HA	1.57	0.84
3:3:158:TYR:HB3	3:3:159:PRO:CD	2.06	0.84
19:A:1799:CLA:C20	16:L:64:LEU:HD21	2.07	0.84
10:F:24:LYS:C	10:F:26:GLN:N	2.30	0.84
16:L:48:ASN:HB3	16:L:49:PRO:HD2	1.56	0.84
5:A:110:LEU:HD11	5:A:239:PRO:HG2	1.57	0.84
19:A:1763:CLA:HAA2	19:A:1763:CLA:C1	2.04	0.84
6:B:427:LEU:HD23	6:B:431:PHE:HZ	1.41	0.84
7:C:62:PHE:CZ	9:E:42:GLU:OE1	2.31	0.84
20:1:1200:LMU:H2'	20:1:1200:LMU:H6D	1.58	0.84
2:2:162:LYS:C	2:2:162:LYS:HD3	1.98	0.84
5:A:133:ASN:ND2	5:A:142:GLY:HA2	1.92	0.84
5:A:207:LEU:HD12	5:A:310:PHE:HD1	1.42	0.84
6:B:202:SER:HB3	6:B:270:LEU:HD11	1.60	0.84
11:G:16:LEU:HD23	11:G:68:ILE:CG2	2.07	0.84
19:1:1308:CLA:H12	19:1:1308:CLA:O1D	1.77	0.84
19:3:1224:CLA:CAA	19:3:1224:CLA:HED2	1.96	0.84
19:1:1196:CLA:CGD	19:1:1196:CLA:HAA2	2.06	0.84
20:A:7038:LMU:C10	20:A:7038:LMU:C6	2.49	0.84
4:4:124:TYR:HB2	4:4:143:PHE:HD1	1.43	0.84
4:4:39:TRP:O	4:4:40:PHE:CD1	2.30	0.84
19:A:1791:CLA:HMA2	19:A:1797:CLA:CBB	2.07	0.84
5:A:393:LEU:HG	5:A:394:SER:N	1.91	0.84
19:1:1308:CLA:CGA	19:1:1308:CLA:CGD	2.54	0.84
19:1:1308:CLA:OBD	19:1:1308:CLA:HED2	1.78	0.84
12:H:25:GLY:HA3	12:H:27:ASP:HB2	1.57	0.84
4:4:57:GLY:O	4:4:60:LEU:HD23	1.78	0.84
5:A:108:ALA:HB1	5:A:138:GLY:HA3	1.58	0.84
11:G:44:PHE:CD2	11:G:44:PHE:O	2.30	0.84
4:4:75:TRP:HE3	4:4:75:TRP:H	1.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:20:GLN:CA	12:H:22:ASP:HB3	2.07	0.84
12:H:28:ALA:N	12:H:29:PRO:HD3	1.89	0.84
19:2:1217:CLA:HED2	19:2:1217:CLA:CAD	2.07	0.84
2:2:41:LEU:O	2:2:41:LEU:HD23	1.78	0.84
4:4:147:LEU:CD1	4:4:148:GLU:HB2	2.08	0.84
4:4:158:ARG:HA	4:4:161:LEU:CD1	2.07	0.84
6:B:167:TRP:HB2	11:G:41:MET:CE	2.08	0.84
25:B:1785:SF4:FE2	25:B:1785:SF4:S4	1.69	0.84
6:B:391:PRO:HB3	6:B:538:ALA:HA	1.59	0.84
11:G:26:PHE:HB2	11:G:27:GLN:HE21	1.41	0.84
1:1:27:LEU:HD22	6:B:314:ARG:HG3	1.59	0.84
19:1:1014:CLA:O2A	19:1:1014:CLA:H51	1.76	0.84
19:1:1149:CLA:HBA2	19:1:1149:CLA:O1D	1.77	0.84
16:L:14:LEU:HA	16:L:24:GLU:HG3	1.59	0.84
4:4:121:PHE:CZ	4:4:122:LYS:O	2.29	0.84
5:A:286:GLY:C	5:A:287:LEU:HD22	1.98	0.84
5:A:373:ALA:HB1	5:A:396:PHE:HD1	1.43	0.84
5:A:470:LEU:HD11	6:B:95:HIS:HB3	1.60	0.84
19:1:1188:CLA:CED	19:1:1188:CLA:CAA	2.54	0.84
19:J:1044:CLA:C7	19:J:1044:CLA:C4	2.30	0.84
15:K:10:ILE:HA	15:K:13:THR:HG21	1.59	0.84
19:A:1772:CLA:CBC	19:A:1772:CLA:HMC1	2.08	0.83
19:A:1811:CLA:CAD	19:A:1811:CLA:HED2	2.07	0.83
5:A:397:THR:HB	5:A:613:ILE:CG1	2.08	0.83
6:B:310:PRO:HG3	19:B:1754:CLA:CMA	2.04	0.83
20:A:7037:LMU:C5	20:A:7037:LMU:H11	2.05	0.83
20:A:7004:LMU:H3'	20:A:7004:LMU:C1	2.07	0.83
20:A:7038:LMU:H101	20:A:7038:LMU:H61	1.58	0.83
4:4:124:TYR:CB	4:4:143:PHE:CD1	2.62	0.83
5:A:393:LEU:CD1	5:A:750:PHE:CE1	2.60	0.83
19:B:1739:CLA:H141	19:B:1758:CLA:H91	1.60	0.83
19:B:1754:CLA:C1A	19:B:1754:CLA:C4	2.40	0.83
6:B:370:ALA:O	19:B:1758:CLA:HMA1	1.77	0.83
6:B:732:LYS:HG3	6:B:733:PHE:C	1.97	0.83
17:N:59:PRO:HB3	17:N:75:TYR:HE1	1.42	0.83
17:N:67:LEU:O	17:N:68:GLU:HG3	1.77	0.83
19:1:1014:CLA:HMA3	19:1:1014:CLA:HED1	1.59	0.83
4:4:106:TRP:HE3	19:4:1209:CLA:HMA1	1.43	0.83
4:4:147:LEU:HD21	4:4:148:GLU:HG3	0.85	0.83
6:B:310:PRO:CG	19:B:1754:CLA:HMA1	2.04	0.83
22:B:1781:BCR:H19C	19:B:1787:CLA:C11	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:105:ARG:HG3	4:4:105:ARG:O	1.75	0.83
5:A:497:ALA:HB2	5:A:515:TRP:HB2	1.59	0.83
19:B:1745:CLA:HMB2	22:B:1777:BCR:C8	2.08	0.83
20:A:7042:LMU:H32	20:A:7042:LMU:C5'	2.08	0.83
18:R:41:UNK:CB	18:R:42:UNK:CB	2.56	0.83
4:4:192:THR:HG21	4:4:195:GLN:H	1.40	0.83
3:3:87:GLU:HB2	22:3:1225:BCR:H382	1.57	0.83
6:B:516:ASP:O	6:B:520:HIS:HB2	1.79	0.83
19:1:1241:CLA:C3C	22:I:1032:BCR:HC22	2.03	0.83
19:A:1783:CLA:H71	22:A:1806:BCR:H372	1.58	0.83
22:B:1777:BCR:H331	22:B:1777:BCR:C8	2.06	0.83
5:A:558:LYS:HZ2	6:B:674:LEU:HB3	1.43	0.83
7:C:7:ILE:HG22	7:C:65:VAL:CG2	2.08	0.83
20:A:7050:LMU:H92	20:A:7050:LMU:H52	0.84	0.83
10:F:61:LEU:HD23	10:F:69:PRO:CB	2.07	0.83
3:3:80:LYS:HD3	3:3:105:ASN:CB	2.07	0.83
4:4:119:PRO:CG	19:4:1208:CLA:C2D	2.56	0.83
5:A:100:GLY:HA3	5:A:153:TRP:HH2	1.40	0.83
19:A:1770:CLA:C3B	22:A:1802:BCR:C19	2.53	0.83
19:A:1787:CLA:H52	19:A:1800:CLA:HHB	1.60	0.83
5:A:693:LEU:HD21	5:A:735:VAL:H	1.43	0.83
1:1:25:ASP:H	6:B:314:ARG:HH22	0.84	0.83
5:A:692:PHE:CE2	19:A:1796:CLA:HBC3	2.14	0.83
10:F:62:LEU:HG	10:F:72:ILE:HD13	1.59	0.83
4:4:69:ILE:CD1	4:4:175:LYS:HB2	1.83	0.83
5:A:21:LEU:HD12	5:A:21:LEU:C	1.90	0.83
20:A:7037:LMU:H51	20:A:7037:LMU:H11	1.57	0.83
8:D:124:ASN:CB	8:D:125:PRO:HD3	2.08	0.83
17:N:18:ASP:HB2	17:N:22:LEU:CG	2.09	0.83
21:B:8054:SUC:H1'1	21:B:8054:SUC:H2	1.61	0.83
3:3:132:TRP:HZ3	3:3:155:GLU:CG	1.60	0.83
17:N:56:LYS:O	17:N:60:PHE:CD1	2.31	0.83
12:H:20:GLN:HB3	12:H:22:ASP:HB2	1.60	0.83
20:R:1056:LMU:H6D	20:R:1056:LMU:O5B	1.79	0.83
4:4:149:ALA:CB	4:4:151:GLU:OE1	2.27	0.83
22:A:1806:BCR:H23C	22:A:1806:BCR:C39	2.09	0.83
6:B:212:PHE:HE1	19:B:1745:CLA:HHB	1.42	0.83
19:B:1769:CLA:H121	22:B:1780:BCR:C31	2.09	0.83
6:B:414:HIS:CD2	19:B:1761:CLA:HMA3	2.13	0.83
11:G:8:ILE:O	11:G:8:ILE:HG13	1.77	0.83
4:4:73:PRO:O	4:4:74:LYS:HG3	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:38:PRO:O	2:2:40:SER:HB2	1.77	0.83
5:A:451:ILE:CD1	19:A:1788:CLA:HED1	2.09	0.83
19:A:1781:CLA:CHC	22:A:1805:BCR:C37	2.56	0.83
5:A:373:ALA:HB1	5:A:396:PHE:CD1	2.14	0.83
6:B:230:TRP:HB3	19:B:1747:CLA:HED3	1.59	0.83
16:L:163:LEU:HD22	16:L:165:TYR:HA	1.61	0.83
17:N:48:GLY:HA3	17:N:49:CYS:CB	2.07	0.83
19:1:1145:CLA:HMA2	19:1:1145:CLA:H61	1.58	0.83
19:1:1145:CLA:H2A	19:1:1145:CLA:O1D	1.79	0.83
15:K:20:PHE:HD2	15:K:20:PHE:C	1.80	0.83
4:4:42:GLN:OE1	4:4:120:ILE:HA	1.79	0.82
4:4:47:ASN:HB3	4:4:161:LEU:HD23	1.59	0.82
6:B:464:GLN:OE1	6:B:469:LYS:HD3	1.78	0.82
6:B:711:VAL:HG12	6:B:711:VAL:O	1.77	0.82
19:L:1168:CLA:CBC	19:L:1168:CLA:CHD	2.55	0.82
16:L:88:ALA:C	16:L:90:GLY:N	2.30	0.82
17:N:58:VAL:HB	17:N:59:PRO:HD2	0.83	0.82
12:H:25:GLY:C	12:H:27:ASP:H	1.74	0.82
8:D:94:TYR:O	8:D:95:LYS:HG2	1.77	0.82
3:3:89:ALA:HB1	3:3:90:LEU:HG	1.61	0.82
22:A:1806:BCR:H312	19:A:1812:CLA:H143	1.61	0.82
23:B:1774:PQN:H161	22:B:1781:BCR:H331	1.60	0.82
8:D:78:ALA:HB3	8:D:82:GLN:NE2	1.93	0.82
19:1:1241:CLA:C3C	22:I:1032:BCR:HC21	2.08	0.82
20:A:7041:LMU:O6B	20:A:7041:LMU:H1B	1.76	0.82
5:A:141:ARG:HH21	5:A:141:ARG:HG3	1.42	0.82
4:4:36:ASN:CB	4:4:39:TRP:CD2	2.62	0.82
5:A:746:THR:HA	5:A:749:PHE:HB3	1.61	0.82
6:B:278:LEU:HD12	19:B:1747:CLA:CMA	2.09	0.82
7:C:2:SER:O	7:C:69:LEU:HB2	1.79	0.82
8:D:39:LYS:HD2	8:D:42:VAL:HG13	1.59	0.82
4:4:75:TRP:CD1	19:4:1205:CLA:C2D	2.62	0.82
17:N:63:ASP:N	17:N:64:ASP:C	2.33	0.82
7:C:17:CYS:CB	7:C:58:CYS:SG	2.66	0.82
3:3:157:ALA:C	3:3:158:TYR:HD2	1.83	0.82
6:B:131:THR:HB	6:B:134:ASP:CB	2.06	0.82
6:B:664:LEU:C	6:B:667:TRP:HZ3	1.81	0.82
20:A:7016:LMU:H91	20:A:7016:LMU:H32	1.60	0.82
20:A:7020:LMU:H6E	20:A:7020:LMU:O6B	1.79	0.82
20:A:7050:LMU:H42	20:A:7050:LMU:O1'	1.67	0.82
16:L:118:LEU:CD1	16:L:119:THR:H	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:85:GLN:OE1	2:2:85:GLN:HA	1.79	0.82
20:A:7006:LMU:H5'	20:A:7006:LMU:O5B	1.74	0.82
19:B:1756:CLA:HBB1	19:B:1770:CLA:HMB2	1.58	0.82
19:B:1756:CLA:HMB3	22:B:1778:BCR:C35	2.10	0.82
6:B:374:HIS:HB2	19:B:1758:CLA:C1B	2.09	0.82
25:B:1785:SF4:S4	25:B:1785:SF4:FE3	1.69	0.82
6:B:337:ALA:HA	19:B:1755:CLA:HAA1	1.61	0.82
14:J:31:ARG:NH2	19:J:1043:CLA:CHC	2.42	0.82
19:4:4007:CLA:HBC2	19:4:4007:CLA:CHD	2.09	0.82
19:1:1149:CLA:HBC2	19:1:1149:CLA:CMC	2.09	0.82
14:J:9:SER:O	14:J:10:VAL:HB	1.80	0.82
5:A:349:ILE:CG2	5:A:349:ILE:O	2.27	0.82
2:2:43:TRP:HZ3	2:2:125:PHE:CG	1.55	0.82
19:3:1212:CLA:HBA2	19:3:1212:CLA:HMA2	1.61	0.82
5:A:244:LEU:HD22	5:A:247:GLU:OE2	1.80	0.82
5:A:747:TRP:CD2	22:A:1806:BCR:C40	2.62	0.82
25:B:1785:SF4:FE2	25:B:1785:SF4:S3	1.71	0.82
11:G:16:LEU:HD12	11:G:17:PHE:CE2	2.14	0.82
11:G:47:GLY:H	11:G:48:ASP:HB3	1.43	0.82
17:N:48:GLY:CA	17:N:49:CYS:O	2.28	0.82
17:N:61:LEU:C	17:N:61:LEU:CD1	2.37	0.82
4:4:36:ASN:HB2	4:4:39:TRP:CH2	2.14	0.82
4:4:36:ASN:OD1	4:4:37:LEU:CA	2.28	0.82
19:A:1760:CLA:H2A	19:A:1760:CLA:O2D	1.80	0.82
5:A:207:LEU:CB	19:A:1776:CLA:HBB2	2.09	0.82
5:A:370:ILE:HD11	19:A:1781:CLA:C3D	2.09	0.82
19:B:1788:CLA:O2A	19:B:1788:CLA:H3A	1.79	0.82
4:4:73:PRO:O	4:4:74:LYS:CG	2.27	0.82
1:1:57:ILE:HD13	1:1:57:ILE:O	1.80	0.82
12:H:50:ARG:HH12	12:H:53:LEU:C	1.83	0.82
19:A:1781:CLA:CHB	22:A:1805:BCR:H363	2.09	0.82
5:A:239:PRO:HA	5:A:242:ILE:HD13	1.62	0.82
6:B:53:GLN:C	6:B:55:ALA:H	1.83	0.82
14:J:23:ALA:O	14:J:26:LEU:HB3	1.80	0.82
19:1:1190:CLA:HBC3	19:1:1190:CLA:HMC1	1.62	0.82
4:4:194:VAL:H	4:4:195:GLN:C	1.83	0.82
19:1:1145:CLA:CAD	19:1:1145:CLA:HED3	2.06	0.82
9:E:45:TRP:HH2	9:E:78:SER:OG	1.63	0.82
4:4:37:LEU:CA	4:4:39:TRP:HB3	2.08	0.82
19:A:1771:CLA:H11	19:A:1771:CLA:HAA2	1.61	0.82
19:A:1781:CLA:HBA2	19:A:1794:CLA:CED	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:401:TRP:CD1	19:A:1783:CLA:CHC	2.62	0.82
5:A:545:HIS:O	5:A:549:ILE:HG13	1.80	0.82
11:G:16:LEU:HD23	11:G:68:ILE:HG23	1.61	0.82
17:N:67:LEU:HB2	17:N:68:GLU:CB	2.09	0.82
19:1:1187:CLA:HMA2	19:1:1187:CLA:CBA	2.08	0.82
2:2:54:TRP:CG	19:2:1222:CLA:O1D	2.33	0.82
2:2:162:LYS:O	2:2:162:LYS:HD3	1.80	0.82
19:4:1199:CLA:CAA	19:F:1157:CLA:H42	2.09	0.82
4:4:169:GLN:CG	19:4:1199:CLA:HAC2	2.10	0.82
19:A:1792:CLA:HBA2	19:A:1792:CLA:HBD	1.59	0.82
8:D:44:GLU:HB2	8:D:46:TYR:CE2	2.14	0.82
9:E:60:LYS:HG3	9:E:61:THR:N	1.95	0.82
11:G:60:SER:OG	11:G:63:PRO:HB2	1.80	0.82
20:A:7020:LMU:C1B	20:A:7020:LMU:O6'	2.28	0.82
20:A:7026:LMU:H41	20:A:7026:LMU:H81	1.62	0.82
20:A:7013:LMU:O6B	20:A:7013:LMU:C1B	2.28	0.82
20:A:7028:LMU:O2'	20:A:7028:LMU:C1	2.28	0.82
2:2:171:MET:SD	2:2:172:LEU:HG	2.19	0.81
2:2:42:ARG:HB3	2:2:43:TRP:CA	2.04	0.81
19:A:1770:CLA:HMC2	22:A:1802:BCR:C16	2.10	0.81
9:E:43:SER:HB2	9:E:82:TYR:HE1	1.44	0.81
1:1:24:PHE:HD2	6:B:314:ARG:HH21	1.22	0.81
20:A:7039:LMU:C6B	20:A:7039:LMU:C4'	2.58	0.81
21:B:8062:SUC:O6'	21:B:8062:SUC:H1'2	1.80	0.81
5:A:370:ILE:CD1	19:A:1781:CLA:CAD	2.58	0.81
5:A:567:ARG:NH1	8:D:35:GLY:CA	2.38	0.81
5:A:711:HIS:NE2	19:A:1795:CLA:HAC1	1.93	0.81
6:B:294:ASN:HB3	11:G:36:PRO:HD2	1.59	0.81
7:C:74:THR:C	7:C:76:SER:N	2.30	0.81
11:G:43:HIS:C	11:G:45:GLU:N	2.29	0.81
16:L:122:GLY:C	16:L:124:LYS:N	2.31	0.81
17:N:47:THR:HB	17:N:52:LEU:O	1.78	0.81
17:N:47:THR:HG21	17:N:54:LYS:HZ2	1.41	0.81
10:F:20:GLN:NE2	10:F:21:ALA:N	2.28	0.81
12:H:53:LEU:HG	12:H:54:LEU:H	1.44	0.81
19:B:1752:CLA:CBC	19:B:1752:CLA:HHD	2.00	0.81
6:B:395:ILE:HD12	6:B:396:ARG:HG2	1.62	0.81
19:A:1811:CLA:C3B	6:B:589:TRP:HH2	1.93	0.81
4:4:114:SER:OG	4:4:120:ILE:HD11	1.81	0.81
4:4:95:PHE:N	4:4:95:PHE:CD1	2.43	0.81
4:4:98:SER:CB	4:4:102:GLU:OE1	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:304:ILE:HD11	19:B:1750:CLA:CED	2.11	0.81
19:B:1735:CLA:C19	10:F:104:TYR:HB3	2.10	0.81
17:N:72:LYS:HZ2	17:N:74:LYS:CG	1.90	0.81
18:R:36:UNK:O	18:R:38:UNK:CB	2.28	0.81
19:J:1044:CLA:C9	19:J:1044:CLA:C15	2.58	0.81
19:1:1146:CLA:CMA	19:1:1146:CLA:O1A	2.27	0.81
10:F:22:LEU:O	10:F:25:LEU:CB	2.28	0.81
10:F:26:GLN:O	10:F:27:ALA:HB3	1.80	0.81
19:4:4007:CLA:HED3	19:4:4007:CLA:O2A	1.79	0.81
1:1:63:LEU:HD12	1:1:63:LEU:H	1.45	0.81
21:3:1226:SUC:O1'	21:3:1226:SUC:C6'	2.28	0.81
21:B:8059:SUC:C3	21:B:8059:SUC:O2'	2.28	0.81
20:A:7017:LMU:H1B	20:A:7017:LMU:O3'	1.78	0.81
1:1:179:THR:HG21	4:4:87:SER:CA	2.09	0.81
19:2:1223:CLA:HMC1	19:2:1223:CLA:HBC3	1.62	0.81
5:A:103:PHE:CZ	19:A:1763:CLA:O1D	2.33	0.81
5:A:621:GLN:HG2	5:A:637:ILE:HD12	1.60	0.81
6:B:255:LEU:HD13	6:B:275:HIS:HB2	1.62	0.81
24:B:1784:LMG:O3	7:C:70:TRP:CE2	2.32	0.81
9:E:88:GLU:O	9:E:90:VAL:CB	2.29	0.81
19:1:1014:CLA:NA	19:1:1014:CLA:HED3	1.93	0.81
20:A:7048:LMU:O5'	20:A:7048:LMU:H32	1.80	0.81
20:A:7021:LMU:C2	20:A:7021:LMU:O6'	2.29	0.81
19:1:1149:CLA:CBC	19:1:1149:CLA:HMC1	2.10	0.81
1:1:184:PRO:C	1:1:185:TRP:CE3	2.53	0.81
4:4:98:SER:O	4:4:102:GLU:CG	2.28	0.81
19:B:1740:CLA:H41	22:B:1782:BCR:H23C	1.62	0.81
6:B:546:LEU:HD11	6:B:567:THR:HG22	1.60	0.81
6:B:294:ASN:OD1	11:G:38:GLN:N	2.13	0.81
19:1:1308:CLA:CMA	19:J:1044:CLA:HED2	2.10	0.81
22:3:1225:BCR:H311	22:3:1225:BCR:HC8	1.61	0.81
4:4:154:ILE:CG1	4:4:155:ALA:H	1.94	0.81
5:A:284:ARG:HA	5:A:284:ARG:CZ	2.09	0.81
5:A:362:LEU:HB3	5:A:410:ALA:HB2	1.62	0.81
5:A:596:ASP:HA	5:A:599:PHE:HB3	1.62	0.81
19:B:1760:CLA:H62	24:B:1784:LMG:H182	1.62	0.81
19:B:1788:CLA:CGA	19:B:1788:CLA:H3A	2.11	0.81
6:B:334:LEU:HG	6:B:334:LEU:O	1.79	0.81
6:B:373:THR:HA	6:B:376:GLN:HB2	1.62	0.81
11:G:45:GLU:CG	11:G:49:THR:HG21	2.11	0.81
17:N:72:LYS:HZ3	17:N:74:LYS:HG2	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:72:LYS:N	17:N:72:LYS:CD	2.41	0.81
10:F:47:GLU:CG	10:F:51:LYS:HE3	2.08	0.81
2:2:137:TYR:CD1	2:2:138:PRO:HD2	2.15	0.81
4:4:144:ALA:HB3	4:4:148:GLU:O	1.81	0.81
6:B:560:ASP:HB2	7:C:66:ARG:HE	1.40	0.81
7:C:74:THR:OG1	7:C:80:ALA:CB	2.29	0.81
11:G:19:GLY:C	11:G:21:PHE:N	2.28	0.81
17:N:66:ASP:O	17:N:67:LEU:CG	2.28	0.81
19:1:1014:CLA:H102	19:1:1014:CLA:H43	1.62	0.81
20:A:7016:LMU:C3	20:A:7016:LMU:O6'	2.29	0.81
19:1:1146:CLA:O1A	19:1:1146:CLA:C3A	2.29	0.81
20:A:7032:LMU:C1	20:A:7032:LMU:O5B	2.29	0.81
20:A:7022:LMU:H21	20:A:7022:LMU:H2'	0.82	0.81
17:N:5:GLU:OE2	17:N:6:TYR:CB	2.28	0.81
2:2:98:GLU:CG	2:2:99:LEU:HD11	2.10	0.81
4:4:99:HIS:CE1	4:4:103:ILE:HD11	2.16	0.81
4:4:36:ASN:C	4:4:39:TRP:CB	2.46	0.81
6:B:331:HIS:CE1	6:B:392:ILE:HG21	2.16	0.81
11:G:17:PHE:O	11:G:20:ARG:HB2	1.81	0.81
17:N:50:GLN:CA	17:N:51:ASP:O	2.28	0.81
20:A:7048:LMU:H21	20:A:7048:LMU:H82	1.61	0.81
20:A:7033:LMU:O2'	20:A:7033:LMU:C6B	2.29	0.81
19:1:1145:CLA:O1A	19:1:1145:CLA:C3A	2.29	0.81
19:4:4007:CLA:CGA	19:4:4007:CLA:O2D	2.29	0.81
21:3:1226:SUC:C5	21:3:1226:SUC:O2'	2.28	0.81
4:4:93:ILE:O	4:4:96:ILE:HD12	1.79	0.81
19:A:1774:CLA:H202	19:A:1782:CLA:H3A	1.62	0.81
19:B:1741:CLA:H52	12:H:65:LEU:HD23	1.63	0.81
16:L:165:TYR:N	16:L:165:TYR:CD2	2.29	0.81
19:1:1148:CLA:CGA	19:1:1148:CLA:O2D	2.29	0.81
19:J:1043:CLA:CHD	19:J:1043:CLA:HBC3	2.11	0.81
20:A:7020:LMU:O5B	20:A:7020:LMU:C6'	2.29	0.81
2:2:196:HIS:NE2	21:2:1225:SUC:O3	2.14	0.81
17:N:4:GLU:O	17:N:4:GLU:CG	2.28	0.81
6:B:317:ARG:NE	6:B:317:ARG:HA	1.94	0.81
7:C:26:LEU:H	7:C:43:PRO:HG3	1.46	0.81
15:K:69:ILE:HA	15:K:72:VAL:HG12	1.63	0.81
2:2:181:HIS:CE1	19:2:1214:CLA:C4D	2.64	0.81
2:2:73:ILE:O	2:2:74:LEU:CG	2.29	0.81
19:4:1198:CLA:O1D	19:4:1198:CLA:C2A	2.29	0.81
19:A:1783:CLA:C7	22:A:1806:BCR:H371	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:203:THR:O	2:2:204:ILE:CG2	2.28	0.81
10:F:26:GLN:CA	10:F:26:GLN:OE1	2.28	0.81
20:A:7039:LMU:H6'2	20:A:7039:LMU:C4'	2.10	0.81
6:B:404:ALA:C	6:B:406:ASN:H	1.84	0.81
17:N:34:THR:OG1	17:N:36:GLU:HB3	1.79	0.81
19:2:1217:CLA:CED	19:2:1217:CLA:OBD	2.29	0.81
2:2:96:ILE:HG13	2:2:97:VAL:N	1.96	0.80
4:4:99:HIS:O	4:4:103:ILE:CD1	2.30	0.80
19:4:1196:CLA:HHD	19:4:1196:CLA:HBC3	1.61	0.80
4:4:145:PRO:O	4:4:147:LEU:CA	2.29	0.80
19:A:1791:CLA:CMA	19:A:1797:CLA:CBB	2.58	0.80
5:A:248:PHE:CD2	5:A:248:PHE:N	2.49	0.80
6:B:128:GLY:HA2	6:B:130:ARG:HE	1.44	0.80
6:B:131:THR:O	6:B:135:LEU:N	2.14	0.80
19:B:1754:CLA:H12	19:B:1754:CLA:HAA1	1.61	0.80
25:B:1785:SF4:FE4	25:B:1785:SF4:S1	1.72	0.80
8:D:102:ARG:NH1	8:D:104:PHE:CD1	2.47	0.80
20:B:1783:LMU:C11	20:B:1783:LMU:H72	2.09	0.80
20:A:7016:LMU:O6'	20:A:7016:LMU:C1	2.29	0.80
19:J:1044:CLA:OBD	19:J:1044:CLA:CED	2.30	0.80
20:A:7037:LMU:O3'	20:A:7037:LMU:C6'	2.28	0.80
19:1:1145:CLA:O1A	19:1:1145:CLA:CMA	2.29	0.80
20:A:7043:LMU:O2B	20:A:7043:LMU:C5'	2.29	0.80
2:2:99:LEU:HB3	19:2:1222:CLA:HBB1	1.62	0.80
4:4:37:LEU:O	4:4:39:TRP:CB	2.27	0.80
19:A:1799:CLA:HBB2	19:B:1771:CLA:HMD1	1.63	0.80
5:A:393:LEU:O	5:A:397:THR:HG23	1.81	0.80
19:B:1756:CLA:CED	19:B:1757:CLA:OBD	2.29	0.80
19:B:1772:CLA:H102	13:I:21:MET:SD	2.21	0.80
19:B:1739:CLA:HMC2	22:B:1781:BCR:H281	1.61	0.80
16:L:164:PRO:HD2	16:L:165:TYR:CD1	2.15	0.80
17:N:66:ASP:O	17:N:67:LEU:CD1	2.29	0.80
20:A:7016:LMU:O6'	20:A:7016:LMU:C1'	2.29	0.80
20:A:7038:LMU:H1B	20:A:7038:LMU:O6'	1.81	0.80
20:A:7038:LMU:O6'	20:A:7038:LMU:C1B	2.29	0.80
4:4:128:ALA:HB1	4:4:141:LEU:HD23	1.62	0.80
5:A:599:PHE:HD1	5:A:600:LEU:HD23	1.44	0.80
6:B:398:TYR:HD1	6:B:542:ARG:HH21	1.27	0.80
21:B:8054:SUC:O2	21:B:8054:SUC:C1'	2.30	0.80
6:B:85:ARG:O	6:B:86:PRO:O	1.98	0.80
7:C:63:LEU:CG	7:C:64:SER:H	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:104:PHE:HB3	8:D:106:SER:H	1.47	0.80
16:L:161:LEU:HD11	16:L:162:ASP:C	2.01	0.80
19:1:1188:CLA:CMA	19:1:1188:CLA:O2A	2.30	0.80
17:N:54:LYS:CB	17:N:57:LYS:CE	2.59	0.80
19:1:1148:CLA:CED	19:1:1148:CLA:C1	2.54	0.80
1:1:60:PRO:O	1:1:61:GLU:HB3	1.81	0.80
3:3:86:GLN:HB2	3:3:88:THR:HB	1.60	0.80
19:4:4007:CLA:HED1	19:4:4007:CLA:CGA	2.07	0.80
20:A:7028:LMU:O6'	20:A:7028:LMU:C1'	2.29	0.80
3:3:83:LEU:CA	19:3:1212:CLA:H43	2.11	0.80
5:A:308:ILE:O	5:A:312:ILE:N	2.15	0.80
6:B:661:PHE:HB2	19:B:1788:CLA:HMC3	1.63	0.80
17:N:45:ASN:HD21	17:N:54:LYS:CB	1.93	0.80
20:A:7032:LMU:O1'	20:A:7032:LMU:C1B	2.30	0.80
20:A:7050:LMU:O3'	20:A:7050:LMU:C6B	2.30	0.80
20:A:7010:LMU:O2B	20:A:7010:LMU:C3'	2.29	0.80
21:B:8060:SUC:O1'	21:B:8060:SUC:C5	2.29	0.80
4:4:128:ALA:CB	4:4:143:PHE:CZ	2.61	0.80
6:B:278:LEU:HD12	19:B:1747:CLA:HMA2	1.63	0.80
19:B:1757:CLA:C8	22:B:1778:BCR:H14C	2.11	0.80
19:B:1763:CLA:HBB2	22:B:1779:BCR:H272	1.64	0.80
5:A:588:GLY:H	6:B:668:ARG:NH1	1.79	0.80
7:C:73:THR:OG1	7:C:76:SER:CB	2.30	0.80
7:C:7:ILE:O	7:C:8:TYR:C	2.18	0.80
11:G:46:ALA:CA	11:G:48:ASP:OD2	2.30	0.80
16:L:123:ARG:HA	16:L:123:ARG:NE	1.95	0.80
4:4:71:ASN:O	4:4:73:PRO:CD	2.29	0.80
4:4:75:TRP:CZ3	4:4:76:TYR:HB3	2.16	0.80
17:N:51:ASP:O	17:N:52:LEU:CD2	2.29	0.80
17:N:61:LEU:CD1	17:N:63:ASP:O	2.29	0.80
18:R:33:UNK:O	18:R:36:UNK:CB	2.29	0.80
10:F:22:LEU:O	10:F:25:LEU:CD1	2.29	0.80
20:A:7032:LMU:C3	20:A:7032:LMU:O5B	2.29	0.80
20:A:7020:LMU:C2B	20:A:7020:LMU:O6'	2.29	0.80
19:R:1055:CLA:CBA	19:R:1055:CLA:O1D	2.29	0.80
5:A:27:ILE:O	5:A:27:ILE:CD1	2.30	0.80
9:E:51:SER:HB3	9:E:68:ARG:NH1	1.96	0.80
3:3:80:LYS:HB2	19:3:1216:CLA:C3D	2.12	0.80
1:1:185:TRP:HB3	1:1:186:HIS:CD2	2.16	0.80
4:4:89:THR:O	4:4:92:VAL:CB	2.29	0.80
5:A:747:TRP:CE3	22:A:1806:BCR:C40	2.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:693:TRP:CD1	19:B:1771:CLA:C2D	2.65	0.80
6:B:382:ILE:HG22	6:B:383:MET:N	1.96	0.80
6:B:586:THR:C	6:B:588:GLY:H	1.85	0.80
9:E:85:ASP:O	9:E:86:GLU:CB	2.30	0.80
11:G:67:ASN:HA	11:G:70:ASP:OD2	1.81	0.80
19:1:1014:CLA:O2A	19:1:1014:CLA:C5	2.30	0.80
19:1:1014:CLA:O2D	19:1:1014:CLA:C2A	2.29	0.80
5:A:23:ASP:OD2	5:A:24:ARG:HD3	1.80	0.80
19:4:1201:CLA:CAA	19:4:1201:CLA:O1D	2.29	0.80
5:A:423:ASP:CB	5:A:424:PRO:HD3	2.09	0.80
11:G:73:ALA:O	11:G:75:GLY:N	2.14	0.80
18:R:26:UNK:O	18:R:28:UNK:CB	2.30	0.80
19:A:1797:CLA:CAA	19:A:1797:CLA:O2D	2.30	0.80
6:B:172:GLU:O	6:B:176:ASN:CB	2.30	0.80
19:L:1167:CLA:HBC3	19:L:1167:CLA:HMC1	1.62	0.80
4:4:69:ILE:HD13	4:4:175:LYS:HB3	1.62	0.80
19:1:1192:CLA:HAA1	20:1:1199:LMU:O3'	1.82	0.80
17:N:65:LEU:CD2	17:N:65:LEU:O	2.30	0.80
19:1:1148:CLA:O2D	19:1:1148:CLA:CBA	2.29	0.80
18:R:38:UNK:O	18:R:42:UNK:CA	2.29	0.80
10:F:24:LYS:O	10:F:27:ALA:CB	2.30	0.80
12:H:25:GLY:CA	12:H:27:ASP:OD2	2.30	0.80
20:A:7026:LMU:H2B	20:A:7026:LMU:O3'	1.80	0.80
15:K:62:ALA:O	15:K:65:ALA:N	2.14	0.80
4:4:147:LEU:HD11	4:4:148:GLU:HB2	1.62	0.80
4:4:81:GLU:O	4:4:82:GLU:CG	2.30	0.80
5:A:210:LEU:HD12	19:A:1769:CLA:HMB2	1.64	0.80
19:A:1781:CLA:O1A	19:A:1782:CLA:HED3	1.82	0.80
6:B:557:PHE:N	6:B:558:PRO:CD	2.44	0.80
8:D:46:TYR:HE1	8:D:80:LYS:HE2	1.45	0.80
9:E:88:GLU:O	9:E:90:VAL:CA	2.29	0.80
20:A:7042:LMU:O6'	20:A:7042:LMU:C3	2.29	0.80
18:R:35:UNK:O	18:R:38:UNK:CB	2.29	0.80
20:A:7050:LMU:C4	20:A:7050:LMU:C9	2.60	0.80
20:A:7039:LMU:C3'	20:A:7039:LMU:O6B	2.30	0.80
1:1:63:LEU:CD2	1:1:63:LEU:O	2.29	0.80
20:A:7021:LMU:O6'	20:A:7021:LMU:C1'	2.30	0.80
20:A:7021:LMU:O6'	20:A:7021:LMU:C3	2.30	0.80
21:B:8053:SUC:O2	21:B:8053:SUC:C5'	2.29	0.80
3:3:107:TRP:CG	3:3:108:ALA:N	2.38	0.80
10:F:12:LYS:HG2	10:F:13:GLN:N	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:151:GLU:O	4:4:154:ILE:N	2.03	0.80
19:A:1799:CLA:C9	22:L:1169:BCR:H321	2.12	0.80
5:A:684:PHE:C	5:A:684:PHE:CD2	2.55	0.80
9:E:90:VAL:CG1	9:E:90:VAL:O	2.29	0.80
5:A:715:LYS:HD2	10:F:153:ASN:OD1	1.82	0.80
11:G:7:VAL:HG22	11:G:8:ILE:H	1.46	0.80
13:I:8:PHE:CB	19:I:1031:CLA:OBD	2.29	0.80
17:N:48:GLY:C	17:N:49:CYS:SG	2.58	0.80
17:N:62:SER:CB	17:N:66:ASP:OD1	2.29	0.80
17:N:72:LYS:HG2	17:N:74:LYS:CG	2.04	0.80
20:A:7016:LMU:C7	20:A:7016:LMU:H112	2.12	0.80
19:1:1146:CLA:O1A	19:1:1146:CLA:C2A	2.30	0.80
20:A:7032:LMU:C1	20:A:7032:LMU:O2'	2.29	0.80
19:1:1145:CLA:C2A	19:1:1145:CLA:O1D	2.30	0.80
21:B:8062:SUC:O6'	21:B:8062:SUC:C1'	2.30	0.80
19:R:1055:CLA:CGA	19:R:1055:CLA:O1D	2.29	0.80
6:B:454:LEU:HD11	10:F:69:PRO:O	1.80	0.80
21:2:1225:SUC:C5'	21:2:1225:SUC:O2	2.29	0.80
16:L:8:TYR:HE1	16:L:11:ILE:HG23	1.47	0.80
20:A:7040:LMU:O3'	20:A:7040:LMU:C1B	2.29	0.80
8:D:93:LYS:HB3	8:D:93:LYS:NZ	1.96	0.80
5:A:107:GLU:OE1	5:A:161:GLU:HG3	1.82	0.80
19:A:1781:CLA:CMA	19:A:1782:CLA:O1A	2.30	0.80
6:B:323:TYR:CE1	19:B:1755:CLA:HBC1	2.17	0.80
11:G:42:SER:OG	11:G:45:GLU:CB	2.29	0.80
11:G:43:HIS:O	11:G:45:GLU:CB	2.29	0.80
20:N:1086:LMU:O6'	20:N:1086:LMU:C4	2.30	0.80
17:N:63:ASP:N	17:N:65:LEU:N	2.30	0.80
2:2:203:THR:O	2:2:204:ILE:CG1	2.29	0.80
18:R:34:UNK:O	18:R:38:UNK:CB	2.29	0.80
20:B:1783:LMU:O6B	20:B:1783:LMU:C3'	2.29	0.80
5:A:24:ARG:O	5:A:26:PRO:CG	2.30	0.80
20:A:7032:LMU:C3	20:A:7032:LMU:H1B	2.09	0.80
20:A:7021:LMU:O6'	20:A:7021:LMU:H1'	1.82	0.80
21:B:8059:SUC:C1	21:B:8059:SUC:O6	2.29	0.80
1:1:185:TRP:O	1:1:186:HIS:CB	2.30	0.79
5:A:711:HIS:HB3	5:A:717:ALA:HB2	1.63	0.79
19:B:1754:CLA:C2A	19:B:1754:CLA:O2D	2.30	0.79
22:B:1782:BCR:H392	19:I:1031:CLA:H142	1.63	0.79
6:B:415:LYS:HE3	6:B:539:LEU:O	1.81	0.79
7:C:1:MET:H2	7:C:3:HIS:CA	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:124:LYS:C	16:L:126:GLN:H	1.85	0.79
16:L:148:VAL:O	16:L:149:SER:HB3	1.80	0.79
20:A:7048:LMU:O2'	20:A:7048:LMU:C2	2.30	0.79
19:3:1224:CLA:CAA	19:3:1224:CLA:O2D	2.30	0.79
19:1:1145:CLA:CAA	19:1:1145:CLA:O1D	2.30	0.79
19:4:4007:CLA:CED	19:4:4007:CLA:O2A	2.30	0.79
9:E:44:TYR:CE1	9:E:73:ASN:HA	2.17	0.79
5:A:726:SER:O	5:A:728:VAL:N	2.15	0.79
2:2:40:SER:O	2:2:41:LEU:CD2	2.30	0.79
2:2:45:VAL:O	2:2:45:VAL:CG1	2.29	0.79
19:A:1771:CLA:O2D	19:A:1771:CLA:C2A	2.30	0.79
19:A:1776:CLA:C2C	19:A:1782:CLA:C17	2.60	0.79
5:A:452:PHE:CE1	19:A:1793:CLA:CBB	2.63	0.79
5:A:747:TRP:CE3	22:A:1806:BCR:H401	2.16	0.79
5:A:207:LEU:O	5:A:310:PHE:HB3	1.80	0.79
5:A:496:HIS:HB3	5:A:515:TRP:CE3	2.17	0.79
19:B:1760:CLA:H72	24:B:1784:LMG:H311	1.64	0.79
11:G:30:ASN:O	11:G:33:LYS:NZ	2.15	0.79
4:4:73:PRO:O	4:4:74:LYS:CB	2.29	0.79
10:F:30:LYS:O	10:F:31:LEU:HB2	1.80	0.79
15:K:8:ASN:O	15:K:12:VAL:HG23	1.81	0.79
6:B:120:VAL:HA	6:B:123:TRP:HD1	1.45	0.79
21:B:8059:SUC:O2	21:B:8059:SUC:C2'	2.30	0.79
17:N:1:GLY:O	17:N:2:VAL:CG1	2.29	0.79
2:2:120:ASN:CB	2:2:121:THR:HB	2.12	0.79
2:2:73:ILE:O	2:2:74:LEU:CD2	2.29	0.79
4:4:103:ILE:O	4:4:106:TRP:HB3	1.82	0.79
4:4:104:ARG:NE	4:4:105:ARG:N	2.29	0.79
19:A:1776:CLA:HAA2	19:A:1780:CLA:HBB2	1.65	0.79
5:A:62:HIS:HB2	19:A:1785:CLA:HBA1	1.63	0.79
5:A:545:HIS:CG	19:A:1792:CLA:HBB2	2.16	0.79
19:A:1781:CLA:O2A	19:A:1794:CLA:O2D	2.00	0.79
19:A:1770:CLA:HMC2	22:A:1802:BCR:C17	2.13	0.79
5:A:78:VAL:O	5:A:82:HIS:HB2	1.82	0.79
6:B:414:HIS:HD2	19:B:1761:CLA:HMA3	1.44	0.79
6:B:672:GLN:HA	6:B:672:GLN:NE2	1.94	0.79
9:E:52:VAL:HG12	9:E:53:VAL:N	1.97	0.79
10:F:103:SER:C	10:F:105:LEU:H	1.86	0.79
20:A:7041:LMU:O6'	20:A:7041:LMU:C1B	2.30	0.79
20:A:7042:LMU:O2B	20:A:7042:LMU:C5'	2.30	0.79
19:1:1148:CLA:O1A	19:1:1148:CLA:CED	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7023:LMU:O6'	20:A:7023:LMU:C1'	2.28	0.79
3:3:194:ILE:CD1	19:3:1214:CLA:CMC	2.50	0.79
19:1:1145:CLA:CMC	19:1:1145:CLA:CBC	2.39	0.79
12:H:21:TRP:N	12:H:22:ASP:HB3	1.96	0.79
20:A:7020:LMU:C5B	20:A:7020:LMU:O6'	2.30	0.79
15:K:10:ILE:HA	15:K:13:THR:HG23	1.57	0.79
20:A:7043:LMU:C6'	20:A:7043:LMU:O2B	2.30	0.79
20:A:7039:LMU:C4'	20:A:7039:LMU:O6B	2.29	0.79
6:B:120:VAL:CA	6:B:123:TRP:CD1	2.63	0.79
1:1:63:LEU:CD1	1:1:63:LEU:O	2.29	0.79
17:N:29:PHE:CD1	17:N:32:ALA:HB3	2.18	0.79
1:1:184:PRO:O	1:1:185:TRP:HE3	1.63	0.79
2:2:70:LYS:HG3	2:2:73:ILE:CG1	2.12	0.79
19:A:1783:CLA:H71	22:A:1806:BCR:C37	2.10	0.79
5:A:157:GLY:HA2	5:A:229:ILE:HG21	1.65	0.79
19:B:1745:CLA:HMA1	22:B:1777:BCR:H313	1.63	0.79
19:G:1099:CLA:C2A	19:G:1099:CLA:O1D	2.30	0.79
11:G:45:GLU:CB	11:G:49:THR:CG2	2.59	0.79
20:A:7036:LMU:O5B	20:A:7036:LMU:C6'	2.30	0.79
20:A:7042:LMU:O6'	20:A:7042:LMU:C4	2.29	0.79
11:G:88:THR:OG1	11:G:92:GLY:HA3	1.82	0.79
20:A:7020:LMU:C3B	20:A:7020:LMU:O6'	2.30	0.79
20:A:7026:LMU:H51	20:A:7026:LMU:H12	1.64	0.79
1:1:185:TRP:O	1:1:186:HIS:HB2	1.81	0.79
2:2:110:TRP:HD1	2:2:113:ILE:CG2	1.92	0.79
2:2:42:ARG:HG3	2:2:45:VAL:CG2	2.05	0.79
4:4:33:ASP:CB	4:4:34:PRO:HD3	2.12	0.79
4:4:92:VAL:HG12	4:4:93:ILE:N	1.98	0.79
22:B:1780:BCR:H321	22:B:1780:BCR:HC8	0.83	0.79
6:B:374:HIS:HB2	19:B:1758:CLA:NB	1.97	0.79
7:C:1:MET:N	7:C:4:SER:N	2.30	0.79
19:B:1772:CLA:C19	13:I:21:MET:HB3	2.11	0.79
20:A:7041:LMU:C5'	20:A:7041:LMU:O2'	2.29	0.79
19:J:1043:CLA:C14	19:J:1043:CLA:O1A	2.30	0.79
21:B:8055:SUC:O6	21:B:8055:SUC:C1	2.29	0.79
12:H:25:GLY:CA	12:H:27:ASP:N	2.27	0.79
20:A:7020:LMU:H3B	20:A:7020:LMU:O6'	1.82	0.79
10:F:102:ARG:HG2	10:F:106:ILE:CD1	2.05	0.79
16:L:152:THR:O	16:L:156:PHE:N	2.11	0.79
4:4:34:PRO:CG	4:4:35:GLU:OE1	2.29	0.79
5:A:581:CYS:SG	25:B:1785:SF4:S2	2.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:1032:BCR:H313	22:I:1032:BCR:HC8	0.83	0.79
20:A:7016:LMU:C5	20:A:7016:LMU:O6'	2.29	0.79
5:A:23:ASP:OD2	5:A:24:ARG:CG	2.30	0.79
19:K:1085:CLA:HMC1	19:K:1085:CLA:HBC2	1.65	0.79
12:H:23:VAL:O	12:H:23:VAL:CG1	2.30	0.79
20:A:7004:LMU:C1	20:A:7004:LMU:O2'	2.30	0.79
3:3:158:TYR:O	3:3:160:GLY:N	2.16	0.79
20:1:1200:LMU:C6'	20:1:1200:LMU:O3'	2.30	0.79
5:A:331:LEU:CD2	5:A:331:LEU:C	2.51	0.79
19:B:1757:CLA:H122	22:B:1778:BCR:C14	2.12	0.79
17:N:45:ASN:CB	17:N:57:LYS:NZ	2.46	0.79
17:N:60:PHE:CA	17:N:61:LEU:O	2.30	0.79
17:N:61:LEU:HD13	17:N:63:ASP:HB2	1.64	0.79
17:N:62:SER:O	17:N:63:ASP:CB	2.30	0.79
4:4:193:ILE:CG2	4:4:195:GLN:O	2.29	0.79
21:B:8055:SUC:C3	21:B:8055:SUC:O2'	2.30	0.79
20:A:7013:LMU:H1B	20:A:7013:LMU:H6B	1.48	0.79
19:4:1198:CLA:O2D	19:4:1198:CLA:CAA	2.30	0.79
4:4:168:ILE:O	4:4:168:ILE:HG13	1.83	0.79
19:A:1776:CLA:C1C	19:A:1782:CLA:H171	2.13	0.79
19:A:1789:CLA:H41	16:L:64:LEU:HD23	1.64	0.79
19:A:1763:CLA:C4B	22:A:1807:BCR:C33	2.60	0.79
19:B:1754:CLA:HBD	19:B:1754:CLA:HAA2	1.65	0.79
19:B:1737:CLA:H43	22:B:1776:BCR:H313	1.63	0.79
19:F:1157:CLA:OBD	19:F:1157:CLA:CED	2.31	0.79
19:1:1241:CLA:HAC1	22:I:1032:BCR:HC32	1.64	0.79
17:N:79:SER:CA	17:N:80:ASN:O	2.27	0.79
19:1:1148:CLA:O2D	19:1:1148:CLA:CAA	2.30	0.79
20:A:7033:LMU:C3'	20:A:7033:LMU:O5B	2.28	0.79
19:1:1145:CLA:OBD	19:1:1145:CLA:CED	2.30	0.79
21:B:8059:SUC:O2	21:B:8059:SUC:C1'	2.30	0.79
4:4:104:ARG:NH1	4:4:105:ARG:HB2	1.90	0.79
4:4:90:LEU:HD22	4:4:90:LEU:N	1.98	0.79
5:A:381:PRO:CB	19:A:1774:CLA:HAA2	2.13	0.79
25:B:1785:SF4:S2	25:B:1785:SF4:FE1	1.71	0.79
21:F:1158:SUC:C5	21:F:1158:SUC:O2	2.27	0.79
3:3:92:TRP:HA	3:3:93:PHE:CG	2.18	0.79
19:1:1148:CLA:O1A	19:1:1148:CLA:C2	2.30	0.79
20:A:7023:LMU:O3B	20:A:7023:LMU:C6B	2.30	0.79
19:1:1014:CLA:H112	19:1:1014:CLA:C3	2.12	0.79
20:A:7016:LMU:C4	20:A:7016:LMU:O6'	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7030:LMU:H92	20:A:7030:LMU:H52	1.64	0.79
19:A:1781:CLA:CBC	19:A:1781:CLA:CHD	2.52	0.79
19:A:1790:CLA:OBD	19:A:1791:CLA:HAC1	1.83	0.79
5:A:40:PHE:HE1	5:A:53:TRP:HD1	1.28	0.79
5:A:491:TRP:CD1	5:A:492:ILE:HG23	2.18	0.79
24:B:1784:LMG:HC61	7:C:70:TRP:CH2	2.17	0.79
19:F:1156:CLA:HBC2	19:F:1156:CLA:HHD	1.64	0.79
17:N:62:SER:O	17:N:63:ASP:HB2	1.79	0.79
19:J:1044:CLA:H151	19:J:1044:CLA:H102	1.64	0.79
20:A:7021:LMU:H41	20:A:7021:LMU:H6D	1.65	0.79
20:A:7026:LMU:H3O1	21:B:8062:SUC:H5'	1.48	0.79
18:R:3:UNK:O	18:R:4:UNK:CB	2.31	0.79
4:4:163:PHE:O	4:4:166:PHE:HB3	1.82	0.78
4:4:44:GLU:O	4:4:47:ASN:N	2.15	0.78
19:A:1797:CLA:O1A	19:A:1797:CLA:CED	2.31	0.78
19:B:1750:CLA:OBD	19:B:1753:CLA:HBC3	1.83	0.78
6:B:438:VAL:HG22	19:B:1764:CLA:HMC3	1.64	0.78
6:B:596:TRP:CD1	6:B:623:TYR:HB2	2.17	0.78
20:N:1086:LMU:O2B	20:N:1086:LMU:H5B	1.82	0.78
17:N:45:ASN:HB2	17:N:57:LYS:NZ	1.99	0.78
17:N:70:GLU:HB3	17:N:72:LYS:H	1.46	0.78
20:A:7048:LMU:H11	20:A:7048:LMU:C5	2.12	0.78
20:A:7016:LMU:O6'	20:A:7016:LMU:C2	2.30	0.78
20:A:7032:LMU:C2	20:A:7032:LMU:O5B	2.30	0.78
1:1:59:VAL:CG1	1:1:60:PRO:O	2.30	0.78
21:B:8060:SUC:H5	21:B:8060:SUC:HO1'	1.46	0.78
5:A:27:ILE:O	5:A:28:LYS:CG	2.30	0.78
7:C:39:ILE:CG1	7:C:40:ALA:H	1.92	0.78
1:1:161:PHE:H	19:1:1189:CLA:CBB	1.95	0.78
10:F:94:ALA:HA	10:F:97:ILE:HG12	1.65	0.78
6:B:558:PRO:CG	6:B:703:VAL:HB	2.13	0.78
10:F:147:GLY:CA	10:F:150:VAL:HB	2.13	0.78
11:G:28:ARG:NH2	11:G:28:ARG:HG2	1.95	0.78
20:A:7033:LMU:C2'	20:A:7033:LMU:H6'2	2.12	0.78
19:3:1224:CLA:O2D	19:3:1224:CLA:CBA	2.31	0.78
5:A:269:PHE:CD1	15:K:14:THR:HG21	2.18	0.78
20:A:7021:LMU:O6'	20:A:7021:LMU:C4	2.30	0.78
19:R:1055:CLA:CBA	19:R:1055:CLA:HBD	2.14	0.78
8:D:48:ILE:HG22	8:D:83:CYS:HB2	1.64	0.78
8:D:32:SER:O	16:L:21:GLY:HA2	1.83	0.78
6:B:317:ARG:HE	6:B:317:ARG:HA	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:126:PRO:HG2	2:2:129:LYS:H	1.47	0.78
5:A:624:VAL:O	5:A:636:HIS:CD2	2.36	0.78
6:B:124:TRP:O	6:B:129:LEU:HB3	1.84	0.78
25:B:1785:SF4:S1	25:B:1785:SF4:FE3	1.74	0.78
4:4:71:ASN:C	4:4:73:PRO:CD	2.52	0.78
17:N:54:LYS:HB2	17:N:57:LYS:HZ1	1.47	0.78
21:B:8062:SUC:C6'	21:B:8062:SUC:C1'	2.49	0.78
5:A:29:THR:CG2	5:A:29:THR:O	2.30	0.78
17:N:5:GLU:OE1	17:N:6:TYR:CE1	2.36	0.78
2:2:38:PRO:CB	2:2:40:SER:OG	2.29	0.78
2:2:41:LEU:C	2:2:41:LEU:CD2	2.28	0.78
4:4:145:PRO:O	4:4:147:LEU:HA	1.84	0.78
5:A:146:THR:O	19:A:1783:CLA:HMA2	1.82	0.78
19:A:1760:CLA:HMC3	19:A:1762:CLA:O2D	1.83	0.78
6:B:189:ALA:HB1	19:B:1759:CLA:H203	1.64	0.78
19:B:1760:CLA:HBC3	19:B:1760:CLA:HMC1	1.65	0.78
6:B:353:TYR:CD2	6:B:594:TRP:CZ3	2.70	0.78
19:G:1099:CLA:O2A	19:G:1099:CLA:C3A	2.30	0.78
11:G:46:ALA:HA	11:G:48:ASP:CG	2.01	0.78
21:B:8052:SUC:O4'	21:B:8052:SUC:C1	2.30	0.78
11:G:93:TYR:HA	11:G:94:ASP:HB2	0.78	0.78
21:B:8055:SUC:C1'	21:B:8055:SUC:O6'	2.30	0.78
20:A:7050:LMU:O3B	20:A:7050:LMU:C6B	2.29	0.78
14:J:11:ALA:CB	14:J:12:PRO:HD2	2.14	0.78
17:N:5:GLU:OE2	17:N:5:GLU:CA	2.29	0.78
10:F:33:ALA:HA	10:F:36:SER:HB2	1.64	0.78
4:4:128:ALA:HB1	4:4:141:LEU:CD2	2.13	0.78
5:A:555:ILE:HG21	19:B:1788:CLA:HMD1	1.65	0.78
6:B:25:ILE:HG21	22:L:1169:BCR:H291	1.53	0.78
19:F:1157:CLA:CAD	19:F:1157:CLA:HED2	2.13	0.78
19:G:1099:CLA:HED3	19:G:1099:CLA:CAD	2.13	0.78
22:L:1170:BCR:H383	22:L:1170:BCR:H23C	1.64	0.78
20:N:1086:LMU:O6'	20:N:1086:LMU:C5	2.30	0.78
17:N:46:PHE:O	17:N:47:THR:CG2	2.28	0.78
19:1:1014:CLA:O2D	19:1:1014:CLA:CBA	2.29	0.78
20:A:7009:LMU:C5B	20:A:7009:LMU:O3'	2.29	0.78
20:A:7005:LMU:C1	20:A:7005:LMU:O2'	2.29	0.78
2:2:126:PRO:CD	2:2:129:LYS:HB2	2.14	0.78
2:2:59:ALA:HB3	2:2:172:LEU:HD13	1.66	0.78
4:4:34:PRO:HB3	4:4:35:GLU:CB	2.14	0.78
5:A:197:GLN:HE22	5:A:351:THR:HB	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:700:TRP:O	5:A:704:ILE:HB	1.83	0.78
6:B:656:VAL:HG22	19:B:1772:CLA:HMB3	1.66	0.78
11:G:21:PHE:O	11:G:23:PHE:HB2	1.82	0.78
19:4:1201:CLA:CMA	19:4:1201:CLA:CBA	2.30	0.78
19:1:1145:CLA:C2A	19:1:1145:CLA:O1A	2.31	0.78
19:R:1054:CLA:CED	19:R:1054:CLA:C1A	2.57	0.78
6:B:475:ASP:HA	6:B:480:SER:O	1.84	0.78
6:B:160:LYS:HG3	6:B:161:TRP:H	1.47	0.78
5:A:242:ILE:HG12	5:A:243:PRO:HD3	1.64	0.78
5:A:402:ILE:HG13	19:A:1784:CLA:CBB	2.12	0.78
6:B:438:VAL:HG21	19:B:1764:CLA:HMC1	1.65	0.78
6:B:280:ILE:HA	6:B:283:LEU:HD12	1.64	0.78
6:B:353:TYR:O	6:B:354:SER:OG	2.01	0.78
5:A:697:ARG:NH2	6:B:566:GLY:O	2.13	0.78
6:B:697:PRO:O	7:C:79:LEU:HD13	1.82	0.78
16:L:99:LEU:CD1	22:L:1169:BCR:HC7	2.14	0.78
5:A:24:ARG:C	5:A:26:PRO:CG	2.46	0.78
20:A:7037:LMU:H72	20:A:7037:LMU:H32	0.79	0.78
2:2:42:ARG:CB	2:2:45:VAL:CG2	2.61	0.78
4:4:37:LEU:O	4:4:39:TRP:HD1	1.67	0.78
19:A:1812:CLA:H11	6:B:431:PHE:CE1	2.18	0.78
19:B:1747:CLA:CBA	19:B:1747:CLA:HED2	2.13	0.78
22:I:1032:BCR:H391	22:L:1169:BCR:H401	1.64	0.78
17:N:45:ASN:HD22	17:N:54:LYS:HG2	0.80	0.78
14:J:31:ARG:NH2	19:J:1043:CLA:C3B	2.46	0.78
20:A:7021:LMU:O3B	20:A:7021:LMU:C6B	2.28	0.78
9:E:44:TYR:CD1	9:E:73:ASN:HB2	2.18	0.78
5:A:259:TYR:CB	5:A:260:PRO:HD2	2.13	0.78
6:B:409:ALA:O	6:B:411:MET:N	2.16	0.78
4:4:123:GLN:O	4:4:143:PHE:CG	2.37	0.78
4:4:39:TRP:O	4:4:40:PHE:HD1	1.64	0.78
19:A:1760:CLA:C1	19:A:1767:CLA:H61	2.10	0.78
5:A:308:ILE:HG22	5:A:309:LEU:N	1.99	0.78
5:A:327:ILE:O	5:A:328:LYS:C	2.16	0.78
6:B:354:SER:O	6:B:355:LEU:HD13	1.84	0.78
7:C:79:LEU:CD2	7:C:81:TYR:O	2.30	0.78
20:A:7042:LMU:C1B	20:A:7042:LMU:O3'	2.28	0.78
20:A:7037:LMU:H61	20:A:7037:LMU:H11	1.65	0.78
2:2:42:ARG:HA	2:2:45:VAL:CB	2.14	0.78
2:2:55:ALA:HB3	2:2:56:MET:HE1	1.63	0.78
22:A:1806:BCR:C23	22:A:1806:BCR:H393	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1783:CLA:C17	22:A:1807:BCR:H15C	2.12	0.78
5:A:80:SER:O	5:A:83:PHE:HB2	1.83	0.78
6:B:188:LEU:O	6:B:191:ALA:N	2.17	0.78
6:B:654:HIS:CE1	19:B:1786:CLA:NB	2.52	0.78
6:B:732:LYS:HB3	6:B:733:PHE:HA	0.79	0.78
7:C:14:CYS:C	7:C:17:CYS:SG	2.61	0.78
3:3:112:THR:O	3:3:114:PHE:N	2.17	0.78
20:A:7025:LMU:O2'	20:A:7025:LMU:H21	1.84	0.78
1:1:185:TRP:HA	1:1:185:TRP:HE3	1.48	0.77
5:A:690:LEU:HD23	5:A:693:LEU:HD12	1.67	0.77
19:B:1762:CLA:CBC	19:B:1762:CLA:CHD	2.63	0.77
6:B:438:VAL:CG2	19:B:1764:CLA:CMC	2.61	0.77
11:G:42:SER:CB	11:G:45:GLU:OE2	2.30	0.77
19:A:1777:CLA:CAD	19:A:1778:CLA:HMA1	2.15	0.77
5:A:392:GLN:HA	5:A:395:LEU:HD23	1.66	0.77
6:B:58:PHE:HB3	6:B:146:SER:HB3	1.65	0.77
11:G:47:GLY:N	11:G:48:ASP:CG	2.37	0.77
17:N:45:ASN:CB	17:N:57:LYS:HZ2	1.97	0.77
21:3:1226:SUC:O1'	21:3:1226:SUC:C4'	2.28	0.77
7:C:12:ILE:HD12	7:C:12:ILE:N	1.98	0.77
1:1:89:VAL:HG12	11:G:77:ILE:HG21	1.65	0.77
5:A:464:ASN:HD22	5:A:464:ASN:N	1.81	0.77
2:2:168:ARG:HH21	2:2:171:MET:CB	1.98	0.77
19:A:1772:CLA:CBA	19:A:1772:CLA:H2	2.14	0.77
5:A:680:LEU:HB3	19:A:1811:CLA:O2A	1.84	0.77
5:A:443:ILE:HG21	5:A:558:LYS:HB2	1.66	0.77
5:A:78:VAL:HG11	19:A:1761:CLA:HBC3	1.65	0.77
6:B:127:ILE:CD1	6:B:198:ALA:HB2	2.13	0.77
19:A:1799:CLA:H92	22:L:1169:BCR:H321	1.64	0.77
5:A:24:ARG:O	5:A:26:PRO:CB	2.32	0.77
19:1:1196:CLA:O1D	19:1:1196:CLA:CAA	2.31	0.77
20:A:7004:LMU:C1B	20:A:7004:LMU:O6B	2.30	0.77
21:B:8060:SUC:C1'	21:B:8060:SUC:O5	2.30	0.77
9:E:48:ASN:ND2	9:E:71:LYS:NZ	2.32	0.77
5:A:58:HIS:CE1	19:A:1759:CLA:ND	2.52	0.77
22:A:1802:BCR:C23	22:A:1802:BCR:C40	2.60	0.77
5:A:723:ARG:HH11	5:A:723:ARG:HG2	1.50	0.77
5:A:737:HIS:HA	5:A:740:LEU:CD2	2.14	0.77
5:A:90:PHE:CE1	19:A:1761:CLA:H91	2.20	0.77
6:B:334:LEU:HB2	19:B:1737:CLA:HMD3	1.66	0.77
7:C:1:MET:N	7:C:4:SER:OG	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:124:LYS:HZ2	16:L:124:LYS:HB2	1.45	0.77
20:A:7023:LMU:H91	20:A:7023:LMU:C3	2.08	0.77
3:3:194:ILE:CG1	19:3:1214:CLA:CMC	2.60	0.77
19:3:1224:CLA:HAA2	19:3:1224:CLA:O2D	1.84	0.77
5:A:168:ALA:O	5:A:171:ALA:HB3	1.82	0.77
2:2:116:PRO:O	2:2:131:THR:CB	2.32	0.77
4:4:90:LEU:CD2	4:4:90:LEU:N	2.47	0.77
4:4:94:GLU:CB	4:4:95:PHE:HD1	1.97	0.77
19:A:1787:CLA:H3A	6:B:685:THR:OG1	1.84	0.77
5:A:281:LEU:HD13	19:A:1772:CLA:H2A	1.65	0.77
5:A:411:ALA:HB2	22:A:1805:BCR:C39	2.15	0.77
19:B:1739:CLA:HMC2	22:B:1781:BCR:C28	2.14	0.77
19:B:1765:CLA:HMD2	19:B:1766:CLA:C2C	2.14	0.77
6:B:394:PHE:O	6:B:542:ARG:NE	2.18	0.77
7:C:70:TRP:O	7:C:72:GLU:HB2	1.84	0.77
11:G:45:GLU:O	11:G:46:ALA:HB3	1.84	0.77
19:1:1188:CLA:C10	19:1:1188:CLA:H41	2.15	0.77
17:N:45:ASN:HD21	17:N:54:LYS:CG	1.93	0.77
3:3:48:PHE:HD2	3:3:49:ILE:CG2	1.82	0.77
4:4:171:ASN:C	4:4:173:THR:N	2.38	0.77
19:4:1211:CLA:HBC3	19:4:1211:CLA:CHD	2.14	0.77
6:B:137:THR:HA	6:B:140:ILE:CG1	2.14	0.77
2:2:73:ILE:O	2:2:74:LEU:HG	1.84	0.77
19:A:1800:CLA:HED1	16:L:32:LEU:HD13	1.67	0.77
19:A:1764:CLA:H111	22:A:1807:BCR:C11	2.13	0.77
5:A:454:GLY:H	5:A:457:SER:CB	1.96	0.77
6:B:664:LEU:O	6:B:667:TRP:CZ3	2.37	0.77
6:B:76:ALA:O	6:B:78:VAL:N	2.18	0.77
10:F:62:LEU:HG	10:F:72:ILE:CD1	2.13	0.77
19:J:1044:CLA:C9	19:J:1044:CLA:H41	2.13	0.77
15:K:27:ALA:CB	15:K:28:PRO:HD3	2.14	0.77
1:1:185:TRP:CE3	1:1:185:TRP:CA	2.67	0.77
4:4:99:HIS:ND1	4:4:103:ILE:HD11	1.99	0.77
19:A:1772:CLA:HBA2	19:A:1772:CLA:C2	2.13	0.77
5:A:442:ILE:CG2	19:A:1786:CLA:HMC3	2.14	0.77
5:A:669:GLY:H	6:B:445:ALA:HA	1.49	0.77
9:E:90:VAL:HG12	9:E:90:VAL:O	1.85	0.77
11:G:42:SER:CB	11:G:45:GLU:OE1	2.29	0.77
17:N:65:LEU:CD2	17:N:66:ASP:O	2.32	0.77
18:R:37:UNK:O	18:R:42:UNK:C	2.33	0.77
20:A:7022:LMU:O2'	20:A:7022:LMU:H5'	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:20:ALA:O	7:C:21:CYS:HB2	1.83	0.77
6:B:503:GLU:HB3	6:B:507:SER:CB	2.15	0.77
19:B:1754:CLA:H43	19:B:1754:CLA:CAA	2.14	0.77
19:B:1756:CLA:CMB	22:B:1778:BCR:H352	2.14	0.77
19:B:1761:CLA:CAA	19:B:1761:CLA:HED2	2.15	0.77
7:C:7:ILE:HG22	7:C:65:VAL:HG23	1.67	0.77
17:N:50:GLN:HA	17:N:51:ASP:O	1.84	0.77
21:B:8052:SUC:H62	21:B:8052:SUC:O3	1.85	0.77
10:F:23:LYS:CB	10:F:24:LYS:HZ3	1.98	0.77
19:A:1783:CLA:C10	22:A:1806:BCR:H372	2.14	0.77
5:A:626:GLY:CA	5:A:636:HIS:HA	2.15	0.77
6:B:196:HIS:CE1	19:B:1746:CLA:HED2	2.19	0.77
20:B:1783:LMU:H3'	20:B:1783:LMU:O6B	1.84	0.77
15:K:9:LEU:O	15:K:12:VAL:HB	1.85	0.77
4:4:34:PRO:HA	4:4:35:GLU:CD	2.06	0.77
19:B:1761:CLA:HAA1	19:B:1761:CLA:HED2	1.67	0.77
6:B:347:LEU:HD22	6:B:351:HIS:CE1	2.20	0.77
6:B:493:TRP:HE1	19:B:1747:CLA:HAC2	1.50	0.77
8:D:78:ALA:CB	8:D:82:GLN:HE22	1.97	0.77
17:N:57:LYS:O	17:N:60:PHE:CD1	2.37	0.77
19:1:1308:CLA:HBA2	19:1:1308:CLA:HBD	0.81	0.77
3:3:64:TYR:CB	19:3:1222:CLA:H42	2.15	0.77
17:N:5:GLU:OE1	17:N:6:TYR:CE2	2.38	0.77
2:2:42:ARG:HD3	2:2:45:VAL:CG2	2.06	0.76
19:B:1757:CLA:HED1	19:B:1765:CLA:CBB	2.14	0.76
16:L:163:LEU:CB	16:L:164:PRO:CA	2.62	0.76
5:A:316:MET:CG	5:A:317:TYR:HD1	1.91	0.76
19:2:1212:CLA:O1A	19:2:1212:CLA:C1A	2.33	0.76
20:A:7022:LMU:O3B	20:A:7022:LMU:C6B	2.29	0.76
15:K:17:LEU:HD22	15:K:17:LEU:C	2.06	0.76
17:N:5:GLU:OE2	17:N:6:TYR:CG	2.38	0.76
8:D:93:LYS:HB3	8:D:93:LYS:HZ3	1.47	0.76
6:B:507:SER:O	6:B:508:LEU:HB2	1.83	0.76
19:A:1769:CLA:HMA2	19:A:1769:CLA:C2	2.15	0.76
6:B:75:GLU:HB2	6:B:132:ASN:HB3	1.67	0.76
19:B:1739:CLA:HBA1	19:B:1758:CLA:OBD	1.86	0.76
6:B:630:GLN:HE21	6:B:731:GLY:HA3	1.49	0.76
6:B:709:GLY:O	6:B:710:LEU:HB2	1.83	0.76
11:G:44:PHE:H	11:G:45:GLU:HB2	1.49	0.76
19:1:1014:CLA:O1D	19:1:1014:CLA:CBA	2.30	0.76
5:A:107:GLU:CD	5:A:161:GLU:HG3	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:588:GLY:N	6:B:668:ARG:HD3	2.00	0.76
19:B:1741:CLA:C5	12:H:65:LEU:HD23	2.14	0.76
19:B:1756:CLA:H72	19:B:1770:CLA:C2D	2.16	0.76
6:B:292:ARG:NH1	6:B:296:GLY:H	1.83	0.76
6:B:437:TYR:HB3	6:B:616:LEU:CD2	2.15	0.76
21:B:8055:SUC:O5	21:B:8055:SUC:C3'	2.30	0.76
10:F:20:GLN:O	10:F:21:ALA:CB	2.30	0.76
10:F:25:LEU:HD22	10:F:46:MET:HB3	1.66	0.76
20:A:7032:LMU:H6'2	20:A:7032:LMU:H22	1.65	0.76
19:4:1206:CLA:H151	19:4:1206:CLA:H8	1.67	0.76
5:A:586:ARG:HG3	7:C:49:VAL:HG21	1.67	0.76
4:4:100:TYR:HA	4:4:103:ILE:HG12	1.67	0.76
19:A:1782:CLA:CGD	19:A:1782:CLA:HBA1	2.16	0.76
5:A:56:ASN:O	5:A:57:LEU:HB3	1.85	0.76
5:A:132:LEU:HD11	5:A:674:ALA:HB2	1.65	0.76
22:B:1779:BCR:C37	10:F:93:ILE:HG21	2.15	0.76
6:B:292:ARG:CZ	6:B:292:ARG:HA	2.14	0.76
8:D:78:ALA:O	8:D:79:ARG:HD3	1.84	0.76
10:F:83:PHE:O	10:F:87:GLY:HA3	1.86	0.76
11:G:41:MET:O	11:G:42:SER:O	2.04	0.76
13:I:23:SER:O	13:I:26:LEU:HD23	1.86	0.76
4:4:70:ILE:C	4:4:72:VAL:N	2.34	0.76
19:1:1192:CLA:HHD	19:1:1192:CLA:HBC2	1.67	0.76
3:3:205:GLY:CA	5:A:252:ARG:HH22	1.99	0.76
19:1:1014:CLA:HMA3	19:1:1014:CLA:CED	2.14	0.76
18:R:34:UNK:H	18:R:36:UNK:CB	1.99	0.76
15:K:58:ALA:HB1	19:K:1085:CLA:HMD3	1.67	0.76
3:3:64:TYR:HB3	19:3:1222:CLA:H43	1.65	0.76
2:2:79:TRP:CD1	2:2:81:THR:HG21	2.20	0.76
4:4:99:HIS:O	4:4:103:ILE:HD13	1.85	0.76
19:A:1795:CLA:HED1	19:B:1735:CLA:H18	1.66	0.76
5:A:591:GLN:HA	5:A:591:GLN:HE21	1.49	0.76
6:B:130:ARG:O	6:B:135:LEU:HD23	1.84	0.76
19:B:1765:CLA:HBB2	22:B:1778:BCR:H381	1.66	0.76
19:B:1756:CLA:HMB3	22:B:1778:BCR:H352	1.68	0.76
6:B:374:HIS:O	6:B:374:HIS:CG	2.38	0.76
7:C:52:LYS:CG	7:C:52:LYS:O	2.34	0.76
17:N:45:ASN:HD22	17:N:57:LYS:HZ3	1.31	0.76
21:2:1225:SUC:C2	21:2:1225:SUC:O2'	2.32	0.76
2:2:41:LEU:CG	2:2:42:ARG:H	1.81	0.76
5:A:281:LEU:CD1	19:A:1772:CLA:H2A	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:54:CYS:SG	25:C:1082:SF4:S3	2.84	0.76
4:4:75:TRP:HB2	19:4:1205:CLA:HMD3	1.67	0.76
17:N:70:GLU:CD	17:N:72:LYS:O	2.24	0.76
19:1:1308:CLA:CBA	19:1:1308:CLA:CBD	2.48	0.76
20:A:7038:LMU:O2B	20:A:7038:LMU:H4'	1.84	0.76
10:F:81:GLY:O	14:J:38:THR:HG23	1.85	0.76
4:4:81:GLU:O	4:4:82:GLU:HG2	1.85	0.76
19:A:1781:CLA:HMA2	19:A:1782:CLA:O1A	1.85	0.76
5:A:233:LEU:O	5:A:235:ALA:N	2.19	0.76
5:A:246:HIS:O	5:A:248:PHE:CD2	2.36	0.76
6:B:29:HIS:CG	19:B:1737:CLA:HBB2	2.21	0.76
6:B:596:TRP:NE1	6:B:623:TYR:HB2	2.00	0.76
5:A:558:LYS:NZ	6:B:674:LEU:HB3	1.99	0.76
17:N:59:PRO:HB3	17:N:75:TYR:CE1	2.20	0.76
19:J:1043:CLA:O1A	19:J:1043:CLA:C15	2.33	0.76
4:4:171:ASN:C	4:4:173:THR:H	1.86	0.76
19:4:1199:CLA:H2A	19:4:1199:CLA:O2A	1.86	0.76
4:4:121:PHE:O	4:4:122:LYS:CB	2.33	0.76
19:A:1771:CLA:HMC1	19:A:1771:CLA:HBC3	0.80	0.76
5:A:214:GLY:HA3	22:A:1803:BCR:H15C	1.68	0.76
5:A:353:SER:O	5:A:354:TRP:HB2	1.85	0.76
5:A:491:TRP:HE1	19:A:1792:CLA:H12	1.50	0.76
5:A:466:THR:HG21	19:B:1740:CLA:CBB	2.16	0.76
6:B:645:VAL:HG11	19:B:1739:CLA:HAC1	1.68	0.76
17:N:65:LEU:HD23	17:N:66:ASP:C	2.06	0.76
2:2:205:PHE:CE1	2:2:206:ALA:HA	2.21	0.76
19:J:1043:CLA:O1A	19:J:1043:CLA:C16	2.34	0.76
5:A:23:ASP:OD1	5:A:24:ARG:CD	2.30	0.76
3:3:173:GLU:CG	3:3:174:LYS:H	1.98	0.76
17:N:11:LYS:HG2	17:N:12:THR:H	1.51	0.76
4:4:126:LEU:HD23	4:4:127:PRO:CD	2.15	0.76
5:A:661:ALA:HA	5:A:664:VAL:HG13	1.67	0.76
20:A:7048:LMU:C9	20:A:7048:LMU:H41	2.15	0.76
6:B:325:THR:O	6:B:329:SER:HB2	1.86	0.76
20:R:1056:LMU:O6B	20:R:1056:LMU:C1B	2.31	0.76
2:2:129:LYS:O	2:2:132:GLY:CA	2.35	0.76
4:4:144:ALA:CB	4:4:147:LEU:O	2.28	0.76
5:A:32:GLU:OE2	19:A:1767:CLA:HMA2	1.86	0.76
6:B:195:VAL:HA	6:B:199:ILE:HG13	1.67	0.76
5:A:668:TYR:OH	6:B:441:ASP:OD1	2.03	0.76
19:1:1188:CLA:HED3	19:1:1188:CLA:CAA	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7037:LMU:C6	20:A:7037:LMU:H11	2.16	0.76
19:3:1222:CLA:O1D	19:3:1222:CLA:C2A	2.33	0.76
2:2:59:ALA:CB	2:2:172:LEU:HD22	2.16	0.75
4:4:106:TRP:CE3	19:4:1209:CLA:HMA1	2.21	0.75
19:A:1776:CLA:C2C	19:A:1782:CLA:H171	2.16	0.75
5:A:342:GLY:HA3	5:A:430:ASP:HB2	0.82	0.75
5:A:459:GLY:O	5:A:462:ILE:HG22	1.86	0.75
5:A:54:ILE:O	5:A:58:HIS:CD2	2.39	0.75
9:E:39:LEU:O	9:E:40:ARG:HD3	1.85	0.75
11:G:44:PHE:H	11:G:45:GLU:CB	1.96	0.75
17:N:42:PHE:H	17:N:43:PRO:HD3	1.50	0.75
20:A:7014:LMU:C1	20:A:7014:LMU:H62	2.09	0.75
8:D:28:ILE:HG12	8:D:67:ILE:HG13	1.69	0.75
4:4:84:PHE:O	4:4:85:ALA:CB	2.28	0.75
19:A:1779:CLA:HBB2	22:A:1804:BCR:H351	1.68	0.75
19:B:1749:CLA:H3A	19:B:1749:CLA:CGA	2.16	0.75
19:B:1754:CLA:H151	19:B:1754:CLA:H102	0.80	0.75
6:B:693:TRP:HD1	19:B:1771:CLA:C1D	1.99	0.75
11:G:46:ALA:H	11:G:49:THR:HG22	1.51	0.75
11:G:47:GLY:N	11:G:48:ASP:CA	2.40	0.75
16:L:63:LEU:HD22	16:L:64:LEU:N	2.00	0.75
17:N:4:GLU:OE2	17:N:5:GLU:HB2	1.86	0.75
19:2:1223:CLA:HMC1	19:2:1223:CLA:CBC	2.15	0.75
4:4:146:THR:O	19:4:1200:CLA:HBA2	1.85	0.75
5:A:636:HIS:C	5:A:638:THR:N	2.39	0.75
6:B:295:PHE:N	6:B:295:PHE:CD2	2.55	0.75
6:B:527:LEU:HD12	19:B:1756:CLA:CHD	2.16	0.75
5:A:555:ILE:HG22	6:B:670:TYR:CE2	2.21	0.75
10:F:96:TRP:CZ3	10:F:134:PHE:HB2	2.20	0.75
11:G:7:VAL:CG2	11:G:8:ILE:N	2.48	0.75
15:K:17:LEU:C	15:K:17:LEU:HD23	1.97	0.75
5:A:259:TYR:CE2	5:A:280:PHE:HA	2.21	0.75
5:A:735:VAL:O	5:A:739:LEU:HG	1.86	0.75
19:B:1743:CLA:HAC1	19:B:1744:CLA:HBB1	1.65	0.75
6:B:711:VAL:HG22	24:B:1784:LMG:H391	1.68	0.75
7:C:1:MET:N	7:C:3:HIS:N	2.29	0.75
16:L:64:LEU:HA	16:L:67:PRO:CG	2.16	0.75
17:N:54:LYS:HG2	17:N:57:LYS:HZ3	1.49	0.75
18:R:35:UNK:O	18:R:36:UNK:C	2.34	0.75
1:1:63:LEU:HD22	1:1:64:GLY:N	2.01	0.75
4:4:30:LEU:O	4:4:30:LEU:CD1	2.30	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:375:HIS:CE1	19:A:1782:CLA:NC	2.55	0.75
6:B:233:TYR:CD2	19:B:1747:CLA:HED1	2.22	0.75
19:B:1759:CLA:OBD	19:B:1759:CLA:O1D	1.93	0.75
22:B:1778:BCR:C23	22:B:1778:BCR:H382	2.09	0.75
6:B:347:LEU:CD2	6:B:351:HIS:CE1	2.70	0.75
5:A:447:ASN:ND2	6:B:678:LEU:HD21	2.01	0.75
14:J:26:LEU:C	14:J:26:LEU:HD23	2.07	0.75
2:2:41:LEU:O	2:2:42:ARG:CG	2.33	0.75
6:B:438:VAL:HG23	19:B:1764:CLA:HAC1	1.67	0.75
6:B:531:THR:HG22	19:B:1756:CLA:CMC	2.09	0.75
6:B:693:TRP:CD1	19:B:1771:CLA:C1D	2.70	0.75
19:B:1772:CLA:H192	13:I:21:MET:HB3	1.68	0.75
19:J:1043:CLA:HED3	19:J:1043:CLA:C2A	2.16	0.75
20:A:7020:LMU:H6E	20:A:7020:LMU:C6B	2.16	0.75
20:A:7020:LMU:O5B	20:A:7020:LMU:H6E	1.85	0.75
15:K:11:MET:SD	15:K:11:MET:O	2.44	0.75
20:A:7026:LMU:H52	20:A:7026:LMU:H12	1.64	0.75
21:B:8060:SUC:H1'2	21:B:8060:SUC:O5	1.86	0.75
16:L:115:ALA:N	16:L:116:PRO:HD2	2.01	0.75
6:B:315:LEU:HD13	6:B:315:LEU:O	1.87	0.75
19:2:1218:CLA:HMD2	19:2:1220:CLA:HMD3	1.66	0.75
4:4:104:ARG:NE	4:4:105:ARG:H	1.83	0.75
4:4:40:PHE:C	4:4:43:ALA:HB3	2.07	0.75
19:A:1783:CLA:H43	19:A:1783:CLA:CBA	2.16	0.75
6:B:122:GLN:HG3	6:B:361:ILE:HG12	1.69	0.75
9:E:39:LEU:C	9:E:40:ARG:HD3	2.06	0.75
16:L:99:LEU:HD11	22:L:1169:BCR:H313	1.69	0.75
17:N:72:LYS:HZ2	17:N:74:LYS:HG3	1.51	0.75
18:R:38:UNK:O	18:R:41:UNK:CB	2.34	0.75
19:2:1212:CLA:O2A	19:2:1212:CLA:C4	2.30	0.75
10:F:7:PRO:HA	10:F:61:LEU:O	1.87	0.75
16:L:49:PRO:HB2	16:L:139:PHE:HB2	1.69	0.75
19:A:1761:CLA:C4	22:A:1803:BCR:H313	2.16	0.75
19:A:1787:CLA:H52	19:A:1800:CLA:CHB	2.16	0.75
5:A:747:TRP:CD2	22:A:1806:BCR:H401	2.22	0.75
5:A:684:PHE:HD2	5:A:685:VAL:N	1.85	0.75
5:A:76:ARG:NH1	5:A:192:LYS:CG	2.44	0.75
1:1:24:PHE:CB	6:B:314:ARG:HH21	2.00	0.75
3:3:194:ILE:HD12	19:3:1214:CLA:HMC2	1.65	0.75
19:4:4007:CLA:O1A	19:4:4007:CLA:CED	2.29	0.75
20:A:7021:LMU:O6'	20:A:7021:LMU:C1	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:112:THR:OG1	3:3:113:LEU:HG	1.87	0.75
3:3:199:VAL:HG22	19:3:1216:CLA:C3C	2.17	0.75
2:2:169:LEU:HD22	19:2:1215:CLA:CBB	2.05	0.75
6:B:124:TRP:CG	6:B:129:LEU:HD13	2.21	0.75
19:B:1739:CLA:H42	19:B:1739:CLA:C4C	2.17	0.75
11:G:47:GLY:H	11:G:48:ASP:HA	1.51	0.75
19:A:1788:CLA:C16	22:L:1169:BCR:H362	2.15	0.75
1:1:63:LEU:HD22	1:1:64:GLY:CA	2.17	0.75
2:2:167:GLY:O	2:2:169:LEU:N	2.20	0.74
4:4:38:ARG:HH11	4:4:38:ARG:HG2	1.50	0.74
4:4:81:GLU:O	4:4:82:GLU:CB	2.35	0.74
19:A:1790:CLA:C3D	19:A:1791:CLA:HAC1	2.16	0.74
19:A:1797:CLA:CMA	19:A:1797:CLA:CBA	2.30	0.74
5:A:224:HIS:O	5:A:225:VAL:HG22	1.87	0.74
19:B:1747:CLA:HED2	19:B:1747:CLA:HBA2	1.67	0.74
1:1:24:PHE:HB3	6:B:314:ARG:NH2	2.01	0.74
19:1:1190:CLA:HMC3	19:1:1195:CLA:CAC	2.17	0.74
15:K:27:ALA:HB3	15:K:28:PRO:HD3	1.68	0.74
2:2:95:PHE:HA	2:2:98:GLU:HG2	1.70	0.74
5:A:393:LEU:HD11	5:A:750:PHE:CE1	2.21	0.74
5:A:648:THR:CG2	5:A:651:GLY:H	2.00	0.74
11:G:40:GLY:C	11:G:41:MET:SD	2.64	0.74
17:N:72:LYS:CG	17:N:74:LYS:H	1.96	0.74
4:4:150:LYS:HG3	4:4:150:LYS:O	1.87	0.74
19:A:1776:CLA:C8	22:A:1804:BCR:H373	2.17	0.74
5:A:284:ARG:HA	5:A:284:ARG:NH1	2.02	0.74
5:A:458:PHE:CD2	19:B:1787:CLA:HMB2	2.21	0.74
6:B:58:PHE:HB2	6:B:146:SER:HB2	1.70	0.74
11:G:13:GLY:CA	11:G:16:LEU:HG	2.17	0.74
17:N:61:LEU:CG	17:N:62:SER:H	1.98	0.74
8:D:111:TYR:CD2	8:D:114:PRO:HB3	2.22	0.74
7:C:31:TRP:O	7:C:33:GLY:N	2.20	0.74
5:A:422:TYR:N	5:A:422:TYR:CD1	2.51	0.74
5:A:452:PHE:HE1	19:A:1793:CLA:HBB2	1.44	0.74
5:A:227:LEU:HD23	5:A:231:GLN:HE22	1.52	0.74
16:L:36:TYR:CG	16:L:36:TYR:O	2.40	0.74
20:A:7043:LMU:H6E	20:A:7043:LMU:O2B	1.88	0.74
19:2:1217:CLA:HMA2	19:2:1217:CLA:H51	1.70	0.74
5:A:220:ARG:O	5:A:221:HIS:HB2	1.86	0.74
1:1:185:TRP:CB	1:1:186:HIS:CG	2.69	0.74
22:A:1805:BCR:HC8	22:A:1805:BCR:H331	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:149:LYS:HB3	19:1:1192:CLA:HMC2	1.68	0.74
11:G:94:ASP:H	11:G:95:PRO:CD	1.99	0.74
12:H:23:VAL:HG12	12:H:23:VAL:O	1.87	0.74
14:J:11:ALA:HB1	14:J:12:PRO:CD	2.16	0.74
2:2:44:ASN:O	2:2:47:ALA:N	2.16	0.74
19:A:1779:CLA:CHD	22:A:1804:BCR:C20	2.65	0.74
5:A:214:GLY:O	5:A:215:SER:HB3	1.86	0.74
5:A:488:PHE:CE2	5:A:533:PRO:HB3	2.23	0.74
5:A:707:ILE:O	5:A:711:HIS:CD2	2.41	0.74
6:B:700:LEU:N	6:B:700:LEU:HD23	2.01	0.74
19:G:1099:CLA:HBC3	19:G:1099:CLA:HHD	0.77	0.74
22:B:1775:BCR:H343	11:G:21:PHE:CD1	2.22	0.74
20:A:7042:LMU:H3'	20:A:7042:LMU:C2B	2.11	0.74
19:1:1148:CLA:HBC2	19:1:1148:CLA:CHD	2.09	0.74
20:A:7037:LMU:H12	20:A:7037:LMU:C5	1.87	0.74
2:2:40:SER:O	2:2:41:LEU:HB3	1.88	0.74
19:4:1199:CLA:HBC3	19:4:1199:CLA:CMC	2.03	0.74
5:A:514:THR:O	5:A:531:PRO:O	2.05	0.74
5:A:691:MET:HE2	23:A:1801:PQN:H2M2	1.70	0.74
6:B:304:ILE:HG22	19:B:1753:CLA:CGD	2.18	0.74
6:B:91:ILE:HD12	6:B:104:PHE:CE2	2.22	0.74
1:1:39:TYR:CD2	19:1:1195:CLA:OBD	2.40	0.74
14:J:31:ARG:HA	14:J:34:PRO:HA	1.69	0.74
10:F:30:LYS:O	10:F:31:LEU:CB	2.36	0.74
19:2:1217:CLA:CBD	19:2:1217:CLA:HBA1	2.18	0.74
2:2:128:ASN:O	2:2:130:LEU:CD1	2.34	0.74
4:4:147:LEU:CD2	4:4:148:GLU:CB	2.66	0.74
6:B:290:MET:HA	19:B:1752:CLA:HAC2	1.68	0.74
6:B:323:TYR:CD1	19:B:1755:CLA:HBC1	2.23	0.74
6:B:269:TRP:CB	6:B:497:TRP:HH2	2.00	0.74
20:A:7048:LMU:H5'	20:A:7048:LMU:H32	0.75	0.74
5:A:755:ILE:O	5:A:756:ALA:HB3	1.85	0.74
6:B:98:GLN:C	6:B:100:ALA:H	1.91	0.74
2:2:42:ARG:HG3	2:2:45:VAL:HG11	1.68	0.74
5:A:364:MET:O	5:A:368:LEU:N	2.20	0.74
6:B:180:SER:HB2	6:B:288:GLY:HA3	1.68	0.74
11:G:13:GLY:O	11:G:16:LEU:HG	1.88	0.74
15:K:17:LEU:HD22	15:K:18:MET:HA	1.69	0.74
7:C:12:ILE:HB	7:C:39:ILE:HA	1.68	0.74
9:E:44:TYR:CG	9:E:73:ASN:HB2	2.22	0.74
20:A:1809:LMU:O6B	20:A:1809:LMU:O1'	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:171:MET:HE1	2:2:175:MET:HB2	1.68	0.74
5:A:103:PHE:N	5:A:103:PHE:CD2	2.56	0.74
19:A:1771:CLA:HMC1	19:A:1771:CLA:HBC2	1.67	0.74
19:A:1787:CLA:O2A	16:L:27:VAL:O	2.05	0.74
5:A:553:VAL:H	5:A:556:LEU:HD12	1.53	0.74
19:B:1738:CLA:H91	19:B:1738:CLA:H193	1.70	0.74
13:I:12:VAL:O	13:I:17:PRO:CD	2.35	0.74
17:N:67:LEU:CA	17:N:68:GLU:HG2	2.18	0.74
3:3:181:LEU:HD13	3:3:182:LYS:HE2	1.68	0.74
19:1:1145:CLA:C2	19:1:1145:CLA:O1A	2.36	0.74
4:4:98:SER:HB2	4:4:102:GLU:OE1	1.87	0.73
4:4:126:LEU:HD23	4:4:127:PRO:HD3	1.68	0.73
19:A:1765:CLA:CBB	19:B:1764:CLA:CMD	2.64	0.73
5:A:691:MET:CE	23:A:1801:PQN:H2M2	2.18	0.73
5:A:328:LYS:HE2	5:A:332:GLU:CD	2.08	0.73
5:A:54:ILE:O	5:A:58:HIS:HD2	1.70	0.73
22:I:1032:BCR:H402	22:I:1032:BCR:H382	1.69	0.73
16:L:124:LYS:O	16:L:126:GLN:N	2.21	0.73
19:1:1190:CLA:CBC	19:1:1190:CLA:HMC1	2.17	0.73
3:3:74:ALA:CA	19:3:1217:CLA:C3D	2.59	0.73
4:4:171:ASN:O	4:4:172:VAL:C	2.25	0.73
20:A:7004:LMU:C1	20:A:7004:LMU:C3'	2.66	0.73
20:A:7010:LMU:O3'	20:A:7010:LMU:H1B	1.88	0.73
14:J:10:VAL:HG13	14:J:14:LEU:HG	1.69	0.73
5:A:479:ASP:HA	5:A:536:THR:HG23	1.70	0.73
2:2:164:ILE:O	2:2:167:GLY:CA	2.36	0.73
19:4:1199:CLA:H2	19:4:1199:CLA:HED1	1.69	0.73
19:A:1769:CLA:HBA1	19:A:1780:CLA:C4	2.16	0.73
19:A:1789:CLA:HBC3	19:A:1789:CLA:HMC1	1.69	0.73
6:B:471:THR:HG23	6:B:502:ASN:ND2	2.02	0.73
9:E:55:VAL:HG23	9:E:65:VAL:HB	1.70	0.73
9:E:88:GLU:O	9:E:90:VAL:HB	1.89	0.73
17:N:47:THR:CB	17:N:52:LEU:O	2.36	0.73
17:N:63:ASP:H	17:N:64:ASP:C	1.90	0.73
17:N:67:LEU:CB	17:N:68:GLU:CG	2.45	0.73
19:4:1211:CLA:CBD	19:4:1211:CLA:HBA1	2.16	0.73
7:C:44:ARG:HH21	8:D:127:ARG:CB	1.99	0.73
12:H:37:SER:HB3	16:L:51:LEU:HG	1.70	0.73
18:R:44:UNK:O	18:R:45:UNK:C	2.35	0.73
2:2:54:TRP:CD1	19:2:1222:CLA:O1D	2.41	0.73
19:4:1198:CLA:O1A	19:4:1198:CLA:C2	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:144:ALA:HB3	4:4:147:LEU:C	2.06	0.73
19:A:1770:CLA:CHC	22:A:1802:BCR:C17	2.66	0.73
19:B:1757:CLA:H8	22:B:1778:BCR:H12C	1.68	0.73
6:B:199:ILE:HG23	6:B:270:LEU:HD22	1.68	0.73
6:B:664:LEU:O	6:B:667:TRP:HZ3	1.71	0.73
16:L:8:TYR:CE1	16:L:11:ILE:HG23	2.24	0.73
6:B:44:GLN:OE1	6:B:163:PRO:HB2	1.88	0.73
4:4:101:VAL:HG13	4:4:104:ARG:HH22	1.49	0.73
4:4:151:GLU:HA	4:4:154:ILE:HG23	1.67	0.73
19:A:1776:CLA:HMD2	19:A:1778:CLA:HBB2	1.66	0.73
22:A:1802:BCR:H341	22:A:1802:BCR:C12	2.16	0.73
5:A:467:MET:HA	5:A:470:LEU:HB2	1.69	0.73
19:B:1753:CLA:H72	19:B:1753:CLA:CBB	2.17	0.73
6:B:421:HIS:NE2	19:B:1762:CLA:C4D	2.52	0.73
6:B:732:LYS:HG3	6:B:734:GLY:CA	2.19	0.73
19:L:1168:CLA:HAA1	19:L:1168:CLA:O1D	1.86	0.73
19:1:1014:CLA:H102	19:1:1014:CLA:C4	2.15	0.73
4:4:193:ILE:H	4:4:193:ILE:HD12	1.52	0.73
1:1:63:LEU:CD2	1:1:64:GLY:C	2.56	0.73
6:B:454:LEU:CD1	10:F:69:PRO:O	2.36	0.73
4:4:58:MET:O	4:4:59:LEU:C	2.26	0.73
12:H:42:THR:HG22	12:H:45:ALA:HB2	1.69	0.73
4:4:104:ARG:HE	4:4:105:ARG:N	1.85	0.73
5:A:217:SER:CB	22:A:1802:BCR:H351	2.18	0.73
23:B:1774:PQN:H192	22:B:1781:BCR:C8	2.19	0.73
22:L:1169:BCR:C27	22:L:1169:BCR:H403	2.17	0.73
20:N:1086:LMU:O5'	20:N:1086:LMU:C3	2.30	0.73
5:A:22:VAL:CG1	5:A:23:ASP:N	2.51	0.73
19:3:1221:CLA:C2A	19:3:3011:CLA:CAC	2.64	0.73
5:A:126:ILE:HG12	19:A:1765:CLA:HMA3	1.71	0.73
5:A:370:ILE:HG22	5:A:400:MET:CA	2.17	0.73
5:A:457:SER:O	5:A:544:ILE:HD13	1.88	0.73
6:B:533:ILE:HD11	6:B:575:ASP:O	1.88	0.73
9:E:58:ASP:OD2	9:E:60:LYS:NZ	2.18	0.73
9:E:86:GLU:HG3	9:E:87:VAL:H	0.71	0.73
4:4:72:VAL:CG1	4:4:72:VAL:O	2.30	0.73
20:N:1086:LMU:C5B	20:N:1086:LMU:O2B	2.30	0.73
17:N:79:SER:CA	17:N:80:ASN:C	2.57	0.73
20:A:7016:LMU:C7	20:A:7016:LMU:C11	2.66	0.73
20:A:7037:LMU:C12	20:A:7051:LMU:H41	2.17	0.73
20:A:7032:LMU:H32	20:A:7032:LMU:H1B	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:4014:CLA:HED3	19:4:4014:CLA:O1A	1.89	0.73
7:C:29:ILE:HG23	8:D:126:GLY:HA2	1.71	0.73
17:N:5:GLU:OE1	17:N:6:TYR:CZ	2.41	0.73
19:A:1760:CLA:H2A	19:A:1760:CLA:CED	2.19	0.73
5:A:187:HIS:CE1	19:A:1767:CLA:C4D	2.68	0.73
5:A:187:HIS:CD2	19:A:1767:CLA:NC	2.38	0.73
19:A:1790:CLA:HMC1	19:A:1790:CLA:HBC2	1.71	0.73
6:B:489:GLY:O	6:B:490:ARG:HG2	1.89	0.73
16:L:163:LEU:HB3	16:L:164:PRO:CA	2.11	0.73
7:C:17:CYS:C	7:C:58:CYS:HB2	2.09	0.73
7:C:26:LEU:N	7:C:43:PRO:HG3	2.03	0.73
2:2:100:VAL:CG2	2:2:101:PHE:N	2.52	0.73
19:A:1783:CLA:H172	22:A:1807:BCR:H17C	1.70	0.73
19:A:1791:CLA:O1A	19:A:1791:CLA:H3A	1.86	0.73
5:A:223:VAL:HG23	5:A:227:LEU:HD13	1.71	0.73
20:A:7006:LMU:C2'	20:A:7006:LMU:H22	2.19	0.73
6:B:190:TRP:HA	19:B:1745:CLA:HBB2	1.70	0.73
6:B:655:LEU:HD21	19:B:1772:CLA:CBB	2.18	0.73
4:4:76:TYR:O	4:4:76:TYR:CD1	2.42	0.73
20:A:7028:LMU:H1'	20:A:7028:LMU:O6'	1.85	0.73
5:A:628:ILE:HG13	5:A:632:GLY:HA2	1.69	0.73
19:A:1776:CLA:C4C	19:A:1782:CLA:H172	2.18	0.73
19:A:1781:CLA:H2	19:A:1782:CLA:CED	2.18	0.73
3:3:92:TRP:HZ2	5:A:250:LEU:HD12	1.54	0.73
2:2:205:PHE:CD1	2:2:206:ALA:CA	2.71	0.73
3:3:50:GLU:N	3:3:51:PRO:CD	2.52	0.73
3:3:52:LYS:O	3:3:56:TYR:HD2	1.63	0.73
20:1:1200:LMU:C1'	20:1:1200:LMU:O6'	2.30	0.73
17:N:5:GLU:CD	17:N:6:TYR:CG	2.62	0.73
3:3:208:PRO:HB3	3:3:210:GLN:OE1	1.89	0.73
1:1:45:ILE:HG22	1:1:48:ARG:HD2	1.71	0.73
19:2:1213:CLA:H93	19:2:1213:CLA:H51	1.69	0.73
19:A:1783:CLA:H102	22:A:1806:BCR:H372	1.70	0.73
19:A:1789:CLA:C4	16:L:64:LEU:HD23	2.18	0.73
5:A:684:PHE:HD2	5:A:684:PHE:C	1.91	0.73
5:A:714:LEU:HD13	22:B:1780:BCR:H392	1.69	0.73
6:B:91:ILE:CD1	6:B:104:PHE:HE2	2.02	0.73
19:B:1750:CLA:C3	19:B:1755:CLA:H92	2.18	0.73
6:B:8:PHE:O	6:B:35:ASP:HB2	1.88	0.73
13:I:11:LEU:HG	22:I:1032:BCR:HC7	1.67	0.73
17:N:61:LEU:HD12	17:N:62:SER:CA	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:192:THR:CG2	4:4:193:ILE:O	2.28	0.73
19:2:1212:CLA:O2A	19:2:1212:CLA:H43	1.89	0.73
2:2:98:GLU:HG3	2:2:99:LEU:CG	2.18	0.72
5:A:218:TRP:O	5:A:222:GLN:HB2	1.88	0.72
19:B:1754:CLA:HMC1	19:B:1754:CLA:HBC3	0.78	0.72
16:L:40:LEU:HB3	16:L:41:PRO:HD3	1.70	0.72
16:L:164:PRO:CA	16:L:165:TYR:CD2	2.71	0.72
17:N:62:SER:CB	17:N:66:ASP:CA	2.65	0.72
19:1:1142:CLA:CMD	19:K:1085:CLA:C1A	2.67	0.72
19:4:1201:CLA:C2	19:4:1201:CLA:O1A	2.29	0.72
15:K:9:LEU:CD2	15:K:9:LEU:H	1.91	0.72
1:1:64:GLY:CA	1:1:66:GLY:O	2.37	0.72
20:R:1056:LMU:O5B	20:R:1056:LMU:C5'	2.33	0.72
8:D:60:MET:SD	8:D:61:PRO:HD2	2.29	0.72
5:A:387:THR:CG2	5:A:523:VAL:HG11	2.19	0.72
2:2:126:PRO:HD2	2:2:129:LYS:HB2	1.70	0.72
4:4:115:VAL:HG13	4:4:116:ASN:H	1.52	0.72
19:A:1771:CLA:CBD	19:A:1771:CLA:HBA1	2.19	0.72
19:A:1781:CLA:H61	19:A:1782:CLA:CED	2.19	0.72
19:A:1799:CLA:C6	19:A:1799:CLA:H112	2.16	0.72
19:A:1787:CLA:HAC2	19:A:1800:CLA:HMC3	1.71	0.72
19:B:1754:CLA:C4	19:B:1754:CLA:HAA1	2.18	0.72
7:C:1:MET:H1	7:C:4:SER:CB	2.01	0.72
20:A:7042:LMU:H1B	20:A:7042:LMU:H3O2	1.51	0.72
20:N:1086:LMU:H52	20:N:1086:LMU:H92	0.73	0.72
17:N:41:LYS:HB2	17:N:42:PHE:HB3	0.80	0.72
17:N:60:PHE:HA	17:N:61:LEU:O	1.88	0.72
6:B:329:SER:O	6:B:330:ILE:HG22	1.88	0.72
17:N:35:VAL:HG12	17:N:37:PHE:CZ	2.25	0.72
19:A:1782:CLA:C4	19:A:1782:CLA:O2A	2.37	0.72
19:A:1797:CLA:HMA2	19:A:1797:CLA:HBA1	0.80	0.72
22:A:1805:BCR:C8	22:A:1805:BCR:H331	2.19	0.72
5:A:368:LEU:HD21	19:A:1774:CLA:H91	1.63	0.72
5:A:41:SER:O	5:A:44:ILE:HA	1.88	0.72
5:A:79:PHE:HE2	5:A:185:HIS:CE1	2.06	0.72
6:B:144:PHE:CD2	6:B:144:PHE:O	2.41	0.72
11:G:68:ILE:HG23	11:G:72:LEU:CD1	2.14	0.72
2:2:120:ASN:CG	14:J:5:LYS:HD2	2.10	0.72
17:N:49:CYS:O	17:N:50:GLN:C	2.28	0.72
17:N:50:GLN:HA	17:N:51:ASP:C	2.09	0.72
2:2:211:LYS:HA	2:2:211:LYS:CE	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:17:LEU:O	15:K:17:LEU:CD2	2.30	0.72
10:F:42:ILE:CG1	10:F:43:LYS:H	1.98	0.72
5:A:29:THR:OG1	5:A:31:PHE:HB2	1.90	0.72
2:2:120:ASN:HB3	2:2:121:THR:CB	2.15	0.72
4:4:144:ALA:CB	4:4:148:GLU:O	2.38	0.72
4:4:37:LEU:CA	4:4:39:TRP:HB2	2.11	0.72
5:A:281:LEU:HA	5:A:297:THR:O	1.89	0.72
5:A:542:HIS:HA	5:A:545:HIS:HD2	1.55	0.72
5:A:85:GLN:O	5:A:89:ILE:HG13	1.90	0.72
6:B:290:MET:HA	19:B:1752:CLA:CAC	2.18	0.72
19:B:1756:CLA:HMB2	19:B:1770:CLA:O1A	1.90	0.72
5:A:668:TYR:CD1	6:B:445:ALA:HB2	2.23	0.72
5:A:555:ILE:HG22	6:B:670:TYR:HE2	1.54	0.72
19:A:1799:CLA:HMB2	19:L:1167:CLA:HBC1	1.70	0.72
16:L:36:TYR:O	16:L:36:TYR:CD1	2.41	0.72
17:N:48:GLY:HA3	17:N:49:CYS:HB2	1.70	0.72
17:N:61:LEU:HG	17:N:62:SER:H	1.54	0.72
17:N:75:TYR:C	17:N:76:LYS:O	2.26	0.72
20:B:1783:LMU:H111	20:B:1783:LMU:C7	2.18	0.72
5:A:27:ILE:CG2	5:A:27:ILE:O	2.30	0.72
10:F:63:CYS:HA	10:F:69:PRO:HA	1.72	0.72
12:H:44:ALA:HB3	16:L:145:PHE:HD1	1.53	0.72
19:4:1206:CLA:H18	19:4:1206:CLA:ND	2.03	0.72
8:D:94:TYR:O	8:D:95:LYS:CG	2.37	0.72
6:B:152:ALA:O	6:B:153:GLY:C	2.26	0.72
3:3:84:ILE:CG1	19:3:1212:CLA:O1A	2.37	0.72
19:B:1757:CLA:H122	22:B:1778:BCR:C13	2.19	0.72
6:B:378:ILE:O	6:B:380:GLY:N	2.21	0.72
5:A:668:TYR:CE2	6:B:617:MET:SD	2.83	0.72
16:L:164:PRO:CB	16:L:165:TYR:CD2	2.73	0.72
20:B:1783:LMU:H5B	20:B:1783:LMU:C4'	2.00	0.72
19:J:1044:CLA:H151	19:J:1044:CLA:H91	1.70	0.72
4:4:192:THR:HG22	4:4:195:GLN:N	2.05	0.72
3:3:106:TYR:CD2	3:3:107:TRP:CD1	2.78	0.72
7:C:11:CYS:SG	7:C:12:ILE:N	2.62	0.72
16:L:48:ASN:HD22	16:L:115:ALA:HB2	1.54	0.72
5:A:289:PRO:O	5:A:290:LEU:HB2	1.90	0.72
22:A:1806:BCR:C32	22:A:1807:BCR:H391	2.19	0.72
5:A:281:LEU:HD12	19:A:1772:CLA:CED	2.17	0.72
19:B:1756:CLA:HED2	19:B:1757:CLA:OBD	1.89	0.72
19:B:1769:CLA:HBC1	10:F:83:PHE:HZ	1.49	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:362:ALA:O	6:B:363:GLN:HG3	1.89	0.72
6:B:444:LEU:O	6:B:445:ALA:HB3	1.89	0.72
6:B:707:LEU:CD1	6:B:711:VAL:HG21	2.19	0.72
9:E:52:VAL:C	9:E:53:VAL:HG23	2.08	0.72
11:G:33:LYS:CA	11:G:33:LYS:HE3	2.14	0.72
6:B:25:ILE:HG22	22:L:1169:BCR:C29	2.14	0.72
17:N:72:LYS:CB	17:N:74:LYS:HB2	2.19	0.72
20:A:7016:LMU:H81	20:A:7016:LMU:H32	1.46	0.72
11:G:92:GLY:C	11:G:94:ASP:OD1	2.28	0.72
8:D:113:HIS:N	8:D:114:PRO:HD2	2.04	0.72
5:A:426:THR:HA	5:A:428:TYR:CE2	2.25	0.72
16:L:118:LEU:HD12	16:L:119:THR:N	2.03	0.72
1:1:45:ILE:HA	1:1:48:ARG:HB2	1.71	0.72
12:H:49:LYS:O	12:H:51:GLY:N	2.22	0.72
19:A:1787:CLA:CBB	19:A:1793:CLA:H192	2.20	0.72
6:B:189:ALA:HB2	19:B:1759:CLA:C20	2.19	0.72
6:B:424:TRP:CZ2	19:B:1762:CLA:HAC1	2.25	0.72
23:B:1774:PQN:H291	24:B:1784:LMG:H201	1.70	0.72
19:A:1799:CLA:HMD3	22:B:1781:BCR:C3	2.20	0.72
6:B:390:GLY:HA3	22:B:1778:BCR:HC22	1.71	0.72
6:B:38:THR:OG1	6:B:41:ARG:HB2	1.90	0.72
7:C:6:LYS:HB3	7:C:63:LEU:HD21	1.72	0.72
11:G:13:GLY:O	11:G:16:LEU:CG	2.38	0.72
19:L:1167:CLA:HHC	22:L:1170:BCR:HC8	1.71	0.72
21:B:8052:SUC:O3	21:B:8052:SUC:C6	2.30	0.72
20:A:7009:LMU:O2'	20:A:7009:LMU:H12	1.88	0.72
5:A:210:LEU:CD1	19:A:1769:CLA:CMB	2.67	0.72
19:A:1781:CLA:HED3	19:A:1782:CLA:CMD	2.10	0.72
19:A:1795:CLA:C1C	19:B:1735:CLA:HBC2	2.20	0.72
5:A:309:LEU:HD21	19:A:1776:CLA:HMC3	1.72	0.72
5:A:334:HIS:HB3	19:A:1777:CLA:CMA	2.19	0.72
19:B:1748:CLA:H52	19:B:1757:CLA:CMB	2.20	0.72
10:F:125:LEU:O	10:F:126:ALA:CB	2.36	0.72
10:F:93:ILE:O	10:F:96:TRP:CD1	2.40	0.72
17:N:72:LYS:NZ	17:N:74:LYS:HG3	2.03	0.72
3:3:52:LYS:HA	3:3:55:ALA:HB3	1.70	0.72
10:F:28:SER:O	10:F:29:LEU:C	2.27	0.72
12:H:21:TRP:H	12:H:22:ASP:HB3	1.55	0.72
16:L:5:LYS:HE2	16:L:5:LYS:HA	1.71	0.72
16:L:107:PHE:HB2	16:L:109:GLU:OE1	1.89	0.72
2:2:54:TRP:HZ2	2:2:109:ARG:CD	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:124:ILE:CG2	2:2:129:LYS:HB3	2.19	0.72
5:A:370:ILE:HD11	19:A:1781:CLA:CAD	2.18	0.72
5:A:79:PHE:CE2	5:A:185:HIS:CE1	2.78	0.72
19:B:1748:CLA:CBD	19:B:1757:CLA:HBB2	2.20	0.72
6:B:615:TYR:HD1	6:B:615:TYR:H	1.38	0.72
11:G:28:ARG:CG	11:G:29:GLU:N	2.52	0.72
19:4:1201:CLA:CMA	19:4:1201:CLA:CGA	2.66	0.72
21:B:8053:SUC:H5	21:B:8053:SUC:O2	1.89	0.72
5:A:76:ARG:O	5:A:186:TYR:HD2	1.72	0.72
5:A:331:LEU:CD2	5:A:331:LEU:O	2.29	0.72
9:E:53:VAL:HG12	9:E:54:ALA:H	1.55	0.72
11:G:42:SER:OG	11:G:45:GLU:CD	2.28	0.72
16:L:66:GLY:N	16:L:67:PRO:HD2	2.05	0.72
20:A:7048:LMU:C3	20:A:7048:LMU:O5'	2.37	0.72
21:B:8055:SUC:H3'	21:B:8055:SUC:O5	1.90	0.72
19:4:4014:CLA:CED	19:4:4014:CLA:O1A	2.38	0.72
4:4:152:LYS:CD	4:4:154:ILE:HD11	2.19	0.71
7:C:1:MET:H2	7:C:3:HIS:C	1.89	0.71
7:C:1:MET:CB	7:C:4:SER:HG	1.86	0.71
11:G:37:GLU:OE2	11:G:42:SER:HA	1.90	0.71
19:A:1787:CLA:H42	16:L:33:ILE:HG12	1.71	0.71
17:N:74:LYS:O	17:N:76:LYS:N	2.23	0.71
10:F:53:PHE:C	10:F:55:ASN:H	1.94	0.71
21:2:1225:SUC:O2	21:2:1225:SUC:H5'	1.88	0.71
6:B:15:ASP:O	6:B:20:ARG:HG2	1.88	0.71
8:D:69:ARG:O	8:D:70:GLU:HB2	1.90	0.71
2:2:42:ARG:HG3	2:2:45:VAL:CG1	2.20	0.71
2:2:91:THR:O	2:2:94:LEU:CB	2.35	0.71
19:A:1782:CLA:H42	19:A:1782:CLA:O2A	1.90	0.71
19:A:1774:CLA:O1A	19:A:1784:CLA:H71	1.90	0.71
22:A:1806:BCR:HC31	22:B:1779:BCR:H17C	1.72	0.71
5:A:340:GLY:O	5:A:343:HIS:N	2.22	0.71
19:B:1746:CLA:O2D	19:B:1746:CLA:OBD	2.06	0.71
19:B:1769:CLA:H61	22:B:1780:BCR:H323	1.71	0.71
7:C:74:THR:CB	7:C:80:ALA:HB2	2.20	0.71
1:1:25:ASP:N	6:B:314:ARG:NH2	2.26	0.71
20:A:7042:LMU:H32	20:A:7042:LMU:O5'	1.90	0.71
10:F:17:ARG:HE	10:F:17:ARG:HA	1.54	0.71
5:A:103:PHE:N	5:A:103:PHE:HD2	1.87	0.71
5:A:121:GLN:NE2	19:A:1765:CLA:HMD1	2.05	0.71
5:A:700:TRP:CZ2	23:A:1801:PQN:H2M3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:708:VAL:HA	5:A:711:HIS:HD2	1.54	0.71
6:B:141:PHE:O	6:B:143:LEU:N	2.23	0.71
22:B:1776:BCR:C33	22:B:1776:BCR:HC8	2.20	0.71
6:B:492:ILE:CD1	6:B:492:ILE:H	2.02	0.71
6:B:687:LEU:HD12	22:L:1170:BCR:HC31	1.72	0.71
10:F:83:PHE:O	10:F:87:GLY:CA	2.38	0.71
16:L:96:SER:OG	16:L:143:PHE:HD2	1.74	0.71
3:3:93:PHE:HD2	3:3:93:PHE:H	1.39	0.71
20:B:1783:LMU:H112	20:B:1783:LMU:H72	1.64	0.71
3:3:52:LYS:O	3:3:56:TYR:N	2.21	0.71
19:J:1043:CLA:H152	19:J:1044:CLA:HMB1	1.72	0.71
4:4:128:ALA:O	4:4:130:GLU:N	2.23	0.71
4:4:37:LEU:HA	4:4:39:TRP:CG	2.26	0.71
4:4:99:HIS:ND1	4:4:99:HIS:C	2.39	0.71
5:A:361:ASN:ND2	19:A:1761:CLA:CED	2.53	0.71
19:B:1757:CLA:H41	19:B:1757:CLA:H72	1.71	0.71
19:B:1769:CLA:H202	22:B:1780:BCR:HC41	1.73	0.71
22:B:1779:BCR:C37	10:F:93:ILE:CG2	2.69	0.71
19:B:1788:CLA:HMC1	19:B:1788:CLA:CBC	2.20	0.71
6:B:463:ILE:O	6:B:464:GLN:HB3	1.91	0.71
9:E:52:VAL:CG1	9:E:53:VAL:H	1.93	0.71
10:F:80:TRP:HE3	19:F:1157:CLA:HMC2	1.55	0.71
11:G:21:PHE:O	11:G:23:PHE:CB	2.38	0.71
19:1:1308:CLA:CED	19:1:1308:CLA:OBD	2.38	0.71
19:1:1187:CLA:CBA	19:1:1187:CLA:CMA	2.60	0.71
4:4:170:HIS:C	4:4:171:ASN:O	2.29	0.71
3:3:84:ILE:N	19:3:1212:CLA:C4	2.46	0.71
22:A:1804:BCR:H382	22:A:1804:BCR:C23	2.09	0.71
6:B:145:LEU:HA	6:B:148:ILE:HD12	1.71	0.71
6:B:594:TRP:C	6:B:594:TRP:CD1	2.64	0.71
9:E:87:VAL:CG1	9:E:87:VAL:O	2.28	0.71
16:L:95:LEU:HA	16:L:98:CYS:HB2	1.71	0.71
19:1:1188:CLA:CHA	19:1:1188:CLA:HED3	2.18	0.71
5:A:249:ILE:O	5:A:251:ASN:N	2.23	0.71
17:N:74:LYS:O	17:N:75:TYR:C	2.29	0.71
5:A:23:ASP:OD2	5:A:24:ARG:CD	2.36	0.71
6:B:504:ASN:ND2	6:B:504:ASN:H	1.88	0.71
26:B:8057:UNL:C6	26:B:8057:UNL:C2	2.63	0.71
15:K:47:ILE:HG23	15:K:48:GLN:H	1.54	0.71
2:2:129:LYS:C	2:2:131:THR:H	1.93	0.71
4:4:36:ASN:C	4:4:39:TRP:CE3	2.64	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1788:CLA:H152	22:L:1169:BCR:C36	2.20	0.71
5:A:462:ILE:CD1	19:B:1787:CLA:H72	2.21	0.71
5:A:690:LEU:HD21	5:A:738:TYR:HE1	1.55	0.71
6:B:230:TRP:HH2	11:G:11:SER:HB2	1.55	0.71
6:B:91:ILE:CD1	6:B:104:PHE:CE2	2.74	0.71
16:L:126:GLN:N	16:L:127:PRO:HD2	2.05	0.71
19:1:1142:CLA:HMD1	19:K:1085:CLA:C1A	2.21	0.71
4:4:172:VAL:O	4:4:173:THR:HG22	1.90	0.71
8:D:28:ILE:HG12	8:D:67:ILE:CG1	2.20	0.71
16:L:10:VAL:O	16:L:10:VAL:HG22	1.90	0.71
6:B:496:GLY:O	6:B:499:ASN:HB2	1.91	0.71
5:A:491:TRP:NE1	19:A:1792:CLA:H12	2.06	0.71
6:B:437:TYR:HB3	6:B:616:LEU:HD23	1.72	0.71
11:G:68:ILE:HG22	11:G:72:LEU:HD13	1.70	0.71
17:N:45:ASN:O	17:N:45:ASN:CG	2.29	0.71
4:4:194:VAL:CG1	4:4:195:GLN:CA	2.64	0.71
5:A:466:THR:O	5:A:470:LEU:HG	1.90	0.71
5:A:396:PHE:CE2	5:A:616:PHE:CG	2.79	0.71
5:A:618:TRP:CZ2	5:A:655:ASP:HB2	2.25	0.71
9:E:39:LEU:H	9:E:40:ARG:HH11	1.38	0.71
20:A:7043:LMU:O2'	20:A:7043:LMU:C1	2.33	0.71
5:A:119:SER:HB2	5:A:136:VAL:HG21	1.71	0.71
5:A:443:ILE:HD11	5:A:557:LEU:HG	1.73	0.71
5:A:550:HIS:O	5:A:552:THR:O	2.07	0.71
6:B:595:HIS:HD2	6:B:623:TYR:OH	1.73	0.71
4:4:192:THR:C	4:4:193:ILE:O	2.28	0.71
1:1:63:LEU:H	1:1:63:LEU:CD1	2.01	0.71
6:B:503:GLU:HB3	6:B:507:SER:HB2	1.71	0.71
5:A:193:LEU:HA	5:A:196:PHE:CE2	2.26	0.71
5:A:202:MET:HG3	19:A:1769:CLA:HBC2	1.71	0.71
17:N:42:PHE:HD1	17:N:43:PRO:N	1.83	0.71
17:N:54:LYS:HG3	17:N:57:LYS:HZ3	1.53	0.71
17:N:54:LYS:HG2	17:N:57:LYS:NZ	2.05	0.71
19:1:1014:CLA:CGA	19:1:1014:CLA:O1D	2.39	0.71
4:4:58:MET:O	4:4:61:PRO:CD	2.39	0.71
5:A:387:THR:HG23	5:A:523:VAL:HG11	1.71	0.71
19:4:1199:CLA:CBC	19:4:1199:CLA:CMC	2.65	0.70
19:A:1783:CLA:H111	22:A:1807:BCR:H353	1.73	0.70
19:B:1754:CLA:HAA2	19:B:1754:CLA:CBD	2.20	0.70
6:B:493:TRP:HB3	19:B:1766:CLA:HED2	1.71	0.70
22:B:1780:BCR:HC32	19:F:1156:CLA:CMA	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:63:ASP:H	17:N:65:LEU:N	1.87	0.70
17:N:65:LEU:O	17:N:66:ASP:C	2.29	0.70
4:4:194:VAL:CB	4:4:195:GLN:CA	2.69	0.70
20:A:7004:LMU:H12	20:A:7004:LMU:C3'	2.01	0.70
9:E:68:ARG:NH2	9:E:69:PHE:HA	2.06	0.70
20:A:7027:LMU:C6B	20:A:7027:LMU:H2B	2.19	0.70
19:3:1219:CLA:HBA1	19:3:1219:CLA:O2D	1.91	0.70
19:2:1218:CLA:H2A	19:2:1218:CLA:O1D	1.91	0.70
2:2:40:SER:C	2:2:41:LEU:CD2	2.58	0.70
4:4:168:ILE:HD11	19:4:1204:CLA:C3C	2.20	0.70
4:4:160:MET:HA	4:4:163:PHE:HB2	1.72	0.70
4:4:164:LEU:O	4:4:165:GLY:C	2.30	0.70
5:A:242:ILE:HG12	5:A:243:PRO:CD	2.19	0.70
5:A:438:HIS:CE1	5:A:442:ILE:HD11	2.25	0.70
7:C:5:VAL:HB	7:C:65:VAL:CA	2.13	0.70
16:L:52:ARG:O	16:L:56:VAL:HG23	1.90	0.70
4:4:70:ILE:HG13	4:4:71:ASN:N	2.06	0.70
20:N:1086:LMU:H91	20:N:1086:LMU:H52	1.65	0.70
10:F:24:LYS:C	10:F:26:GLN:H	1.93	0.70
3:3:106:TYR:O	3:3:108:ALA:HB2	1.91	0.70
4:4:124:TYR:HB3	4:4:143:PHE:CE1	2.25	0.70
19:A:1760:CLA:H12	19:A:1767:CLA:C6	2.14	0.70
19:A:1783:CLA:C7	22:A:1806:BCR:H372	2.16	0.70
19:A:1797:CLA:C3D	19:A:1797:CLA:O1D	2.30	0.70
5:A:211:LEU:O	5:A:214:GLY:O	2.09	0.70
5:A:207:LEU:HD12	5:A:310:PHE:CD1	2.25	0.70
5:A:368:LEU:HD22	19:A:1774:CLA:H92	1.74	0.70
5:A:431:LEU:O	5:A:435:VAL:HG12	1.90	0.70
5:A:445:HIS:O	5:A:446:LEU:CB	2.39	0.70
5:A:497:ALA:HB2	5:A:515:TRP:CB	2.20	0.70
5:A:397:THR:HB	5:A:613:ILE:HD11	1.73	0.70
23:A:1801:PQN:C13	22:B:1779:BCR:H322	2.21	0.70
6:B:545:LYS:HG2	6:B:546:LEU:N	2.03	0.70
7:C:1:MET:SD	7:C:4:SER:CB	2.79	0.70
6:B:542:ARG:NH2	8:D:143:PRO:HG3	2.05	0.70
1:1:25:ASP:HB3	1:1:26:PRO:CD	2.20	0.70
20:A:7027:LMU:H6'1	20:A:7027:LMU:H2B	1.73	0.70
5:A:485:GLN:O	5:A:487:VAL:N	2.24	0.70
5:A:625:TRP:CB	5:A:637:ILE:HD11	2.20	0.70
6:B:174:ARG:NH1	19:B:1755:CLA:CMD	2.54	0.70
11:G:46:ALA:C	11:G:48:ASP:OD1	2.29	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:42:PHE:O	17:N:43:PRO:C	2.30	0.70
21:B:8055:SUC:H3	21:B:8055:SUC:C5'	2.21	0.70
12:H:21:TRP:H	12:H:22:ASP:CB	2.03	0.70
19:3:3011:CLA:HMA2	19:3:3011:CLA:C1	2.14	0.70
8:D:48:ILE:CG2	8:D:83:CYS:HB2	2.21	0.70
17:N:18:ASP:HB3	17:N:22:LEU:HG	1.73	0.70
17:N:11:LYS:HD2	17:N:12:THR:O	1.92	0.70
2:2:110:TRP:HA	2:2:113:ILE:CG2	2.21	0.70
5:A:216:LEU:HD12	22:A:1802:BCR:H353	1.73	0.70
5:A:663:GLN:HB3	5:A:752:ALA:O	1.90	0.70
6:B:130:ARG:HG2	6:B:130:ARG:HH11	1.57	0.70
19:A:1799:CLA:HMC2	19:B:1771:CLA:H11	1.74	0.70
22:B:1779:BCR:H371	10:F:93:ILE:CG2	2.22	0.70
6:B:295:PHE:N	6:B:295:PHE:HD2	1.85	0.70
6:B:375:HIS:HE1	19:B:1759:CLA:NC	1.89	0.70
7:C:5:VAL:CB	7:C:65:VAL:HG22	2.22	0.70
8:D:47:VAL:HB	8:D:76:LYS:HA	1.73	0.70
17:N:70:GLU:C	17:N:72:LYS:N	2.34	0.70
21:B:8059:SUC:HO2	21:B:8059:SUC:H1'2	1.55	0.70
5:A:423:ASP:HB3	5:A:424:PRO:CD	2.08	0.70
3:3:157:ALA:C	3:3:158:TYR:CD2	2.64	0.70
8:D:91:ARG:HH12	8:D:119:TYR:HE1	1.38	0.70
9:E:44:TYR:CZ	9:E:73:ASN:HA	2.27	0.70
17:N:4:GLU:C	17:N:4:GLU:OE2	2.30	0.70
5:A:479:ASP:OD2	5:A:536:THR:HG23	1.90	0.70
4:4:38:ARG:HH11	4:4:38:ARG:CG	2.02	0.70
19:A:1774:CLA:OBD	19:A:1784:CLA:H43	1.91	0.70
5:A:396:PHE:HE2	5:A:616:PHE:CB	2.04	0.70
6:B:172:GLU:HG3	6:B:301:ILE:HG13	1.72	0.70
19:B:1756:CLA:H72	19:B:1770:CLA:C3D	2.22	0.70
23:B:1774:PQN:H2M1	23:B:1774:PQN:H142	1.74	0.70
22:L:1170:BCR:C33	22:L:1170:BCR:HC8	2.22	0.70
4:4:75:TRP:CB	19:4:1205:CLA:HMD3	2.22	0.70
12:H:45:ALA:O	12:H:47:PHE:N	2.25	0.70
2:2:113:ILE:HG13	2:2:114:LEU:N	2.06	0.70
19:4:1200:CLA:CBC	19:4:1200:CLA:CMC	2.33	0.70
4:4:97:LEU:C	4:4:99:HIS:N	2.36	0.70
19:A:1779:CLA:HBB2	22:A:1804:BCR:C35	2.17	0.70
5:A:225:VAL:O	5:A:229:ILE:HB	1.90	0.70
5:A:454:GLY:N	5:A:457:SER:HB3	2.00	0.70
5:A:545:HIS:CE1	5:A:612:VAL:HG22	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:59:ALA:O	5:A:61:ALA:N	2.23	0.70
18:R:37:UNK:O	18:R:43:UNK:N	2.24	0.70
20:A:7016:LMU:H12	20:A:7016:LMU:O6'	1.90	0.70
19:1:1142:CLA:HMD1	19:K:1085:CLA:C4A	2.21	0.70
8:D:28:ILE:HG21	8:D:67:ILE:HG13	1.74	0.70
12:H:45:ALA:HB3	12:H:46:PRO:CD	2.21	0.70
19:L:1166:CLA:HED2	19:L:1166:CLA:HAA2	1.74	0.70
19:A:1782:CLA:HBD	19:A:1782:CLA:HBA1	1.72	0.70
5:A:470:LEU:HD13	6:B:95:HIS:HB3	1.72	0.70
6:B:174:ARG:NH1	19:B:1755:CLA:HMD1	2.07	0.70
19:B:1765:CLA:HMD2	19:B:1766:CLA:C1C	2.21	0.70
6:B:730:SER:C	6:B:731:GLY:O	2.29	0.70
9:E:42:GLU:HG2	9:E:43:SER:H	1.54	0.70
1:1:57:ILE:O	1:1:59:VAL:C	2.30	0.70
12:H:14:ILE:HG13	12:H:17:THR:OG1	1.92	0.70
6:B:369:ALA:O	6:B:725:LEU:CD1	2.38	0.70
3:3:163:PHE:O	3:3:164:PHE:HB2	1.91	0.70
1:1:179:THR:OG1	4:4:87:SER:OG	2.09	0.70
2:2:38:PRO:C	2:2:40:SER:OG	2.29	0.70
2:2:98:GLU:HG3	2:2:99:LEU:HG	1.73	0.70
19:4:1198:CLA:CAA	19:4:1198:CLA:CGD	2.70	0.70
4:4:31:ALA:O	4:4:32:GLU:C	2.30	0.70
5:A:385:LEU:O	5:A:386:ALA:CB	2.38	0.70
5:A:475:ASP:HB3	19:A:1789:CLA:HED3	1.73	0.70
6:B:568:CYS:O	6:B:570:ILE:N	2.25	0.70
6:B:612:SER:HA	6:B:615:TYR:CE1	2.21	0.70
9:E:34:SER:O	9:E:35:LYS:HB3	1.91	0.70
19:J:1044:CLA:H72	19:J:1044:CLA:H42	1.72	0.70
21:B:8059:SUC:C2	21:B:8059:SUC:O2'	2.35	0.70
6:B:607:SER:HA	6:B:610:ASN:HD22	1.57	0.70
12:H:10:ASP:HB3	12:H:13:ASP:HB2	1.72	0.70
10:F:116:GLN:C	10:F:118:GLU:H	1.92	0.70
5:A:723:ARG:NH1	5:A:723:ARG:HG2	2.06	0.70
19:B:1760:CLA:CMC	19:B:1760:CLA:HBC2	2.10	0.70
6:B:576:PHE:CE2	19:B:1760:CLA:HAC1	2.26	0.70
7:C:1:MET:CA	7:C:4:SER:OG	2.40	0.70
13:I:20:ALA:O	13:I:24:LEU:HB3	1.92	0.70
13:I:9:VAL:HG12	13:I:10:PRO:HD3	1.73	0.70
4:4:69:ILE:O	4:4:70:ILE:C	2.27	0.70
5:A:21:LEU:CD1	5:A:21:LEU:O	2.30	0.70
1:1:142:GLU:OE1	19:1:1187:CLA:C2D	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:195:ALA:HB1	2:2:197:LEU:HG	1.73	0.70
2:2:113:ILE:HG13	2:2:114:LEU:H	1.57	0.69
2:2:102:ILE:HG13	19:2:1223:CLA:HMD2	1.74	0.69
5:A:157:GLY:HA2	5:A:229:ILE:CG2	2.22	0.69
5:A:736:THR:HG21	19:A:1785:CLA:H91	1.74	0.69
6:B:293:THR:HG22	6:B:294:ASN:ND2	2.07	0.69
6:B:655:LEU:CD2	19:B:1772:CLA:CBB	2.69	0.69
13:I:7:LEU:HD12	22:I:1032:BCR:H333	0.89	0.69
5:A:141:ARG:HD3	10:F:39:ALA:HA	1.74	0.69
6:B:160:LYS:HZ3	6:B:160:LYS:HB2	1.56	0.69
5:A:164:LEU:HA	5:A:167:THR:HG23	1.73	0.69
22:B:1781:BCR:H17C	19:B:1787:CLA:C10	2.18	0.69
16:L:163:LEU:HB3	16:L:164:PRO:CD	2.11	0.69
22:3:1225:BCR:H23C	22:3:1225:BCR:H393	0.77	0.69
20:A:7043:LMU:O2B	20:A:7043:LMU:H5'	1.92	0.69
20:A:7022:LMU:O2'	20:A:7022:LMU:C5'	2.30	0.69
4:4:106:TRP:C	4:4:108:ASP:N	2.42	0.69
4:4:121:PHE:HD1	4:4:128:ALA:HB3	1.57	0.69
4:4:93:ILE:O	4:4:94:GLU:C	2.29	0.69
4:4:98:SER:C	4:4:102:GLU:OE1	2.30	0.69
5:A:308:ILE:HG13	19:A:1772:CLA:HBB1	1.74	0.69
19:A:1776:CLA:H61	22:A:1805:BCR:H19C	1.73	0.69
5:A:453:LEU:HD13	5:A:547:PHE:HA	1.74	0.69
5:A:685:VAL:HG12	5:A:741:GLY:HA2	1.74	0.69
9:E:90:VAL:O	9:E:91:ALA:C	2.30	0.69
20:A:7042:LMU:O6'	20:A:7042:LMU:H41	1.91	0.69
17:N:76:LYS:HG3	17:N:77:CYS:N	2.00	0.69
20:R:1056:LMU:O5B	20:R:1056:LMU:C6'	2.39	0.69
8:D:111:TYR:HD2	8:D:114:PRO:CB	2.05	0.69
7:C:44:ARG:HH22	8:D:127:ARG:NE	1.90	0.69
16:L:43:TYR:O	16:L:44:ARG:HB2	1.91	0.69
19:I:1241:CLA:C2C	22:I:1032:BCR:HC21	2.22	0.69
19:A:1811:CLA:CAD	19:A:1811:CLA:CED	2.70	0.69
5:A:370:ILE:HD12	19:A:1781:CLA:O1D	1.92	0.69
6:B:269:TRP:HE3	6:B:270:LEU:H	1.38	0.69
5:A:567:ARG:HH11	8:D:35:GLY:CA	2.02	0.69
20:R:1056:LMU:O6'	20:R:1056:LMU:C1'	2.40	0.69
12:H:53:LEU:CG	12:H:54:LEU:H	2.04	0.69
16:L:158:MET:CG	16:L:159:TYR:H	2.04	0.69
19:B:1750:CLA:HBB2	19:B:1755:CLA:H41	1.75	0.69
16:L:64:LEU:HA	16:L:67:PRO:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:34:UNK:C	18:R:38:UNK:CB	2.71	0.69
10:F:22:LEU:C	10:F:24:LYS:H	1.93	0.69
2:2:100:VAL:HG22	2:2:101:PHE:N	2.07	0.69
19:A:1796:CLA:H71	19:A:1812:CLA:H171	1.72	0.69
5:A:449:VAL:HG22	19:A:1794:CLA:HMC3	1.75	0.69
6:B:124:TRP:HE1	6:B:129:LEU:HD22	1.57	0.69
19:B:1756:CLA:HBC3	19:B:1756:CLA:HHD	1.74	0.69
10:F:15:ALA:O	10:F:18:GLU:HB2	1.92	0.69
10:F:47:GLU:HG3	10:F:51:LYS:CE	2.09	0.69
7:C:31:TRP:HB2	7:C:39:ILE:HG21	1.75	0.69
6:B:409:ALA:C	6:B:411:MET:H	1.96	0.69
4:4:121:PHE:O	4:4:143:PHE:HD2	1.74	0.69
4:4:81:GLU:HA	4:4:81:GLU:OE2	1.92	0.69
19:A:1764:CLA:C4	22:A:1806:BCR:H383	2.23	0.69
22:B:1780:BCR:H333	19:F:1156:CLA:HBB	1.74	0.69
6:B:25:ILE:HG21	22:L:1169:BCR:H292	0.70	0.69
6:B:336:LEU:HD13	19:B:1755:CLA:HBB1	1.75	0.69
7:C:78:GLY:O	7:C:81:TYR:CE1	2.42	0.69
10:F:21:ALA:O	10:F:22:LEU:C	2.28	0.69
21:B:8056:SUC:C3'	21:B:8056:SUC:O2	2.30	0.69
5:A:263:ALA:O	5:A:264:GLU:HG3	1.93	0.69
2:2:98:GLU:HG2	2:2:99:LEU:CD1	2.21	0.69
22:A:1806:BCR:H311	19:A:1812:CLA:H142	1.73	0.69
5:A:436:LEU:O	5:A:439:ARG:HB3	1.93	0.69
23:B:1774:PQN:H192	22:B:1781:BCR:C10	2.09	0.69
19:B:1787:CLA:H91	19:B:1788:CLA:C9	2.22	0.69
6:B:178:HIS:C	6:B:180:SER:H	1.94	0.69
6:B:438:VAL:O	6:B:441:ASP:N	2.26	0.69
11:G:62:ASP:HB2	11:G:63:PRO:HD3	1.73	0.69
4:4:121:PHE:CD1	4:4:143:PHE:CE2	2.81	0.69
5:A:615:HIS:CE1	19:A:1792:CLA:HBC3	2.28	0.69
6:B:124:TRP:HD1	6:B:124:TRP:O	1.76	0.69
22:B:1781:BCR:C23	22:B:1781:BCR:H382	2.11	0.69
6:B:692:ARG:HH22	6:B:694:ARG:HG2	1.57	0.69
7:C:2:SER:O	7:C:3:HIS:ND1	2.26	0.69
4:4:70:ILE:C	4:4:72:VAL:H	1.94	0.69
20:N:1086:LMU:H6E	20:N:1086:LMU:H51	0.72	0.69
3:3:52:LYS:C	3:3:56:TYR:CD2	2.65	0.69
19:J:1044:CLA:C9	19:J:1044:CLA:H152	2.22	0.69
20:A:7037:LMU:C1	20:A:7037:LMU:C6	2.71	0.69
6:B:404:ALA:C	6:B:406:ASN:N	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:12:ILE:HB	7:C:38:GLN:O	1.93	0.69
16:L:25:THR:O	16:L:28:THR:HB	1.92	0.69
6:B:242:HIS:O	6:B:243:LEU:HG	1.93	0.69
4:4:146:THR:O	4:4:146:THR:HG22	1.92	0.69
4:4:97:LEU:O	4:4:98:SER:C	2.31	0.69
6:B:292:ARG:NH2	6:B:297:ILE:HG13	2.07	0.69
7:C:55:GLU:C	7:C:57:ALA:H	1.96	0.69
8:D:102:ARG:NE	8:D:110:GLN:HB2	2.07	0.69
4:4:73:PRO:HB2	4:4:75:TRP:HB2	1.73	0.69
19:1:1014:CLA:CGD	19:1:1014:CLA:C2A	2.71	0.69
5:A:259:TYR:CD2	5:A:280:PHE:HA	2.28	0.69
16:L:113:SER:O	16:L:116:PRO:HD2	1.92	0.69
5:A:582:ASP:OD1	5:A:586:ARG:NH1	2.18	0.69
5:A:585:GLY:O	5:A:589:THR:OG1	2.11	0.69
2:2:100:VAL:HG22	2:2:101:PHE:H	1.56	0.69
19:A:1771:CLA:CED	19:A:1771:CLA:C2A	2.70	0.69
19:A:1810:CLA:HBC3	19:A:1810:CLA:HHD	1.75	0.69
5:A:390:ALA:HA	5:A:393:LEU:HD23	1.75	0.69
5:A:472:ARG:O	5:A:474:GLN:HG3	1.93	0.69
6:B:124:TRP:CD1	6:B:129:LEU:HD13	2.28	0.69
19:B:1763:CLA:H51	22:B:1780:BCR:H401	1.75	0.69
19:B:1739:CLA:CMC	22:B:1781:BCR:H282	2.22	0.69
6:B:561:GLY:HA3	7:C:52:LYS:CG	2.21	0.69
11:G:13:GLY:HA2	11:G:16:LEU:CG	2.23	0.69
3:3:97:PHE:CD2	3:3:97:PHE:N	2.59	0.69
17:N:55:GLN:O	17:N:56:LYS:CG	2.41	0.69
3:3:182:LYS:O	3:3:186:ASN:N	2.23	0.69
20:A:7016:LMU:C7	20:A:7016:LMU:C2	2.71	0.69
18:R:51:UNK:O	18:R:52:UNK:CB	2.41	0.69
20:A:7026:LMU:H3'	20:A:7026:LMU:H11	1.73	0.69
14:J:10:VAL:CG1	14:J:11:ALA:N	2.56	0.69
4:4:121:PHE:HZ	4:4:125:SER:O	1.76	0.68
19:A:1764:CLA:HMB1	19:A:1765:CLA:H11	1.75	0.68
19:B:1749:CLA:C3A	19:B:1749:CLA:CGA	2.70	0.68
19:B:1751:CLA:H2	19:B:1751:CLA:NB	2.08	0.68
19:B:1745:CLA:HMB3	22:B:1777:BCR:H311	1.73	0.68
11:G:28:ARG:HD2	11:G:33:LYS:HE2	1.75	0.68
10:F:52:ARG:NH1	10:F:55:ASN:OD1	2.26	0.68
6:B:468:GLY:O	6:B:470:THR:N	2.26	0.68
4:4:124:TYR:HB2	4:4:143:PHE:CD1	2.26	0.68
5:A:396:PHE:HE2	5:A:616:PHE:CG	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:347:LEU:HD13	6:B:351:HIS:HD1	1.58	0.68
7:C:65:VAL:HG12	7:C:66:ARG:H	1.57	0.68
17:N:67:LEU:CA	17:N:68:GLU:CG	2.70	0.68
19:R:1055:CLA:H91	20:R:1056:LMU:H4O1	1.58	0.68
19:3:1218:CLA:HAC2	19:3:1219:CLA:H91	1.75	0.68
12:H:32:TYR:OH	16:L:44:ARG:NE	2.18	0.68
2:2:51:HIS:O	2:2:54:TRP:HB2	1.94	0.68
4:4:128:ALA:H	4:4:143:PHE:HZ	1.36	0.68
4:4:169:GLN:HG2	19:4:1199:CLA:HAC2	1.75	0.68
19:A:1781:CLA:HBB2	19:A:1794:CLA:H3A	1.75	0.68
5:A:206:HIS:O	5:A:211:LEU:HD23	1.93	0.68
5:A:370:ILE:HG23	5:A:403:GLY:CA	2.22	0.68
6:B:188:LEU:HD11	19:B:1746:CLA:CBB	2.23	0.68
6:B:299:HIS:CE1	19:B:1753:CLA:HMD1	2.29	0.68
16:L:69:VAL:HG11	16:L:84:GLY:H	1.58	0.68
20:B:1783:LMU:C10	20:B:1783:LMU:H61	2.23	0.68
4:4:192:THR:HG21	4:4:195:GLN:CA	2.21	0.68
4:4:192:THR:CG2	4:4:195:GLN:H	1.99	0.68
5:A:269:PHE:CE1	15:K:14:THR:CG2	2.74	0.68
16:L:77:THR:HG21	16:L:82:ALA:HB1	1.74	0.68
20:A:7027:LMU:O2'	20:A:7027:LMU:C1	2.39	0.68
5:A:520:LEU:HD22	20:A:1808:LMU:O2'	1.92	0.68
4:4:36:ASN:C	4:4:39:TRP:CG	2.67	0.68
4:4:97:LEU:C	4:4:99:HIS:H	1.94	0.68
5:A:51:THR:CG2	19:A:1795:CLA:HBB2	2.18	0.68
5:A:206:HIS:C	5:A:211:LEU:HD23	2.14	0.68
5:A:408:VAL:HG11	5:A:602:LEU:HD23	1.75	0.68
6:B:711:VAL:CG1	6:B:711:VAL:O	2.42	0.68
24:B:1784:LMG:O3	7:C:70:TRP:NE1	2.26	0.68
13:I:10:PRO:HA	13:I:14:LEU:HB2	1.74	0.68
16:L:65:VAL:C	16:L:67:PRO:HD2	2.12	0.68
5:A:472:ARG:HH22	16:L:74:LEU:HD21	1.58	0.68
4:4:71:ASN:O	4:4:72:VAL:C	2.30	0.68
17:N:65:LEU:HD23	17:N:66:ASP:O	1.93	0.68
20:B:1783:LMU:C10	20:B:1783:LMU:C6	2.66	0.68
19:J:1044:CLA:H93	19:J:1044:CLA:H41	1.75	0.68
3:3:197:TYR:OH	19:3:1214:CLA:CHC	2.41	0.68
16:L:13:PRO:O	16:L:14:LEU:HB2	1.93	0.68
5:A:464:ASN:HD22	5:A:464:ASN:H	1.39	0.68
7:C:20:ALA:O	7:C:21:CYS:CB	2.41	0.68
5:A:170:GLY:O	5:A:173:VAL:CG2	2.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:174:PHE:CE2	19:A:1761:CLA:H152	2.27	0.68
19:A:1788:CLA:O1A	19:A:1799:CLA:C1	2.41	0.68
5:A:475:ASP:OD2	16:L:74:LEU:HA	1.93	0.68
5:A:620:MET:HG3	5:A:625:TRP:CE2	2.28	0.68
6:B:469:LYS:HE2	6:B:471:THR:OG1	1.93	0.68
10:F:95:GLY:O	10:F:99:TRP:HB2	1.93	0.68
19:1:1192:CLA:H61	19:1:1192:CLA:H122	1.76	0.68
17:N:40:CYS:N	17:N:41:LYS:HA	2.09	0.68
5:A:22:VAL:C	5:A:23:ASP:O	2.29	0.68
3:3:87:GLU:CB	22:3:1225:BCR:H382	2.22	0.68
5:A:720:THR:HG22	5:A:720:THR:O	1.93	0.68
4:4:117:GLN:O	4:4:122:LYS:C	2.31	0.68
19:A:1763:CLA:C3B	22:A:1807:BCR:H332	2.11	0.68
5:A:472:ARG:HH12	16:L:74:LEU:CG	1.96	0.68
19:B:1735:CLA:NC	19:B:1735:CLA:H52	2.09	0.68
19:B:1743:CLA:HAC1	19:B:1744:CLA:CBB	2.16	0.68
6:B:294:ASN:OD1	11:G:38:GLN:CA	2.37	0.68
6:B:696:LYS:HG2	7:C:80:ALA:HA	1.75	0.68
17:N:61:LEU:HD12	17:N:63:ASP:HB2	1.74	0.68
20:A:1809:LMU:O5B	20:A:1809:LMU:H5'	1.93	0.68
2:2:39:GLU:HA	2:2:40:SER:HB2	1.73	0.68
19:A:1782:CLA:H101	19:A:1782:CLA:H143	1.74	0.68
19:A:1781:CLA:H172	22:A:1804:BCR:H332	1.75	0.68
19:A:1811:CLA:HMB3	19:B:1786:CLA:C18	2.22	0.68
5:A:374:GLN:O	5:A:377:TYR:HD2	1.77	0.68
5:A:603:PHE:HZ	5:A:693:LEU:HD21	1.59	0.68
19:B:1763:CLA:HBB2	22:B:1779:BCR:C27	2.24	0.68
6:B:269:TRP:CD1	6:B:497:TRP:CH2	2.82	0.68
13:I:14:LEU:C	13:I:17:PRO:HD2	2.14	0.68
3:3:93:PHE:N	3:3:95:THR:H	1.89	0.68
3:3:181:LEU:CA	3:3:182:LYS:HG3	2.20	0.68
20:A:7016:LMU:H71	20:A:7016:LMU:C11	2.23	0.68
5:A:425:THR:O	5:A:427:ARG:NE	2.26	0.68
4:4:40:PHE:O	4:4:43:ALA:CB	2.29	0.68
5:A:158:ILE:HG22	19:A:1770:CLA:HED3	1.75	0.68
5:A:207:LEU:HA	5:A:211:LEU:CG	2.23	0.68
5:A:400:MET:O	5:A:609:ILE:HD12	1.94	0.68
5:A:88:ILE:HG22	5:A:89:ILE:N	2.09	0.68
6:B:697:PRO:HB3	19:B:1771:CLA:HBC3	1.76	0.68
6:B:273:VAL:O	6:B:277:HIS:HD2	1.75	0.68
6:B:388:ALA:C	6:B:391:PRO:CD	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:70:TRP:O	7:C:72:GLU:CB	2.41	0.68
9:E:53:VAL:O	9:E:55:VAL:N	2.25	0.68
11:G:12:THR:HG22	11:G:72:LEU:CD1	2.24	0.68
3:3:63:ARG:CZ	3:3:185:LYS:HG2	2.24	0.68
1:1:57:ILE:O	1:1:57:ILE:CD1	2.39	0.68
3:3:88:THR:N	22:3:1225:BCR:H383	2.09	0.68
15:K:4:GLY:HA2	15:K:7:THR:HB	1.75	0.68
4:4:164:LEU:O	4:4:167:ILE:N	2.27	0.68
4:4:36:ASN:OD1	4:4:39:TRP:CD1	2.47	0.68
19:A:1771:CLA:CBA	19:A:1771:CLA:HED2	2.24	0.68
5:A:244:LEU:HB2	5:A:247:GLU:HB2	1.76	0.68
5:A:309:LEU:O	5:A:310:PHE:HB2	1.93	0.68
5:A:624:VAL:O	5:A:636:HIS:HD2	1.75	0.68
19:B:1756:CLA:HED2	19:B:1757:CLA:HMD1	1.76	0.68
6:B:178:HIS:O	6:B:180:SER:N	2.27	0.68
6:B:595:HIS:CD2	6:B:623:TYR:OH	2.47	0.68
6:B:689:ASN:O	6:B:691:ILE:N	2.26	0.68
2:2:127:ASN:HB3	14:J:1:MET:O	1.94	0.68
3:3:93:PHE:H	3:3:95:THR:N	1.89	0.68
17:N:40:CYS:H	17:N:41:LYS:HA	1.58	0.68
19:3:1224:CLA:H143	19:3:1224:CLA:H102	1.76	0.68
10:F:25:LEU:HD23	10:F:46:MET:HB3	1.73	0.68
8:D:49:THR:HG22	8:D:99:GLN:HB3	1.75	0.68
17:N:33:TYR:O	17:N:34:THR:HG22	1.94	0.68
6:B:160:LYS:HE3	6:B:161:TRP:CD2	2.28	0.68
5:A:68:THR:C	5:A:70:ASP:H	1.97	0.68
5:A:131:ILE:HD13	6:B:446:PHE:C	2.14	0.68
19:A:1776:CLA:H162	19:A:1776:CLA:H111	1.76	0.68
6:B:46:ILE:HG21	19:B:1737:CLA:HBC3	1.74	0.68
19:B:1759:CLA:H101	22:B:1777:BCR:H343	1.76	0.68
6:B:187:SER:O	6:B:189:ALA:N	2.27	0.68
6:B:267:SER:HA	6:B:356:PRO:O	1.94	0.68
22:L:1170:BCR:C38	22:L:1170:BCR:H23C	2.24	0.68
3:3:92:TRP:CA	3:3:93:PHE:CG	2.74	0.68
19:1:1148:CLA:H2	19:1:1148:CLA:H72	1.76	0.68
21:B:8052:SUC:O4'	21:B:8052:SUC:H2	1.94	0.68
4:4:193:ILE:O	4:4:194:VAL:C	2.29	0.68
2:2:124:ILE:HB	2:2:129:LYS:HB3	1.74	0.67
4:4:147:LEU:HD22	4:4:148:GLU:CG	2.21	0.67
5:A:207:LEU:HB2	19:A:1776:CLA:HBB2	1.75	0.67
19:A:1811:CLA:C1	6:B:616:LEU:HG	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1796:CLA:H142	19:A:1812:CLA:H143	1.76	0.67
5:A:204:ASN:O	5:A:205:HIS:CB	2.36	0.67
5:A:618:TRP:O	5:A:622:SER:HB3	1.94	0.67
6:B:174:ARG:O	6:B:175:LEU:HB3	1.95	0.67
22:B:1782:BCR:C4	19:B:1788:CLA:H142	2.24	0.67
6:B:633:ASN:ND2	6:B:636:THR:HB	2.09	0.67
14:J:22:LEU:O	14:J:25:LEU:N	2.27	0.67
20:A:7041:LMU:O6B	20:A:7041:LMU:C1B	2.42	0.67
12:H:74:GLN:OE1	12:H:74:GLN:O	2.12	0.67
19:A:1785:CLA:H101	19:A:1785:CLA:H152	1.76	0.67
19:A:1811:CLA:C3B	6:B:589:TRP:CH2	2.77	0.67
6:B:141:PHE:HD2	6:B:144:PHE:CE1	2.12	0.67
19:B:1754:CLA:H42	19:B:1754:CLA:CHB	2.23	0.67
22:B:1781:BCR:C20	19:B:1787:CLA:H151	2.24	0.67
6:B:347:LEU:HD21	6:B:351:HIS:HE1	1.59	0.67
7:C:73:THR:N	7:C:76:SER:OG	2.27	0.67
7:C:75:ARG:HH22	8:D:110:GLN:CD	1.96	0.67
11:G:28:ARG:NH2	11:G:29:GLU:O	2.28	0.67
3:3:50:GLU:O	3:3:53:TRP:N	2.27	0.67
20:A:7020:LMU:O2'	20:A:7020:LMU:H5'	1.92	0.67
8:D:28:ILE:CG2	8:D:67:ILE:HG13	2.25	0.67
6:B:140:ILE:HD13	6:B:140:ILE:H	1.59	0.67
4:4:37:LEU:CA	4:4:39:TRP:CG	2.77	0.67
5:A:118:PRO:HB3	5:A:150:PHE:CE2	2.29	0.67
19:A:1794:CLA:CMC	19:A:1794:CLA:HBC3	2.21	0.67
5:A:154:ARG:HH21	5:A:233:LEU:HD13	1.58	0.67
5:A:390:ALA:HA	5:A:393:LEU:CD2	2.24	0.67
5:A:680:LEU:HD21	6:B:617:MET:CE	2.24	0.67
23:A:1801:PQN:H142	22:B:1779:BCR:HC22	1.75	0.67
6:B:450:GLU:O	6:B:452:GLN:N	2.25	0.67
5:A:705:GLU:HB3	6:B:545:LYS:HZ1	1.58	0.67
6:B:598:HIS:HB3	6:B:602:TRP:CZ3	2.30	0.67
6:B:649:MET:O	6:B:653:GLY:N	2.26	0.67
6:B:552:ASP:HA	8:D:144:ILE:HG22	1.76	0.67
19:A:1799:CLA:H152	22:L:1170:BCR:H352	1.76	0.67
4:4:70:ILE:O	4:4:72:VAL:N	2.27	0.67
3:3:92:TRP:HZ2	5:A:250:LEU:HB2	1.60	0.67
17:N:44:GLU:O	17:N:46:PHE:N	2.27	0.67
17:N:62:SER:HB2	17:N:66:ASP:OD1	1.94	0.67
17:N:18:ASP:HB2	17:N:22:LEU:CD1	2.23	0.67
12:H:63:SER:O	12:H:67:TYR:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:97:VAL:O	2:2:100:VAL:HG13	1.94	0.67
19:A:1791:CLA:C2A	19:A:1797:CLA:HBB1	2.25	0.67
6:B:30:ASP:OD2	6:B:396:ARG:NH1	2.26	0.67
6:B:398:TYR:HD1	6:B:542:ARG:NH2	1.91	0.67
19:1:1148:CLA:O1A	19:1:1148:CLA:HED3	1.94	0.67
5:A:25:ASP:N	5:A:26:PRO:CD	2.56	0.67
20:A:7022:LMU:H1B	20:A:7022:LMU:O2'	1.95	0.67
8:D:60:MET:HG3	8:D:61:PRO:O	1.94	0.67
20:A:7005:LMU:H32	20:A:7005:LMU:H71	1.77	0.67
12:H:54:LEU:HD13	12:H:55:LYS:HG3	1.76	0.67
19:A:1782:CLA:HBC2	19:A:1782:CLA:CMC	2.16	0.67
19:A:1783:CLA:H202	22:A:1807:BCR:C15	2.24	0.67
19:B:1748:CLA:CAD	19:B:1757:CLA:CBB	2.71	0.67
19:B:1788:CLA:HHB	19:B:1788:CLA:C4	2.23	0.67
8:D:39:LYS:CD	8:D:42:VAL:CG1	2.72	0.67
16:L:60:HIS:HD2	19:L:1167:CLA:HED1	1.57	0.67
17:N:61:LEU:HD12	17:N:62:SER:O	1.92	0.67
19:1:1014:CLA:HAA2	19:1:1014:CLA:CBD	2.25	0.67
19:1:1014:CLA:CHA	19:1:1014:CLA:CED	2.72	0.67
1:1:64:GLY:C	1:1:66:GLY:O	2.33	0.67
20:A:7021:LMU:O6'	20:A:7021:LMU:H12	1.94	0.67
2:2:98:GLU:HG2	2:2:99:LEU:HD11	1.76	0.67
19:B:1765:CLA:HMB3	19:B:1768:CLA:HED3	1.77	0.67
11:G:28:ARG:HG2	11:G:29:GLU:H	1.56	0.67
11:G:49:THR:OG1	11:G:50:ARG:N	2.28	0.67
4:4:194:VAL:CA	4:4:195:GLN:C	2.61	0.67
8:D:126:GLY:C	8:D:127:ARG:HG2	2.14	0.67
19:1:1241:CLA:CAC	22:I:1032:BCR:C2	2.71	0.67
2:2:127:ASN:OD1	14:J:2:ARG:HA	1.93	0.67
4:4:118:ASP:N	4:4:118:ASP:OD1	2.27	0.67
4:4:88:SER:C	4:4:90:LEU:HD22	2.14	0.67
19:A:1764:CLA:H43	22:A:1806:BCR:H383	1.77	0.67
19:A:1782:CLA:CBD	19:A:1782:CLA:HBA1	2.25	0.67
19:A:1793:CLA:H11	19:A:1793:CLA:ND	2.10	0.67
5:A:270:PHE:CZ	19:A:1797:CLA:O2A	2.47	0.67
22:B:1781:BCR:C33	22:B:1781:BCR:HC8	2.24	0.67
6:B:349:ALA:HB2	6:B:375:HIS:HB3	1.77	0.67
10:F:140:ALA:O	10:F:144:LEU:HB3	1.95	0.67
19:1:1188:CLA:O2D	19:1:1188:CLA:CBA	2.38	0.67
20:N:1086:LMU:H32	20:N:1086:LMU:C5'	2.24	0.67
19:K:1085:CLA:O2A	19:K:1085:CLA:H43	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:74:ALA:CA	19:3:1217:CLA:C1D	2.70	0.67
16:L:108:LYS:O	16:L:132:SER:CB	2.40	0.67
17:N:2:VAL:O	17:N:2:VAL:HG23	1.95	0.67
2:2:189:ILE:HD13	2:2:189:ILE:H	1.58	0.67
12:H:67:TYR:O	12:H:70:ALA:O	2.13	0.67
6:B:426:SER:O	6:B:430:GLY:N	2.26	0.67
15:K:31:ASN:H	15:K:32:ARG:HH11	1.39	0.67
4:4:106:TRP:O	4:4:108:ASP:N	2.28	0.67
19:4:1198:CLA:HAA2	19:4:1198:CLA:HED3	0.72	0.67
4:4:34:PRO:CB	4:4:35:GLU:OE1	2.43	0.67
5:A:107:GLU:OE1	5:A:161:GLU:CG	2.43	0.67
5:A:203:LEU:H	5:A:203:LEU:HD12	1.59	0.67
5:A:618:TRP:CZ2	5:A:655:ASP:CB	2.77	0.67
6:B:127:ILE:CD1	6:B:193:HIS:CE1	2.78	0.67
19:B:1743:CLA:HAC2	19:B:1744:CLA:HBB2	0.67	0.67
22:B:1781:BCR:H19C	19:B:1787:CLA:C15	2.22	0.67
7:C:60:THR:CG2	7:C:63:LEU:O	2.43	0.67
10:F:123:VAL:HB	10:F:126:ALA:C	2.15	0.67
20:B:1783:LMU:H111	20:B:1783:LMU:H72	1.77	0.67
3:3:47:GLY:O	3:3:49:ILE:N	2.27	0.67
19:1:1145:CLA:C2	19:1:1145:CLA:HMA2	2.19	0.67
12:H:30:SER:O	12:H:31:PRO:O	2.11	0.67
2:2:102:ILE:HD11	19:2:1223:CLA:HMD1	1.76	0.67
4:4:101:VAL:O	4:4:104:ARG:HB3	1.94	0.67
4:4:121:PHE:CZ	4:4:125:SER:O	2.48	0.67
19:A:1781:CLA:O1A	19:A:1781:CLA:C2	2.41	0.67
5:A:207:LEU:CD2	5:A:314:GLY:HA2	2.25	0.67
6:B:646:TRP:CH2	6:B:726:ILE:HD13	2.29	0.67
7:C:66:ARG:NH2	7:C:66:ARG:HG2	1.95	0.67
22:I:1032:BCR:H311	22:I:1032:BCR:C8	2.22	0.67
3:3:63:ARG:NH1	3:3:185:LYS:O	2.28	0.67
19:1:1149:CLA:CBA	19:1:1149:CLA:O1D	2.43	0.67
3:3:107:TRP:CD1	3:3:108:ALA:CA	2.77	0.67
2:2:189:ILE:O	2:2:190:ASP:HB3	1.95	0.67
6:B:98:GLN:O	6:B:100:ALA:N	2.28	0.67
4:4:169:GLN:CD	19:4:1199:CLA:HHD	2.14	0.67
19:A:1785:CLA:C10	19:A:1785:CLA:H152	2.25	0.67
5:A:692:PHE:CZ	19:A:1796:CLA:HBC3	2.29	0.67
5:A:217:SER:HA	22:A:1802:BCR:C35	2.23	0.67
19:F:1157:CLA:CED	19:F:1157:CLA:CAD	2.73	0.67
3:3:173:GLU:CG	3:3:174:LYS:N	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:629:ASN:HD21	5:A:633:VAL:HG23	1.59	0.67
1:1:179:THR:HG21	4:4:87:SER:O	1.94	0.66
2:2:102:ILE:C	19:2:1222:CLA:CBB	2.55	0.66
4:4:36:ASN:CA	4:4:39:TRP:CE3	2.78	0.66
19:A:1771:CLA:HBB1	22:A:1802:BCR:H352	1.76	0.66
19:A:1810:CLA:HBC3	19:A:1810:CLA:CHD	2.25	0.66
19:B:1756:CLA:CAD	19:B:1768:CLA:HBB1	2.25	0.66
19:B:1772:CLA:C19	13:I:21:MET:CB	2.72	0.66
7:C:66:ARG:HH21	7:C:66:ARG:CG	2.03	0.66
9:E:87:VAL:O	9:E:89:GLU:N	2.27	0.66
10:F:130:LEU:HD12	10:F:131:PHE:HD1	1.60	0.66
10:F:130:LEU:HD12	10:F:131:PHE:CD1	2.30	0.66
3:3:97:PHE:O	3:3:98:ILE:HG23	1.95	0.66
21:B:8052:SUC:O4'	21:B:8052:SUC:C2	2.42	0.66
19:K:1085:CLA:O2A	19:K:1085:CLA:C4	2.42	0.66
5:A:27:ILE:C	5:A:27:ILE:CD1	2.63	0.66
3:3:106:TYR:CG	3:3:107:TRP:CD1	2.84	0.66
19:4:1200:CLA:HBD	19:4:1200:CLA:HAA2	1.77	0.66
5:A:114:THR:CG2	5:A:115:HIS:CE1	2.75	0.66
19:A:1771:CLA:O1A	19:A:1771:CLA:NA	2.28	0.66
19:A:1811:CLA:H122	19:A:1811:CLA:H92	1.77	0.66
5:A:397:THR:HB	5:A:613:ILE:CD1	2.26	0.66
5:A:708:VAL:HA	5:A:711:HIS:CD2	2.30	0.66
6:B:292:ARG:NH2	6:B:297:ILE:H	1.93	0.66
6:B:418:ILE:O	6:B:422:LEU:HD12	1.94	0.66
6:B:576:PHE:HE2	19:B:1760:CLA:HAC1	1.58	0.66
7:C:55:GLU:O	7:C:57:ALA:N	2.21	0.66
19:1:1308:CLA:HBC2	19:1:1308:CLA:CMC	2.23	0.66
6:B:247:THR:CG2	6:B:250:ALA:HB3	2.25	0.66
6:B:154:TRP:HD1	6:B:158:GLN:HG2	1.59	0.66
5:A:160:SER:HB2	5:A:163:GLN:OE1	1.96	0.66
5:A:98:PHE:O	5:A:99:HIS:HB2	1.94	0.66
6:B:127:ILE:CD1	6:B:193:HIS:HE1	2.08	0.66
19:B:1735:CLA:H191	10:F:104:TYR:CB	2.22	0.66
9:E:89:GLU:HG2	9:E:92:ALA:H	1.60	0.66
10:F:104:TYR:O	10:F:104:TYR:CD2	2.47	0.66
16:L:99:LEU:HD11	22:L:1169:BCR:C31	2.26	0.66
1:1:25:ASP:HB3	1:1:26:PRO:HD2	1.77	0.66
17:N:65:LEU:O	17:N:67:LEU:N	2.29	0.66
17:N:80:ASN:OD1	17:N:82:PHE:HA	1.95	0.66
7:C:14:CYS:O	7:C:14:CYS:SG	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:22:VAL:CG1	5:A:23:ASP:H	2.08	0.66
5:A:631:GLN:HG3	5:A:631:GLN:O	1.96	0.66
21:B:8061:SUC:H1'2	21:B:8061:SUC:O5	1.94	0.66
4:4:108:ASP:C	4:4:108:ASP:OD2	2.30	0.66
4:4:34:PRO:CA	4:4:35:GLU:OE1	2.44	0.66
4:4:93:ILE:O	4:4:95:PHE:N	2.27	0.66
5:A:173:VAL:HG23	5:A:174:PHE:HD1	1.61	0.66
19:A:1811:CLA:H11	6:B:616:LEU:CG	2.23	0.66
5:A:42:ARG:C	5:A:44:ILE:H	1.98	0.66
5:A:458:PHE:CD2	19:B:1787:CLA:CMB	2.78	0.66
5:A:660:GLN:O	5:A:661:ALA:CB	2.42	0.66
6:B:141:PHE:HA	6:B:144:PHE:CD1	2.31	0.66
19:B:1747:CLA:CHD	19:B:1747:CLA:CBC	2.74	0.66
6:B:530:THR:HG22	19:B:1756:CLA:HMC1	1.76	0.66
6:B:81:PRO:HG2	6:B:360:PHE:CD1	2.30	0.66
6:B:414:HIS:O	6:B:414:HIS:CG	2.49	0.66
8:D:44:GLU:CB	8:D:46:TYR:HE2	2.04	0.66
10:F:80:TRP:HZ3	19:F:1156:CLA:CMC	2.08	0.66
19:A:1788:CLA:C15	22:L:1169:BCR:C36	2.74	0.66
16:L:99:LEU:HD11	22:L:1169:BCR:HC7	1.76	0.66
17:N:45:ASN:HD21	17:N:54:LYS:HB2	1.51	0.66
17:N:81:VAL:O	17:N:83:TRP:N	2.29	0.66
5:A:129:GLN:O	5:A:130:GLU:HB2	1.95	0.66
5:A:123:VAL:HG22	5:A:133:ASN:OD1	1.94	0.66
5:A:229:ILE:CG1	5:A:243:PRO:HB3	2.25	0.66
5:A:578:ARG:O	5:A:579:PHE:CD1	2.49	0.66
19:B:1744:CLA:CBC	19:B:1744:CLA:HMC1	2.22	0.66
19:B:1736:CLA:HBC3	19:B:1760:CLA:H51	1.77	0.66
13:I:14:LEU:O	13:I:17:PRO:HD2	1.95	0.66
4:4:69:ILE:O	4:4:71:ASN:N	2.29	0.66
5:A:269:PHE:HE1	15:K:14:THR:CG2	2.09	0.66
12:H:44:ALA:HB2	16:L:145:PHE:CE1	2.29	0.66
20:A:7031:LMU:H4'	20:A:7031:LMU:O2B	1.94	0.66
19:A:1776:CLA:CBC	19:A:1776:CLA:HMC1	2.24	0.66
19:A:1777:CLA:H2A	19:A:1777:CLA:O1D	1.95	0.66
5:A:711:HIS:CG	19:A:1795:CLA:HBC1	2.30	0.66
19:A:1811:CLA:HED1	19:B:1786:CLA:H61	1.77	0.66
5:A:432:LEU:HA	5:A:435:VAL:HG13	1.78	0.66
11:G:23:PHE:CD2	11:G:24:PHE:HB2	2.31	0.66
1:1:27:LEU:HD21	6:B:314:ARG:HD3	1.75	0.66
20:A:7042:LMU:O6'	20:A:7042:LMU:H32	1.91	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:82:PHE:O	17:N:84:LYS:N	2.29	0.66
19:1:1014:CLA:HBD	19:1:1014:CLA:HAA2	1.76	0.66
20:A:7016:LMU:H112	20:A:7016:LMU:H71	1.78	0.66
19:1:1308:CLA:H2	19:1:1308:CLA:HMA2	1.76	0.66
20:A:7026:LMU:C4	20:A:7026:LMU:C8	2.65	0.66
2:2:171:MET:SD	2:2:172:LEU:HA	2.36	0.66
4:4:86:SER:O	4:4:88:SER:N	2.29	0.66
19:B:1740:CLA:H12	19:B:1740:CLA:HAA1	1.76	0.66
6:B:510:LEU:HD21	19:B:1768:CLA:HHD	1.77	0.66
6:B:349:ALA:CB	6:B:375:HIS:HB3	2.26	0.66
7:C:74:THR:O	7:C:76:SER:N	2.29	0.66
8:D:39:LYS:NZ	8:D:43:GLU:OE2	2.28	0.66
9:E:89:GLU:O	9:E:90:VAL:HB	1.96	0.66
10:F:131:PHE:HE1	21:F:1158:SUC:HO3'	1.37	0.66
11:G:60:SER:HG	11:G:63:PRO:HB2	1.58	0.66
14:J:2:ARG:NH1	14:J:8:LEU:HD13	2.04	0.66
16:L:64:LEU:HD22	16:L:91:LEU:HD22	1.78	0.66
17:N:62:SER:HB3	17:N:66:ASP:OD1	1.89	0.66
19:K:1085:CLA:C3A	19:K:1085:CLA:CGA	2.73	0.66
19:K:1085:CLA:C3A	19:K:1085:CLA:O1A	2.32	0.66
21:B:8055:SUC:H1'1	21:B:8055:SUC:O6'	1.91	0.66
20:A:7026:LMU:H52	20:A:7026:LMU:C1	2.22	0.66
5:A:255:LEU:CD1	5:A:280:PHE:HZ	2.09	0.66
16:L:10:VAL:O	16:L:10:VAL:CG2	2.44	0.66
5:A:539:PHE:HD2	5:A:539:PHE:O	1.78	0.66
2:2:103:GLY:CA	19:2:1222:CLA:CBB	2.72	0.66
4:4:145:PRO:O	4:4:147:LEU:N	2.29	0.66
19:A:1760:CLA:HBC3	19:A:1760:CLA:HHD	1.76	0.66
19:A:1790:CLA:O1A	19:A:1791:CLA:HBC3	1.96	0.66
5:A:606:TYR:O	5:A:610:SER:CB	2.43	0.66
6:B:124:TRP:CD1	6:B:124:TRP:O	2.48	0.66
19:B:1740:CLA:H91	22:B:1782:BCR:H361	1.76	0.66
16:L:69:VAL:HG11	16:L:84:GLY:N	2.10	0.66
17:N:61:LEU:O	17:N:62:SER:HB2	1.93	0.66
19:1:1014:CLA:HAA2	19:1:1014:CLA:CGD	2.26	0.66
11:G:93:TYR:N	11:G:94:ASP:OD1	2.28	0.66
19:1:1146:CLA:H2A	19:1:1146:CLA:O1A	1.95	0.66
10:F:22:LEU:O	10:F:25:LEU:N	2.29	0.66
6:B:247:THR:HG23	6:B:250:ALA:HB3	1.77	0.66
20:A:7038:LMU:H1B	20:A:7038:LMU:C6'	2.26	0.66
2:2:42:ARG:CB	2:2:45:VAL:HG21	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:93:THR:O	2:2:97:VAL:HG22	1.95	0.66
4:4:144:ALA:C	4:4:145:PRO:O	2.29	0.66
4:4:151:GLU:C	4:4:154:ILE:N	2.38	0.66
5:A:58:HIS:HB3	19:A:1760:CLA:HBC1	1.77	0.66
19:A:1777:CLA:HBC3	19:A:1779:CLA:HED1	1.77	0.66
19:A:1781:CLA:C4B	22:A:1805:BCR:C37	2.66	0.66
5:A:636:HIS:O	5:A:638:THR:N	2.29	0.66
19:B:1757:CLA:HED1	19:B:1765:CLA:HBB1	1.76	0.66
19:B:1760:CLA:CMC	19:B:1760:CLA:CBC	2.56	0.66
19:B:1757:CLA:H71	22:B:1778:BCR:H14C	1.77	0.66
6:B:203:ARG:H	6:B:270:LEU:HD11	1.61	0.66
5:A:128:GLY:HA3	6:B:446:PHE:CD2	2.31	0.66
11:G:24:PHE:CE1	11:G:27:GLN:O	2.49	0.66
17:N:49:CYS:C	17:N:51:ASP:O	2.34	0.66
20:A:7037:LMU:H121	20:A:7051:LMU:H32	1.76	0.66
19:4:4007:CLA:HED1	19:4:4007:CLA:C1	2.11	0.66
2:2:106:GLU:O	19:2:1222:CLA:HMA3	1.95	0.66
2:2:43:TRP:O	2:2:44:ASN:C	2.30	0.66
4:4:150:LYS:CG	4:4:150:LYS:O	2.41	0.66
5:A:101:ALA:O	5:A:104:SER:HA	1.96	0.66
6:B:55:ALA:HB1	6:B:150:LEU:CD1	2.26	0.66
7:C:74:THR:O	7:C:75:ARG:C	2.30	0.66
11:G:13:GLY:O	11:G:16:LEU:CB	2.44	0.66
11:G:28:ARG:HH21	11:G:29:GLU:H	1.44	0.66
17:N:70:GLU:HB3	17:N:72:LYS:CA	2.26	0.66
19:J:1044:CLA:C4A	19:J:1044:CLA:HBA2	2.25	0.66
10:F:22:LEU:O	10:F:24:LYS:N	2.29	0.66
1:1:57:ILE:O	1:1:59:VAL:N	2.28	0.66
19:R:1054:CLA:H2A	19:R:1054:CLA:O1A	1.94	0.66
8:D:101:TYR:CD1	8:D:114:PRO:HD3	2.31	0.66
4:4:101:VAL:O	4:4:104:ARG:CZ	2.45	0.65
19:A:1776:CLA:H8	22:A:1805:BCR:H19C	1.76	0.65
5:A:353:SER:HB2	5:A:356:ALA:HB3	1.78	0.65
5:A:625:TRP:HB2	5:A:637:ILE:HD11	1.78	0.65
5:A:645:SER:HB3	6:B:637:PRO:HG3	1.77	0.65
19:B:1788:CLA:HED3	19:B:1788:CLA:CBA	2.27	0.65
6:B:292:ARG:HH22	6:B:297:ILE:HG13	1.60	0.65
6:B:538:ALA:O	6:B:540:ASP:N	2.29	0.65
6:B:73:ASN:HB3	6:B:76:ALA:HB3	1.76	0.65
13:I:12:VAL:CG2	19:I:1031:CLA:O1A	2.42	0.65
22:I:1032:BCR:C27	22:I:1032:BCR:H403	2.20	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:71:ASN:O	4:4:73:PRO:N	2.28	0.65
17:N:58:VAL:O	17:N:60:PHE:N	2.29	0.65
18:R:36:UNK:O	18:R:38:UNK:N	2.29	0.65
20:A:7048:LMU:O5'	20:A:7048:LMU:C2	2.30	0.65
5:A:23:ASP:OD2	5:A:24:ARG:N	2.29	0.65
5:A:23:ASP:OD1	5:A:24:ARG:NE	2.29	0.65
5:A:25:ASP:O	5:A:26:PRO:C	2.29	0.65
20:A:7037:LMU:C1	20:A:7037:LMU:H61	2.25	0.65
10:F:21:ALA:O	10:F:23:LYS:N	2.29	0.65
20:A:7050:LMU:C4	20:A:7050:LMU:H92	2.18	0.65
14:J:10:VAL:HG13	14:J:11:ALA:H	1.59	0.65
4:4:36:ASN:C	4:4:39:TRP:CD2	2.69	0.65
4:4:52:MET:HE1	4:4:156:ASN:HB2	1.77	0.65
4:4:91:PHE:CG	4:4:92:VAL:N	2.60	0.65
5:A:664:VAL:CG2	5:A:665:ILE:HG23	2.26	0.65
6:B:708:VAL:O	6:B:710:LEU:O	2.15	0.65
6:B:366:THR:HG23	6:B:729:THR:HG22	1.78	0.65
7:C:7:ILE:HG22	7:C:65:VAL:HG21	1.76	0.65
14:J:2:ARG:HH12	14:J:8:LEU:CD1	2.04	0.65
16:L:63:LEU:CD2	16:L:64:LEU:H	2.08	0.65
4:4:69:ILE:CG1	4:4:175:LYS:HB2	2.26	0.65
17:N:54:LYS:O	17:N:57:LYS:N	2.29	0.65
17:N:69:CYS:O	17:N:72:LYS:CE	2.44	0.65
19:1:1145:CLA:C6	19:1:1145:CLA:CMA	2.69	0.65
19:2:1212:CLA:NA	19:2:1212:CLA:O1A	2.29	0.65
2:2:143:PHE:HD1	2:2:144:ASP:N	1.95	0.65
4:4:92:VAL:HG12	4:4:93:ILE:H	1.60	0.65
5:A:187:HIS:CD2	19:A:1767:CLA:C4C	2.79	0.65
5:A:390:ALA:HB1	5:A:754:ILE:HD13	1.79	0.65
5:A:362:LEU:CB	5:A:410:ALA:HB2	2.26	0.65
7:C:79:LEU:CD2	7:C:81:TYR:C	2.65	0.65
16:L:128:ASP:OD2	16:L:129:GLN:N	2.28	0.65
3:3:93:PHE:HD2	3:3:95:THR:H	1.41	0.65
17:N:80:ASN:OD1	17:N:82:PHE:N	2.30	0.65
3:3:52:LYS:O	3:3:56:TYR:CG	2.50	0.65
5:A:22:VAL:N	5:A:23:ASP:O	2.30	0.65
15:K:59:ASP:OD1	15:K:59:ASP:C	2.34	0.65
2:2:41:LEU:O	2:2:42:ARG:NE	2.28	0.65
19:A:1764:CLA:HMC3	19:A:1765:CLA:HHD	1.76	0.65
5:A:370:ILE:HD13	19:A:1781:CLA:CAD	2.26	0.65
19:A:1784:CLA:CHD	22:A:1803:BCR:H333	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1781:CLA:C3B	22:A:1805:BCR:H373	2.27	0.65
5:A:697:ARG:HD3	6:B:566:GLY:O	1.97	0.65
6:B:388:ALA:O	6:B:391:PRO:HD2	1.95	0.65
7:C:1:MET:CG	7:C:4:SER:HG	2.02	0.65
8:D:102:ARG:HE	8:D:110:GLN:CB	2.08	0.65
9:E:65:VAL:HG13	9:E:82:TYR:O	1.96	0.65
10:F:147:GLY:HA2	10:F:150:VAL:HB	1.79	0.65
11:G:16:LEU:HA	11:G:68:ILE:HG13	1.77	0.65
21:3:1226:SUC:O1'	21:3:1226:SUC:H4'	1.95	0.65
4:4:58:MET:SD	4:4:59:LEU:HA	2.36	0.65
3:3:163:PHE:C	3:3:163:PHE:HD1	1.99	0.65
17:N:24:THR:O	17:N:26:GLY:N	2.29	0.65
5:A:109:TRP:HA	5:A:116:ILE:HG13	1.78	0.65
19:A:1776:CLA:HMD1	19:A:1777:CLA:HHD	1.79	0.65
5:A:732:ALA:HB1	19:A:1796:CLA:HED2	1.79	0.65
5:A:328:LYS:O	5:A:330:ILE:N	2.30	0.65
6:B:171:ALA:O	6:B:172:GLU:HB2	1.97	0.65
6:B:663:PHE:O	6:B:664:LEU:CB	2.34	0.65
10:F:123:VAL:HB	10:F:126:ALA:O	1.97	0.65
18:R:38:UNK:C	18:R:39:UNK:O	2.43	0.65
20:A:7033:LMU:C3'	20:A:7033:LMU:O6B	2.44	0.65
1:1:59:VAL:CG1	1:1:60:PRO:HD2	2.26	0.65
19:1:1196:CLA:OBD	19:1:1196:CLA:HMD1	1.95	0.65
10:F:151:ASP:C	10:F:154:PHE:HB3	2.16	0.65
16:L:13:PRO:HG2	16:L:18:PRO:HB3	1.77	0.65
15:K:27:ALA:HB3	15:K:28:PRO:CD	2.25	0.65
11:G:83:TYR:O	11:G:83:TYR:CG	2.48	0.65
2:2:42:ARG:O	2:2:44:ASN:N	2.29	0.65
4:4:30:LEU:HD13	20:4:1212:LMU:C12	2.25	0.65
19:A:1811:CLA:H152	19:A:1811:CLA:H91	1.77	0.65
6:B:119:GLY:O	6:B:121:TYR:N	2.29	0.65
6:B:646:TRP:CH2	6:B:726:ILE:HG21	2.32	0.65
7:C:1:MET:N	7:C:4:SER:CB	2.60	0.65
10:F:62:LEU:CG	10:F:72:ILE:HD13	2.25	0.65
11:G:16:LEU:HD23	11:G:68:ILE:HG21	1.79	0.65
2:2:205:PHE:HD1	2:2:206:ALA:H	0.67	0.65
20:A:7048:LMU:C9	20:A:7048:LMU:C4	2.67	0.65
15:K:20:PHE:HD2	15:K:21:ALA:CA	2.08	0.65
3:3:107:TRP:CD1	3:3:108:ALA:HA	2.32	0.65
6:B:324:ASP:O	6:B:328:ASN:HB2	1.96	0.65
2:2:161:THR:HB	2:2:165:LYS:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:43:TRP:O	2:2:45:VAL:N	2.29	0.65
4:4:88:SER:C	4:4:89:THR:HG22	2.17	0.65
19:A:1771:CLA:CBB	22:A:1802:BCR:H352	2.27	0.65
5:A:362:LEU:HD11	19:A:1785:CLA:HBB2	1.78	0.65
5:A:618:TRP:CH2	5:A:655:ASP:HB2	2.32	0.65
5:A:679:PHE:CE2	5:A:683:HIS:HD2	2.14	0.65
22:B:1780:BCR:H333	19:F:1156:CLA:HMA1	1.78	0.65
9:E:40:ARG:HB2	9:E:42:GLU:OE2	1.97	0.65
14:J:4:PHE:O	14:J:5:LYS:HB2	1.95	0.65
16:L:40:LEU:HB3	16:L:41:PRO:CD	2.27	0.65
19:1:1014:CLA:C4A	19:1:1014:CLA:HED3	2.26	0.65
20:A:7033:LMU:H3'	20:A:7033:LMU:O5B	1.78	0.65
19:3:1217:CLA:HHC	19:3:1222:CLA:H11	1.79	0.65
6:B:247:THR:C	6:B:250:ALA:HB2	2.16	0.65
14:J:10:VAL:HG13	14:J:11:ALA:N	2.12	0.65
10:F:42:ILE:C	10:F:43:LYS:HE3	2.17	0.65
1:1:161:PHE:N	19:1:1189:CLA:HBB2	2.12	0.65
2:2:81:THR:O	2:2:83:GLY:N	2.30	0.65
12:H:63:SER:O	12:H:67:TYR:CB	2.45	0.65
6:B:62:SER:OG	6:B:63:GLY:N	2.29	0.65
2:2:110:TRP:CA	2:2:113:ILE:HG23	2.25	0.65
19:2:1213:CLA:HBC2	19:2:1213:CLA:CHD	2.22	0.65
19:A:1790:CLA:CAD	19:A:1791:CLA:HAC1	2.26	0.65
5:A:705:GLU:HA	5:A:708:VAL:HB	1.79	0.65
5:A:393:LEU:HD11	5:A:750:PHE:CD1	2.31	0.65
19:B:1735:CLA:CBC	22:B:1779:BCR:H332	2.27	0.65
19:B:1737:CLA:H121	19:B:1744:CLA:OBD	1.95	0.65
19:B:1756:CLA:HBB1	19:B:1770:CLA:HBB	1.79	0.65
19:B:1763:CLA:HBB2	22:B:1779:BCR:C26	2.26	0.65
2:2:203:THR:HG23	2:2:204:ILE:N	2.12	0.65
4:4:136:GLY:O	4:4:137:ILE:HB	1.96	0.65
2:2:120:ASN:OD1	2:2:120:ASN:N	2.28	0.65
19:3:1212:CLA:HMC3	19:A:1770:CLA:CBA	2.25	0.65
19:A:1781:CLA:C6	19:A:1782:CLA:HED2	2.25	0.65
5:A:197:GLN:NE2	5:A:351:THR:HB	2.11	0.65
5:A:514:THR:HB	5:A:532:ILE:HG23	1.79	0.65
5:A:691:MET:CE	23:A:1801:PQN:C2M	2.74	0.65
20:A:7006:LMU:C5'	20:A:7006:LMU:O5B	2.42	0.65
6:B:556:SER:C	6:B:558:PRO:CD	2.61	0.65
6:B:625:TRP:HE3	6:B:626:LEU:N	1.94	0.65
7:C:55:GLU:C	7:C:57:ALA:N	2.50	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:7:ILE:C	7:C:8:TYR:O	2.35	0.65
11:G:47:GLY:N	11:G:48:ASP:OD1	2.30	0.65
20:A:7042:LMU:C1	20:A:7042:LMU:H71	2.25	0.65
1:1:59:VAL:HG12	1:1:60:PRO:C	2.18	0.65
3:3:114:PHE:CD1	19:3:1220:CLA:CHA	2.80	0.65
19:1:1149:CLA:CAA	19:1:1149:CLA:O1D	2.45	0.65
6:B:317:ARG:NE	6:B:317:ARG:CA	2.55	0.65
6:B:607:SER:HA	6:B:610:ASN:ND2	2.12	0.65
1:1:185:TRP:O	1:1:186:HIS:ND1	2.30	0.65
2:2:97:VAL:HG23	2:2:98:GLU:H	1.62	0.65
4:4:101:VAL:O	4:4:104:ARG:NH2	2.30	0.65
4:4:121:PHE:CD1	4:4:128:ALA:HB3	2.32	0.65
5:A:402:ILE:HD11	19:A:1784:CLA:HBB2	1.78	0.65
6:B:131:THR:CB	6:B:134:ASP:HB2	2.11	0.65
6:B:493:TRP:HH2	19:B:1766:CLA:HMA2	1.61	0.65
6:B:188:LEU:HD11	19:B:1746:CLA:HBB2	1.79	0.65
6:B:190:TRP:HE3	19:B:1745:CLA:CBB	2.09	0.65
6:B:527:LEU:HD13	6:B:586:THR:HG21	1.78	0.65
11:G:28:ARG:NH2	11:G:29:GLU:H	1.94	0.65
11:G:60:SER:CA	11:G:63:PRO:HD2	2.26	0.65
20:A:7042:LMU:C3	20:A:7042:LMU:O5'	2.45	0.65
17:N:65:LEU:HD23	17:N:66:ASP:N	2.11	0.65
6:B:20:ARG:HB3	6:B:20:ARG:HH11	1.61	0.65
2:2:54:TRP:HZ2	2:2:109:ARG:HB3	1.62	0.64
2:2:55:ALA:CB	2:2:56:MET:HE1	2.24	0.64
4:4:101:VAL:CG1	4:4:104:ARG:HH22	2.07	0.64
4:4:93:ILE:O	4:4:96:ILE:N	2.29	0.64
19:A:1760:CLA:HBB2	19:A:1762:CLA:C4D	2.26	0.64
19:A:1787:CLA:HBB1	19:A:1793:CLA:C19	2.27	0.64
5:A:281:LEU:HD11	19:A:1772:CLA:HED2	1.79	0.64
5:A:361:ASN:HD22	5:A:362:LEU:N	1.95	0.64
5:A:40:PHE:CE1	5:A:53:TRP:CD1	2.75	0.64
19:B:1757:CLA:H41	19:B:1757:CLA:C7	2.27	0.64
6:B:432:HIS:CE1	19:B:1763:CLA:NB	2.62	0.64
6:B:438:VAL:CG2	19:B:1764:CLA:HAC1	2.27	0.64
6:B:666:SER:O	6:B:667:TRP:HB2	1.96	0.64
16:L:36:TYR:O	16:L:37:LEU:HB3	1.95	0.64
17:N:54:LYS:O	17:N:56:LYS:N	2.29	0.64
10:F:12:LYS:HG2	10:F:13:GLN:H	1.59	0.64
1:1:140:LEU:H	1:1:140:LEU:HD23	1.63	0.64
6:B:224:PRO:HA	6:B:227:THR:OG1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:42:ARG:CG	2:2:45:VAL:CB	2.70	0.64
4:4:103:ILE:HG13	19:4:1197:CLA:HMD1	1.78	0.64
5:A:382:TYR:CE2	19:A:1784:CLA:HED3	2.32	0.64
6:B:174:ARG:HH11	19:B:1755:CLA:HMD1	1.61	0.64
6:B:175:LEU:O	6:B:179:LEU:HG	1.97	0.64
6:B:545:LYS:HD3	6:B:546:LEU:H	1.61	0.64
6:B:558:PRO:HG2	6:B:703:VAL:CB	2.21	0.64
11:G:33:LYS:NZ	11:G:33:LYS:HA	2.12	0.64
4:4:192:THR:HG21	4:4:195:GLN:HA	1.79	0.64
19:1:1145:CLA:CMC	19:1:1145:CLA:HBC2	2.13	0.64
2:2:45:VAL:O	2:2:45:VAL:HG13	1.97	0.64
4:4:40:PHE:CA	4:4:43:ALA:HB2	2.24	0.64
19:B:1752:CLA:CHD	19:B:1752:CLA:CBC	2.64	0.64
6:B:451:LYS:HD2	19:B:1764:CLA:O2D	1.98	0.64
11:G:48:ASP:N	11:G:48:ASP:OD1	2.29	0.64
19:4:4014:CLA:CBC	19:4:4014:CLA:CMC	2.73	0.64
12:H:14:ILE:O	12:H:16:ASN:N	2.29	0.64
3:3:74:ALA:N	19:3:1217:CLA:C2D	2.60	0.64
20:A:7043:LMU:O3'	20:A:7043:LMU:H1B	1.97	0.64
9:E:44:TYR:HB3	9:E:45:TRP:CE3	2.32	0.64
8:D:93:LYS:CB	8:D:93:LYS:NZ	2.60	0.64
4:4:121:PHE:HB2	4:4:128:ALA:HB3	1.79	0.64
4:4:158:ARG:CA	4:4:161:LEU:HD12	2.22	0.64
4:4:44:GLU:O	4:4:46:VAL:N	2.30	0.64
19:A:1770:CLA:CHC	22:A:1802:BCR:C18	2.75	0.64
19:A:1786:CLA:HMB2	19:A:1787:CLA:C1D	2.27	0.64
5:A:216:LEU:HD12	22:A:1802:BCR:C35	2.27	0.64
5:A:281:LEU:O	5:A:283:PHE:N	2.29	0.64
5:A:53:TRP:HA	5:A:56:ASN:CB	2.27	0.64
6:B:387:PHE:O	6:B:391:PRO:HD3	1.97	0.64
8:D:79:ARG:O	8:D:82:GLN:HB2	1.97	0.64
19:J:1043:CLA:O1A	19:J:1043:CLA:H152	1.97	0.64
19:1:1142:CLA:OBD	19:K:1085:CLA:CHB	2.46	0.64
12:H:16:ASN:HD22	12:H:19:GLY:HA2	1.63	0.64
20:A:7010:LMU:C2B	20:A:7010:LMU:C3'	2.75	0.64
3:3:198:PHE:HA	3:3:201:ALA:CB	2.18	0.64
19:4:1198:CLA:O2D	19:4:1198:CLA:HAA1	1.96	0.64
4:4:39:TRP:CA	4:4:40:PHE:HD1	2.09	0.64
19:A:1771:CLA:CMC	19:A:1771:CLA:HBC2	2.24	0.64
19:A:1781:CLA:H43	19:A:1793:CLA:HBA1	1.80	0.64
5:A:368:LEU:CD1	19:A:1782:CLA:C6	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1756:CLA:HMB3	22:B:1778:BCR:H351	1.78	0.64
19:B:1769:CLA:HHB	19:B:1770:CLA:OBD	1.97	0.64
16:L:30:SER:HG	16:L:32:LEU:HB2	1.63	0.64
19:1:1188:CLA:H2	19:1:1188:CLA:HED2	1.78	0.64
19:3:1221:CLA:C2A	19:3:3011:CLA:CBC	2.76	0.64
15:K:52:PRO:O	15:K:56:THR:CG2	2.45	0.64
8:D:118:VAL:CG1	8:D:119:TYR:N	2.60	0.64
8:D:113:HIS:CD2	8:D:118:VAL:HG21	2.32	0.64
10:F:151:ASP:O	10:F:154:PHE:CB	2.40	0.64
4:4:58:MET:SD	4:4:59:LEU:CA	2.85	0.64
6:B:67:HIS:O	6:B:68:VAL:HG23	1.97	0.64
12:H:50:ARG:HG2	16:L:137:ALA:HB1	1.78	0.64
6:B:42:LEU:O	6:B:43:TYR:C	2.35	0.64
12:H:75:ASP:CG	12:H:77:LEU:HG	2.18	0.64
19:A:1779:CLA:NC	22:A:1804:BCR:H17C	2.12	0.64
5:A:340:GLY:O	5:A:343:HIS:CB	2.43	0.64
5:A:514:THR:HB	5:A:532:ILE:CG2	2.28	0.64
19:B:1741:CLA:H2	12:H:69:SER:OG	1.97	0.64
6:B:142:LEU:HD21	22:B:1777:BCR:H333	1.77	0.64
19:B:1787:CLA:CBB	19:B:1788:CLA:CHB	2.73	0.64
9:E:35:LYS:CE	9:E:89:GLU:OE2	2.46	0.64
10:F:100:VAL:CA	10:F:103:SER:OG	2.44	0.64
4:4:68:GLY:O	4:4:71:ASN:CB	2.29	0.64
20:A:7036:LMU:O5B	20:A:7036:LMU:H6E	1.95	0.64
17:N:39:SER:OG	17:N:40:CYS:N	2.30	0.64
17:N:41:LYS:HB2	17:N:42:PHE:CA	2.26	0.64
8:D:32:SER:H	16:L:23:LEU:HG	1.61	0.64
19:A:1796:CLA:NC	19:A:1796:CLA:C4	2.61	0.64
5:A:401:TRP:O	5:A:405:PHE:HB2	1.98	0.64
5:A:544:ILE:O	5:A:548:THR:OG1	2.09	0.64
23:B:1774:PQN:H162	22:B:1781:BCR:H332	1.63	0.64
22:B:1781:BCR:C35	19:B:1788:CLA:H111	2.27	0.64
19:A:1811:CLA:HED1	19:B:1786:CLA:H2	1.79	0.64
10:F:62:LEU:CD2	10:F:72:ILE:HD13	2.27	0.64
17:N:80:ASN:C	17:N:82:PHE:H	2.00	0.64
17:N:83:TRP:O	17:N:83:TRP:HE3	1.80	0.64
1:1:64:GLY:HA3	1:1:66:GLY:O	1.97	0.64
15:K:51:ASP:C	15:K:51:ASP:OD1	2.35	0.64
9:E:45:TRP:CZ3	9:E:78:SER:OG	2.51	0.64
12:H:45:ALA:HB3	12:H:46:PRO:HD3	1.78	0.64
17:N:5:GLU:OE2	17:N:6:TYR:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:161:PHE:CD1	19:1:1189:CLA:HBB1	2.33	0.64
6:B:37:ILE:HD12	6:B:37:ILE:O	1.97	0.64
6:B:49:SER:O	6:B:52:GLY:N	2.31	0.64
6:B:211:ASN:HB2	6:B:214:ASP:HB3	1.79	0.64
10:F:11:SER:OG	10:F:14:PHE:HB3	1.97	0.64
2:2:124:ILE:CB	2:2:129:LYS:HB3	2.27	0.64
4:4:128:ALA:HB3	4:4:143:PHE:HE2	1.61	0.64
4:4:163:PHE:O	4:4:167:ILE:N	2.28	0.64
19:A:1759:CLA:O1D	19:A:1759:CLA:HBA2	1.97	0.64
19:A:1790:CLA:HMC1	19:A:1790:CLA:HBC3	1.80	0.64
19:B:1743:CLA:H11	19:B:1743:CLA:H61	1.80	0.64
19:B:1772:CLA:HED1	24:B:1784:LMG:C21	2.28	0.64
6:B:282:PHE:O	6:B:286:ILE:HG13	1.97	0.64
6:B:334:LEU:CG	6:B:334:LEU:O	2.46	0.64
9:E:36:VAL:C	9:E:49:VAL:HG13	2.18	0.64
11:G:37:GLU:OE2	11:G:42:SER:N	2.31	0.64
7:C:59:PRO:HB3	7:C:61:ASP:OD1	1.98	0.64
16:L:48:ASN:HB3	16:L:49:PRO:CD	2.27	0.64
5:A:418:MET:O	5:A:564:ARG:HD2	1.98	0.64
2:2:74:LEU:O	2:2:75:ASN:ND2	2.29	0.64
4:4:154:ILE:O	4:4:157:GLY:HA3	1.97	0.64
5:A:691:MET:HE3	23:A:1801:PQN:C2M	2.27	0.64
5:A:370:ILE:CD1	19:A:1781:CLA:O1D	2.44	0.64
5:A:657:LEU:HD23	19:A:1810:CLA:C1D	2.28	0.64
6:B:103:ALA:O	6:B:104:PHE:CB	2.34	0.64
19:B:1744:CLA:C4	19:B:1749:CLA:CBC	2.75	0.64
6:B:535:VAL:HG13	6:B:536:LYS:N	2.13	0.64
6:B:608:GLN:O	6:B:612:SER:HB3	1.97	0.64
10:F:147:GLY:C	10:F:150:VAL:HB	2.18	0.64
11:G:68:ILE:O	11:G:72:LEU:HB2	1.96	0.64
17:N:63:ASP:CA	17:N:64:ASP:O	2.41	0.64
21:B:8060:SUC:C1'	21:B:8060:SUC:C5	2.75	0.64
6:B:475:ASP:CA	6:B:480:SER:HA	2.27	0.64
17:N:11:LYS:HG2	17:N:12:THR:N	2.13	0.64
5:A:66:SER:O	5:A:67:HIS:HB2	1.98	0.64
5:A:113:PRO:C	5:A:115:HIS:H	2.01	0.64
5:A:733:VAL:HG11	19:A:1796:CLA:C2D	2.28	0.64
5:A:281:LEU:HG	5:A:282:THR:H	1.62	0.64
5:A:558:LYS:HZ2	6:B:674:LEU:CB	2.11	0.64
5:A:744:ALA:CB	22:A:1806:BCR:C39	2.36	0.64
19:B:1735:CLA:HMD3	22:B:1779:BCR:C4	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:494:LEU:HD12	19:B:1766:CLA:HED1	1.80	0.64
6:B:555:TYR:CD2	6:B:573:TRP:HB2	2.32	0.64
10:F:153:ASN:C	10:F:153:ASN:ND2	2.48	0.64
17:N:80:ASN:O	17:N:82:PHE:N	2.28	0.64
17:N:81:VAL:O	17:N:82:PHE:C	2.37	0.64
19:J:1043:CLA:O2A	19:J:1043:CLA:C16	2.45	0.64
8:D:90:LEU:O	8:D:90:LEU:HD13	1.98	0.64
8:D:31:GLY:HA2	16:L:13:PRO:HB3	1.80	0.64
19:3:1218:CLA:HAC2	19:3:1219:CLA:C9	2.28	0.64
3:3:163:PHE:C	3:3:163:PHE:CD1	2.72	0.64
19:2:1213:CLA:H42	19:2:1213:CLA:C4C	2.28	0.63
5:A:132:LEU:HD11	5:A:674:ALA:CB	2.27	0.63
6:B:366:THR:HG23	6:B:729:THR:CG2	2.28	0.63
8:D:36:LEU:HD12	8:D:78:ALA:H	1.62	0.63
10:F:125:LEU:O	10:F:126:ALA:HB2	1.98	0.63
11:G:28:ARG:HG3	11:G:29:GLU:CG	2.28	0.63
16:L:128:ASP:CG	16:L:129:GLN:H	2.01	0.63
4:4:69:ILE:CD1	4:4:175:LYS:CD	2.75	0.63
17:N:57:LYS:HG3	17:N:58:VAL:H	0.61	0.63
6:B:475:ASP:HA	6:B:480:SER:HA	1.78	0.63
19:2:1217:CLA:O1D	19:2:1217:CLA:HBA2	1.96	0.63
2:2:40:SER:O	2:2:41:LEU:CB	2.47	0.63
4:4:91:PHE:CE2	19:4:1207:CLA:C3C	2.81	0.63
5:A:346:LEU:HD11	19:A:1779:CLA:CHD	2.28	0.63
5:A:492:ILE:HA	5:A:495:THR:HG23	1.78	0.63
5:A:612:VAL:O	5:A:615:HIS:HB3	1.98	0.63
5:A:377:TYR:CD1	5:A:616:PHE:HE1	2.16	0.63
6:B:77:TRP:CZ2	6:B:122:GLN:NE2	2.67	0.63
19:B:1743:CLA:HMC1	22:B:1776:BCR:H373	1.79	0.63
6:B:530:THR:CG2	19:B:1756:CLA:HMC1	2.29	0.63
6:B:334:LEU:CA	19:B:1737:CLA:HMD3	2.29	0.63
10:F:130:LEU:CD1	10:F:131:PHE:HD1	2.12	0.63
13:I:22:ALA:O	13:I:23:SER:C	2.35	0.63
17:N:59:PRO:C	17:N:66:ASP:OD1	2.37	0.63
17:N:77:CYS:O	17:N:79:SER:N	2.30	0.63
3:3:181:LEU:HD12	3:3:182:LYS:HE2	1.79	0.63
10:F:22:LEU:O	10:F:25:LEU:HD12	1.97	0.63
20:A:7032:LMU:H12	20:A:7032:LMU:H2O2	1.60	0.63
3:3:106:TYR:HB3	3:3:107:TRP:CD1	2.32	0.63
4:4:123:GLN:HG2	4:4:124:TYR:N	2.13	0.63
5:A:114:THR:CG2	5:A:115:HIS:ND1	2.59	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:187:HIS:CE1	19:A:1767:CLA:C1A	2.71	0.63
19:A:1771:CLA:CGA	19:A:1771:CLA:C1A	2.66	0.63
5:A:302:HIS:HB2	19:A:1773:CLA:C1B	2.28	0.63
5:A:207:LEU:O	5:A:310:PHE:CB	2.46	0.63
5:A:360:ILE:O	5:A:361:ASN:CB	2.45	0.63
5:A:434:ARG:O	5:A:437:ARG:HB2	1.99	0.63
20:A:7006:LMU:C2'	20:A:7006:LMU:C2	2.77	0.63
6:B:269:TRP:HD1	6:B:497:TRP:CH2	2.17	0.63
6:B:17:THR:HA	6:B:696:LYS:H	1.63	0.63
11:G:42:SER:OG	11:G:43:HIS:C	2.37	0.63
11:G:7:VAL:HG23	11:G:8:ILE:N	2.12	0.63
16:L:99:LEU:O	16:L:102:TYR:N	2.29	0.63
17:N:66:ASP:N	17:N:66:ASP:OD2	2.29	0.63
19:1:1308:CLA:CMA	19:1:1308:CLA:H2	2.28	0.63
20:A:7010:LMU:O3'	20:A:7010:LMU:C1B	2.47	0.63
19:2:1217:CLA:HBD	19:2:1217:CLA:CBA	2.28	0.63
6:B:92:TRP:O	6:B:92:TRP:CD1	2.51	0.63
4:4:97:LEU:O	4:4:99:HIS:N	2.32	0.63
19:A:1770:CLA:H2A	19:A:1770:CLA:HED2	1.81	0.63
19:A:1788:CLA:C14	19:A:1788:CLA:H101	2.29	0.63
5:A:530:LEU:HB2	5:A:531:PRO:HD2	1.81	0.63
19:B:1743:CLA:CMC	22:B:1776:BCR:H373	2.27	0.63
6:B:203:ARG:HG2	6:B:204:GLY:H	1.63	0.63
6:B:577:TYR:HE2	6:B:578:LEU:HD12	1.64	0.63
6:B:732:LYS:CG	6:B:733:PHE:O	2.41	0.63
22:I:1032:BCR:C39	22:L:1169:BCR:H401	2.28	0.63
20:N:1086:LMU:H32	20:N:1086:LMU:C6'	2.29	0.63
19:1:1148:CLA:O2A	19:1:1148:CLA:HED1	1.98	0.63
21:B:8059:SUC:C1'	21:B:8059:SUC:HO2	2.10	0.63
19:1:1193:CLA:H43	19:1:1193:CLA:CGA	2.28	0.63
6:B:216:LEU:O	6:B:218:TYR:N	2.31	0.63
2:2:103:GLY:O	2:2:104:TRP:C	2.36	0.63
2:2:98:GLU:CG	2:2:99:LEU:HD12	2.27	0.63
19:A:1774:CLA:H193	19:A:1774:CLA:H93	1.79	0.63
19:A:1781:CLA:HBB2	19:A:1794:CLA:CMA	2.29	0.63
5:A:229:ILE:HG12	5:A:243:PRO:HB3	1.81	0.63
5:A:284:ARG:HH12	5:A:507:ALA:HB1	1.63	0.63
19:B:1761:CLA:HMB2	19:B:1762:CLA:CHB	2.28	0.63
22:B:1781:BCR:C17	19:B:1787:CLA:H101	2.22	0.63
6:B:447:GLY:O	6:B:449:PRO:HD3	1.98	0.63
6:B:551:LYS:CE	8:D:143:PRO:HA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:79:GLN:O	6:B:80:ASP:HB3	1.96	0.63
8:D:46:TYR:HE1	8:D:80:LYS:CE	2.11	0.63
17:N:41:LYS:CB	17:N:42:PHE:CB	2.56	0.63
17:N:72:LYS:N	17:N:72:LYS:HD2	2.07	0.63
17:N:72:LYS:CB	17:N:73:ASP:C	2.56	0.63
19:1:1148:CLA:HAA1	19:1:1148:CLA:CED	2.27	0.63
19:1:1308:CLA:HMC1	19:1:1308:CLA:CBC	2.25	0.63
4:4:194:VAL:HG12	4:4:195:GLN:N	2.07	0.63
19:1:1145:CLA:C2	19:1:1145:CLA:CMA	2.76	0.63
5:A:520:LEU:O	5:A:522:ALA:N	2.27	0.63
4:4:52:MET:HE3	4:4:156:ASN:CB	2.28	0.63
5:A:174:PHE:O	5:A:175:ALA:HB2	1.97	0.63
5:A:224:HIS:CE1	19:A:1771:CLA:C4C	2.82	0.63
5:A:210:LEU:HD12	19:A:1769:CLA:CMB	2.27	0.63
5:A:308:ILE:CG2	5:A:309:LEU:N	2.61	0.63
19:B:1739:CLA:HMC1	22:B:1781:BCR:H282	1.80	0.63
19:B:1769:CLA:C12	22:B:1780:BCR:C31	2.76	0.63
7:C:62:PHE:CE2	8:D:137:ILE:HB	2.33	0.63
19:1:1192:CLA:HHD	19:1:1192:CLA:HBC3	1.76	0.63
3:3:50:GLU:N	3:3:51:PRO:HD3	2.13	0.63
5:A:425:THR:OG1	5:A:428:TYR:HE1	1.73	0.63
17:N:29:PHE:CE1	17:N:32:ALA:HB3	2.33	0.63
6:B:224:PRO:CB	6:B:227:THR:HB	2.28	0.63
1:1:179:THR:HG21	4:4:87:SER:C	2.19	0.63
19:A:1783:CLA:H102	22:A:1806:BCR:C37	2.29	0.63
5:A:664:VAL:HG23	5:A:665:ILE:HG23	1.80	0.63
5:A:690:LEU:CD2	6:B:661:PHE:HE1	2.12	0.63
5:A:701:GLN:O	5:A:704:ILE:N	2.32	0.63
5:A:87:SER:OG	5:A:179:LEU:HB2	1.98	0.63
19:B:1757:CLA:H8	22:B:1778:BCR:H14C	1.80	0.63
6:B:655:LEU:HD21	19:B:1772:CLA:HBB1	1.81	0.63
6:B:715:VAL:HG23	6:B:719:PHE:HD2	1.62	0.63
4:4:76:TYR:O	4:4:77:ALA:HB3	1.96	0.63
19:J:1043:CLA:CGA	19:J:1043:CLA:C16	2.77	0.63
10:F:20:GLN:C	10:F:20:GLN:CD	2.54	0.63
20:A:7050:LMU:C4	20:A:7050:LMU:O1'	2.30	0.63
6:B:247:THR:HG23	6:B:250:ALA:CB	2.28	0.63
17:N:34:THR:C	17:N:36:GLU:H	2.01	0.63
8:D:31:GLY:HA3	16:L:23:LEU:HD21	1.80	0.63
2:2:63:PHE:HD2	2:2:172:LEU:HD21	1.63	0.63
5:A:304:LEU:CD2	19:A:1772:CLA:HBB2	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1781:CLA:HMA3	19:A:1782:CLA:O1A	1.98	0.63
5:A:439:ARG:NH1	5:A:565:SER:O	2.32	0.63
5:A:472:ARG:N	5:A:473:PRO:HD2	2.12	0.63
5:A:508:THR:O	5:A:509:ALA:CB	2.47	0.63
5:A:599:PHE:CD2	5:A:735:VAL:HG21	2.34	0.63
5:A:705:GLU:HB3	6:B:545:LYS:NZ	2.14	0.63
7:C:77:MET:O	7:C:79:LEU:N	2.29	0.63
19:F:1156:CLA:CHD	19:F:1156:CLA:HBC2	2.26	0.63
13:I:11:LEU:HD11	22:I:1032:BCR:C10	2.29	0.63
16:L:122:GLY:O	16:L:124:LYS:N	2.32	0.63
4:4:70:ILE:CG1	4:4:71:ASN:N	2.62	0.63
19:1:1188:CLA:C2	19:1:1188:CLA:CED	2.62	0.63
5:A:249:ILE:C	5:A:251:ASN:H	2.01	0.63
5:A:254:LEU:C	5:A:256:ALA:H	2.02	0.63
19:1:1014:CLA:C3A	19:1:1014:CLA:HED3	2.29	0.63
11:G:92:GLY:O	11:G:93:TYR:C	2.36	0.63
11:G:93:TYR:CA	11:G:94:ASP:CG	2.59	0.63
20:A:7020:LMU:H92	20:A:7020:LMU:C5	2.18	0.63
19:R:1054:CLA:NA	19:R:1054:CLA:HED3	2.12	0.63
20:A:7030:LMU:C2'	20:A:7030:LMU:C6'	2.63	0.63
7:C:28:MET:HG2	7:C:38:GLN:HE21	1.64	0.63
2:2:72:GLY:O	2:2:74:LEU:N	2.28	0.63
4:4:40:PHE:HB3	4:4:43:ALA:HB3	1.70	0.63
4:4:99:HIS:O	4:4:99:HIS:ND1	2.30	0.63
19:A:1781:CLA:C3B	22:A:1805:BCR:C22	2.77	0.63
22:A:1806:BCR:H353	19:A:1811:CLA:H41	1.81	0.63
5:A:455:PHE:HD1	19:A:1788:CLA:CMA	2.12	0.63
5:A:691:MET:O	23:A:1801:PQN:O1	2.17	0.63
5:A:707:ILE:C	5:A:711:HIS:CD2	2.73	0.63
19:B:1759:CLA:H142	22:B:1777:BCR:C10	2.24	0.63
19:B:1756:CLA:H52	19:B:1770:CLA:CBD	2.28	0.63
13:I:8:PHE:CE1	19:I:1031:CLA:H43	2.33	0.63
17:N:62:SER:CA	17:N:66:ASP:H	2.12	0.63
5:A:27:ILE:HG23	5:A:28:LYS:HG3	1.81	0.63
7:C:12:ILE:CB	7:C:39:ILE:HA	2.29	0.63
4:4:93:ILE:CG2	4:4:94:GLU:N	2.61	0.62
19:A:1771:CLA:CGA	19:A:1771:CLA:NA	2.62	0.62
5:A:201:SER:O	5:A:204:ASN:HB2	1.99	0.62
5:A:665:ILE:C	5:A:665:ILE:HD12	2.19	0.62
5:A:711:HIS:HB3	5:A:717:ALA:CB	2.29	0.62
22:B:1777:BCR:H331	22:B:1777:BCR:HC8	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:378:ILE:HG22	6:B:379:ALA:H	1.63	0.62
6:B:464:GLN:HA	6:B:467:HIS:HB2	1.80	0.62
6:B:670:TYR:C	6:B:670:TYR:CD1	2.72	0.62
9:E:61:THR:HG22	9:E:62:ARG:N	2.11	0.62
10:F:80:TRP:HB3	19:F:1157:CLA:HHC	1.81	0.62
13:I:26:LEU:HD13	13:I:30:LYS:HB3	1.80	0.62
22:L:1170:BCR:C23	22:L:1170:BCR:C38	2.76	0.62
19:L:1167:CLA:CHC	22:L:1170:BCR:HC8	2.28	0.62
17:N:54:LYS:CB	17:N:57:LYS:HE2	2.12	0.62
5:A:109:TRP:CH2	5:A:154:ARG:HD3	2.34	0.62
19:A:1779:CLA:C1B	22:A:1804:BCR:C15	2.77	0.62
19:A:1764:CLA:H142	22:A:1807:BCR:H14C	1.79	0.62
5:A:210:LEU:HD13	19:A:1769:CLA:CMB	2.23	0.62
5:A:281:LEU:O	5:A:282:THR:C	2.36	0.62
19:B:1748:CLA:CBD	19:B:1757:CLA:CBB	2.77	0.62
6:B:392:ILE:HD13	19:B:1760:CLA:CED	2.30	0.62
6:B:704:GLN:O	6:B:708:VAL:HG23	1.99	0.62
7:C:60:THR:HG23	7:C:63:LEU:O	1.99	0.62
8:D:48:ILE:CB	8:D:100:PHE:HB3	2.28	0.62
5:A:426:THR:HA	5:A:428:TYR:CZ	2.34	0.62
20:A:7028:LMU:H11	20:A:7028:LMU:O2'	1.98	0.62
4:4:106:TRP:CE3	19:4:1209:CLA:CMA	2.82	0.62
4:4:89:THR:N	4:4:90:LEU:CD2	2.52	0.62
5:A:406:LEU:HD11	19:A:1762:CLA:HMB3	1.80	0.62
5:A:360:ILE:HD13	22:A:1804:BCR:H371	1.79	0.62
5:A:398:HIS:CD2	19:A:1783:CLA:ND	2.67	0.62
5:A:412:ALA:HA	5:A:598:VAL:HG21	1.80	0.62
5:A:604:TRP:O	5:A:607:ASN:N	2.27	0.62
19:B:1739:CLA:CMC	22:B:1781:BCR:C28	2.76	0.62
6:B:493:TRP:NE1	19:B:1747:CLA:HAC2	2.13	0.62
6:B:545:LYS:CG	6:B:546:LEU:N	2.61	0.62
6:B:689:ASN:OD1	6:B:689:ASN:N	2.31	0.62
6:B:732:LYS:CD	6:B:734:GLY:N	2.60	0.62
7:C:73:THR:C	7:C:76:SER:OG	2.37	0.62
6:B:120:VAL:CA	6:B:123:TRP:HD1	2.08	0.62
15:K:53:ALA:HA	15:K:56:THR:HG23	1.80	0.62
4:4:62:GLU:O	4:4:65:THR:HG22	1.99	0.62
6:B:221:GLY:C	6:B:223:GLY:H	2.03	0.62
2:2:42:ARG:HA	2:2:45:VAL:HG23	0.72	0.62
19:A:1765:CLA:HBD	19:A:1765:CLA:HBA2	1.80	0.62
5:A:224:HIS:HE1	19:A:1771:CLA:CHD	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1765:CLA:H51	22:A:1807:BCR:H10C	1.82	0.62
5:A:697:ARG:C	5:A:699:TYR:H	2.02	0.62
5:A:555:ILE:HG23	19:B:1788:CLA:OBD	1.99	0.62
6:B:429:LEU:HB3	6:B:525:LEU:HB2	1.80	0.62
6:B:53:GLN:C	6:B:55:ALA:N	2.53	0.62
19:B:1741:CLA:HBB2	13:I:13:GLY:C	2.18	0.62
13:I:24:LEU:C	13:I:26:LEU:N	2.51	0.62
20:A:7036:LMU:H92	20:A:7036:LMU:H11	1.80	0.62
18:R:31:UNK:C	18:R:32:UNK:O	2.47	0.62
19:J:1043:CLA:C2	19:J:1043:CLA:C16	2.75	0.62
10:F:22:LEU:CA	10:F:25:LEU:HD13	2.29	0.62
20:A:7032:LMU:C1B	20:A:7032:LMU:H32	2.25	0.62
1:1:57:ILE:CG1	1:1:57:ILE:O	2.44	0.62
12:H:41:GLU:OE2	12:H:42:THR:OG1	2.15	0.62
19:4:1198:CLA:H2A	19:4:1198:CLA:CGD	2.18	0.62
5:A:158:ILE:CG2	19:A:1770:CLA:HED3	2.30	0.62
19:A:1782:CLA:HMC1	19:A:1782:CLA:HBC3	1.76	0.62
19:A:1783:CLA:H72	22:A:1806:BCR:C37	2.20	0.62
5:A:330:ILE:O	5:A:330:ILE:HG22	1.99	0.62
5:A:401:TRP:HD1	19:A:1783:CLA:CHC	2.12	0.62
5:A:702:GLU:HA	6:B:545:LYS:HE2	1.81	0.62
5:A:79:PHE:HE2	5:A:185:HIS:CG	2.17	0.62
19:B:1757:CLA:C7	22:B:1778:BCR:H14C	2.30	0.62
6:B:467:HIS:NE2	19:B:1765:CLA:C1A	2.63	0.62
8:D:37:LEU:O	8:D:39:LYS:N	2.32	0.62
8:D:78:ALA:O	8:D:79:ARG:NH1	2.33	0.62
6:B:25:ILE:CB	22:L:1169:BCR:H292	2.28	0.62
3:3:59:ILE:O	3:3:63:ARG:HG3	1.99	0.62
5:A:348:GLU:O	5:A:350:LEU:N	2.33	0.62
4:4:145:PRO:O	4:4:146:THR:C	2.31	0.62
5:A:122:VAL:HA	5:A:133:ASN:HD21	1.65	0.62
5:A:553:VAL:HG22	22:A:1805:BCR:H401	1.81	0.62
5:A:553:VAL:O	5:A:557:LEU:N	2.29	0.62
19:B:1738:CLA:HBB2	19:B:1759:CLA:HHC	1.79	0.62
19:B:1747:CLA:HBA1	19:B:1747:CLA:HED2	1.81	0.62
6:B:289:LEU:HD22	22:B:1775:BCR:H352	1.80	0.62
6:B:284:PHE:O	6:B:288:GLY:N	2.28	0.62
6:B:661:PHE:HB3	19:B:1788:CLA:HBC3	1.81	0.62
10:F:103:SER:C	10:F:105:LEU:N	2.53	0.62
16:L:64:LEU:HA	16:L:67:PRO:HG3	1.80	0.62
4:4:69:ILE:HD11	4:4:175:LYS:CD	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:73:PRO:O	4:4:74:LYS:HB2	1.99	0.62
1:1:28:GLY:O	19:1:1197:CLA:C3C	2.47	0.62
17:N:58:VAL:C	17:N:60:PHE:H	2.03	0.62
20:A:7016:LMU:H1'	20:A:7016:LMU:H31	1.81	0.62
12:H:21:TRP:N	12:H:22:ASP:CB	2.61	0.62
6:B:456:GLU:HG2	10:F:70:HIS:HB3	1.80	0.62
17:N:4:GLU:CD	17:N:5:GLU:HB2	2.20	0.62
8:D:94:TYR:O	8:D:95:LYS:CB	2.48	0.62
6:B:40:GLY:HA2	6:B:165:VAL:HG23	1.80	0.62
2:2:168:ARG:HH11	2:2:168:ARG:HG2	1.64	0.62
2:2:44:ASN:ND2	14:J:1:MET:CB	2.62	0.62
2:2:56:MET:O	2:2:57:LEU:C	2.36	0.62
2:2:72:GLY:C	2:2:74:LEU:H	2.03	0.62
19:A:1763:CLA:HBA1	19:A:1763:CLA:NA	2.05	0.62
19:A:1760:CLA:HBA2	19:A:1767:CLA:H62	1.82	0.62
5:A:308:ILE:HG22	5:A:309:LEU:H	1.64	0.62
5:A:399:HIS:O	5:A:400:MET:HB2	1.97	0.62
5:A:669:GLY:N	6:B:445:ALA:HA	2.15	0.62
19:B:1756:CLA:H11	19:B:1770:CLA:CBD	2.29	0.62
6:B:697:PRO:CB	19:B:1771:CLA:HBC3	2.30	0.62
6:B:527:LEU:HB3	19:B:1756:CLA:C4C	2.29	0.62
17:N:66:ASP:C	17:N:67:LEU:CG	2.68	0.62
10:F:40:LEU:HA	10:F:42:ILE:CG1	2.26	0.62
8:D:87:GLY:N	8:D:90:LEU:HB3	2.15	0.62
2:2:54:TRP:CZ2	2:2:109:ARG:CG	2.82	0.62
19:A:1768:CLA:C3D	19:A:1769:CLA:HMC3	2.30	0.62
19:A:1796:CLA:H161	22:A:1806:BCR:HC22	1.82	0.62
5:A:40:PHE:CZ	5:A:56:ASN:HB3	2.35	0.62
19:B:1748:CLA:HBD	19:B:1757:CLA:HBB2	1.80	0.62
5:A:558:LYS:NZ	6:B:674:LEU:HD23	2.15	0.62
16:L:30:SER:O	16:L:32:LEU:N	2.33	0.62
4:4:74:LYS:H	4:4:75:TRP:CB	2.13	0.62
19:1:1308:CLA:O1D	19:1:1308:CLA:CGA	2.47	0.62
19:1:1308:CLA:HMA3	19:J:1044:CLA:CED	2.27	0.62
1:1:57:ILE:C	1:1:59:VAL:N	2.51	0.62
12:H:14:ILE:O	12:H:14:ILE:HD13	1.99	0.62
20:A:7039:LMU:O2'	20:A:7039:LMU:H5'	2.00	0.62
10:F:151:ASP:HA	10:F:154:PHE:HB3	1.80	0.62
19:A:1783:CLA:C18	22:A:1807:BCR:H17C	2.29	0.62
6:B:190:TRP:HE3	19:B:1745:CLA:HBB2	1.64	0.62
19:A:1810:CLA:CAA	19:B:1786:CLA:HBB2	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:560:ASP:CG	6:B:561:GLY:N	2.53	0.62
6:B:622:ASP:HA	6:B:626:LEU:HB3	1.82	0.62
6:B:715:VAL:O	6:B:719:PHE:N	2.32	0.62
10:F:84:ILE:O	10:F:87:GLY:N	2.26	0.62
19:1:1187:CLA:HBC3	19:1:1187:CLA:HMC1	0.70	0.62
2:2:196:HIS:HE1	21:2:1225:SUC:O3	1.78	0.62
3:3:173:GLU:HG2	3:3:174:LYS:N	2.08	0.62
6:B:216:LEU:HD21	6:B:221:GLY:CA	2.30	0.62
15:K:27:ALA:CB	15:K:28:PRO:CD	2.78	0.62
16:L:158:MET:SD	16:L:159:TYR:N	2.69	0.62
6:B:213:LEU:HD12	6:B:214:ASP:N	2.15	0.62
12:H:57:LEU:HD13	12:H:57:LEU:O	1.99	0.62
5:A:448:TRP:CD1	19:A:1788:CLA:HED2	2.35	0.62
5:A:711:HIS:NE2	19:A:1795:CLA:HBC1	2.11	0.62
5:A:302:HIS:HE1	19:A:1774:CLA:CHB	2.13	0.62
19:B:1735:CLA:HBB1	10:F:101:GLY:HA3	1.81	0.62
6:B:334:LEU:CB	19:B:1737:CLA:HMD3	2.29	0.62
19:B:1739:CLA:H142	19:B:1739:CLA:C10	2.29	0.62
6:B:347:LEU:CD2	6:B:351:HIS:HE1	2.11	0.62
6:B:439:HIS:CD2	6:B:453:ILE:HG22	2.35	0.62
6:B:462:TRP:HZ3	19:B:1765:CLA:CBC	2.12	0.62
6:B:664:LEU:C	6:B:667:TRP:CZ3	2.70	0.62
6:B:91:ILE:HD11	6:B:104:PHE:CD2	2.34	0.62
16:L:30:SER:C	16:L:32:LEU:H	2.03	0.62
17:N:67:LEU:HB2	17:N:68:GLU:HB3	1.82	0.62
3:3:181:LEU:HD13	3:3:181:LEU:N	2.11	0.62
19:1:1308:CLA:HBA2	19:1:1308:CLA:CGD	2.29	0.62
3:3:194:ILE:HG13	19:3:1214:CLA:C2C	2.30	0.62
12:H:25:GLY:CA	12:H:27:ASP:HB2	2.28	0.62
12:H:26:SER:C	12:H:27:ASP:O	2.34	0.62
9:E:73:ASN:C	9:E:73:ASN:HD22	2.04	0.62
2:2:187:GLY:O	2:2:189:ILE:HG12	2.00	0.62
6:B:31:PHE:HB2	6:B:42:LEU:CD1	2.28	0.62
2:2:166:ASN:OD1	2:2:169:LEU:HD12	2.00	0.61
3:3:83:LEU:C	19:3:1212:CLA:H43	2.20	0.61
4:4:129:GLY:C	4:4:131:VAL:H	2.02	0.61
19:A:1774:CLA:C20	19:A:1782:CLA:H3A	2.30	0.61
19:A:1783:CLA:H171	22:A:1807:BCR:H351	1.81	0.61
5:A:445:HIS:O	5:A:446:LEU:HB2	1.99	0.61
5:A:578:ARG:HA	5:A:595:TRP:HB2	1.80	0.61
19:B:1769:CLA:C1A	19:B:1769:CLA:CGA	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:654:HIS:HE1	19:B:1786:CLA:NB	1.96	0.61
6:B:633:ASN:ND2	6:B:636:THR:CB	2.63	0.61
19:L:1167:CLA:CMC	19:L:1167:CLA:HBC3	2.30	0.61
8:D:118:VAL:HG12	8:D:119:TYR:N	2.15	0.61
5:A:27:ILE:C	5:A:27:ILE:HD13	2.19	0.61
7:C:44:ARG:NH2	8:D:127:ARG:CB	2.60	0.61
1:1:44:LEU:HD22	1:1:154:ALA:HB3	1.80	0.61
3:3:62:GLY:HA2	3:3:65:ALA:HB3	1.82	0.61
19:A:1788:CLA:HAA1	22:L:1170:BCR:C13	2.30	0.61
19:A:1811:CLA:CED	19:B:1786:CLA:H2	2.30	0.61
5:A:307:ALA:O	5:A:308:ILE:C	2.39	0.61
6:B:458:ILE:HG23	19:B:1769:CLA:CMD	2.30	0.61
9:E:32:ARG:HH22	9:E:53:VAL:HA	1.64	0.61
3:3:52:LYS:CA	3:3:55:ALA:HB3	2.30	0.61
4:4:194:VAL:N	4:4:195:GLN:O	2.29	0.61
20:R:1056:LMU:H6'	20:R:1056:LMU:H1'	1.65	0.61
6:B:82:PHE:O	6:B:84:VAL:N	2.33	0.61
5:A:451:ILE:HD11	19:A:1788:CLA:HED1	1.81	0.61
5:A:662:SER:HA	5:A:665:ILE:HD11	1.81	0.61
19:B:1757:CLA:C10	22:B:1778:BCR:H14C	2.30	0.61
6:B:196:HIS:CE1	19:B:1746:CLA:ND	2.68	0.61
18:R:41:UNK:CA	18:R:42:UNK:CB	2.76	0.61
20:A:7040:LMU:H3O2	20:A:7040:LMU:C1B	2.13	0.61
2:2:208:PHE:CG	2:2:209:THR:N	2.68	0.61
6:B:166:SER:O	6:B:168:PHE:N	2.33	0.61
19:2:1215:CLA:H2	19:2:1218:CLA:HMD3	1.81	0.61
4:4:118:ASP:HB2	19:4:1200:CLA:HMB3	1.82	0.61
4:4:147:LEU:HD22	4:4:148:GLU:CB	2.29	0.61
4:4:99:HIS:HD1	4:4:99:HIS:C	2.03	0.61
5:A:143:ILE:HD12	5:A:144:GLN:H	1.66	0.61
19:A:1796:CLA:H101	19:A:1812:CLA:H152	1.81	0.61
5:A:308:ILE:HG13	19:A:1772:CLA:CBB	2.29	0.61
5:A:472:ARG:O	5:A:474:GLN:CG	2.47	0.61
19:B:1754:CLA:CMC	19:B:1754:CLA:HBC2	2.30	0.61
19:B:1756:CLA:CMB	22:B:1778:BCR:C35	2.76	0.61
6:B:592:PHE:HA	6:B:721:TYR:OH	2.01	0.61
6:B:658:ALA:O	6:B:661:PHE:HD2	1.84	0.61
6:B:692:ARG:NH2	6:B:694:ARG:HG2	2.15	0.61
3:3:194:ILE:HD11	19:3:1214:CLA:CMC	2.16	0.61
10:F:17:ARG:HA	10:F:17:ARG:NE	2.14	0.61
1:1:161:PHE:CD1	19:1:1189:CLA:CBB	2.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:10:GLU:OE1	10:F:11:SER:N	2.33	0.61
4:4:104:ARG:HA	4:4:107:GLN:HB2	1.83	0.61
4:4:40:PHE:CA	4:4:43:ALA:CB	2.79	0.61
19:B:1762:CLA:HBC2	19:B:1762:CLA:CHD	2.20	0.61
6:B:433:THR:O	6:B:436:LEU:O	2.17	0.61
19:B:1772:CLA:H191	13:I:21:MET:HB2	1.83	0.61
19:1:1145:CLA:CAD	19:1:1145:CLA:CED	2.75	0.61
20:A:7050:LMU:H101	20:A:7050:LMU:H32	1.39	0.61
5:A:337:PRO:CD	19:A:1798:CLA:HHC	2.31	0.61
6:B:98:GLN:C	6:B:100:ALA:N	2.53	0.61
5:A:261:SER:O	5:A:262:PHE:CD2	2.54	0.61
4:4:143:PHE:CB	4:4:150:LYS:HE2	2.29	0.61
5:A:105:ASN:HB2	5:A:140:PHE:HZ	1.66	0.61
5:A:308:ILE:HG21	19:A:1772:CLA:HMC2	1.83	0.61
5:A:207:LEU:HB3	19:A:1776:CLA:HBB2	1.83	0.61
5:A:711:HIS:NE2	19:A:1795:CLA:CBC	2.62	0.61
6:B:127:ILE:HG12	6:B:193:HIS:HE1	1.65	0.61
7:C:1:MET:H2	7:C:3:HIS:H	1.42	0.61
8:D:102:ARG:NH2	8:D:109:VAL:O	2.33	0.61
11:G:37:GLU:OE2	11:G:42:SER:CA	2.49	0.61
17:N:57:LYS:O	17:N:60:PHE:N	2.33	0.61
18:R:35:UNK:C	18:R:38:UNK:CB	2.79	0.61
15:K:17:LEU:HG	15:K:56:THR:CB	2.30	0.61
5:A:582:ASP:HB3	5:A:589:THR:HG22	1.81	0.61
4:4:37:LEU:O	4:4:39:TRP:CG	2.53	0.61
19:A:1796:CLA:H43	19:A:1796:CLA:NC	2.15	0.61
19:A:1771:CLA:HBB1	22:A:1802:BCR:C13	2.31	0.61
19:B:1772:CLA:HMC3	19:B:1788:CLA:HMB3	1.83	0.61
6:B:310:PRO:HB2	6:B:311:PRO:CD	2.31	0.61
6:B:371:LEU:HD21	19:B:1759:CLA:HED3	1.82	0.61
6:B:668:ARG:HG3	6:B:700:LEU:O	2.00	0.61
22:B:1779:BCR:C39	10:F:90:PHE:HA	2.31	0.61
14:J:2:ARG:HB3	14:J:7:TYR:CZ	2.36	0.61
17:N:65:LEU:HD21	17:N:66:ASP:O	2.00	0.61
20:B:1783:LMU:H5'	20:B:1783:LMU:O5B	2.01	0.61
17:N:1:GLY:C	17:N:2:VAL:HG13	2.21	0.61
2:2:187:GLY:O	2:2:188:PRO:C	2.38	0.61
5:A:170:GLY:C	5:A:173:VAL:HG22	2.20	0.61
19:A:1799:CLA:H112	19:A:1799:CLA:H61	1.81	0.61
5:A:358:LEU:HD21	5:A:413:HIS:ND1	2.15	0.61
6:B:212:PHE:CZ	19:B:1745:CLA:HAC1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1748:CLA:HBD	19:B:1757:CLA:CBB	2.30	0.61
19:B:1763:CLA:H71	22:B:1780:BCR:H402	1.83	0.61
22:I:1032:BCR:H382	22:I:1032:BCR:C40	2.31	0.61
17:N:39:SER:O	17:N:40:CYS:CB	2.48	0.61
20:A:7048:LMU:H31	20:A:7048:LMU:H3'	1.81	0.61
4:4:194:VAL:CG1	4:4:195:GLN:HB3	2.30	0.61
10:F:20:GLN:O	10:F:21:ALA:HB2	2.01	0.61
2:2:159:LEU:O	2:2:160:ARG:C	2.39	0.61
19:A:1781:CLA:HAA2	19:A:1782:CLA:CAD	2.31	0.61
19:A:1781:CLA:HMA1	22:A:1805:BCR:H16C	1.81	0.61
5:A:229:ILE:CG2	5:A:229:ILE:O	2.48	0.61
5:A:281:LEU:HD22	19:A:1772:CLA:HMA3	1.83	0.61
5:A:84:GLY:O	5:A:87:SER:O	2.18	0.61
6:B:124:TRP:C	6:B:124:TRP:CD1	2.73	0.61
6:B:130:ARG:CG	6:B:130:ARG:HH11	2.13	0.61
6:B:143:LEU:C	6:B:145:LEU:H	2.03	0.61
6:B:290:MET:HG3	19:B:1752:CLA:C2C	2.31	0.61
6:B:623:TYR:O	6:B:624:LEU:HB2	1.99	0.61
14:J:20:GLY:O	14:J:21:SER:HB2	2.01	0.61
17:N:73:ASP:N	17:N:73:ASP:OD1	2.32	0.61
17:N:72:LYS:HZ3	17:N:74:LYS:CG	2.02	0.61
8:D:84:LEU:HD12	8:D:100:PHE:HZ	1.65	0.61
6:B:456:GLU:OE1	10:F:70:HIS:ND1	2.33	0.61
9:E:73:ASN:ND2	9:E:75:ALA:H	1.99	0.61
17:N:5:GLU:CD	17:N:6:TYR:CD2	2.74	0.61
18:R:4:UNK:O	18:R:5:UNK:CB	2.49	0.61
2:2:79:TRP:CD1	2:2:81:THR:CG2	2.84	0.61
5:A:527:VAL:CG1	5:A:528:ALA:N	2.64	0.61
2:2:98:GLU:OE2	19:2:1223:CLA:ND	2.33	0.61
2:2:37:ASP:OD2	3:3:41:ASP:CB	2.49	0.61
4:4:94:GLU:HG2	4:4:95:PHE:CG	2.35	0.61
19:A:1787:CLA:C4	16:L:33:ILE:HG12	2.30	0.61
5:A:389:TYR:HE1	5:A:625:TRP:CD1	2.19	0.61
5:A:581:CYS:CB	5:A:590:CYS:O	2.49	0.61
6:B:289:LEU:HD21	19:B:1751:CLA:NA	2.16	0.61
6:B:459:PHE:O	6:B:463:ILE:HD13	2.01	0.61
5:A:705:GLU:HG2	6:B:545:LYS:HZ2	1.66	0.61
6:B:707:LEU:HD12	6:B:711:VAL:HG21	1.81	0.61
8:D:46:TYR:CD2	8:D:46:TYR:N	2.69	0.61
6:B:231:ASN:OD1	11:G:5:SER:HB2	2.01	0.61
5:A:249:ILE:CG1	5:A:250:LEU:N	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:28:MET:HB3	8:D:122:LYS:O	2.00	0.61
2:2:85:GLN:OE1	2:2:86:GLU:N	2.34	0.61
1:1:183:ASP:OD1	4:4:89:THR:HB	2.01	0.60
19:4:1196:CLA:HBC3	19:4:1196:CLA:CHD	2.24	0.60
5:A:123:VAL:O	5:A:124:TRP:HB2	2.01	0.60
19:A:1783:CLA:C17	22:A:1807:BCR:H17C	2.30	0.60
5:A:394:SER:HB2	19:A:1783:CLA:CMA	2.20	0.60
5:A:39:HIS:O	5:A:40:PHE:HB3	2.01	0.60
6:B:534:LEU:HD21	6:B:579:ALA:CB	2.31	0.60
6:B:295:PHE:HE2	11:G:38:GLN:NE2	1.99	0.60
2:2:128:ASN:ND2	14:J:4:PHE:H	1.97	0.60
16:L:46:ALA:HB2	16:L:52:ARG:NH2	2.16	0.60
19:1:1146:CLA:CBC	19:1:1146:CLA:HMC1	2.20	0.60
8:D:117:GLY:O	8:D:118:VAL:CG2	2.39	0.60
3:3:106:TYR:CD1	3:3:107:TRP:N	2.68	0.60
12:H:39:PHE:O	12:H:40:PHE:CD1	2.54	0.60
13:I:2:ILE:HG12	13:I:3:ASN:ND2	2.16	0.60
2:2:128:ASN:CG	2:2:130:LEU:HB2	2.21	0.60
5:A:360:ILE:O	5:A:361:ASN:HB3	2.01	0.60
5:A:446:LEU:CD1	5:A:554:LEU:HA	2.30	0.60
6:B:275:HIS:HD1	19:B:1748:CLA:HMB1	1.64	0.60
19:B:1754:CLA:C1	19:B:1754:CLA:HAA1	2.31	0.60
19:B:1759:CLA:C14	22:B:1777:BCR:H10C	2.25	0.60
6:B:555:TYR:O	6:B:571:SER:HB2	2.01	0.60
6:B:632:ILE:C	6:B:634:GLY:H	2.04	0.60
7:C:74:THR:C	7:C:76:SER:H	2.01	0.60
9:E:39:LEU:H	9:E:40:ARG:CZ	2.14	0.60
9:E:37:LYS:HB2	9:E:49:VAL:HG22	1.81	0.60
4:4:70:ILE:O	4:4:73:PRO:HD2	2.00	0.60
16:L:161:LEU:CD1	16:L:162:ASP:HA	2.16	0.60
1:1:32:VAL:HG21	19:1:1197:CLA:ND	2.16	0.60
1:1:185:TRP:HE3	1:1:185:TRP:CA	2.12	0.60
2:2:37:ASP:CG	2:2:38:PRO:HD3	2.21	0.60
2:2:68:LEU:O	2:2:70:LYS:N	2.35	0.60
19:A:1786:CLA:HMB2	19:A:1787:CLA:C2D	2.30	0.60
19:A:1779:CLA:HBC1	22:A:1804:BCR:C39	2.31	0.60
6:B:348:VAL:HG12	6:B:349:ALA:N	2.16	0.60
20:A:7016:LMU:H92	20:A:7016:LMU:H32	1.77	0.60
19:1:1308:CLA:C1	19:1:1308:CLA:O1D	2.47	0.60
3:3:64:TYR:CB	19:3:1222:CLA:C4	2.73	0.60
15:K:51:ASP:OD1	15:K:55:PHE:CD1	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:71:VAL:O	11:G:73:ALA:O	2.19	0.60
4:4:107:GLN:O	19:4:1196:CLA:HMA3	1.82	0.60
4:4:36:ASN:O	4:4:38:ARG:NH1	2.35	0.60
19:A:1781:CLA:H61	19:A:1782:CLA:HED2	1.83	0.60
5:A:154:ARG:NH2	5:A:233:LEU:HD13	2.16	0.60
5:A:346:LEU:O	5:A:347:TYR:HB2	2.02	0.60
23:A:1801:PQN:H251	19:B:1735:CLA:HMC1	1.81	0.60
5:A:466:THR:HG22	19:B:1740:CLA:HHC	1.82	0.60
16:L:124:LYS:C	16:L:126:GLN:N	2.54	0.60
20:A:7023:LMU:H21	20:A:7023:LMU:H91	0.65	0.60
18:R:39:UNK:CB	18:R:40:UNK:HA	2.31	0.60
3:3:181:LEU:N	3:3:182:LYS:CD	2.64	0.60
1:1:160:GLY:CA	19:1:1189:CLA:HBB2	2.31	0.60
6:B:500:ALA:HB2	6:B:508:LEU:HD22	1.83	0.60
2:2:103:GLY:HA2	19:2:1222:CLA:CBB	2.32	0.60
2:2:73:ILE:HD13	2:2:75:ASN:HA	1.82	0.60
19:A:1781:CLA:CAA	19:A:1781:CLA:HED2	2.31	0.60
19:A:1783:CLA:H172	22:A:1807:BCR:C17	2.31	0.60
5:A:295:TRP:HB2	5:A:298:ASP:OD2	2.01	0.60
19:B:1739:CLA:C14	19:B:1739:CLA:H102	2.30	0.60
6:B:493:TRP:CB	19:B:1766:CLA:HED2	2.31	0.60
6:B:392:ILE:HG12	6:B:555:TYR:CD1	2.36	0.60
6:B:559:CYS:HB2	6:B:702:ILE:HD12	1.82	0.60
13:I:10:PRO:O	13:I:15:LEU:N	2.34	0.60
22:3:1225:BCR:C23	22:3:1225:BCR:C39	2.37	0.60
21:B:8056:SUC:H1	21:B:8056:SUC:C5'	2.31	0.60
15:K:17:LEU:HD23	15:K:21:ALA:HB2	1.84	0.60
10:F:151:ASP:OD2	10:F:154:PHE:CD1	2.54	0.60
9:E:48:ASN:ND2	9:E:71:LYS:HZ2	1.99	0.60
19:A:1765:CLA:HMC1	19:A:1765:CLA:HBC3	1.82	0.60
5:A:452:PHE:CD1	19:A:1793:CLA:HBB2	2.36	0.60
19:A:1779:CLA:NC	22:A:1804:BCR:C19	2.56	0.60
6:B:212:PHE:HZ	19:B:1745:CLA:HAC1	1.67	0.60
6:B:569:ASP:HB3	6:B:574:ASP:HB3	1.84	0.60
6:B:646:TRP:O	6:B:649:MET:HB2	2.01	0.60
8:D:79:ARG:H	8:D:82:GLN:NE2	2.00	0.60
7:C:62:PHE:CE1	9:E:42:GLU:HB2	2.37	0.60
11:G:34:GLN:O	11:G:35:VAL:C	2.39	0.60
11:G:42:SER:OG	11:G:44:PHE:N	2.35	0.60
11:G:45:GLU:O	11:G:46:ALA:CB	2.49	0.60
16:L:33:ILE:CD1	16:L:36:TYR:HD1	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7050:LMU:O3'	20:A:7050:LMU:H6'2	2.00	0.60
9:E:72:VAL:O	9:E:73:ASN:CB	2.39	0.60
8:D:86:LEU:C	8:D:90:LEU:HB3	2.22	0.60
6:B:488:ALA:HB1	19:B:1767:CLA:C1C	2.32	0.60
4:4:128:ALA:O	4:4:130:GLU:HG2	2.02	0.60
5:A:389:TYR:CE1	5:A:625:TRP:CD1	2.89	0.60
19:B:1769:CLA:C12	22:B:1780:BCR:H312	2.32	0.60
6:B:661:PHE:CB	19:B:1788:CLA:HMC1	2.31	0.60
6:B:194:LEU:O	6:B:198:ALA:HB3	2.01	0.60
6:B:551:LYS:CG	6:B:552:ASP:H	2.14	0.60
6:B:593:TYR:O	6:B:596:TRP:O	2.18	0.60
22:3:1225:BCR:H321	22:3:1225:BCR:HC8	1.84	0.60
16:L:9:GLN:C	16:L:11:ILE:H	2.04	0.60
2:2:124:ILE:HG22	2:2:129:LYS:HB3	1.83	0.60
4:4:109:ILE:HG22	4:4:120:ILE:HG23	1.84	0.60
4:4:94:GLU:CB	4:4:95:PHE:HE1	1.89	0.60
5:A:131:ILE:CG2	5:A:132:LEU:N	2.65	0.60
19:A:1790:CLA:H2A	19:A:1790:CLA:O1D	2.00	0.60
19:A:1787:CLA:H92	19:A:1800:CLA:H2	1.82	0.60
5:A:98:PHE:O	5:A:99:HIS:CB	2.49	0.60
6:B:625:TRP:CE3	6:B:626:LEU:N	2.69	0.60
9:E:41:ARG:HG3	9:E:46:PHE:CZ	2.37	0.60
2:2:128:ASN:HD21	14:J:4:PHE:H	1.50	0.60
2:2:203:THR:O	2:2:204:ILE:CB	2.48	0.60
18:R:35:UNK:N	18:R:38:UNK:CB	2.65	0.60
20:A:7016:LMU:C7	20:A:7016:LMU:C3	2.75	0.60
19:J:1043:CLA:H141	19:J:1044:CLA:HMB3	1.83	0.60
15:K:1:ASP:CA	15:K:5:SER:HB3	2.25	0.60
9:E:56:ASP:HB2	9:E:64:PRO:CB	2.28	0.60
6:B:154:TRP:CD1	6:B:158:GLN:CG	2.85	0.60
2:2:209:THR:HG23	2:2:209:THR:O	2.02	0.60
17:N:28:ASN:HA	17:N:30:ALA:H	1.66	0.60
2:2:129:LYS:HA	2:2:131:THR:HG23	1.84	0.60
19:A:1780:CLA:H112	19:A:1780:CLA:OBD	2.01	0.60
19:A:1783:CLA:C4	19:A:1783:CLA:HBA1	2.29	0.60
5:A:499:ALA:HB3	19:A:1790:CLA:O2D	2.02	0.60
19:A:1770:CLA:CMB	22:A:1802:BCR:H382	2.19	0.60
5:A:334:HIS:HB3	19:A:1777:CLA:HMA1	1.83	0.60
19:B:1742:CLA:HBD	19:B:1742:CLA:O2A	2.01	0.60
6:B:374:HIS:HB2	19:B:1758:CLA:C4B	2.30	0.60
6:B:353:TYR:C	6:B:355:LEU:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:357:ALA:O	6:B:358:TYR:CD1	2.54	0.60
6:B:393:PHE:CD2	6:B:397:ASP:OD1	2.47	0.60
6:B:8:PHE:O	6:B:35:ASP:CB	2.49	0.60
16:L:163:LEU:HB2	16:L:164:PRO:HG3	1.77	0.60
19:1:1192:CLA:CBC	19:1:1192:CLA:CHD	2.76	0.60
2:2:205:PHE:CE1	2:2:206:ALA:CA	2.85	0.60
11:G:93:TYR:CA	11:G:94:ASP:OD1	2.49	0.60
11:G:94:ASP:H	11:G:95:PRO:HD2	1.66	0.60
20:A:7033:LMU:C1B	20:A:7033:LMU:C6'	2.73	0.60
1:1:89:VAL:O	11:G:77:ILE:HD11	1.98	0.60
19:2:1217:CLA:CBD	19:2:1217:CLA:CBA	2.80	0.60
5:A:631:GLN:O	20:A:1808:LMU:H6E	2.02	0.60
2:2:61:GLY:O	2:2:65:PRO:CG	2.49	0.60
19:A:1765:CLA:CHA	19:A:1765:CLA:HBA2	2.31	0.60
5:A:243:PRO:O	5:A:244:LEU:O	2.19	0.60
5:A:653:LEU:HD23	19:B:1786:CLA:HBC2	1.84	0.60
5:A:693:LEU:HD11	5:A:738:TYR:CD1	2.37	0.60
6:B:657:TRP:O	6:B:660:GLY:N	2.25	0.60
6:B:666:SER:HB3	6:B:671:TRP:NE1	2.12	0.60
11:G:30:ASN:HD22	11:G:30:ASN:C	2.04	0.60
10:F:23:LYS:HB3	10:F:24:LYS:HZ3	1.67	0.60
10:F:46:MET:O	10:F:48:LYS:N	2.35	0.60
20:A:7043:LMU:H6D	20:A:7050:LMU:H3'	1.84	0.60
5:A:257:GLN:O	5:A:258:LEU:HB2	2.02	0.60
16:L:58:LEU:HD21	16:L:153:TRP:CZ2	2.37	0.60
19:2:1213:CLA:H2A	19:2:1213:CLA:O1D	2.02	0.59
19:3:1212:CLA:HBA2	19:3:1212:CLA:CMA	2.19	0.59
4:4:169:GLN:CD	19:4:1199:CLA:HAC2	2.22	0.59
5:A:110:LEU:O	5:A:113:PRO:HD3	2.02	0.59
5:A:109:TRP:HH2	5:A:154:ARG:HD3	1.66	0.59
5:A:174:PHE:O	5:A:175:ALA:CB	2.49	0.59
5:A:451:ILE:HD11	19:A:1788:CLA:CED	2.32	0.59
19:A:1788:CLA:CBC	19:A:1793:CLA:HBC2	2.32	0.59
5:A:472:ARG:N	5:A:473:PRO:CD	2.64	0.59
5:A:636:HIS:C	5:A:638:THR:H	2.04	0.59
5:A:684:PHE:CD2	5:A:685:VAL:N	2.69	0.59
19:B:1739:CLA:H42	19:B:1739:CLA:CHD	2.32	0.59
19:B:1750:CLA:OBD	19:B:1753:CLA:CBC	2.48	0.59
6:B:436:LEU:O	6:B:437:TYR:HB2	2.02	0.59
6:B:652:PHE:O	6:B:656:VAL:HG23	2.01	0.59
6:B:697:PRO:O	7:C:79:LEU:HD11	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:707:LEU:O	6:B:710:LEU:HB3	2.02	0.59
7:C:74:THR:O	7:C:77:MET:N	2.30	0.59
11:G:26:PHE:HB2	11:G:27:GLN:NE2	2.16	0.59
17:N:58:VAL:C	17:N:60:PHE:N	2.51	0.59
2:2:204:ILE:O	2:2:205:PHE:HB3	2.02	0.59
16:L:14:LEU:HD21	16:L:20:ILE:HG22	1.84	0.59
5:A:535:GLY:O	5:A:539:PHE:HB2	2.01	0.59
3:3:141:GLN:HG2	3:3:142:TYR:N	2.16	0.59
2:2:41:LEU:O	2:2:42:ARG:HD3	2.01	0.59
4:4:103:ILE:O	4:4:107:GLN:HB2	2.02	0.59
5:A:165:TYR:O	5:A:165:TYR:CD2	2.55	0.59
5:A:309:LEU:HA	5:A:312:ILE:O	2.01	0.59
5:A:42:ARG:C	5:A:44:ILE:N	2.55	0.59
5:A:491:TRP:HE1	19:A:1792:CLA:C1	2.15	0.59
5:A:604:TRP:HE1	19:B:1788:CLA:C1D	2.15	0.59
5:A:737:HIS:HA	5:A:740:LEU:HD23	1.83	0.59
19:B:1788:CLA:HED3	19:B:1788:CLA:HBA2	1.84	0.59
6:B:187:SER:O	6:B:188:LEU:C	2.39	0.59
4:4:76:TYR:C	4:4:76:TYR:CD1	2.72	0.59
12:H:25:GLY:C	12:H:27:ASP:N	2.37	0.59
19:4:4007:CLA:C2	19:4:4007:CLA:HED3	2.31	0.59
5:A:755:ILE:O	5:A:756:ALA:CB	2.50	0.59
5:A:218:TRP:CA	19:A:1770:CLA:HBB2	2.31	0.59
22:A:1806:BCR:H322	22:A:1807:BCR:H391	1.84	0.59
19:A:1812:CLA:CGA	19:A:1812:CLA:H3A	2.32	0.59
5:A:373:ALA:O	5:A:396:PHE:CD1	2.54	0.59
5:A:678:PHE:O	5:A:680:LEU:N	2.35	0.59
5:A:708:VAL:CA	5:A:711:HIS:HD2	2.16	0.59
19:B:1738:CLA:C19	19:B:1758:CLA:H141	2.32	0.59
22:B:1782:BCR:H392	19:I:1031:CLA:C14	2.32	0.59
6:B:400:PRO:HD2	8:D:143:PRO:HD3	1.85	0.59
16:L:36:TYR:OH	19:L:1167:CLA:HBA2	2.02	0.59
17:N:39:SER:OG	17:N:41:LYS:HA	2.02	0.59
20:A:7032:LMU:C4B	20:A:7032:LMU:H31	2.33	0.59
15:K:7:THR:HA	15:K:10:ILE:CG1	2.32	0.59
21:B:8053:SUC:C5	21:B:8053:SUC:O2	2.48	0.59
20:A:7030:LMU:H2'	20:A:7030:LMU:H6E	1.82	0.59
6:B:482:ASN:OD1	6:B:485:ALA:HB2	2.01	0.59
8:D:58:PHE:HD2	8:D:59:GLU:H	1.47	0.59
17:N:33:TYR:O	17:N:34:THR:CG2	2.50	0.59
1:1:161:PHE:N	19:1:1189:CLA:CBB	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:185:TRP:HB2	1:1:186:HIS:NE2	2.14	0.59
19:A:1779:CLA:C1B	22:A:1804:BCR:H15C	2.33	0.59
5:A:746:THR:OG1	19:A:1810:CLA:O1D	2.20	0.59
5:A:230:ASN:HA	5:A:233:LEU:HB2	1.84	0.59
5:A:413:HIS:ND1	5:A:416:ILE:HD12	2.17	0.59
6:B:670:TYR:OH	19:B:1788:CLA:CAD	2.50	0.59
6:B:53:GLN:HA	6:B:53:GLN:OE1	1.91	0.59
20:A:7021:LMU:C4	20:A:7021:LMU:C6'	2.75	0.59
19:1:1193:CLA:HAA2	19:1:1193:CLA:CGD	2.32	0.59
6:B:498:LEU:HD12	6:B:498:LEU:O	2.02	0.59
2:2:43:TRP:CZ3	2:2:125:PHE:HB2	2.37	0.59
2:2:42:ARG:C	2:2:44:ASN:N	2.52	0.59
2:2:97:VAL:HA	2:2:100:VAL:CG1	2.33	0.59
5:A:302:HIS:HB2	19:A:1773:CLA:CHB	2.31	0.59
5:A:455:PHE:HD1	19:A:1788:CLA:HMA2	1.67	0.59
5:A:547:PHE:HE2	19:B:1788:CLA:O1A	1.86	0.59
19:B:1758:CLA:HBC3	19:B:1758:CLA:HMC1	1.85	0.59
6:B:412:LEU:O	6:B:415:LYS:HB3	2.03	0.59
6:B:557:PHE:CD1	6:B:571:SER:HB3	2.37	0.59
6:B:727:ALA:C	6:B:728:SER:OG	2.40	0.59
10:F:103:SER:O	10:F:105:LEU:N	2.34	0.59
11:G:64:VAL:O	11:G:64:VAL:HG12	2.02	0.59
5:A:478:SER:HB3	5:A:644:GLN:CD	2.21	0.59
7:C:49:VAL:HG22	7:C:50:GLY:H	1.68	0.59
14:J:32:PHE:HE2	14:J:33:PHE:CZ	2.21	0.59
16:L:135:GLY:O	16:L:138:LYS:HG2	2.02	0.59
2:2:127:ASN:O	2:2:128:ASN:HB2	2.02	0.59
2:2:50:VAL:O	2:2:54:TRP:CD1	2.44	0.59
6:B:661:PHE:CB	19:B:1788:CLA:CMC	2.80	0.59
6:B:282:PHE:HE2	19:B:1747:CLA:H3A	1.66	0.59
6:B:594:TRP:C	6:B:594:TRP:HD1	2.06	0.59
6:B:707:LEU:HD11	6:B:711:VAL:HG21	1.84	0.59
6:B:715:VAL:O	6:B:716:GLY:C	2.40	0.59
6:B:295:PHE:CE2	11:G:38:GLN:NE2	2.71	0.59
14:J:26:LEU:HD23	14:J:26:LEU:O	2.02	0.59
17:N:62:SER:O	17:N:66:ASP:CG	2.40	0.59
19:1:1142:CLA:HMD3	19:K:1085:CLA:ND	2.17	0.59
8:D:111:TYR:CD2	8:D:114:PRO:CB	2.84	0.59
19:4:1206:CLA:C19	19:4:1206:CLA:H152	2.22	0.59
2:2:198:ALA:O	2:2:199:ASP:CB	2.50	0.59
6:B:409:ALA:C	6:B:411:MET:N	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:115:GLU:HG3	1:1:116:LYS:H	1.67	0.59
19:2:1218:CLA:C1B	19:2:1218:CLA:H2	2.32	0.59
4:4:118:ASP:CA	4:4:123:GLN:N	2.60	0.59
4:4:36:ASN:O	4:4:39:TRP:CD2	2.56	0.59
19:A:1760:CLA:H12	19:A:1767:CLA:H92	1.83	0.59
19:A:1773:CLA:H52	19:A:1790:CLA:HBA1	1.84	0.59
5:A:370:ILE:CD1	19:A:1781:CLA:C3D	2.78	0.59
5:A:432:LEU:C	5:A:434:ARG:N	2.55	0.59
19:B:1739:CLA:CGA	19:B:1739:CLA:C1A	2.81	0.59
19:B:1788:CLA:HMC1	19:B:1788:CLA:HBC3	1.85	0.59
6:B:50:HIS:HA	6:B:53:GLN:HB2	1.85	0.59
6:B:557:PHE:HE2	7:C:66:ARG:HE	1.48	0.59
19:G:1099:CLA:CED	19:G:1099:CLA:CAD	2.79	0.59
22:L:1170:BCR:C8	22:L:1170:BCR:C33	2.73	0.59
5:A:259:TYR:HB3	5:A:260:PRO:CD	2.30	0.59
3:3:90:LEU:HD12	3:3:90:LEU:H	1.67	0.59
6:B:154:TRP:CD1	6:B:158:GLN:HG2	2.38	0.59
1:1:34:ALA:HB3	1:1:137:PRO:HB3	1.85	0.59
2:2:45:VAL:O	2:2:45:VAL:HG12	2.01	0.59
2:2:50:VAL:CG1	2:2:50:VAL:O	2.50	0.59
4:4:116:ASN:O	4:4:123:GLN:HG3	2.03	0.59
5:A:122:VAL:HG22	5:A:142:GLY:HA2	1.84	0.59
5:A:368:LEU:HD12	19:A:1782:CLA:C6	2.33	0.59
22:A:1803:BCR:H403	22:A:1803:BCR:C23	2.14	0.59
5:A:309:LEU:HD23	5:A:309:LEU:C	2.23	0.59
5:A:497:ALA:O	5:A:498:LEU:HB2	2.02	0.59
5:A:502:THR:H	5:A:504:ALA:HB3	1.68	0.59
5:A:592:VAL:HG23	5:A:593:SER:H	1.66	0.59
5:A:681:GLY:HA2	5:A:684:PHE:HB3	1.84	0.59
19:B:1762:CLA:HHD	19:B:1762:CLA:HBC3	1.80	0.59
6:B:278:LEU:O	6:B:281:ALA:N	2.36	0.59
6:B:36:ASP:O	6:B:41:ARG:NE	2.36	0.59
6:B:442:VAL:HG21	19:B:1764:CLA:CAC	2.28	0.59
10:F:83:PHE:O	10:F:87:GLY:N	2.36	0.59
22:B:1779:BCR:H23C	10:F:90:PHE:CD1	2.38	0.59
11:G:63:PRO:HG2	19:G:1099:CLA:HMC1	1.84	0.59
18:R:37:UNK:C	18:R:42:UNK:O	2.50	0.59
5:A:22:VAL:HG12	5:A:23:ASP:H	1.65	0.59
5:A:23:ASP:CB	5:A:24:ARG:HD3	2.29	0.59
20:A:7037:LMU:C7	20:A:7037:LMU:C3	2.30	0.59
3:3:86:GLN:HB2	3:3:88:THR:CB	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:21:TRP:N	12:H:22:ASP:CA	2.61	0.59
20:A:7050:LMU:C10	20:A:7050:LMU:H31	2.13	0.59
15:K:17:LEU:CG	15:K:56:THR:OG1	2.38	0.59
6:B:261:PHE:CZ	6:B:500:ALA:HB2	2.38	0.59
2:2:39:GLU:N	2:2:40:SER:CA	2.66	0.59
2:2:57:LEU:HD23	2:2:58:GLY:N	2.18	0.59
4:4:104:ARG:HE	4:4:105:ARG:CA	2.16	0.59
4:4:121:PHE:O	4:4:143:PHE:CD2	2.55	0.59
19:A:1773:CLA:HBC3	19:A:1773:CLA:HMC1	1.83	0.59
20:A:7006:LMU:C5B	20:A:7006:LMU:H3'	2.33	0.59
6:B:310:PRO:CB	6:B:311:PRO:CD	2.81	0.59
6:B:732:LYS:CG	6:B:733:PHE:HA	2.22	0.59
5:A:567:ARG:NH2	8:D:82:GLN:OE1	2.34	0.59
19:B:1769:CLA:CBC	10:F:83:PHE:CZ	2.84	0.59
4:4:70:ILE:CG1	4:4:71:ASN:H	2.16	0.59
17:N:53:ALA:O	17:N:54:LYS:CD	2.51	0.59
17:N:72:LYS:N	17:N:72:LYS:HD3	2.18	0.59
3:3:194:ILE:HG23	3:3:197:TYR:OH	2.02	0.59
20:A:7033:LMU:H2O2	20:A:7033:LMU:C6B	2.14	0.59
19:3:1222:CLA:O1D	19:3:1222:CLA:HAA2	2.03	0.59
21:B:8062:SUC:O6	21:B:8062:SUC:C2'	2.50	0.59
20:R:1056:LMU:H1B	20:R:1056:LMU:H6B	1.63	0.59
6:B:454:LEU:N	6:B:454:LEU:HD12	2.18	0.59
8:D:61:PRO:HD3	8:D:86:LEU:HD21	1.85	0.59
4:4:49:ARG:O	4:4:53:LEU:CD1	2.51	0.59
2:2:98:GLU:HG3	2:2:99:LEU:HD12	1.85	0.59
5:A:210:LEU:HD13	19:A:1769:CLA:HHB	1.85	0.59
19:A:1783:CLA:H18	19:A:1811:CLA:H18	1.85	0.59
5:A:193:LEU:O	5:A:194:ALA:C	2.41	0.59
5:A:44:ILE:O	5:A:46:LYS:HA	2.03	0.59
5:A:500:PRO:HB3	5:A:506:GLY:HA2	1.85	0.59
5:A:555:ILE:CG2	19:B:1788:CLA:OBD	2.50	0.59
5:A:98:PHE:HD1	5:A:99:HIS:HD2	1.50	0.59
19:B:1738:CLA:H191	19:B:1758:CLA:H141	1.85	0.59
9:E:40:ARG:HH22	9:E:87:VAL:HG22	1.68	0.59
19:1:1241:CLA:CHD	22:I:1032:BCR:HC22	2.33	0.59
14:J:26:LEU:HA	14:J:29:ILE:HG22	1.85	0.59
16:L:40:LEU:CB	16:L:41:PRO:CD	2.81	0.59
11:G:93:TYR:C	11:G:95:PRO:HD3	2.22	0.59
16:L:50:LEU:HG	16:L:51:LEU:HD23	1.85	0.59
2:2:38:PRO:O	2:2:40:SER:CB	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:588:GLY:N	6:B:668:ARG:NH1	2.50	0.58
6:B:277:HIS:HE1	19:B:1749:CLA:NC	2.01	0.58
19:B:1738:CLA:H71	24:B:1784:LMG:H381	1.84	0.58
6:B:551:LYS:O	6:B:553:PHE:CD2	2.56	0.58
6:B:694:ARG:HE	16:L:105:ALA:HA	1.67	0.58
16:L:45:THR:HA	16:L:52:ARG:HH12	1.66	0.58
19:1:1308:CLA:O1D	19:1:1308:CLA:H2A	2.03	0.58
4:4:192:THR:HG22	4:4:194:VAL:C	2.23	0.58
20:A:7037:LMU:H61	20:A:7037:LMU:C2	2.33	0.58
10:F:40:LEU:CA	10:F:42:ILE:HG12	2.30	0.58
19:1:1505:CLA:C10	19:1:1505:CLA:H41	2.33	0.58
19:2:1215:CLA:HBC2	19:2:1215:CLA:HMC1	1.84	0.58
2:2:57:LEU:O	2:2:60:ALA:CB	2.51	0.58
19:4:1196:CLA:H2A	19:4:1196:CLA:O1D	2.03	0.58
19:4:1198:CLA:O1A	19:4:1198:CLA:H2	2.01	0.58
4:4:38:ARG:CG	4:4:39:TRP:H	2.06	0.58
5:A:308:ILE:HD12	19:A:1772:CLA:C8	2.34	0.58
19:A:1776:CLA:C3C	19:A:1782:CLA:C17	2.75	0.58
19:A:1782:CLA:HBA2	22:A:1805:BCR:H12C	1.85	0.58
5:A:396:PHE:O	5:A:396:PHE:CG	2.55	0.58
5:A:625:TRP:HB3	5:A:637:ILE:HD11	1.84	0.58
5:A:651:GLY:O	5:A:655:ASP:N	2.36	0.58
19:B:1769:CLA:C6	22:B:1780:BCR:H323	2.32	0.58
6:B:376:GLN:HA	6:B:376:GLN:OE1	2.03	0.58
14:J:13:VAL:HG12	14:J:15:SER:HB2	1.85	0.58
17:N:63:ASP:N	17:N:64:ASP:CA	2.54	0.58
19:J:1044:CLA:H93	19:J:1044:CLA:C4	2.33	0.58
6:B:70:TRP:NE1	6:B:71:GLN:OE1	2.36	0.58
2:2:181:HIS:CE1	19:2:1214:CLA:CHA	2.86	0.58
6:B:156:HIS:O	6:B:163:PRO:HB3	2.03	0.58
4:4:183:GLN:HG2	4:4:183:GLN:O	2.03	0.58
4:4:67:ILE:HG22	4:4:67:ILE:O	2.02	0.58
19:3:1212:CLA:HBC3	19:A:1770:CLA:C2D	2.33	0.58
4:4:81:GLU:O	4:4:82:GLU:HB3	2.03	0.58
5:A:163:GLN:O	5:A:166:CYS:N	2.36	0.58
19:A:1787:CLA:H93	16:L:36:TYR:CE1	2.37	0.58
22:A:1806:BCR:H312	19:A:1812:CLA:C14	2.17	0.58
19:B:1756:CLA:CHB	19:B:1770:CLA:HAA2	2.33	0.58
6:B:415:LYS:CE	6:B:539:LEU:O	2.50	0.58
7:C:7:ILE:O	7:C:60:THR:HA	2.03	0.58
9:E:36:VAL:CG2	9:E:52:VAL:HG22	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:75:TRP:CD1	19:4:1205:CLA:C1D	2.86	0.58
3:3:157:ALA:O	3:3:158:TYR:HB2	2.02	0.58
10:F:151:ASP:CA	10:F:154:PHE:HB3	2.33	0.58
20:A:7013:LMU:H41	20:A:7013:LMU:H1'	1.84	0.58
4:4:49:ARG:O	4:4:53:LEU:HD12	2.02	0.58
8:D:31:GLY:O	8:D:32:SER:CB	2.52	0.58
2:2:51:HIS:C	2:2:54:TRP:HB2	2.24	0.58
19:A:1796:CLA:C10	19:A:1812:CLA:H152	2.33	0.58
5:A:225:VAL:HG12	5:A:248:PHE:CD1	2.39	0.58
5:A:298:ASP:OD2	5:A:298:ASP:N	2.37	0.58
19:B:1755:CLA:H61	19:B:1755:CLA:HMA2	1.84	0.58
6:B:186:SER:C	6:B:187:SER:O	2.42	0.58
6:B:193:HIS:HB2	19:B:1745:CLA:CHC	2.33	0.58
5:A:705:GLU:CB	6:B:545:LYS:NZ	2.66	0.58
7:C:1:MET:SD	7:C:4:SER:HB2	2.43	0.58
6:B:551:LYS:CD	8:D:143:PRO:HA	2.34	0.58
9:E:51:SER:O	9:E:68:ARG:N	2.27	0.58
9:E:69:PHE:CD2	9:E:71:LYS:HG2	2.38	0.58
4:4:62:GLU:C	4:4:65:THR:HG22	2.24	0.58
5:A:112:ASP:O	5:A:116:ILE:HG12	2.02	0.58
19:A:1763:CLA:C1	19:A:1765:CLA:HED1	2.31	0.58
19:A:1796:CLA:H192	14:J:19:PHE:CD2	2.39	0.58
5:A:184:PHE:CE2	19:A:1766:CLA:C2D	2.87	0.58
5:A:390:ALA:CB	5:A:754:ILE:HD13	2.33	0.58
5:A:473:PRO:O	5:A:475:ASP:N	2.36	0.58
5:A:284:ARG:HH22	5:A:507:ALA:C	2.06	0.58
5:A:40:PHE:CE1	5:A:53:TRP:HD1	2.16	0.58
5:A:704:ILE:HA	5:A:707:ILE:HG13	1.85	0.58
6:B:615:TYR:HD1	6:B:615:TYR:N	2.01	0.58
8:D:45:PHE:C	8:D:46:TYR:HD2	2.06	0.58
11:G:33:LYS:CA	11:G:33:LYS:CE	2.61	0.58
3:3:52:LYS:N	3:3:55:ALA:HB3	2.19	0.58
19:1:1308:CLA:CBA	19:1:1308:CLA:CGD	2.81	0.58
6:B:481:THR:O	6:B:482:ASN:HB2	2.03	0.58
8:D:31:GLY:HA2	16:L:13:PRO:CB	2.34	0.58
4:4:126:LEU:HD23	4:4:127:PRO:HG3	1.86	0.58
4:4:154:ILE:CG1	4:4:155:ALA:N	2.56	0.58
4:4:163:PHE:O	4:4:164:LEU:C	2.40	0.58
5:A:157:GLY:O	5:A:158:ILE:HB	2.04	0.58
5:A:218:TRP:HA	19:A:1770:CLA:HBB2	1.85	0.58
5:A:239:PRO:CA	5:A:242:ILE:HD11	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:55:ALA:HB1	6:B:150:LEU:HD11	1.84	0.58
6:B:276:HIS:HB2	19:B:1748:CLA:C1B	2.33	0.58
19:B:1759:CLA:C17	22:B:1776:BCR:H363	2.34	0.58
6:B:421:HIS:CE1	19:B:1762:CLA:C4D	2.86	0.58
6:B:662:MET:HG2	23:B:1774:PQN:O1	2.03	0.58
6:B:710:LEU:C	6:B:712:HIS:N	2.55	0.58
7:C:6:LYS:N	7:C:65:VAL:HG22	2.19	0.58
10:F:78:ARG:O	10:F:80:TRP:HD1	1.86	0.58
13:I:28:VAL:O	13:I:29:GLU:CD	2.42	0.58
19:1:1148:CLA:H12	19:1:1148:CLA:HED1	1.78	0.58
5:A:22:VAL:HG13	5:A:23:ASP:N	2.19	0.58
19:3:1224:CLA:H142	19:3:1224:CLA:H102	1.64	0.58
2:2:211:LYS:HG2	3:3:113:LEU:CD1	2.31	0.58
9:E:48:ASN:ND2	9:E:71:LYS:HZ1	2.02	0.58
2:2:42:ARG:HG3	2:2:45:VAL:HB	1.85	0.58
2:2:65:PRO:O	2:2:66:GLU:O	2.21	0.58
4:4:158:ARG:O	4:4:159:LEU:C	2.41	0.58
4:4:90:LEU:H	4:4:90:LEU:CD2	2.16	0.58
19:A:1765:CLA:CBD	19:A:1765:CLA:HBA2	2.33	0.58
23:A:1801:PQN:H272	23:A:1801:PQN:H241	1.86	0.58
6:B:144:PHE:HD2	6:B:144:PHE:O	1.85	0.58
6:B:189:ALA:HA	19:B:1746:CLA:HBB1	1.86	0.58
19:B:1750:CLA:HBA1	19:B:1750:CLA:HBD	1.86	0.58
6:B:390:GLY:N	6:B:391:PRO:CD	2.67	0.58
6:B:458:ILE:HG13	6:B:459:PHE:N	2.16	0.58
6:B:460:ALA:O	6:B:461:GLN:C	2.42	0.58
6:B:628:SER:O	6:B:631:LEU:HD23	2.03	0.58
11:G:46:ALA:CA	11:G:48:ASP:HB3	2.33	0.58
17:N:61:LEU:HD13	17:N:63:ASP:CB	2.28	0.58
18:R:35:UNK:C	18:R:36:UNK:O	2.51	0.58
12:H:27:ASP:C	12:H:29:PRO:HD3	2.23	0.58
21:3:1226:SUC:H1'1	21:3:1226:SUC:C6'	1.98	0.58
1:1:34:ALA:HB3	1:1:137:PRO:CB	2.33	0.58
2:2:64:ILE:HD13	19:2:1213:CLA:HMB1	1.86	0.58
2:2:43:TRP:C	2:2:45:VAL:N	2.50	0.58
4:4:115:VAL:HG13	4:4:116:ASN:N	2.19	0.58
4:4:115:VAL:O	4:4:117:GLN:HG3	2.04	0.58
4:4:165:GLY:O	4:4:169:GLN:CG	2.48	0.58
19:A:1763:CLA:CBA	19:A:1763:CLA:NA	2.56	0.58
19:A:1795:CLA:OBD	10:F:105:LEU:HD11	2.03	0.58
5:A:362:LEU:HB3	5:A:406:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:592:VAL:HG23	5:A:593:SER:N	2.19	0.58
5:A:59:ALA:C	5:A:61:ALA:H	2.07	0.58
6:B:95:HIS:CE1	19:B:1740:CLA:HMB3	2.39	0.58
19:B:1760:CLA:H201	19:B:1772:CLA:HBA1	1.86	0.58
6:B:336:LEU:CD1	19:B:1755:CLA:HBB1	2.32	0.58
6:B:378:ILE:HA	6:B:381:PHE:HB2	1.84	0.58
16:L:125:LYS:C	16:L:127:PRO:HD2	2.24	0.58
1:1:25:ASP:CB	1:1:26:PRO:CD	2.81	0.58
19:1:1142:CLA:HMD3	19:K:1085:CLA:NA	2.18	0.58
6:B:224:PRO:O	6:B:226:LEU:N	2.37	0.58
5:A:195:TRP:CZ2	19:A:1766:CLA:CMA	2.83	0.58
19:A:1771:CLA:HBB1	22:A:1802:BCR:C11	2.34	0.58
5:A:701:GLN:NE2	5:A:701:GLN:HA	2.19	0.58
6:B:555:TYR:CE2	6:B:573:TRP:HA	2.39	0.58
6:B:646:TRP:CZ2	6:B:726:ILE:HG21	2.39	0.58
10:F:23:LYS:O	10:F:24:LYS:NZ	2.27	0.58
5:A:468:SER:HB2	5:A:476:MET:SD	2.44	0.58
19:4:1199:CLA:H2	19:4:1199:CLA:CED	2.34	0.58
5:A:105:ASN:HB2	5:A:140:PHE:CZ	2.39	0.58
5:A:740:LEU:HD13	19:A:1796:CLA:HMA1	1.86	0.58
19:A:1810:CLA:H192	19:B:1787:CLA:C2B	2.34	0.58
5:A:185:HIS:O	5:A:188:LYS:N	2.37	0.58
5:A:284:ARG:HG3	5:A:295:TRP:CG	2.39	0.58
5:A:154:ARG:HG3	5:A:383:PRO:HB2	1.86	0.58
5:A:51:THR:HG21	19:A:1795:CLA:CBB	2.23	0.58
5:A:470:LEU:HG	19:B:1740:CLA:HMC3	1.85	0.58
19:B:1741:CLA:HAC2	22:B:1782:BCR:H342	1.85	0.58
19:B:1754:CLA:H2	19:B:1754:CLA:H71	1.81	0.58
19:B:1760:CLA:H93	24:B:1784:LMG:H311	1.85	0.58
22:B:1782:BCR:HC41	19:B:1788:CLA:H142	1.85	0.58
6:B:178:HIS:HE1	19:B:1744:CLA:NC	2.00	0.58
6:B:305:LEU:O	6:B:306:GLU:C	2.43	0.58
6:B:649:MET:CE	6:B:723:ALA:HB2	2.34	0.58
14:J:18:TRP:CH2	14:J:22:LEU:HD22	2.39	0.58
19:1:1308:CLA:HBA2	19:1:1308:CLA:CHA	2.28	0.58
20:A:7043:LMU:C1B	20:A:7043:LMU:O3'	2.51	0.58
18:R:52:UNK:CB	18:R:53:UNK:CB	2.82	0.58
9:E:69:PHE:CD2	9:E:70:ALA:N	2.71	0.58
19:2:1213:CLA:CBC	19:2:1213:CLA:HHD	2.26	0.57
19:A:1770:CLA:HMC2	22:A:1802:BCR:C15	2.33	0.57
5:A:223:VAL:O	5:A:228:PRO:HD3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:462:ILE:HD11	19:B:1787:CLA:C5	2.29	0.57
5:A:146:THR:HG21	5:A:751:LEU:HD22	1.86	0.57
6:B:175:LEU:HA	6:B:178:HIS:HB2	1.86	0.57
6:B:722:ALA:O	6:B:726:ILE:HD12	2.04	0.57
6:B:91:ILE:HG22	19:B:1740:CLA:CAD	2.34	0.57
7:C:52:LYS:C	7:C:54:CYS:N	2.56	0.57
11:G:31:MET:O	11:G:34:GLN:N	2.35	0.57
17:N:80:ASN:C	17:N:82:PHE:N	2.58	0.57
19:J:1044:CLA:C9	19:J:1044:CLA:H151	2.32	0.57
10:F:22:LEU:O	10:F:25:LEU:HD13	2.02	0.57
19:4:4007:CLA:HED3	19:4:4007:CLA:H12	1.39	0.57
2:2:210:PRO:O	2:2:211:LYS:HB2	2.04	0.57
6:B:5:ILE:CB	6:B:6:PRO:HD2	2.31	0.57
10:F:2:ILE:HG22	10:F:3:ALA:N	2.19	0.57
1:1:185:TRP:CB	1:1:186:HIS:NE2	2.66	0.57
2:2:126:PRO:HG2	2:2:129:LYS:N	2.17	0.57
5:A:341:GLN:HB3	5:A:434:ARG:NH1	2.19	0.57
5:A:81:ALA:CB	19:A:1760:CLA:HMA3	2.28	0.57
19:B:1756:CLA:HBC3	19:B:1756:CLA:CHD	2.33	0.57
6:B:257:ILE:HA	6:B:272:ASP:OD2	2.04	0.57
6:B:266:GLN:HE21	6:B:363:GLN:HG2	1.69	0.57
6:B:510:LEU:HD22	6:B:510:LEU:H	1.69	0.57
6:B:549:ASP:OD1	7:C:63:LEU:HB3	2.05	0.57
7:C:79:LEU:HD22	7:C:81:TYR:C	2.24	0.57
17:N:48:GLY:HA3	17:N:49:CYS:C	2.14	0.57
17:N:67:LEU:CB	17:N:68:GLU:CB	2.80	0.57
18:R:38:UNK:C	18:R:42:UNK:O	2.52	0.57
20:A:7051:LMU:H31	20:A:7051:LMU:H82	1.84	0.57
5:A:316:MET:CA	5:A:317:TYR:HD1	2.16	0.57
6:B:321:GLY:O	6:B:325:THR:HG22	2.04	0.57
8:D:101:TYR:CE1	8:D:114:PRO:HD3	2.39	0.57
16:L:97:MET:HA	16:L:100:THR:HG23	1.86	0.57
20:A:7038:LMU:C10	20:A:7038:LMU:H61	2.21	0.57
3:3:162:PRO:HG2	3:3:164:PHE:CD1	2.39	0.57
2:2:77:PRO:O	17:N:3:ILE:CD1	2.52	0.57
5:A:513:LEU:HB3	5:A:529:LEU:HD13	1.85	0.57
4:4:114:SER:O	4:4:117:GLN:HG3	2.04	0.57
5:A:158:ILE:O	5:A:243:PRO:HG2	2.03	0.57
19:A:1790:CLA:C1B	22:A:1805:BCR:H333	2.34	0.57
5:A:595:TRP:HE3	5:A:596:ASP:OD2	1.87	0.57
5:A:699:TYR:HD1	5:A:700:TRP:CD1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:391:PRO:HB3	6:B:538:ALA:CA	2.34	0.57
6:B:53:GLN:O	6:B:55:ALA:N	2.33	0.57
6:B:553:PHE:O	6:B:554:GLY:C	2.41	0.57
6:B:594:TRP:CD2	6:B:598:HIS:CE1	2.93	0.57
13:I:12:VAL:HG21	19:I:1031:CLA:CGA	2.35	0.57
1:I:27:LEU:HD22	6:B:314:ARG:CG	2.14	0.57
17:N:72:LYS:CD	17:N:74:LYS:H	2.17	0.57
10:F:50:LYS:O	10:F:52:ARG:C	2.43	0.57
8:D:99:GLN:OE1	8:D:101:TYR:OH	2.21	0.57
14:J:9:SER:O	14:J:10:VAL:CB	2.52	0.57
10:F:7:PRO:HB3	10:F:60:GLY:O	2.04	0.57
5:A:464:ASN:H	5:A:464:ASN:ND2	2.01	0.57
5:A:583:GLY:O	5:A:585:GLY:N	2.37	0.57
1:I:185:TRP:C	1:I:186:HIS:HD1	2.03	0.57
5:A:146:THR:HA	5:A:391:THR:HG23	1.85	0.57
19:A:1760:CLA:CBA	19:A:1767:CLA:H62	2.34	0.57
19:A:1812:CLA:HMA1	19:A:1812:CLA:H2	1.86	0.57
5:A:328:LYS:CG	5:A:332:GLU:CB	2.59	0.57
5:A:402:ILE:C	5:A:404:GLY:H	2.07	0.57
5:A:708:VAL:O	5:A:711:HIS:HB2	2.05	0.57
6:B:351:HIS:NE2	19:B:1757:CLA:NC	2.53	0.57
6:B:486:LEU:O	6:B:487:ASN:HB3	2.05	0.57
6:B:422:LEU:CD1	6:B:535:VAL:HG11	2.27	0.57
9:E:40:ARG:CB	9:E:42:GLU:OE2	2.52	0.57
16:L:95:LEU:HD11	16:L:143:PHE:CZ	2.39	0.57
16:L:164:PRO:CB	16:L:165:TYR:HB3	2.19	0.57
17:N:52:LEU:HB3	17:N:53:ALA:CA	2.34	0.57
2:2:203:THR:HG23	2:2:204:ILE:H	1.69	0.57
19:3:1224:CLA:HBC3	19:3:1224:CLA:HMC1	0.67	0.57
15:K:5:SER:O	15:K:9:LEU:CD2	2.52	0.57
20:A:7021:LMU:H6D	20:A:7021:LMU:C4	2.34	0.57
20:A:7021:LMU:H3O1	20:A:7021:LMU:C6B	2.14	0.57
8:D:118:VAL:CG1	8:D:119:TYR:H	2.17	0.57
20:A:7005:LMU:C3	20:A:7005:LMU:H71	2.34	0.57
8:D:29:PHE:O	8:D:30:ALA:HB3	2.04	0.57
19:A:1788:CLA:HAA1	22:L:1170:BCR:C14	2.35	0.57
19:A:1779:CLA:C4B	22:A:1804:BCR:H15C	2.34	0.57
19:A:1811:CLA:C3D	19:A:1811:CLA:HED2	2.35	0.57
19:B:1740:CLA:HBB2	19:B:1787:CLA:C13	2.30	0.57
6:B:674:LEU:HD12	6:B:674:LEU:C	2.25	0.57
16:L:63:LEU:O	16:L:64:LEU:C	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:80:ASN:O	17:N:82:PHE:HD2	1.88	0.57
21:B:8052:SUC:O5	21:B:8052:SUC:H5'	2.04	0.57
19:3:1212:CLA:HBC2	19:A:1770:CLA:C4D	2.34	0.57
4:4:101:VAL:HG12	4:4:102:GLU:N	2.20	0.57
5:A:156:SER:O	5:A:158:ILE:N	2.37	0.57
19:A:1761:CLA:HMC3	19:A:1785:CLA:HMA1	1.86	0.57
19:A:1797:CLA:O2D	19:A:1797:CLA:HAA2	2.05	0.57
5:A:232:PHE:CZ	5:A:242:ILE:HG22	2.38	0.57
5:A:401:TRP:HB3	19:A:1783:CLA:HMC3	1.86	0.57
5:A:679:PHE:HE1	5:A:749:PHE:HB2	1.69	0.57
6:B:707:LEU:HD11	19:B:1760:CLA:C9	2.34	0.57
6:B:651:LEU:HB3	19:B:1787:CLA:O2A	2.05	0.57
19:B:1787:CLA:NB	19:B:1788:CLA:HBB2	2.18	0.57
6:B:378:ILE:CA	6:B:381:PHE:HB2	2.35	0.57
6:B:545:LYS:CD	6:B:546:LEU:H	2.17	0.57
6:B:551:LYS:HE2	8:D:143:PRO:HA	1.86	0.57
17:N:50:GLN:N	17:N:51:ASP:O	2.37	0.57
17:N:61:LEU:HD21	17:N:63:ASP:C	2.15	0.57
19:4:1201:CLA:C2A	19:4:1201:CLA:O1D	2.52	0.57
21:B:8056:SUC:H1	21:B:8056:SUC:H5'	1.87	0.57
21:B:8059:SUC:HO2	21:B:8059:SUC:C2'	2.16	0.57
8:D:49:THR:OG1	8:D:74:LEU:HD12	2.05	0.57
7:C:29:ILE:CG2	8:D:126:GLY:HA2	2.34	0.57
2:2:86:GLU:HA	2:2:86:GLU:OE2	2.03	0.57
6:B:399:ASN:O	6:B:401:GLU:N	2.38	0.57
1:1:185:TRP:O	1:1:186:HIS:CG	2.57	0.57
19:A:1797:CLA:C4D	19:A:1797:CLA:O1D	2.33	0.57
19:A:1783:CLA:C11	22:A:1807:BCR:H353	2.34	0.57
5:A:694:PHE:HZ	6:B:661:PHE:CD1	2.22	0.57
5:A:83:PHE:CE1	19:A:1769:CLA:HED1	2.40	0.57
19:B:1748:CLA:C1A	19:B:1748:CLA:H12	2.35	0.57
19:B:1766:CLA:CBB	22:B:1778:BCR:H281	2.34	0.57
11:G:32:ALA:O	11:G:33:LYS:C	2.42	0.57
6:B:25:ILE:HG22	22:L:1169:BCR:H291	1.81	0.57
19:3:3011:CLA:H3A	19:3:3011:CLA:CGA	2.34	0.57
8:D:125:PRO:HG2	8:D:127:ARG:HD3	1.86	0.57
16:L:14:LEU:CD2	16:L:21:GLY:O	2.53	0.57
5:A:265:GLY:CA	5:A:272:LEU:HD21	2.34	0.57
20:2:1224:LMU:H41	20:2:1224:LMU:H6D	1.87	0.57
4:4:100:TYR:O	4:4:103:ILE:HG12	2.05	0.57
5:A:123:VAL:HB	5:A:129:GLN:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1787:CLA:H142	19:A:1800:CLA:H43	1.86	0.57
5:A:532:ILE:N	5:A:533:PRO:HD3	2.19	0.57
5:A:56:ASN:O	5:A:57:LEU:CB	2.50	0.57
5:A:81:ALA:HB1	19:A:1760:CLA:HMA3	1.81	0.57
19:B:1746:CLA:H2A	19:B:1746:CLA:O1D	2.05	0.57
22:A:1806:BCR:C3	22:B:1779:BCR:H17C	2.34	0.57
6:B:127:ILE:HD13	6:B:193:HIS:CE1	2.40	0.57
5:A:587:GLY:HA3	6:B:668:ARG:CZ	2.33	0.57
9:E:32:ARG:NH2	9:E:53:VAL:HA	2.20	0.57
9:E:39:LEU:N	9:E:40:ARG:HH11	1.94	0.57
19:1:1188:CLA:O2D	19:1:1188:CLA:CAA	2.53	0.57
19:1:1193:CLA:HBC3	19:1:1193:CLA:CMC	2.32	0.57
1:1:141:GLU:O	1:1:143:LEU:O	2.23	0.57
16:L:17:ASP:OD1	16:L:17:ASP:O	2.23	0.57
5:A:158:ILE:HG23	5:A:163:GLN:NE2	2.20	0.57
5:A:354:TRP:CZ2	19:A:1780:CLA:H171	2.40	0.57
5:A:431:LEU:O	5:A:435:VAL:CG1	2.53	0.57
5:A:114:THR:HG1	5:A:525:ASN:HB2	1.65	0.57
19:B:1752:CLA:HMA3	19:B:1753:CLA:C4D	2.34	0.57
19:B:1757:CLA:C4	19:B:1757:CLA:H72	2.35	0.57
19:B:1769:CLA:H203	22:B:1780:BCR:HC41	1.87	0.57
24:B:1784:LMG:HC91	24:B:1784:LMG:H111	1.87	0.57
19:B:1787:CLA:H91	19:B:1788:CLA:H92	1.87	0.57
6:B:428:PHE:HA	19:B:1763:CLA:O1D	2.05	0.57
6:B:486:LEU:HB2	6:B:489:GLY:O	2.05	0.57
6:B:615:TYR:CD1	6:B:615:TYR:N	2.72	0.57
8:D:140:ASN:HA	8:D:142:SER:OG	2.05	0.57
17:N:50:GLN:OE1	17:N:51:ASP:HA	2.04	0.57
2:2:205:PHE:O	2:2:206:ALA:CB	2.53	0.57
20:A:7051:LMU:O2'	20:A:7051:LMU:H12	2.05	0.57
2:2:50:VAL:HG12	2:2:50:VAL:O	2.03	0.57
4:4:47:ASN:HB3	4:4:161:LEU:CD2	2.31	0.57
5:A:240:LYS:H	5:A:243:PRO:HD3	1.69	0.57
5:A:435:VAL:HA	5:A:438:HIS:CE1	2.40	0.57
5:A:547:PHE:O	5:A:551:VAL:CG1	2.46	0.57
5:A:619:LYS:HG2	5:A:642:PHE:CE1	2.40	0.57
6:B:262:HIS:O	6:B:265:THR:O	2.23	0.57
6:B:305:LEU:HD22	19:B:1754:CLA:O1D	2.05	0.57
6:B:34:HIS:O	6:B:36:ASP:N	2.37	0.57
6:B:351:HIS:HB3	19:B:1748:CLA:CED	2.30	0.57
10:F:72:ILE:HG22	10:F:73:VAL:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:65:VAL:H	16:L:67:PRO:HD2	1.69	0.57
16:L:65:VAL:N	16:L:67:PRO:HD2	2.20	0.57
16:L:88:ALA:O	16:L:90:GLY:N	2.37	0.57
17:N:80:ASN:OD1	17:N:82:PHE:CA	2.53	0.57
8:D:91:ARG:NH1	8:D:119:TYR:HE1	2.03	0.57
19:A:1798:CLA:HBA2	19:A:1798:CLA:O2D	2.04	0.57
5:A:258:LEU:O	5:A:280:PHE:CE1	2.58	0.57
15:K:43:ARG:NE	15:K:43:ARG:HA	2.20	0.57
2:2:37:ASP:CG	3:3:41:ASP:HB2	2.25	0.56
19:A:1764:CLA:H142	22:A:1807:BCR:C13	2.35	0.56
19:A:1771:CLA:C4	19:A:1771:CLA:HAA2	2.29	0.56
5:A:544:ILE:HD11	19:A:1810:CLA:H193	1.87	0.56
5:A:369:THR:HG21	5:A:402:ILE:CG2	2.35	0.56
5:A:442:ILE:HG23	19:A:1786:CLA:CMC	2.25	0.56
5:A:733:VAL:HG11	19:A:1796:CLA:C1D	2.35	0.56
24:B:1784:LMG:C9	24:B:1784:LMG:H111	2.35	0.56
6:B:444:LEU:O	6:B:445:ALA:CB	2.53	0.56
6:B:630:GLN:HE21	6:B:731:GLY:CA	2.15	0.56
16:L:164:PRO:CG	16:L:165:TYR:CE1	2.84	0.56
1:1:28:GLY:HA2	19:1:1197:CLA:C3C	2.35	0.56
17:N:52:LEU:HB3	17:N:53:ALA:HA	1.86	0.56
17:N:76:LYS:CG	17:N:77:CYS:H	2.07	0.56
2:2:182:ILE:CG2	2:2:205:PHE:HB2	2.35	0.56
4:4:193:ILE:HG21	14:J:42:PHE:HD1	1.69	0.56
3:3:197:TYR:OH	19:3:1214:CLA:C4B	2.53	0.56
19:R:1055:CLA:H92	20:R:1056:LMU:C4B	2.35	0.56
15:K:53:ALA:O	15:K:54:GLY:C	2.41	0.56
9:E:44:TYR:CD2	9:E:45:TRP:HE3	2.23	0.56
1:1:160:GLY:HA3	19:1:1189:CLA:HBB2	1.86	0.56
6:B:48:ALA:CB	6:B:157:LEU:HD22	2.34	0.56
17:N:25:THR:CG2	17:N:26:GLY:N	2.68	0.56
4:4:100:TYR:CA	4:4:103:ILE:HG12	2.34	0.56
5:A:205:HIS:CE1	19:A:1769:CLA:HMC2	2.40	0.56
19:A:1771:CLA:HAA1	19:A:1771:CLA:H42	1.85	0.56
19:A:1781:CLA:C11	19:A:1781:CLA:H162	2.35	0.56
19:A:1799:CLA:H201	16:L:64:LEU:CD2	2.31	0.56
10:F:131:PHE:O	10:F:133:GLY:N	2.38	0.56
16:L:30:SER:C	16:L:32:LEU:N	2.59	0.56
17:N:45:ASN:HA	17:N:57:LYS:NZ	2.19	0.56
3:3:181:LEU:HD12	3:3:182:LYS:CE	2.35	0.56
19:1:1308:CLA:O2A	19:1:1308:CLA:H2A	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:20:PHE:CE2	15:K:52:PRO:HA	2.40	0.56
4:4:93:ILE:C	4:4:95:PHE:N	2.54	0.56
19:A:1776:CLA:C1C	19:A:1782:CLA:C17	2.80	0.56
19:A:1799:CLA:H202	16:L:64:LEU:HD21	1.86	0.56
5:A:40:PHE:H	5:A:44:ILE:HG21	1.71	0.56
5:A:462:ILE:HD11	19:B:1787:CLA:H72	1.85	0.56
6:B:561:GLY:CA	7:C:52:LYS:HG2	2.29	0.56
19:B:1769:CLA:CB	10:F:83:PHE:HZ	2.17	0.56
1:1:185:TRP:HE3	1:1:185:TRP:N	2.04	0.56
2:2:118:CYS:C	2:2:119:VAL:HG13	2.15	0.56
19:A:1761:CLA:H201	22:A:1803:BCR:C18	2.35	0.56
5:A:733:VAL:CG1	19:A:1796:CLA:C3D	2.83	0.56
5:A:214:GLY:HA3	22:A:1803:BCR:C15	2.36	0.56
5:A:284:ARG:NH1	5:A:507:ALA:HB1	2.19	0.56
19:B:1757:CLA:C4	19:B:1757:CLA:C7	2.84	0.56
19:B:1755:CLA:C8	19:B:1757:CLA:H43	2.35	0.56
19:B:1768:CLA:HBC3	19:B:1768:CLA:CMC	2.25	0.56
24:B:1784:LMG:C9	24:B:1784:LMG:C11	2.83	0.56
6:B:284:PHE:CE1	19:B:1750:CLA:HHC	2.41	0.56
6:B:553:PHE:O	6:B:555:TYR:N	2.39	0.56
6:B:597:LYS:O	6:B:598:HIS:HB2	2.05	0.56
9:E:41:ARG:HG3	9:E:46:PHE:CE1	2.41	0.56
10:F:76:ASP:O	10:F:78:ARG:N	2.39	0.56
16:L:66:GLY:C	19:L:1168:CLA:HMC3	2.25	0.56
17:N:66:ASP:CA	17:N:67:LEU:HD12	2.32	0.56
2:2:178:TRP:O	2:2:182:ILE:N	2.25	0.56
20:A:7048:LMU:C3	20:A:7048:LMU:C3'	2.78	0.56
4:4:193:ILE:CG2	4:4:194:VAL:N	2.61	0.56
3:3:194:ILE:HA	3:3:197:TYR:CE1	2.40	0.56
3:3:87:GLU:C	22:3:1225:BCR:H383	2.22	0.56
6:B:455:ILE:HD12	6:B:517:PHE:CZ	2.40	0.56
6:B:247:THR:CG2	6:B:250:ALA:CB	2.82	0.56
7:C:31:TRP:CB	7:C:39:ILE:HG21	2.35	0.56
6:B:500:ALA:CB	6:B:508:LEU:HD22	2.35	0.56
1:1:48:ARG:O	1:1:52:LEU:HB2	2.05	0.56
12:H:36:GLN:HG2	12:H:36:GLN:O	2.05	0.56
16:L:54:VAL:O	16:L:58:LEU:HB2	2.04	0.56
11:G:78:GLY:O	11:G:79:HIS:ND1	2.38	0.56
19:A:1797:CLA:H93	19:A:1797:CLA:C5	2.31	0.56
19:A:1799:CLA:H141	16:L:95:LEU:HD22	1.87	0.56
19:A:1784:CLA:H51	22:A:1803:BCR:H331	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:372:VAL:O	5:A:374:GLN:N	2.38	0.56
5:A:374:GLN:O	5:A:376:MET:N	2.38	0.56
6:B:559:CYS:SG	6:B:560:ASP:N	2.79	0.56
14:J:13:VAL:CG1	14:J:15:SER:HB2	2.36	0.56
20:A:7016:LMU:C3	20:A:7016:LMU:C9	2.62	0.56
19:J:1043:CLA:C15	19:J:1044:CLA:HMB1	2.36	0.56
1:1:57:ILE:O	1:1:57:ILE:HG12	2.04	0.56
11:G:69:VAL:O	11:G:73:ALA:HB3	2.05	0.56
4:4:123:GLN:HG2	4:4:124:TYR:H	1.70	0.56
19:A:1781:CLA:HMA2	19:A:1782:CLA:CGA	2.35	0.56
5:A:207:LEU:HA	5:A:211:LEU:HB2	1.86	0.56
5:A:223:VAL:HA	5:A:227:LEU:HB2	1.88	0.56
5:A:157:GLY:O	5:A:248:PHE:HE1	1.88	0.56
19:B:1760:CLA:C20	19:B:1772:CLA:HBA1	2.35	0.56
6:B:266:GLN:O	6:B:267:SER:CB	2.45	0.56
6:B:486:LEU:HD13	19:B:1766:CLA:HMD3	1.88	0.56
20:1:1199:LMU:H1B	20:1:1199:LMU:C6'	2.34	0.56
17:N:70:GLU:CB	17:N:72:LYS:H	2.15	0.56
5:A:316:MET:HA	5:A:317:TYR:HD1	1.70	0.56
10:F:24:LYS:N	10:F:26:GLN:H	2.04	0.56
4:4:58:MET:SD	4:4:59:LEU:N	2.78	0.56
6:B:37:ILE:HD12	6:B:37:ILE:C	2.26	0.56
1:1:54:VAL:C	1:1:56:GLY:H	2.09	0.56
4:4:100:TYR:CA	4:4:103:ILE:HD11	2.31	0.56
19:A:1760:CLA:HBB2	19:A:1762:CLA:CAD	2.35	0.56
5:A:309:LEU:O	5:A:310:PHE:CB	2.52	0.56
19:B:1760:CLA:H62	24:B:1784:LMG:C18	2.34	0.56
22:B:1781:BCR:H351	19:B:1788:CLA:H111	1.85	0.56
6:B:388:ALA:HA	6:B:391:PRO:CG	2.35	0.56
6:B:633:ASN:O	6:B:636:THR:HB	2.06	0.56
8:D:39:LYS:HG3	8:D:43:GLU:HG2	1.88	0.56
9:E:39:LEU:HA	9:E:46:PHE:CE1	2.40	0.56
19:4:1205:CLA:HBD	19:4:1205:CLA:HBA2	1.88	0.56
17:N:47:THR:HG21	17:N:54:LYS:CE	2.30	0.56
3:3:48:PHE:CD2	3:3:49:ILE:CG2	2.69	0.56
20:A:7033:LMU:C2'	20:A:7033:LMU:C6B	2.80	0.56
10:F:102:ARG:CD	10:F:106:ILE:HD11	2.36	0.56
12:H:67:TYR:C	12:H:67:TYR:HD1	2.09	0.56
19:A:1759:CLA:HMB1	19:A:1767:CLA:H18	1.87	0.56
5:A:42:ARG:HA	5:A:44:ILE:HG12	1.88	0.56
19:B:1761:CLA:HAA2	19:B:1761:CLA:HED2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1763:CLA:H51	22:B:1780:BCR:C40	2.35	0.56
6:B:275:HIS:O	6:B:278:LEU:HB3	2.05	0.56
5:A:131:ILE:HD13	6:B:447:GLY:N	2.20	0.56
6:B:560:ASP:OD1	7:C:52:LYS:NZ	2.36	0.56
10:F:126:ALA:O	10:F:128:SER:N	2.38	0.56
16:L:62:PHE:HB2	16:L:154:ALA:HB2	1.86	0.56
2:2:203:THR:C	2:2:204:ILE:HG13	2.23	0.56
6:B:479:SER:O	6:B:481:THR:N	2.28	0.56
9:E:48:ASN:HD21	9:E:71:LYS:NZ	2.04	0.56
16:L:25:THR:HB	16:L:26:PRO:HD2	1.88	0.56
6:B:408:LEU:O	6:B:411:MET:HB3	2.05	0.56
4:4:67:ILE:CG2	4:4:67:ILE:O	2.52	0.56
4:4:152:LYS:HA	4:4:154:ILE:HG12	1.87	0.56
5:A:133:ASN:HD22	5:A:142:GLY:HA2	1.69	0.56
5:A:287:LEU:N	5:A:295:TRP:HE1	2.04	0.56
19:B:1754:CLA:CGD	19:B:1754:CLA:C2A	2.83	0.56
19:B:1756:CLA:HED2	19:B:1757:CLA:CAD	2.35	0.56
19:B:1769:CLA:H121	22:B:1780:BCR:H311	1.88	0.56
6:B:291:TYR:O	6:B:292:ARG:O	2.24	0.56
6:B:340:SER:O	6:B:344:ILE:HG13	2.06	0.56
6:B:363:GLN:HA	6:B:365:PHE:CE1	2.40	0.56
6:B:574:ASP:OD2	6:B:706:ARG:NE	2.39	0.56
10:F:80:TRP:CE3	19:F:1157:CLA:HMC2	2.37	0.56
11:G:46:ALA:CA	11:G:48:ASP:CB	2.81	0.56
19:A:1789:CLA:O1D	16:L:73:PRO:HA	2.06	0.56
19:1:1192:CLA:O1D	20:1:1199:LMU:O2'	2.23	0.56
17:N:62:SER:O	17:N:63:ASP:CG	2.44	0.56
20:B:1783:LMU:C4'	20:B:1783:LMU:C5B	2.72	0.56
20:A:7048:LMU:C5'	20:A:7048:LMU:C2	2.84	0.56
5:A:582:ASP:HB3	5:A:589:THR:CG2	2.36	0.56
5:A:527:VAL:CG1	5:A:528:ALA:H	2.18	0.56
2:2:60:ALA:HA	2:2:63:PHE:CE2	2.41	0.56
4:4:94:GLU:CA	4:4:95:PHE:HD1	2.18	0.56
19:A:1800:CLA:HED1	16:L:32:LEU:CD1	2.35	0.56
6:B:132:ASN:OD1	6:B:132:ASN:C	2.45	0.56
19:B:1740:CLA:H193	19:B:1772:CLA:C4	2.36	0.56
6:B:197:VAL:O	6:B:198:ALA:HB2	2.06	0.56
6:B:398:TYR:CD1	6:B:542:ARG:NH2	2.73	0.56
6:B:661:PHE:HB2	19:B:1788:CLA:HMC1	1.84	0.56
9:E:88:GLU:O	9:E:90:VAL:HG23	2.06	0.56
10:F:22:LEU:CB	10:F:23:LYS:HD3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:69:ILE:HA	15:K:72:VAL:CG1	2.34	0.56
12:H:36:GLN:HE22	19:L:1166:CLA:CAD	2.19	0.56
19:1:1241:CLA:HAC2	22:I:1032:BCR:C3	2.12	0.56
2:2:171:MET:SD	2:2:172:LEU:N	2.79	0.56
4:4:104:ARG:HA	4:4:107:GLN:HE21	1.70	0.56
4:4:118:ASP:HA	4:4:122:LYS:CA	2.36	0.56
5:A:157:GLY:O	5:A:248:PHE:CE1	2.59	0.56
19:A:1812:CLA:HBC2	19:A:1812:CLA:HMC1	1.88	0.56
5:A:578:ARG:NH1	5:A:578:ARG:HB2	2.20	0.56
5:A:603:PHE:HZ	5:A:693:LEU:CD2	2.19	0.56
5:A:75:SER:HB3	5:A:354:TRP:CZ2	2.41	0.56
19:B:1754:CLA:H72	19:B:1754:CLA:C2	2.31	0.56
6:B:340:SER:CA	19:B:1757:CLA:H51	2.25	0.56
6:B:352:MET:SD	19:B:1759:CLA:OBD	2.64	0.56
22:B:1776:BCR:C8	22:B:1776:BCR:C33	2.84	0.56
6:B:646:TRP:CZ3	6:B:726:ILE:HD13	2.41	0.56
7:C:51:CYS:N	25:C:1082:SF4:S1	2.74	0.56
6:B:542:ARG:NH2	8:D:141:VAL:O	2.39	0.56
11:G:27:GLN:O	11:G:28:ARG:HB3	2.05	0.56
13:I:19:VAL:O	13:I:23:SER:N	2.39	0.56
8:D:124:ASN:CB	8:D:125:PRO:CD	2.82	0.56
9:E:73:ASN:C	9:E:73:ASN:ND2	2.60	0.56
16:L:25:THR:HB	16:L:26:PRO:CD	2.36	0.56
8:D:69:ARG:O	8:D:70:GLU:CB	2.54	0.56
6:B:42:LEU:O	6:B:45:ASN:N	2.39	0.56
4:4:106:TRP:HE3	19:4:1209:CLA:CMA	2.14	0.55
5:A:150:PHE:H	5:A:153:TRP:HE3	1.49	0.55
19:A:1789:CLA:HBC3	19:A:1789:CLA:CMC	2.35	0.55
19:A:1781:CLA:CBA	19:A:1794:CLA:HED1	2.19	0.55
22:A:1806:BCR:H15C	19:A:1811:CLA:H151	1.88	0.55
19:B:1761:CLA:HMB2	19:B:1762:CLA:C4A	2.37	0.55
22:B:1781:BCR:C20	19:B:1787:CLA:C15	2.84	0.55
6:B:255:LEU:HD12	19:B:1747:CLA:O2D	2.06	0.55
8:D:75:LEU:HD21	16:L:19:PHE:CZ	2.40	0.55
3:3:94:ARG:C	3:3:97:PHE:HE1	2.09	0.55
1:1:112:ARG:HH11	19:1:1195:CLA:CGD	2.08	0.55
3:3:202:LEU:HB3	3:3:204:THR:HG23	1.87	0.55
2:2:42:ARG:HD2	2:2:45:VAL:CG2	2.19	0.55
4:4:37:LEU:HA	4:4:39:TRP:CD1	2.41	0.55
19:A:1787:CLA:H12	6:B:686:PRO:HG2	1.86	0.55
5:A:358:LEU:O	5:A:361:ASN:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:409:GLY:C	5:A:411:ALA:H	2.10	0.55
5:A:559:GLY:HA2	5:A:597:HIS:ND1	2.21	0.55
5:A:88:ILE:CG2	5:A:89:ILE:N	2.69	0.55
5:A:249:ILE:HG23	5:A:251:ASN:OD1	2.06	0.55
20:N:1086:LMU:H41	20:N:1086:LMU:O6'	2.05	0.55
3:3:49:ILE:HA	3:3:51:PRO:HD2	1.88	0.55
20:A:7048:LMU:H51	20:A:7048:LMU:C1	2.33	0.55
20:A:7048:LMU:C5	20:A:7048:LMU:H12	2.15	0.55
5:A:425:THR:O	5:A:428:TYR:CE1	2.59	0.55
20:A:7038:LMU:H6'	20:A:7038:LMU:C1B	2.18	0.55
19:A:1769:CLA:C1	19:A:1769:CLA:HMA2	2.36	0.55
19:A:1772:CLA:CMC	19:A:1772:CLA:CBC	2.81	0.55
19:A:1776:CLA:H43	19:A:1779:CLA:H2	1.88	0.55
19:A:1781:CLA:HBB2	19:A:1794:CLA:C3A	2.36	0.55
5:A:177:LEU:C	5:A:179:LEU:H	2.10	0.55
19:B:1756:CLA:C7	19:B:1770:CLA:C3D	2.84	0.55
19:B:1738:CLA:C4	24:B:1784:LMG:H321	2.36	0.55
6:B:343:VAL:CG1	19:B:1757:CLA:H2	2.36	0.55
5:A:447:ASN:ND2	6:B:678:LEU:CD2	2.69	0.55
6:B:715:VAL:HA	6:B:718:ILE:HG22	1.88	0.55
11:G:19:GLY:C	11:G:21:PHE:HA	2.26	0.55
16:L:66:GLY:HA2	16:L:69:VAL:HG22	1.89	0.55
4:4:70:ILE:O	4:4:73:PRO:CD	2.53	0.55
1:1:63:LEU:HD23	1:1:64:GLY:O	2.05	0.55
21:B:8062:SUC:H1	21:B:8062:SUC:O3'	2.07	0.55
3:3:158:TYR:OH	19:3:1215:CLA:C3B	2.53	0.55
6:B:117:TYR:O	6:B:367:THR:HG23	2.07	0.55
1:1:111:GLN:HE21	1:1:111:GLN:HA	1.72	0.55
4:4:126:LEU:HD23	4:4:127:PRO:CG	2.36	0.55
5:A:158:ILE:HG23	5:A:163:GLN:HE22	1.72	0.55
19:A:1800:CLA:HMA3	16:L:27:VAL:CA	2.12	0.55
19:A:1781:CLA:C3B	22:A:1805:BCR:C21	2.85	0.55
19:B:1741:CLA:CHD	22:B:1782:BCR:H342	2.36	0.55
6:B:427:LEU:HB3	19:B:1763:CLA:HED1	1.89	0.55
7:C:75:ARG:NH1	8:D:110:GLN:OE1	2.38	0.55
8:D:75:LEU:HD22	8:D:76:LYS:H	1.72	0.55
2:2:182:ILE:HG23	2:2:205:PHE:HB2	1.89	0.55
3:3:50:GLU:H	3:3:51:PRO:HD3	1.71	0.55
20:A:7030:LMU:C9	20:A:7030:LMU:H51	2.14	0.55
3:3:201:ALA:C	3:3:202:LEU:HD22	2.27	0.55
6:B:476:ILE:O	6:B:479:SER:OG	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:89:VAL:CG1	11:G:77:ILE:HG21	2.37	0.55
2:2:143:PHE:CD1	2:2:144:ASP:N	2.75	0.55
5:A:536:THR:HA	5:A:539:PHE:CB	2.37	0.55
1:1:167:ALA:C	1:1:169:PRO:HD3	2.26	0.55
8:D:64:GLY:O	8:D:65:ALA:CB	2.55	0.55
2:2:51:HIS:O	2:2:55:ALA:N	2.29	0.55
2:2:67:PHE:O	2:2:68:LEU:C	2.45	0.55
19:A:1765:CLA:H51	22:A:1807:BCR:C10	2.35	0.55
19:A:1777:CLA:C2D	19:A:1778:CLA:HMB3	2.36	0.55
5:A:361:ASN:HD22	5:A:361:ASN:C	2.10	0.55
5:A:472:ARG:O	5:A:474:GLN:N	2.40	0.55
5:A:88:ILE:HG22	5:A:89:ILE:H	1.72	0.55
6:B:310:PRO:CB	6:B:311:PRO:HD2	2.35	0.55
6:B:594:TRP:HD1	6:B:595:HIS:HB2	1.72	0.55
6:B:596:TRP:CZ3	6:B:613:SER:HB3	2.41	0.55
6:B:649:MET:HE3	6:B:723:ALA:HB2	1.89	0.55
9:E:40:ARG:NH2	9:E:87:VAL:HG22	2.21	0.55
10:F:123:VAL:HG13	14:J:7:TYR:H	1.71	0.55
17:N:63:ASP:H	17:N:64:ASP:HB2	1.65	0.55
19:1:1148:CLA:O1A	19:1:1148:CLA:H2	2.05	0.55
5:A:141:ARG:HH21	5:A:141:ARG:CG	2.14	0.55
10:F:117:LYS:N	10:F:118:GLU:OE2	2.39	0.55
6:B:14:GLN:H	6:B:14:GLN:HE21	1.55	0.55
2:2:129:LYS:C	2:2:131:THR:N	2.60	0.55
2:2:129:LYS:O	2:2:132:GLY:HA3	2.05	0.55
2:2:57:LEU:CD2	2:2:58:GLY:N	2.69	0.55
4:4:120:ILE:HD12	4:4:120:ILE:H	1.72	0.55
4:4:30:LEU:CD1	20:4:1212:LMU:H121	2.32	0.55
5:A:100:GLY:HA3	5:A:153:TRP:CZ3	2.42	0.55
5:A:412:ALA:O	5:A:415:ALA:HB3	2.07	0.55
5:A:438:HIS:HB2	5:A:441:ALA:HB3	1.89	0.55
5:A:471:GLY:O	5:A:472:ARG:HG2	2.07	0.55
5:A:46:LYS:HG3	5:A:48:PRO:HB2	1.87	0.55
5:A:397:THR:HB	5:A:613:ILE:HG12	1.86	0.55
5:A:678:PHE:O	5:A:681:GLY:O	2.25	0.55
20:A:7006:LMU:H3'	20:A:7006:LMU:O6B	2.06	0.55
5:A:711:HIS:O	5:A:716:VAL:HG22	2.06	0.55
6:B:102:GLU:O	6:B:103:ALA:C	2.45	0.55
6:B:597:LYS:HG2	19:B:1768:CLA:HBC1	1.89	0.55
6:B:416:GLU:H	6:B:416:GLU:CD	2.09	0.55
6:B:586:THR:C	6:B:588:GLY:N	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7023:LMU:C1B	20:A:7023:LMU:O4'	2.53	0.55
3:3:181:LEU:CD1	3:3:182:LYS:CE	2.84	0.55
3:3:56:TYR:HD1	3:3:185:LYS:HZ1	1.51	0.55
10:F:46:MET:O	10:F:49:THR:N	2.38	0.55
19:2:1212:CLA:CMC	19:2:1212:CLA:HBC3	2.28	0.55
6:B:15:ASP:O	6:B:20:ARG:CG	2.55	0.55
1:1:129:ASP:OD2	1:1:133:TYR:HA	2.07	0.55
20:A:7019:LMU:O2'	20:A:7019:LMU:H32	2.06	0.55
2:2:163:GLU:OE1	2:2:163:GLU:HA	2.07	0.55
19:A:1762:CLA:HBA2	19:A:1762:CLA:HED2	1.88	0.55
19:A:1771:CLA:H2A	19:A:1771:CLA:CGD	2.36	0.55
19:A:1782:CLA:C14	19:A:1782:CLA:H101	2.37	0.55
5:A:334:HIS:HB3	19:A:1777:CLA:HMA3	1.88	0.55
5:A:650:ASN:O	5:A:653:LEU:N	2.30	0.55
19:B:1772:CLA:CHD	23:B:1774:PQN:H18	2.36	0.55
19:B:1738:CLA:H43	24:B:1784:LMG:H321	1.89	0.55
6:B:577:TYR:CE2	6:B:578:LEU:HD12	2.41	0.55
6:B:732:LYS:HG3	6:B:733:PHE:O	2.04	0.55
6:B:76:ALA:O	6:B:79:GLN:N	2.39	0.55
11:G:5:SER:O	11:G:7:VAL:HG13	2.05	0.55
14:J:19:PHE:O	14:J:23:ALA:HB3	2.06	0.55
16:L:56:VAL:HA	19:L:1167:CLA:HED1	1.89	0.55
19:1:1188:CLA:C7	19:1:1188:CLA:H41	2.20	0.55
17:N:46:PHE:O	17:N:47:THR:CB	2.53	0.55
19:1:1190:CLA:HBA1	19:1:1190:CLA:CHA	2.36	0.55
19:J:1043:CLA:H152	19:J:1044:CLA:CMB	2.36	0.55
4:4:192:THR:HG23	4:4:193:ILE:C	2.24	0.55
10:F:23:LYS:CA	10:F:24:LYS:NZ	2.69	0.55
3:3:74:ALA:HA	19:3:1217:CLA:ND	2.21	0.55
20:A:7009:LMU:H3O2	20:A:7009:LMU:H5B	1.68	0.55
10:F:40:LEU:HD12	10:F:42:ILE:HD11	1.89	0.55
2:2:192:LEU:HG	2:2:193:PHE:N	2.22	0.55
1:1:54:VAL:O	1:1:56:GLY:N	2.40	0.55
1:1:85:LEU:HD13	1:1:85:LEU:H	1.70	0.55
2:2:63:PHE:HE2	2:2:168:ARG:CD	2.20	0.55
19:A:1771:CLA:H2A	19:A:1771:CLA:CED	2.32	0.55
5:A:210:LEU:N	5:A:213:LEU:H	2.05	0.55
19:B:1757:CLA:H142	19:B:1757:CLA:C10	2.35	0.55
19:B:1788:CLA:CMB	19:B:1788:CLA:H41	2.37	0.55
6:B:361:ILE:C	6:B:362:ALA:O	2.44	0.55
6:B:493:TRP:CH2	19:B:1748:CLA:H122	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:519:VAL:HG11	6:B:593:TYR:HB2	1.89	0.55
6:B:75:GLU:CB	6:B:132:ASN:HD22	2.19	0.55
7:C:69:LEU:HD23	7:C:70:TRP:N	2.21	0.55
7:C:74:THR:OG1	7:C:75:ARG:N	2.33	0.55
22:L:1169:BCR:H331	22:L:1169:BCR:C8	2.36	0.55
16:L:33:ILE:HD11	16:L:36:TYR:HD1	1.72	0.55
16:L:41:PRO:HG3	16:L:52:ARG:HD3	1.88	0.55
17:N:59:PRO:C	17:N:61:LEU:O	2.45	0.55
19:4:1206:CLA:H151	19:4:1206:CLA:C8	2.35	0.55
16:L:14:LEU:HD22	16:L:21:GLY:O	2.07	0.55
5:A:262:PHE:O	5:A:264:GLU:N	2.40	0.55
1:1:50:ALA:O	1:1:54:VAL:HG23	2.07	0.55
3:3:134:LYS:O	3:3:135:PRO:C	2.44	0.55
19:1:1241:CLA:O1D	19:1:1241:CLA:H2A	2.06	0.55
4:4:36:ASN:C	4:4:36:ASN:OD1	2.45	0.55
19:A:1760:CLA:CHD	19:A:1760:CLA:HBC3	2.36	0.55
19:A:1764:CLA:H2A	19:A:1764:CLA:O2D	2.06	0.55
19:A:1762:CLA:O1A	19:A:1785:CLA:HMB2	2.07	0.55
19:A:1800:CLA:HBA1	16:L:33:ILE:HD13	1.89	0.55
5:A:451:ILE:HD12	19:A:1788:CLA:CED	2.07	0.55
5:A:408:VAL:HG21	5:A:602:LEU:HG	1.88	0.55
5:A:679:PHE:O	5:A:683:HIS:HB2	2.07	0.55
6:B:275:HIS:ND1	19:B:1748:CLA:HMB1	2.21	0.55
7:C:1:MET:H1	7:C:4:SER:CA	2.20	0.55
16:L:87:ALA:O	16:L:89:ALA:N	2.40	0.55
3:3:92:TRP:CZ2	5:A:250:LEU:HB2	2.40	0.55
6:B:330:ILE:HD12	6:B:330:ILE:O	2.05	0.55
5:A:278:ALA:O	5:A:279:ASP:O	2.25	0.55
19:1:1193:CLA:HBA2	19:1:1193:CLA:HMA3	1.88	0.55
5:A:520:LEU:HD22	20:A:1808:LMU:O1'	2.07	0.55
16:L:111:GLU:OE1	20:L:1171:LMU:O6B	2.18	0.55
19:A:1788:CLA:H101	19:A:1788:CLA:H142	1.88	0.55
19:A:1787:CLA:H141	19:A:1800:CLA:H93	1.89	0.55
5:A:211:LEU:HB3	5:A:310:PHE:CD2	2.43	0.55
5:A:697:ARG:C	5:A:699:TYR:N	2.60	0.55
5:A:82:HIS:O	5:A:84:GLY:N	2.40	0.55
6:B:91:ILE:HD11	6:B:104:PHE:CE2	2.42	0.55
19:B:1759:CLA:H62	22:B:1777:BCR:H321	1.88	0.55
6:B:427:LEU:HD13	19:B:1735:CLA:OBD	2.07	0.55
6:B:616:LEU:O	6:B:619:TRP:HB2	2.06	0.55
6:B:633:ASN:HD22	6:B:636:THR:HB	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:121:THR:OG1	16:L:122:GLY:N	2.38	0.55
17:N:82:PHE:HD2	17:N:82:PHE:H	1.55	0.55
20:A:7016:LMU:H31	20:A:7016:LMU:C1'	2.36	0.55
10:F:20:GLN:O	10:F:21:ALA:HB3	2.05	0.55
10:F:25:LEU:HD21	10:F:46:MET:HB3	1.84	0.55
12:H:25:GLY:HA3	12:H:27:ASP:CG	2.27	0.55
6:B:475:ASP:HA	6:B:480:SER:C	2.27	0.55
4:4:58:MET:C	4:4:58:MET:SD	2.85	0.55
5:A:478:SER:C	5:A:480:THR:H	2.11	0.55
16:L:50:LEU:HG	16:L:51:LEU:CD2	2.37	0.55
15:K:72:VAL:HG13	15:K:73:GLY:N	2.22	0.55
15:K:62:ALA:O	15:K:65:ALA:CB	2.55	0.55
19:A:1762:CLA:H51	19:A:1785:CLA:C4C	2.37	0.54
19:A:1787:CLA:HMB1	19:A:1799:CLA:HAA2	1.88	0.54
19:A:1796:CLA:H62	19:A:1812:CLA:H193	1.89	0.54
5:A:541:VAL:CG1	5:A:615:HIS:CD2	2.72	0.54
19:B:1739:CLA:H2	19:B:1739:CLA:H71	1.89	0.54
6:B:197:VAL:O	6:B:197:VAL:HG12	2.06	0.54
6:B:575:ASP:O	6:B:579:ALA:N	2.37	0.54
7:C:75:ARG:NH2	8:D:110:GLN:OE1	2.36	0.54
5:A:24:ARG:O	5:A:25:ASP:C	2.46	0.54
19:1:1187:CLA:HBA2	19:1:1187:CLA:CMA	2.26	0.54
20:R:1056:LMU:O5B	20:R:1056:LMU:H5'	2.07	0.54
6:B:476:ILE:HG22	6:B:479:SER:OG	2.08	0.54
8:D:30:ALA:O	16:L:18:PRO:CB	2.51	0.54
6:B:154:TRP:O	6:B:157:LEU:N	2.30	0.54
4:4:114:SER:O	4:4:117:GLN:N	2.40	0.54
4:4:89:THR:CA	4:4:90:LEU:HD22	2.37	0.54
5:A:160:SER:O	5:A:163:GLN:CG	2.36	0.54
6:B:299:HIS:HE1	19:B:1753:CLA:HMD1	1.72	0.54
6:B:707:LEU:HD13	24:B:1784:LMG:H301	1.88	0.54
6:B:437:TYR:CG	6:B:616:LEU:HD22	2.41	0.54
6:B:596:TRP:O	6:B:597:LYS:CB	2.54	0.54
10:F:104:TYR:HD2	10:F:104:TYR:O	1.88	0.54
11:G:18:LEU:C	11:G:21:PHE:H	2.10	0.54
11:G:19:GLY:O	11:G:22:VAL:N	2.40	0.54
3:3:94:ARG:C	3:3:97:PHE:CE1	2.81	0.54
17:N:63:ASP:N	17:N:64:ASP:HB2	2.22	0.54
17:N:63:ASP:N	17:N:64:ASP:HB3	2.10	0.54
19:R:1054:CLA:HBA2	19:R:1054:CLA:HBD	1.89	0.54
3:3:156:PRO:O	3:3:157:ALA:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:338:PHE:CE1	19:A:1798:CLA:HBB1	2.42	0.54
5:A:337:PRO:HD2	19:A:1798:CLA:HHC	1.88	0.54
16:L:58:LEU:HA	16:L:146:GLY:O	2.07	0.54
4:4:41:VAL:CG1	4:4:41:VAL:O	2.48	0.54
2:2:166:ASN:OD1	2:2:169:LEU:CD1	2.55	0.54
2:2:170:ALA:O	2:2:171:MET:C	2.45	0.54
4:4:104:ARG:HA	4:4:107:GLN:NE2	2.22	0.54
4:4:163:PHE:O	4:4:166:PHE:N	2.40	0.54
5:A:700:TRP:CZ3	19:A:1812:CLA:O1D	2.60	0.54
5:A:216:LEU:CD1	22:A:1802:BCR:H352	2.38	0.54
5:A:229:ILE:HG13	5:A:243:PRO:HB3	1.90	0.54
19:B:1755:CLA:H61	19:B:1755:CLA:CMA	2.37	0.54
6:B:172:GLU:C	6:B:176:ASN:HB2	2.27	0.54
19:B:1788:CLA:H41	19:B:1788:CLA:HMB2	1.88	0.54
5:A:668:TYR:CE1	6:B:445:ALA:HB2	2.41	0.54
6:B:463:ILE:O	6:B:464:GLN:CB	2.55	0.54
6:B:625:TRP:C	6:B:625:TRP:CE3	2.81	0.54
6:B:732:LYS:HG3	6:B:734:GLY:HA2	1.87	0.54
5:A:714:LEU:HA	10:F:149:LEU:HD11	1.89	0.54
4:4:68:GLY:C	4:4:69:ILE:O	2.46	0.54
4:4:69:ILE:CG2	4:4:70:ILE:N	2.52	0.54
16:L:160:VAL:O	16:L:160:VAL:CG2	2.29	0.54
1:1:29:LEU:O	1:1:31:GLU:N	2.41	0.54
2:2:182:ILE:C	2:2:204:ILE:O	2.46	0.54
12:H:27:ASP:O	12:H:29:PRO:HD3	2.06	0.54
9:E:48:ASN:OD1	9:E:48:ASN:C	2.45	0.54
5:A:479:ASP:OD1	5:A:536:THR:O	2.26	0.54
16:L:55:GLU:HG3	19:L:1166:CLA:C1A	2.37	0.54
12:H:67:TYR:CD1	12:H:67:TYR:C	2.81	0.54
4:4:42:GLN:NE2	4:4:119:PRO:HB2	2.23	0.54
5:A:124:TRP:HA	5:A:124:TRP:CE3	2.41	0.54
5:A:137:GLY:C	5:A:139:GLY:H	2.10	0.54
19:A:1764:CLA:CMB	19:A:1765:CLA:H11	2.38	0.54
19:A:1783:CLA:H43	19:A:1783:CLA:CGA	2.36	0.54
5:A:308:ILE:CD1	19:A:1772:CLA:C8	2.85	0.54
5:A:618:TRP:HB2	5:A:656:PHE:CE1	2.43	0.54
5:A:672:LEU:HD23	5:A:672:LEU:H	1.71	0.54
5:A:83:PHE:HA	5:A:86:LEU:HD23	1.90	0.54
22:B:1779:BCR:C33	22:B:1779:BCR:HC8	2.36	0.54
19:B:1769:CLA:C12	22:B:1780:BCR:H311	2.37	0.54
6:B:462:TRP:CZ3	19:B:1765:CLA:CBC	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:VAL:HG21	19:1:1197:CLA:C1D	2.37	0.54
1:1:149:LYS:HB3	19:1:1192:CLA:CMC	2.37	0.54
20:N:1086:LMU:H32	20:N:1086:LMU:O6'	2.07	0.54
17:N:41:LYS:CB	17:N:42:PHE:CA	2.83	0.54
19:1:1142:CLA:HHD	19:1:1142:CLA:HBC3	1.89	0.54
21:3:1226:SUC:O1'	21:3:1226:SUC:C5'	2.54	0.54
7:C:39:ILE:HG23	7:C:40:ALA:N	2.23	0.54
6:B:475:ASP:O	6:B:479:SER:OG	2.26	0.54
10:F:152:ASN:H	10:F:152:ASN:ND2	2.05	0.54
4:4:99:HIS:HD1	4:4:103:ILE:CD1	2.21	0.54
4:4:119:PRO:HD2	4:4:120:ILE:HD12	1.89	0.54
4:4:36:ASN:O	4:4:39:TRP:CG	2.60	0.54
4:4:38:ARG:CG	4:4:38:ARG:NH1	2.65	0.54
4:4:99:HIS:O	4:4:103:ILE:HD11	2.02	0.54
19:A:1759:CLA:C4	19:A:1796:CLA:H8	2.37	0.54
19:A:1762:CLA:C7	19:A:1762:CLA:H2	2.36	0.54
5:A:705:GLU:CB	6:B:545:LYS:HZ2	2.20	0.54
6:B:124:TRP:CZ2	6:B:135:LEU:HD22	2.43	0.54
19:B:1738:CLA:HHB	19:B:1760:CLA:HBB2	1.90	0.54
6:B:431:PHE:HE2	19:B:1763:CLA:CED	2.20	0.54
6:B:25:ILE:HG22	22:L:1169:BCR:C28	2.28	0.54
18:R:32:UNK:CB	18:R:33:UNK:CA	2.76	0.54
15:K:17:LEU:HD22	15:K:18:MET:CA	2.36	0.54
3:3:106:TYR:HB3	3:3:107:TRP:HD1	1.71	0.54
2:2:198:ALA:O	2:2:199:ASP:CG	2.46	0.54
2:2:137:TYR:CD1	2:2:138:PRO:CD	2.89	0.54
6:B:224:PRO:HB3	6:B:227:THR:HB	1.89	0.54
1:1:183:ASP:HB3	1:1:184:PRO:HD2	1.90	0.54
2:2:54:TRP:CD2	19:2:1222:CLA:O1D	2.60	0.54
4:4:88:SER:HB3	4:4:89:THR:HG22	1.90	0.54
19:A:1783:CLA:H171	19:A:1783:CLA:H122	1.89	0.54
5:A:733:VAL:HG11	19:A:1796:CLA:C3D	2.37	0.54
19:A:1771:CLA:HBB1	22:A:1802:BCR:C35	2.38	0.54
5:A:378:SER:OG	19:A:1782:CLA:HBC2	2.08	0.54
5:A:618:TRP:CD1	5:A:618:TRP:O	2.60	0.54
5:A:622:SER:OG	5:A:642:PHE:HB2	2.07	0.54
5:A:731:ARG:O	5:A:735:VAL:HG23	2.08	0.54
19:B:1735:CLA:H52	19:B:1735:CLA:C4C	2.38	0.54
19:B:1771:CLA:HMC1	19:B:1771:CLA:HBC2	1.90	0.54
19:B:1772:CLA:CBC	19:B:1772:CLA:HMC1	2.27	0.54
19:B:1763:CLA:CBB	22:B:1779:BCR:H272	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:544:SER:O	6:B:546:LEU:N	2.41	0.54
6:B:550:LYS:CG	6:B:550:LYS:O	2.54	0.54
16:L:39:ASN:O	16:L:52:ARG:NH2	2.24	0.54
17:N:62:SER:C	17:N:66:ASP:H	2.10	0.54
17:N:65:LEU:CG	17:N:65:LEU:O	2.54	0.54
10:F:23:LYS:HD3	10:F:23:LYS:N	2.20	0.54
19:4:4014:CLA:H2A	19:4:4014:CLA:HED2	0.71	0.54
6:B:120:VAL:HA	6:B:123:TRP:HE1	1.66	0.54
20:A:7010:LMU:C2B	20:A:7010:LMU:H3'	2.34	0.54
20:A:7013:LMU:H3O2	20:A:7013:LMU:C1B	2.21	0.54
6:B:166:SER:C	6:B:168:PHE:H	2.09	0.54
19:1:1505:CLA:HAA1	19:1:1505:CLA:H42	1.90	0.54
11:G:85:ILE:O	11:G:86:LEU:HB2	2.08	0.54
2:2:171:MET:SD	2:2:172:LEU:CA	2.95	0.54
4:4:107:GLN:CA	19:4:1196:CLA:HMA2	2.31	0.54
5:A:162:LEU:C	5:A:165:TYR:HB3	2.28	0.54
5:A:680:LEU:HD21	6:B:617:MET:HE3	1.89	0.54
19:B:1761:CLA:HAA2	19:B:1761:CLA:CED	2.37	0.54
6:B:304:ILE:HD11	19:B:1750:CLA:HED2	1.86	0.54
6:B:596:TRP:O	6:B:597:LYS:HB3	2.07	0.54
8:D:46:TYR:CE1	8:D:80:LYS:HE2	2.34	0.54
9:E:61:THR:CG2	9:E:62:ARG:H	2.08	0.54
4:4:70:ILE:HG13	4:4:71:ASN:H	1.71	0.54
3:3:95:THR:HB	3:3:96:GLY:O	2.08	0.54
17:N:46:PHE:C	17:N:47:THR:HG23	2.17	0.54
19:1:1014:CLA:CMA	19:1:1014:CLA:CED	2.86	0.54
3:3:53:TRP:HA	3:3:56:TYR:HD2	1.73	0.54
22:3:1225:BCR:C8	22:3:1225:BCR:C31	2.72	0.54
3:3:66:MET:HG2	3:3:195:LEU:HD11	1.88	0.54
4:4:40:PHE:HB3	4:4:43:ALA:HB1	1.75	0.54
4:4:92:VAL:CG1	4:4:93:ILE:N	2.69	0.54
5:A:207:LEU:HD13	19:A:1776:CLA:HBB2	1.88	0.54
19:A:1779:CLA:ND	22:A:1804:BCR:C19	2.71	0.54
5:A:455:PHE:O	19:A:1789:CLA:CBB	2.56	0.54
5:A:591:GLN:OE1	5:A:600:LEU:HD21	2.07	0.54
19:B:1735:CLA:H71	19:B:1735:CLA:HMC2	1.90	0.54
19:B:1744:CLA:C4	19:B:1749:CLA:HBC1	2.37	0.54
6:B:278:LEU:HD12	19:B:1747:CLA:HMA1	1.87	0.54
19:B:1740:CLA:H143	19:B:1758:CLA:H18	1.90	0.54
6:B:373:THR:O	6:B:377:TYR:N	2.31	0.54
6:B:415:LYS:CG	6:B:416:GLU:OE2	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:462:TRP:HZ3	19:B:1765:CLA:HBC1	1.72	0.54
6:B:545:LYS:HG2	9:E:74:TYR:CE2	2.43	0.54
19:A:1788:CLA:H162	22:L:1169:BCR:H362	1.88	0.54
16:L:60:HIS:HD2	19:L:1167:CLA:CED	2.20	0.54
20:A:7041:LMU:O4'	20:A:7042:LMU:O1'	2.26	0.54
19:1:1188:CLA:O2A	19:1:1188:CLA:HMA3	2.08	0.54
5:A:250:LEU:O	5:A:252:ARG:HG2	2.08	0.54
20:A:7023:LMU:C1B	20:A:7023:LMU:H4O1	2.20	0.54
4:4:191:ASN:C	4:4:191:ASN:OD1	2.44	0.54
12:H:14:ILE:HD11	12:H:17:THR:H	1.73	0.54
8:D:87:GLY:H	8:D:90:LEU:H	1.56	0.54
1:1:185:TRP:CA	1:1:186:HIS:HD1	2.18	0.54
2:2:125:PHE:O	2:2:126:PRO:C	2.46	0.54
2:2:42:ARG:CB	2:2:45:VAL:HB	2.37	0.54
4:4:40:PHE:CD1	4:4:40:PHE:N	2.72	0.54
5:A:144:GLN:CG	5:A:145:ILE:H	2.20	0.54
19:A:1789:CLA:O1D	16:L:73:PRO:O	2.26	0.54
5:A:723:ARG:O	19:A:1795:CLA:CBB	2.56	0.54
5:A:84:GLY:C	5:A:87:SER:O	2.46	0.54
19:B:1748:CLA:H112	19:B:1766:CLA:H3A	1.90	0.54
22:B:1778:BCR:H311	22:B:1778:BCR:C8	2.38	0.54
6:B:301:ILE:O	6:B:301:ILE:CG2	2.56	0.54
6:B:308:HIS:HD1	6:B:309:ILE:N	2.05	0.54
10:F:22:LEU:C	10:F:25:LEU:HD13	2.27	0.54
5:A:629:ASN:HD21	5:A:633:VAL:CG2	2.20	0.54
19:2:1218:CLA:HBA1	20:A:7003:LMU:H51	1.89	0.54
5:A:118:PRO:HB3	5:A:150:PHE:CD2	2.43	0.54
19:A:1776:CLA:CAA	19:A:1780:CLA:HBB2	2.37	0.54
19:A:1781:CLA:HAA2	19:A:1782:CLA:OBD	2.08	0.54
19:A:1799:CLA:CGA	19:A:1799:CLA:C1A	2.86	0.54
5:A:242:ILE:HG12	5:A:243:PRO:HG3	1.90	0.54
5:A:328:LYS:CD	5:A:332:GLU:HG3	2.28	0.54
5:A:361:ASN:O	5:A:365:LEU:N	2.39	0.54
5:A:656:PHE:O	5:A:659:ALA:N	2.40	0.54
19:B:1735:CLA:H2A	19:B:1735:CLA:CED	2.31	0.54
6:B:167:TRP:CZ2	19:B:1742:CLA:HMA1	2.43	0.54
6:B:190:TRP:CA	19:B:1745:CLA:HBB2	2.38	0.54
6:B:655:LEU:HD22	19:B:1772:CLA:CBB	2.37	0.54
6:B:233:TYR:HB3	6:B:254:ILE:O	2.08	0.54
6:B:546:LEU:HD12	6:B:570:ILE:HD13	1.89	0.54
8:D:102:ARG:HH21	8:D:110:GLN:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1188:CLA:CHA	19:1:1188:CLA:CED	2.84	0.54
4:4:193:ILE:HG21	14:J:42:PHE:CD1	2.42	0.54
20:A:7014:LMU:C6	20:A:7014:LMU:C1	2.76	0.54
6:B:456:GLU:HA	6:B:514:PRO:HD3	1.90	0.54
5:A:255:LEU:HD11	5:A:280:PHE:HZ	1.72	0.54
6:B:513:GLY:O	6:B:515:GLY:N	2.41	0.54
1:1:161:PHE:HD1	19:1:1189:CLA:CBB	2.21	0.54
1:1:160:GLY:O	1:1:162:CYS:N	2.41	0.54
12:H:77:LEU:HB3	12:H:78:PRO:CD	2.36	0.54
16:L:58:LEU:HD11	16:L:153:TRP:HZ2	1.73	0.54
7:C:35:LYS:C	7:C:37:LYS:H	2.10	0.54
6:B:681:ALA:O	6:B:684:ARG:N	2.33	0.54
2:2:116:PRO:HB2	2:2:136:GLY:CA	2.35	0.53
2:2:102:ILE:CG1	19:2:1223:CLA:HMD2	2.36	0.53
4:4:147:LEU:HD21	4:4:148:GLU:CB	2.30	0.53
4:4:154:ILE:HG22	19:4:1203:CLA:CHA	2.38	0.53
19:A:1760:CLA:O2D	19:A:1760:CLA:C2A	2.55	0.53
19:3:1212:CLA:CMC	19:A:1770:CLA:HBA2	2.29	0.53
19:A:1779:CLA:NB	22:A:1804:BCR:H15C	2.22	0.53
6:B:626:LEU:O	6:B:627:ASN:HB2	2.08	0.53
6:B:580:VAL:CG1	6:B:710:LEU:HD21	2.37	0.53
7:C:5:VAL:C	7:C:65:VAL:CG2	2.68	0.53
18:R:36:UNK:C	18:R:38:UNK:N	2.65	0.53
20:A:7039:LMU:H6B	20:A:7039:LMU:H4'	1.71	0.53
13:I:2:ILE:HG13	13:I:3:ASN:OD1	2.08	0.53
2:2:56:MET:SD	2:2:169:LEU:HA	2.49	0.53
4:4:42:GLN:O	4:4:43:ALA:C	2.47	0.53
5:A:163:GLN:O	5:A:166:CYS:SG	2.66	0.53
19:A:1776:CLA:C9	22:A:1804:BCR:H371	2.21	0.53
19:A:1779:CLA:C1C	22:A:1804:BCR:H17C	2.38	0.53
5:A:453:LEU:HD21	19:A:1793:CLA:CBB	2.38	0.53
5:A:214:GLY:CA	22:A:1803:BCR:H15C	2.38	0.53
19:A:1810:CLA:HMB3	19:A:1811:CLA:CAD	2.38	0.53
5:A:308:ILE:O	5:A:311:LEU:HB2	2.08	0.53
5:A:638:THR:OG1	5:A:641:ASN:ND2	2.41	0.53
5:A:78:VAL:O	5:A:82:HIS:CB	2.55	0.53
6:B:132:ASN:HA	6:B:135:LEU:HG	1.90	0.53
6:B:174:ARG:HH12	19:B:1755:CLA:CMD	2.20	0.53
19:B:1739:CLA:C14	19:B:1758:CLA:H91	2.35	0.53
6:B:203:ARG:HB3	6:B:270:LEU:HD12	1.89	0.53
6:B:50:HIS:HA	6:B:53:GLN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:40:ARG:H	9:E:46:PHE:HE1	1.55	0.53
10:F:123:VAL:HG21	10:F:128:SER:OG	2.08	0.53
19:G:1099:CLA:O1D	19:G:1099:CLA:CAA	2.56	0.53
11:G:47:GLY:N	11:G:48:ASP:HA	2.16	0.53
13:I:29:GLU:HA	13:I:29:GLU:OE2	2.08	0.53
16:L:56:VAL:HG13	19:L:1167:CLA:HED3	1.88	0.53
2:2:205:PHE:HE1	2:2:206:ALA:HA	1.71	0.53
6:B:160:LYS:HE3	6:B:161:TRP:CE2	2.43	0.53
1:1:136:ASP:HB2	1:1:140:LEU:HB3	1.88	0.53
5:A:527:VAL:HG13	5:A:528:ALA:H	1.73	0.53
5:A:148:GLY:C	5:A:149:PHE:O	2.43	0.53
19:A:1763:CLA:HHB	19:A:1764:CLA:HMB3	1.89	0.53
19:A:1796:CLA:HBA2	19:A:1796:CLA:C4A	2.32	0.53
5:A:439:ARG:HG2	5:A:562:PHE:CE2	2.43	0.53
5:A:449:VAL:CG2	19:A:1794:CLA:HMC3	2.38	0.53
5:A:723:ARG:HH11	5:A:723:ARG:HG3	1.68	0.53
6:B:648:TRP:CZ2	19:B:1787:CLA:H62	2.43	0.53
5:A:709:TRP:CH2	6:B:417:ALA:HB2	2.44	0.53
6:B:533:ILE:O	6:B:537:GLY:N	2.30	0.53
19:L:1167:CLA:HAC2	22:L:1169:BCR:HC42	1.89	0.53
3:3:56:TYR:O	3:3:60:ILE:HD12	2.07	0.53
6:B:406:ASN:HD22	6:B:406:ASN:C	2.11	0.53
9:E:50:GLY:HA3	9:E:69:PHE:HB2	1.91	0.53
20:A:7038:LMU:C10	20:A:7038:LMU:H62	2.29	0.53
6:B:222:LEU:O	6:B:222:LEU:HD23	2.07	0.53
2:2:137:TYR:O	2:2:143:PHE:CE2	2.61	0.53
2:2:181:HIS:CE1	19:2:1214:CLA:ND	2.75	0.53
6:B:20:ARG:HH11	6:B:20:ARG:CG	2.21	0.53
5:A:187:HIS:NE2	19:A:1767:CLA:C4C	2.53	0.53
19:A:1783:CLA:C20	22:A:1807:BCR:C16	2.87	0.53
22:B:1781:BCR:C33	22:B:1781:BCR:C8	2.85	0.53
6:B:304:ILE:HD11	19:B:1750:CLA:HED3	1.90	0.53
6:B:573:TRP:O	6:B:577:TYR:N	2.31	0.53
22:I:1032:BCR:C38	22:I:1032:BCR:C40	2.73	0.53
1:1:27:LEU:CD2	6:B:314:ARG:CD	2.69	0.53
20:A:7042:LMU:C4'	20:A:7042:LMU:O2B	2.52	0.53
17:N:61:LEU:HG	17:N:62:SER:N	2.12	0.53
3:3:49:ILE:HG13	3:3:52:LYS:HB2	1.90	0.53
20:A:7051:LMU:H1B	20:A:7051:LMU:O6B	2.06	0.53
10:F:44:ALA:HB1	10:F:48:LYS:HB3	1.91	0.53
7:C:31:TRP:HD1	7:C:32:GLY:N	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:161:PHE:H	19:1:1189:CLA:HBB2	1.66	0.53
6:B:503:GLU:HB3	6:B:507:SER:CA	2.39	0.53
10:F:2:ILE:HG22	10:F:3:ALA:H	1.73	0.53
1:1:105:ILE:O	1:1:108:VAL:HG12	2.08	0.53
2:2:97:VAL:HA	2:2:100:VAL:HG13	1.89	0.53
19:A:1763:CLA:HBC2	19:A:1763:CLA:CHD	2.38	0.53
19:A:1783:CLA:C17	19:A:1783:CLA:H122	2.37	0.53
5:A:389:TYR:CE1	5:A:625:TRP:CG	2.96	0.53
5:A:448:TRP:CD1	19:A:1788:CLA:CED	2.92	0.53
19:B:1747:CLA:CHD	19:B:1747:CLA:HBC2	2.27	0.53
6:B:492:ILE:HD13	6:B:492:ILE:N	2.14	0.53
6:B:87:ILE:O	6:B:121:TYR:HE2	1.91	0.53
11:G:48:ASP:HB3	11:G:49:THR:HG21	1.86	0.53
16:L:123:ARG:O	16:L:124:LYS:HE3	2.09	0.53
16:L:96:SER:HG	16:L:143:PHE:HD2	1.48	0.53
5:A:253:ASP:O	5:A:256:ALA:CB	2.57	0.53
14:J:31:ARG:HH21	19:J:1043:CLA:C3B	2.21	0.53
20:A:7050:LMU:O3'	20:A:7050:LMU:C5B	2.57	0.53
8:D:28:ILE:O	8:D:66:ALA:HB3	2.08	0.53
16:L:48:ASN:HB2	16:L:50:LEU:HD22	1.91	0.53
5:A:586:ARG:CG	7:C:49:VAL:HG21	2.38	0.53
12:H:34:SER:OG	12:H:36:GLN:NE2	2.41	0.53
2:2:148:TRP:HH2	20:2:1224:LMU:H12	1.72	0.53
4:4:128:ALA:CA	4:4:143:PHE:CZ	2.91	0.53
5:A:308:ILE:HD13	19:A:1772:CLA:H91	1.72	0.53
19:A:1782:CLA:CBC	19:A:1782:CLA:CMC	2.63	0.53
5:A:615:HIS:ND1	19:A:1792:CLA:HBC3	2.22	0.53
5:A:466:THR:O	5:A:470:LEU:CG	2.57	0.53
5:A:467:MET:HE1	5:A:475:ASP:O	2.09	0.53
5:A:379:MET:SD	5:A:512:SER:HB2	2.49	0.53
5:A:650:ASN:O	5:A:653:LEU:HD13	2.08	0.53
5:A:707:ILE:C	5:A:711:HIS:HD2	2.12	0.53
6:B:75:GLU:HB2	6:B:132:ASN:HD22	1.73	0.53
19:B:1756:CLA:CGA	19:B:1770:CLA:HAA1	2.37	0.53
22:B:1781:BCR:C19	19:B:1787:CLA:H112	2.28	0.53
19:B:1787:CLA:CBB	19:B:1788:CLA:C1B	2.80	0.53
22:B:1782:BCR:HC42	19:B:1788:CLA:H142	1.88	0.53
6:B:529:THR:HA	6:B:532:LEU:HD23	1.89	0.53
6:B:551:LYS:O	6:B:553:PHE:CE2	2.61	0.53
6:B:668:ARG:HH12	6:B:672:GLN:HG2	1.71	0.53
7:C:74:THR:OG1	7:C:80:ALA:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:126:ALA:O	10:F:128:SER:OG	2.17	0.53
11:G:19:GLY:HA2	11:G:22:VAL:H	1.74	0.53
12:H:65:LEU:HD11	16:L:90:GLY:HA2	1.90	0.53
10:F:23:LYS:CA	10:F:24:LYS:HZ3	2.22	0.53
19:2:1212:CLA:HBC2	19:2:1212:CLA:CMC	2.32	0.53
8:D:31:GLY:O	8:D:32:SER:HB2	2.09	0.53
11:G:69:VAL:O	11:G:73:ALA:CB	2.57	0.53
6:B:20:ARG:CB	6:B:20:ARG:HH11	2.20	0.53
5:A:291:THR:O	5:A:293:GLY:N	2.36	0.53
2:2:42:ARG:C	2:2:45:VAL:H	2.11	0.53
4:4:94:GLU:HG2	4:4:95:PHE:CZ	2.38	0.53
19:A:1783:CLA:C1A	19:A:1783:CLA:CGA	2.87	0.53
19:A:1763:CLA:HMB2	22:A:1807:BCR:HC7	1.88	0.53
5:A:420:ARG:HG2	5:A:421:ASP:N	2.23	0.53
5:A:64:PHE:HE2	19:A:1761:CLA:HMC1	1.74	0.53
5:A:55:TRP:CD2	5:A:729:GLN:NE2	2.77	0.53
6:B:174:ARG:CB	19:B:1744:CLA:HBC2	2.27	0.53
22:B:1782:BCR:H272	22:I:1032:BCR:H352	1.90	0.53
6:B:189:ALA:CB	19:B:1759:CLA:C20	2.69	0.53
6:B:188:LEU:HG	6:B:189:ALA:N	2.24	0.53
6:B:431:PHE:HE2	19:B:1763:CLA:HED3	1.73	0.53
10:F:144:LEU:HG	10:F:145:LEU:HD23	1.91	0.53
10:F:149:LEU:HD23	10:F:153:ASN:ND2	2.23	0.53
6:B:302:LYS:HD3	11:G:49:THR:HA	1.91	0.53
22:I:1032:BCR:H291	22:L:1169:BCR:H281	1.89	0.53
4:4:75:TRP:HD1	19:4:1205:CLA:HMD3	1.63	0.53
4:4:68:GLY:C	4:4:71:ASN:HB2	2.20	0.53
16:L:162:ASP:HB2	16:L:163:LEU:HA	1.91	0.53
5:A:253:ASP:O	5:A:256:ALA:HB3	2.09	0.53
17:N:69:CYS:O	17:N:70:GLU:O	2.26	0.53
17:N:69:CYS:O	17:N:72:LYS:CD	2.57	0.53
5:A:22:VAL:HG12	5:A:23:ASP:N	2.22	0.53
19:4:4007:CLA:CHD	19:4:4007:CLA:CBC	2.80	0.53
6:B:330:ILE:CD1	6:B:330:ILE:O	2.57	0.53
7:C:28:MET:SD	8:D:122:LYS:C	2.87	0.53
17:N:37:PHE:N	17:N:37:PHE:CD2	2.76	0.53
2:2:51:HIS:HA	2:2:54:TRP:HB2	1.91	0.53
19:A:1780:CLA:C9	19:A:1780:CLA:OBD	2.42	0.53
5:A:281:LEU:HB2	5:A:301:HIS:HD2	1.73	0.53
5:A:567:ARG:NH2	5:A:567:ARG:HB3	2.23	0.53
19:B:1756:CLA:C2B	22:B:1778:BCR:C35	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:271:THR:OG1	6:B:272:ASP:N	2.41	0.53
6:B:302:LYS:O	6:B:303:TYR:CB	2.35	0.53
6:B:606:VAL:C	6:B:608:GLN:H	2.12	0.53
10:F:128:SER:O	10:F:130:LEU:HD23	2.09	0.53
11:G:13:GLY:O	11:G:16:LEU:HB2	2.07	0.53
6:B:294:ASN:CB	11:G:36:PRO:HD2	2.35	0.53
19:1:1192:CLA:CGD	20:1:1199:LMU:O2'	2.57	0.53
17:N:42:PHE:H	17:N:43:PRO:HD2	1.71	0.53
17:N:44:GLU:C	17:N:46:PHE:H	2.11	0.53
12:H:23:VAL:O	12:H:24:TYR:C	2.47	0.53
15:K:51:ASP:O	15:K:52:PRO:C	2.46	0.53
10:F:58:LYS:O	10:F:60:GLY:N	2.42	0.53
11:G:14:LEU:HG	11:G:14:LEU:O	2.07	0.53
5:A:438:HIS:HB2	5:A:441:ALA:CB	2.39	0.53
5:A:40:PHE:N	5:A:44:ILE:HG21	2.24	0.53
5:A:473:PRO:O	5:A:474:GLN:C	2.48	0.53
6:B:143:LEU:C	6:B:145:LEU:N	2.62	0.53
6:B:390:GLY:CA	22:B:1778:BCR:HC22	2.38	0.53
22:B:1781:BCR:C19	19:B:1787:CLA:C15	2.80	0.53
19:B:1787:CLA:H71	19:B:1787:CLA:C12	2.38	0.53
6:B:78:VAL:HG23	6:B:78:VAL:O	2.08	0.53
8:D:40:ALA:HA	8:D:44:GLU:O	2.08	0.53
12:H:25:GLY:CA	12:H:27:ASP:CB	2.75	0.53
10:F:61:LEU:CD2	10:F:69:PRO:HB2	2.31	0.53
16:L:108:LYS:C	16:L:108:LYS:HE2	2.29	0.53
6:B:44:GLN:CD	6:B:163:PRO:HB2	2.28	0.53
19:A:1782:CLA:CBA	19:A:1782:CLA:O1D	2.46	0.53
19:A:1799:CLA:H92	22:L:1169:BCR:C32	2.36	0.53
5:A:441:ALA:HA	5:A:444:SER:HB3	1.91	0.53
6:B:22:TRP:CE2	19:B:1771:CLA:HMB1	2.44	0.53
6:B:127:ILE:CG1	6:B:193:HIS:HE1	2.21	0.53
6:B:295:PHE:O	11:G:33:LYS:HB2	2.09	0.53
6:B:338:LEU:O	6:B:339:ALA:HB3	2.09	0.53
6:B:378:ILE:HG22	6:B:379:ALA:N	2.24	0.53
6:B:717:TYR:O	19:B:1786:CLA:HED3	2.09	0.53
6:B:719:PHE:CZ	19:B:1758:CLA:H71	2.44	0.53
9:E:86:GLU:CG	9:E:87:VAL:N	2.30	0.53
17:N:45:ASN:CA	17:N:57:LYS:NZ	2.72	0.53
17:N:58:VAL:CG1	17:N:59:PRO:CD	2.87	0.53
20:A:7023:LMU:C1	20:A:7023:LMU:H91	2.31	0.53
20:A:7016:LMU:H21	20:A:7016:LMU:H61	1.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:57:ILE:O	1:1:59:VAL:CA	2.56	0.53
20:A:7030:LMU:H2'	20:A:7030:LMU:C6'	2.39	0.53
19:1:1193:CLA:HAA2	19:1:1193:CLA:CBD	2.39	0.53
2:2:79:TRP:CG	2:2:79:TRP:O	2.62	0.53
15:K:31:ASN:H	15:K:32:ARG:NH1	2.07	0.53
19:1:1241:CLA:C4C	22:I:1032:BCR:C2	2.66	0.52
2:2:64:ILE:CG2	2:2:65:PRO:HD3	2.39	0.52
4:4:121:PHE:CD2	4:4:122:LYS:N	2.77	0.52
4:4:147:LEU:CD1	4:4:148:GLU:CB	2.85	0.52
4:4:152:LYS:CA	4:4:154:ILE:HG12	2.32	0.52
5:A:114:THR:O	5:A:525:ASN:ND2	2.42	0.52
5:A:725:LEU:HD21	19:A:1796:CLA:HMD3	1.91	0.52
22:A:1806:BCR:H17C	19:A:1811:CLA:H172	1.91	0.52
5:A:197:GLN:OE1	5:A:351:THR:O	2.27	0.52
5:A:430:ASP:H	5:A:433:ASP:CG	2.12	0.52
5:A:44:ILE:O	5:A:45:ALA:C	2.47	0.52
19:B:1736:CLA:CHD	22:I:1032:BCR:H401	2.40	0.52
19:B:1763:CLA:CBB	22:B:1779:BCR:C23	2.87	0.52
22:B:1779:BCR:H392	10:F:90:PHE:HA	1.91	0.52
6:B:193:HIS:HD2	19:B:1745:CLA:NC	2.07	0.52
6:B:431:PHE:CE2	19:B:1763:CLA:HED3	2.44	0.52
19:G:1099:CLA:H3A	19:G:1099:CLA:C1	2.38	0.52
11:G:43:HIS:O	11:G:45:GLU:CA	2.56	0.52
4:4:69:ILE:O	4:4:71:ASN:CB	2.56	0.52
3:3:132:TRP:CZ3	3:3:155:GLU:OE1	2.57	0.52
3:3:52:LYS:C	3:3:56:TYR:HD2	2.10	0.52
8:D:86:LEU:HD13	8:D:90:LEU:HG	1.90	0.52
2:2:181:HIS:NE2	19:2:1214:CLA:C4D	2.72	0.52
5:A:293:GLY:O	5:A:294:LEU:HB3	2.08	0.52
10:F:92:TYR:CD2	10:F:92:TYR:C	2.82	0.52
2:2:64:ILE:HG22	2:2:65:PRO:HD3	1.91	0.52
19:A:1781:CLA:CHC	22:A:1805:BCR:H371	2.38	0.52
19:A:1799:CLA:C11	19:A:1799:CLA:H61	2.38	0.52
5:A:242:ILE:HG12	5:A:243:PRO:CG	2.39	0.52
6:B:431:PHE:CE2	19:B:1763:CLA:CED	2.92	0.52
19:B:1756:CLA:H52	19:B:1770:CLA:HBD	1.90	0.52
6:B:376:GLN:HB3	6:B:587:ILE:HD12	1.91	0.52
6:B:707:LEU:HD11	19:B:1760:CLA:H91	1.91	0.52
6:B:458:ILE:HD11	19:F:1156:CLA:CED	2.39	0.52
10:F:73:VAL:HG11	10:F:83:PHE:HB2	1.89	0.52
19:G:1099:CLA:O1D	19:G:1099:CLA:HAA2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:25:LEU:HA	14:J:28:GLU:HB2	1.92	0.52
20:N:1086:LMU:C3	20:N:1086:LMU:O6'	2.56	0.52
18:R:39:UNK:CA	18:R:41:UNK:CB	2.88	0.52
19:J:1043:CLA:CBC	19:J:1043:CLA:CHD	2.83	0.52
19:2:1212:CLA:C3A	19:2:1212:CLA:CGA	2.85	0.52
19:R:1054:CLA:C4D	19:R:1054:CLA:HED3	2.34	0.52
4:4:53:LEU:O	4:4:54:GLY:C	2.48	0.52
3:3:208:PRO:HB3	3:3:210:GLN:CD	2.29	0.52
2:2:161:THR:HB	2:2:165:LYS:HB2	1.91	0.52
4:4:81:GLU:CA	4:4:81:GLU:OE2	2.50	0.52
5:A:368:LEU:HD12	19:A:1782:CLA:H61	1.89	0.52
5:A:214:GLY:O	5:A:215:SER:CB	2.56	0.52
5:A:40:PHE:H	5:A:44:ILE:CG2	2.22	0.52
5:A:91:LEU:O	19:A:1763:CLA:HMC3	2.09	0.52
19:B:1744:CLA:H41	19:B:1749:CLA:HBC1	1.85	0.52
19:B:1754:CLA:HMD2	19:B:1755:CLA:HBB2	1.88	0.52
6:B:185:VAL:CG2	22:B:1776:BCR:H272	2.39	0.52
8:D:43:GLU:HG3	8:D:44:GLU:H	1.74	0.52
6:B:228:GLY:HA3	11:G:8:ILE:HB	1.90	0.52
16:L:66:GLY:N	16:L:67:PRO:CD	2.72	0.52
20:A:7036:LMU:C1B	20:A:7036:LMU:H6E	2.39	0.52
20:A:7042:LMU:C6'	20:A:7042:LMU:C4	2.88	0.52
17:N:42:PHE:CD1	17:N:43:PRO:CA	2.92	0.52
19:3:3011:CLA:C12	19:3:3011:CLA:H172	2.29	0.52
7:C:29:ILE:HG23	8:D:126:GLY:CA	2.39	0.52
8:D:122:LYS:NZ	8:D:124:ASN:OD1	2.43	0.52
5:A:265:GLY:HA2	5:A:272:LEU:HD21	1.92	0.52
2:2:148:TRP:CH2	20:2:1224:LMU:H12	2.44	0.52
1:1:183:ASP:HB3	1:1:184:PRO:CD	2.40	0.52
1:1:183:ASP:OD1	4:4:89:THR:CB	2.57	0.52
2:2:97:VAL:CA	2:2:100:VAL:HG13	2.39	0.52
4:4:147:LEU:HD13	4:4:148:GLU:HB2	1.89	0.52
5:A:716:VAL:O	19:A:1795:CLA:HMD3	2.09	0.52
5:A:351:THR:HA	19:A:1780:CLA:H191	1.92	0.52
5:A:641:ASN:H	5:A:641:ASN:HD22	1.57	0.52
6:B:486:LEU:HD12	19:B:1766:CLA:OBD	2.09	0.52
5:A:690:LEU:HD21	6:B:661:PHE:HE1	1.75	0.52
7:C:1:MET:SD	7:C:4:SER:OG	2.67	0.52
19:A:1788:CLA:H152	22:L:1169:BCR:H363	1.90	0.52
4:4:75:TRP:CD2	4:4:76:TYR:N	2.77	0.52
3:3:182:LYS:O	3:3:185:LYS:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7050:LMU:C3	20:A:7050:LMU:H92	2.23	0.52
8:D:116:ASP:HB3	8:D:127:ARG:HH12	1.73	0.52
8:D:86:LEU:CD1	8:D:90:LEU:HG	2.39	0.52
20:A:7027:LMU:C2B	20:A:7027:LMU:C6B	2.88	0.52
10:F:91:LEU:O	10:F:94:ALA:O	2.26	0.52
6:B:98:GLN:O	6:B:98:GLN:NE2	2.43	0.52
5:A:536:THR:HA	5:A:539:PHE:HB3	1.91	0.52
12:H:70:ALA:O	12:H:71:ASN:HB2	2.09	0.52
19:A:1764:CLA:HBB2	19:A:1765:CLA:C4D	2.39	0.52
19:A:1811:CLA:H152	19:A:1811:CLA:H101	1.90	0.52
19:3:1212:CLA:O1D	5:A:246:HIS:CD2	2.62	0.52
5:A:378:SER:OG	5:A:378:SER:O	2.28	0.52
5:A:545:HIS:ND1	19:A:1792:CLA:CBB	2.68	0.52
5:A:603:PHE:CZ	5:A:735:VAL:HG22	2.45	0.52
19:B:1754:CLA:H12	19:B:1754:CLA:CAA	2.23	0.52
19:B:1765:CLA:C1D	19:B:1766:CLA:HBB2	2.39	0.52
19:B:1765:CLA:HMC3	19:B:1768:CLA:H2	1.91	0.52
6:B:18:THR:O	6:B:21:ILE:N	2.29	0.52
6:B:274:ALA:O	6:B:278:LEU:HB2	2.08	0.52
9:E:80:ASN:HB3	9:E:82:TYR:CE2	2.44	0.52
11:G:28:ARG:HH21	11:G:29:GLU:N	2.06	0.52
11:G:45:GLU:CA	11:G:49:THR:CG2	2.77	0.52
11:G:44:PHE:H	11:G:45:GLU:HB3	1.73	0.52
19:A:1788:CLA:C15	22:L:1169:BCR:H361	2.38	0.52
4:4:73:PRO:CB	4:4:75:TRP:HB2	2.38	0.52
17:N:62:SER:O	17:N:66:ASP:OD2	2.28	0.52
3:3:47:GLY:C	3:3:49:ILE:H	2.10	0.52
7:C:11:CYS:C	7:C:13:GLY:H	2.12	0.52
2:2:168:ARG:NE	2:2:168:ARG:HA	2.25	0.52
19:A:1783:CLA:HAA1	19:A:1783:CLA:HBD	1.91	0.52
5:A:453:LEU:CB	5:A:547:PHE:HB2	2.34	0.52
5:A:710:ALA:CB	19:B:1735:CLA:HED2	2.40	0.52
19:B:1763:CLA:CBB	22:B:1779:BCR:H23C	2.39	0.52
6:B:188:LEU:HG	6:B:189:ALA:H	1.75	0.52
6:B:207:VAL:O	6:B:208:ARG:O	2.27	0.52
6:B:273:VAL:O	6:B:277:HIS:CD2	2.61	0.52
6:B:387:PHE:O	6:B:391:PRO:HG3	2.09	0.52
6:B:464:GLN:OE1	6:B:469:LYS:CD	2.54	0.52
6:B:700:LEU:N	6:B:700:LEU:CD2	2.72	0.52
20:A:7036:LMU:H22	20:A:7036:LMU:C9	2.38	0.52
17:N:80:ASN:O	17:N:80:ASN:OD1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:49:ILE:CG1	3:3:52:LYS:HB2	2.39	0.52
20:A:7020:LMU:O1B	20:A:7020:LMU:O6'	2.28	0.52
7:C:12:ILE:O	7:C:38:GLN:HG2	2.09	0.52
7:C:39:ILE:CG1	7:C:40:ALA:N	2.65	0.52
17:N:34:THR:C	17:N:36:GLU:N	2.63	0.52
2:2:167:GLY:O	2:2:168:ARG:C	2.48	0.52
19:4:1198:CLA:HBC3	19:4:1198:CLA:HMC1	1.91	0.52
4:4:36:ASN:OD1	4:4:39:TRP:CE2	2.56	0.52
19:3:1212:CLA:CMC	19:A:1770:CLA:CBA	2.87	0.52
5:A:62:HIS:O	19:A:1785:CLA:HAA2	2.10	0.52
5:A:223:VAL:CG1	5:A:224:HIS:N	2.72	0.52
5:A:310:PHE:H	5:A:313:ALA:HB3	1.74	0.52
5:A:353:SER:O	5:A:354:TRP:CB	2.58	0.52
5:A:472:ARG:NE	5:A:474:GLN:HG3	2.14	0.52
19:B:1736:CLA:HBC2	19:B:1736:CLA:HMC1	1.92	0.52
19:B:1747:CLA:O2A	19:B:1747:CLA:HMA2	2.09	0.52
19:B:1735:CLA:HBC1	22:B:1779:BCR:C33	2.40	0.52
6:B:326:ILE:O	6:B:326:ILE:HG12	2.09	0.52
6:B:427:LEU:C	19:B:1763:CLA:HED2	2.30	0.52
6:B:8:PHE:O	6:B:35:ASP:CG	2.48	0.52
5:A:701:GLN:OE1	9:E:74:TYR:HE1	1.92	0.52
11:G:13:GLY:C	11:G:16:LEU:HG	2.30	0.52
16:L:56:VAL:CA	19:L:1167:CLA:HED2	2.33	0.52
16:L:162:ASP:OD2	16:L:162:ASP:N	2.35	0.52
17:N:65:LEU:C	17:N:66:ASP:OD2	2.48	0.52
3:3:60:ILE:HA	3:3:63:ARG:HD2	1.92	0.52
20:A:7022:LMU:O3B	20:A:7022:LMU:O6B	2.28	0.52
8:D:113:HIS:HD2	8:D:118:VAL:HG21	1.72	0.52
4:4:58:MET:O	4:4:60:LEU:N	2.43	0.52
8:D:33:THR:HG23	16:L:23:LEU:HD12	1.92	0.52
17:N:5:GLU:OE2	17:N:6:TYR:CA	2.57	0.52
6:B:160:LYS:HG3	6:B:161:TRP:N	2.20	0.52
2:2:98:GLU:OE2	19:2:1223:CLA:C4D	2.57	0.52
4:4:118:ASP:CG	4:4:123:GLN:CB	2.75	0.52
4:4:123:GLN:CG	4:4:124:TYR:H	2.23	0.52
5:A:691:MET:HB2	19:A:1812:CLA:C1C	2.39	0.52
5:A:207:LEU:HA	5:A:211:LEU:CB	2.39	0.52
5:A:341:GLN:O	5:A:344:LYS:HB2	2.10	0.52
5:A:331:LEU:CD1	5:A:346:LEU:CB	2.60	0.52
5:A:703:LEU:O	5:A:707:ILE:HG12	2.09	0.52
6:B:122:GLN:O	6:B:126:THR:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:124:TRP:C	6:B:124:TRP:HD1	2.11	0.52
6:B:393:PHE:CE1	6:B:394:PHE:CE2	2.98	0.52
8:D:36:LEU:HD21	8:D:45:PHE:CZ	2.44	0.52
9:E:90:VAL:O	9:E:91:ALA:O	2.28	0.52
19:B:1735:CLA:H191	10:F:104:TYR:CG	2.45	0.52
10:F:96:TRP:CE3	10:F:134:PHE:N	2.78	0.52
11:G:28:ARG:CG	11:G:29:GLU:HB2	2.39	0.52
11:G:68:ILE:HD12	11:G:68:ILE:H	1.75	0.52
13:I:17:PRO:O	13:I:18:ALA:C	2.48	0.52
17:N:46:PHE:O	17:N:47:THR:OG1	2.28	0.52
17:N:53:ALA:HB3	17:N:55:GLN:NE2	2.24	0.52
4:4:192:THR:HG23	4:4:193:ILE:CA	2.40	0.52
10:F:23:LYS:O	10:F:24:LYS:HE2	2.07	0.52
6:B:454:LEU:HD22	10:F:70:HIS:CD2	2.45	0.52
7:C:19:ARG:NE	8:D:121:GLU:OE2	2.43	0.52
2:2:119:VAL:O	2:2:120:ASN:O	2.28	0.52
19:4:1196:CLA:OBD	19:4:1196:CLA:O2D	2.28	0.52
4:4:128:ALA:HB3	4:4:143:PHE:CE2	2.35	0.52
5:A:149:PHE:O	5:A:150:PHE:HB2	2.09	0.52
19:A:1762:CLA:CED	19:A:1762:CLA:HBA2	2.40	0.52
19:A:1781:CLA:HBB2	19:A:1794:CLA:HMA1	1.92	0.52
5:A:32:GLU:HG3	5:A:33:GLN:N	2.25	0.52
5:A:393:LEU:O	5:A:397:THR:CG2	2.55	0.52
5:A:389:TYR:CD1	5:A:625:TRP:CG	2.97	0.52
19:B:1756:CLA:H11	19:B:1770:CLA:HBD	1.92	0.52
7:C:72:GLU:O	7:C:73:THR:O	2.27	0.52
17:N:42:PHE:N	17:N:43:PRO:HD3	2.22	0.52
17:N:67:LEU:N	17:N:67:LEU:CD1	2.53	0.52
17:N:76:LYS:O	17:N:77:CYS:O	2.27	0.52
20:A:7023:LMU:O1B	20:A:7023:LMU:O4'	2.27	0.52
19:2:1212:CLA:O1A	19:2:1212:CLA:C4A	2.57	0.52
8:D:131:GLY:O	8:D:132:LEU:HB2	2.08	0.52
3:3:106:TYR:CB	3:3:107:TRP:CD1	2.92	0.52
7:C:31:TRP:CD1	7:C:32:GLY:N	2.78	0.52
16:L:8:TYR:HE1	16:L:11:ILE:CG2	2.20	0.52
5:A:631:GLN:O	5:A:632:GLY:C	2.48	0.52
11:G:96:SER:C	11:G:98:PHE:H	2.13	0.52
19:A:1776:CLA:HBC2	19:A:1782:CLA:H18	1.90	0.52
19:A:1781:CLA:HHB	22:A:1805:BCR:H363	1.87	0.52
5:A:398:HIS:HD2	19:A:1783:CLA:ND	2.07	0.52
19:A:1797:CLA:CBA	19:A:1797:CLA:HMA3	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:553:VAL:CG2	22:A:1805:BCR:H401	2.38	0.52
5:A:216:LEU:O	5:A:219:ALA:N	2.43	0.52
5:A:598:VAL:HG12	5:A:598:VAL:O	2.10	0.52
19:B:1771:CLA:HBA1	22:L:1169:BCR:H362	1.91	0.52
9:E:89:GLU:O	9:E:90:VAL:CB	2.58	0.52
10:F:124:PRO:C	10:F:126:ALA:H	2.13	0.52
21:B:8055:SUC:C3'	21:B:8055:SUC:O6'	2.55	0.52
21:3:1226:SUC:H5'	21:3:1226:SUC:O6	2.09	0.52
15:K:55:PHE:N	15:K:55:PHE:HD1	2.07	0.52
19:A:1798:CLA:CED	19:A:1798:CLA:CBA	2.88	0.52
12:H:54:LEU:CD1	12:H:55:LYS:HG3	2.40	0.52
5:A:630:ASP:C	5:A:632:GLY:N	2.60	0.52
15:K:32:ARG:HA	15:K:32:ARG:NE	2.25	0.52
2:2:54:TRP:HZ2	2:2:109:ARG:HD3	1.76	0.51
19:A:1759:CLA:CGA	19:A:1796:CLA:H2	2.40	0.51
5:A:301:HIS:NE2	19:A:1772:CLA:CHA	2.73	0.51
5:A:216:LEU:CD1	22:A:1802:BCR:C35	2.88	0.51
5:A:38:GLY:O	5:A:39:HIS:HB3	2.10	0.51
5:A:473:PRO:C	5:A:475:ASP:N	2.61	0.51
5:A:654:ARG:HA	6:B:632:ILE:HD13	1.91	0.51
5:A:734:GLY:O	5:A:736:THR:N	2.43	0.51
6:B:290:MET:HG3	19:B:1752:CLA:HMC3	1.92	0.51
6:B:530:THR:HG22	19:B:1756:CLA:CMC	2.39	0.51
6:B:525:LEU:HD22	6:B:529:THR:OG1	2.10	0.51
6:B:556:SER:O	24:B:1784:LMG:HC2	2.10	0.51
6:B:55:ALA:HB1	6:B:150:LEU:HD12	1.91	0.51
11:G:47:GLY:N	11:G:48:ASP:HB3	2.08	0.51
16:L:102:TYR:C	16:L:104:ILE:H	2.13	0.51
8:D:75:LEU:HD21	16:L:19:PHE:CE2	2.45	0.51
17:N:63:ASP:OD1	17:N:66:ASP:OD2	2.28	0.51
18:R:35:UNK:O	18:R:42:UNK:O	2.29	0.51
20:A:7051:LMU:O2'	20:A:7051:LMU:C1	2.58	0.51
21:3:1226:SUC:C5'	21:3:1226:SUC:O6	2.59	0.51
2:2:198:ALA:O	2:2:199:ASP:OD2	2.28	0.51
1:1:136:ASP:O	1:1:138:LYS:N	2.43	0.51
1:1:115:GLU:O	1:1:116:LYS:HB2	2.10	0.51
4:4:103:ILE:HG13	19:4:1197:CLA:CMD	2.39	0.51
4:4:34:PRO:CB	4:4:35:GLU:CB	2.61	0.51
19:A:1763:CLA:HMB3	19:A:1764:CLA:HHB	1.92	0.51
19:A:1781:CLA:H111	19:A:1781:CLA:H162	1.92	0.51
19:A:1783:CLA:H92	22:A:1806:BCR:H373	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:218:TRP:N	19:A:1770:CLA:HBB2	2.25	0.51
5:A:211:LEU:HB3	5:A:310:PHE:CE2	2.44	0.51
5:A:393:LEU:HD13	5:A:750:PHE:CE1	2.43	0.51
5:A:366:GLY:O	5:A:403:GLY:HA2	2.10	0.51
5:A:435:VAL:O	5:A:438:HIS:ND1	2.40	0.51
6:B:130:ARG:NH1	6:B:130:ARG:CG	2.72	0.51
19:B:1741:CLA:HMA2	19:B:1741:CLA:C1	2.40	0.51
19:B:1742:CLA:HAA2	19:B:1742:CLA:H12	1.92	0.51
22:B:1779:BCR:C37	10:F:93:ILE:HG22	2.39	0.51
6:B:292:ARG:NE	6:B:297:ILE:O	2.43	0.51
6:B:440:ASN:ND2	6:B:453:ILE:O	2.43	0.51
6:B:560:ASP:OD1	7:C:66:ARG:HB3	2.09	0.51
6:B:697:PRO:HB3	19:B:1771:CLA:CBC	2.41	0.51
9:E:40:ARG:N	9:E:46:PHE:HE1	2.08	0.51
9:E:88:GLU:O	9:E:90:VAL:CG2	2.57	0.51
11:G:58:LEU:O	11:G:60:SER:N	2.43	0.51
16:L:33:ILE:O	16:L:36:TYR:N	2.44	0.51
16:L:160:VAL:O	16:L:161:LEU:O	2.29	0.51
17:N:62:SER:O	17:N:66:ASP:OD1	2.28	0.51
17:N:70:GLU:O	17:N:72:LYS:N	2.40	0.51
17:N:75:TYR:HH	20:N:1086:LMU:H4O1	1.58	0.51
19:1:1148:CLA:O1A	19:1:1148:CLA:HED1	2.01	0.51
18:R:37:UNK:O	18:R:42:UNK:O	2.28	0.51
20:B:1783:LMU:O3'	20:B:1783:LMU:C5B	2.47	0.51
15:K:17:LEU:CD2	15:K:21:ALA:HB2	2.40	0.51
17:N:4:GLU:CD	17:N:4:GLU:C	2.69	0.51
5:A:635:THR:HG22	5:A:635:THR:O	2.10	0.51
2:2:68:LEU:O	2:2:69:THR:C	2.48	0.51
4:4:127:PRO:HB2	4:4:143:PHE:CE1	2.46	0.51
4:4:149:ALA:CB	4:4:151:GLU:CD	2.48	0.51
19:A:1770:CLA:CAB	22:A:1802:BCR:H19C	2.33	0.51
5:A:227:LEU:HD23	5:A:231:GLN:NE2	2.24	0.51
5:A:361:ASN:ND2	19:A:1761:CLA:HED1	2.23	0.51
5:A:450:CYS:O	5:A:453:LEU:O	2.27	0.51
5:A:685:VAL:O	5:A:688:PHE:HB3	2.10	0.51
6:B:289:LEU:HA	19:B:1751:CLA:O1D	2.10	0.51
6:B:563:GLY:C	6:B:564:ARG:O	2.46	0.51
6:B:599:ILE:O	6:B:734:GLY:C	2.48	0.51
7:C:7:ILE:CG2	7:C:65:VAL:HG21	2.41	0.51
6:B:16:PRO:HG3	7:C:74:THR:CG2	2.39	0.51
19:4:1204:CLA:C4B	19:F:1157:CLA:H43	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:16:LEU:CD2	11:G:68:ILE:HG21	2.40	0.51
17:N:49:CYS:O	17:N:51:ASP:O	2.29	0.51
18:R:39:UNK:CA	18:R:42:UNK:CB	2.85	0.51
19:R:1054:CLA:C4D	19:R:1054:CLA:CED	2.89	0.51
3:3:157:ALA:O	3:3:158:TYR:CD2	2.63	0.51
7:C:12:ILE:HG21	7:C:39:ILE:C	2.31	0.51
9:E:69:PHE:HD2	9:E:71:LYS:HG2	1.76	0.51
16:L:5:LYS:N	16:L:6:PRO:CD	2.73	0.51
12:H:50:ARG:NH1	12:H:53:LEU:C	2.61	0.51
5:A:519:ASP:C	5:A:520:LEU:HG	2.30	0.51
19:A:1776:CLA:HMC1	19:A:1776:CLA:HBC2	1.92	0.51
19:A:1783:CLA:O1D	19:A:1783:CLA:H2A	2.10	0.51
5:A:207:LEU:HB3	19:A:1776:CLA:CBB	2.40	0.51
5:A:281:LEU:HD22	19:A:1772:CLA:CMA	2.40	0.51
5:A:73:GLU:HA	5:A:76:ARG:HD2	1.91	0.51
6:B:299:HIS:NE2	6:B:304:ILE:HG21	2.25	0.51
6:B:536:LYS:O	6:B:537:GLY:C	2.48	0.51
6:B:570:ILE:O	6:B:570:ILE:HG13	2.10	0.51
5:A:571:ASP:OD2	8:D:88:THR:HG21	2.10	0.51
11:G:21:PHE:O	11:G:23:PHE:N	2.43	0.51
11:G:38:GLN:O	11:G:40:GLY:O	2.28	0.51
11:G:43:HIS:O	11:G:45:GLU:N	2.44	0.51
16:L:161:LEU:HD11	16:L:163:LEU:N	2.26	0.51
17:N:42:PHE:HD1	17:N:43:PRO:CA	2.23	0.51
19:1:1014:CLA:O1A	19:1:1014:CLA:O1D	2.28	0.51
3:3:63:ARG:NH2	3:3:189:LEU:HD23	2.19	0.51
4:4:191:ASN:O	4:4:192:THR:O	2.29	0.51
5:A:25:ASP:N	5:A:26:PRO:HD2	2.22	0.51
20:K:1086:LMU:O4'	20:K:1086:LMU:O6B	2.28	0.51
12:H:20:GLN:C	12:H:22:ASP:HB3	2.31	0.51
20:A:7039:LMU:O2'	20:A:7039:LMU:C5'	2.43	0.51
6:B:317:ARG:NH2	6:B:410:ARG:HG2	2.25	0.51
4:4:169:GLN:NE2	19:4:1199:CLA:CHD	2.69	0.51
5:A:744:ALA:HB2	22:A:1806:BCR:H391	0.59	0.51
5:A:183:TRP:O	5:A:185:HIS:N	2.44	0.51
5:A:209:GLY:C	5:A:213:LEU:HB2	2.31	0.51
5:A:334:HIS:CB	19:A:1777:CLA:HMA3	2.40	0.51
5:A:401:TRP:CZ3	5:A:609:ILE:HB	2.44	0.51
5:A:661:ALA:O	5:A:665:ILE:HG13	2.10	0.51
5:A:741:GLY:O	5:A:743:ILE:N	2.44	0.51
19:B:1769:CLA:C6	22:B:1780:BCR:C32	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1788:CLA:HBC2	19:B:1788:CLA:HMC1	1.92	0.51
6:B:362:ALA:C	6:B:364:ASP:H	2.14	0.51
6:B:353:TYR:HB2	6:B:594:TRP:HH2	1.76	0.51
6:B:606:VAL:C	6:B:608:GLN:N	2.62	0.51
7:C:5:VAL:HB	7:C:65:VAL:HG22	1.91	0.51
10:F:100:VAL:C	10:F:103:SER:HG	2.12	0.51
10:F:104:TYR:C	10:F:104:TYR:CD2	2.84	0.51
16:L:123:ARG:C	16:L:124:LYS:HE3	2.31	0.51
18:R:30:UNK:O	18:R:32:UNK:N	2.43	0.51
18:R:38:UNK:O	18:R:42:UNK:C	2.59	0.51
21:B:8062:SUC:O6	21:B:8062:SUC:O2'	2.29	0.51
8:D:58:PHE:CD2	8:D:59:GLU:N	2.78	0.51
6:B:70:TRP:HB3	6:B:136:TYR:OH	2.09	0.51
17:N:27:ALA:O	17:N:28:ASN:O	2.29	0.51
3:3:153:SER:OG	3:3:154:GLY:N	2.43	0.51
4:4:37:LEU:O	4:4:38:ARG:O	2.27	0.51
5:A:361:ASN:OD1	19:A:1761:CLA:OBD	2.29	0.51
19:A:1773:CLA:H51	19:A:1782:CLA:HMB1	1.93	0.51
19:A:1797:CLA:H91	15:K:61:LEU:CD1	2.36	0.51
22:A:1807:BCR:C23	22:A:1807:BCR:C39	2.65	0.51
5:A:619:LYS:O	5:A:621:GLN:N	2.43	0.51
19:B:1756:CLA:HBD	19:B:1768:CLA:HMB3	1.92	0.51
6:B:337:ALA:O	6:B:339:ALA:O	2.29	0.51
6:B:729:THR:CG2	6:B:729:THR:O	2.30	0.51
9:E:63:TYR:HA	9:E:83:ALA:HB2	1.92	0.51
10:F:104:TYR:HD2	10:F:104:TYR:C	2.13	0.51
11:G:43:HIS:O	11:G:45:GLU:OE1	2.28	0.51
4:4:174:GLY:O	4:4:175:LYS:CG	2.40	0.51
19:J:1043:CLA:NA	19:J:1043:CLA:HED3	2.12	0.51
20:A:7026:LMU:C2B	20:A:7026:LMU:O3'	2.57	0.51
6:B:247:THR:O	6:B:248:GLN:O	2.27	0.51
5:A:335:LYS:CG	5:A:336:GLY:N	2.60	0.51
2:2:98:GLU:HG2	2:2:99:LEU:HD12	1.91	0.51
4:4:128:ALA:CA	4:4:143:PHE:HZ	2.23	0.51
5:A:212:GLY:C	5:A:214:GLY:H	2.13	0.51
5:A:298:ASP:O	5:A:301:HIS:N	2.44	0.51
5:A:356:ALA:O	5:A:360:ILE:HG22	2.10	0.51
5:A:369:THR:HG21	5:A:402:ILE:HG22	1.90	0.51
5:A:40:PHE:HZ	5:A:56:ASN:HB3	1.72	0.51
5:A:701:GLN:OE1	9:E:74:TYR:CE1	2.64	0.51
5:A:746:THR:O	5:A:750:PHE:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:124:TRP:CE2	6:B:129:LEU:HD22	2.45	0.51
19:B:1758:CLA:CGA	19:B:1758:CLA:H3A	2.35	0.51
6:B:197:VAL:O	6:B:198:ALA:CB	2.59	0.51
6:B:440:ASN:CG	6:B:614:THR:O	2.49	0.51
5:A:654:ARG:HH21	6:B:637:PRO:HD2	1.75	0.51
6:B:662:MET:O	6:B:663:PHE:C	2.48	0.51
6:B:730:SER:O	6:B:731:GLY:O	2.29	0.51
10:F:104:TYR:OH	10:F:122:ASP:N	2.33	0.51
11:G:33:LYS:O	11:G:34:GLN:O	2.28	0.51
11:G:58:LEU:HD12	11:G:59:LYS:HE3	1.92	0.51
16:L:128:ASP:CG	16:L:129:GLN:N	2.63	0.51
4:4:72:VAL:O	4:4:73:PRO:O	2.28	0.51
17:N:47:THR:O	17:N:48:GLY:O	2.29	0.51
12:H:26:SER:O	12:H:27:ASP:O	2.29	0.51
8:D:72:PRO:HB2	8:D:74:LEU:HB2	1.93	0.51
12:H:40:PHE:O	12:H:43:PHE:N	2.44	0.51
20:A:7017:LMU:O3'	20:A:7017:LMU:C1B	2.56	0.51
12:H:77:LEU:HB3	12:H:78:PRO:HD2	1.93	0.51
5:A:527:VAL:HG12	5:A:528:ALA:N	2.26	0.51
6:B:681:ALA:O	6:B:683:GLU:N	2.44	0.51
3:3:116:PHE:O	3:3:120:LEU:HB2	2.10	0.51
2:2:183:TYR:O	2:2:184:THR:C	2.49	0.51
1:1:183:ASP:CB	1:1:184:PRO:CD	2.87	0.51
19:A:1772:CLA:C2	19:A:1772:CLA:CBA	2.77	0.51
19:A:1773:CLA:H12	19:A:1773:CLA:C4A	2.41	0.51
5:A:575:LEU:CD1	5:A:576:GLY:H	2.24	0.51
5:A:725:LEU:HD12	5:A:725:LEU:N	2.26	0.51
6:B:86:PRO:C	6:B:115:ASN:HB3	2.31	0.51
6:B:202:SER:CB	6:B:270:LEU:HD21	2.41	0.51
6:B:510:LEU:CD2	6:B:510:LEU:H	2.23	0.51
6:B:710:LEU:C	6:B:712:HIS:H	2.12	0.51
10:F:80:TRP:CH2	19:F:1156:CLA:HAC2	2.46	0.51
16:L:96:SER:OG	16:L:143:PHE:CD2	2.57	0.51
17:N:38:GLY:HA3	17:N:46:PHE:CD1	2.46	0.51
17:N:72:LYS:HZ3	17:N:74:LYS:HA	1.76	0.51
7:C:9:ASP:CB	25:C:1083:SF4:S2	2.99	0.51
10:F:26:GLN:O	10:F:28:SER:OG	2.28	0.51
15:K:10:ILE:O	15:K:13:THR:CG2	2.41	0.51
19:3:1222:CLA:O1D	19:3:1222:CLA:CAA	2.58	0.51
8:D:132:LEU:HD23	8:D:133:ASN:O	2.10	0.51
8:D:113:HIS:N	8:D:114:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:62:ALA:O	15:K:65:ALA:HB2	2.11	0.51
2:2:101:PHE:O	2:2:102:ILE:C	2.49	0.51
4:4:31:ALA:O	4:4:32:GLU:O	2.29	0.51
4:4:98:SER:O	4:4:102:GLU:CD	2.49	0.51
19:A:1782:CLA:HBD	19:A:1782:CLA:CBA	2.41	0.51
19:B:1757:CLA:H101	22:B:1778:BCR:H14C	1.92	0.51
6:B:665:ILE:HD12	19:B:1788:CLA:HBC1	1.93	0.51
6:B:467:HIS:NE2	19:B:1765:CLA:CHA	2.74	0.51
6:B:74:PHE:C	6:B:76:ALA:H	2.14	0.51
7:C:73:THR:OG1	7:C:76:SER:OG	2.29	0.51
19:F:1156:CLA:O1D	19:F:1156:CLA:H2A	2.11	0.51
19:A:1787:CLA:H93	16:L:36:TYR:HE1	1.76	0.51
16:L:164:PRO:HD3	16:L:165:TYR:CZ	2.37	0.51
20:A:7023:LMU:H92	20:A:7023:LMU:C4	2.03	0.51
2:2:204:ILE:O	2:2:205:PHE:CB	2.59	0.51
4:4:191:ASN:O	4:4:191:ASN:OD1	2.29	0.51
17:N:35:VAL:HG12	17:N:37:PHE:CE1	2.45	0.51
5:A:574:ASN:N	5:A:574:ASN:OD1	2.43	0.51
2:2:121:THR:OG1	2:2:121:THR:O	2.28	0.51
4:4:98:SER:OG	4:4:102:GLU:OE1	2.29	0.51
4:4:46:VAL:HG21	4:4:105:ARG:NH1	2.26	0.51
4:4:88:SER:C	4:4:89:THR:CG2	2.79	0.51
4:4:90:LEU:H	4:4:90:LEU:HD23	1.75	0.51
4:4:98:SER:O	4:4:102:GLU:OE1	2.29	0.51
19:A:1770:CLA:C4B	22:A:1802:BCR:C20	2.87	0.51
5:A:224:HIS:HE1	19:A:1771:CLA:C4C	2.24	0.51
5:A:509:ALA:O	5:A:510:SER:OG	2.17	0.51
5:A:592:VAL:O	5:A:597:HIS:CD2	2.64	0.51
5:A:655:ASP:O	5:A:660:GLN:NE2	2.44	0.51
5:A:747:TRP:CD2	22:A:1806:BCR:H403	2.46	0.51
6:B:414:HIS:NE2	19:B:1761:CLA:NA	2.59	0.51
19:B:1769:CLA:C16	22:B:1780:BCR:H311	2.37	0.51
23:B:1774:PQN:C29	24:B:1784:LMG:H201	2.40	0.51
6:B:228:GLY:HA3	11:G:8:ILE:HD13	1.92	0.51
6:B:309:ILE:HD12	6:B:312:GLY:HA3	1.93	0.51
6:B:436:LEU:O	6:B:437:TYR:CB	2.59	0.51
6:B:535:VAL:HG13	6:B:536:LYS:H	1.76	0.51
6:B:77:TRP:CE2	6:B:81:PRO:HB3	2.45	0.51
10:F:83:PHE:C	10:F:86:PRO:HD2	2.32	0.51
22:I:1032:BCR:H271	22:I:1032:BCR:H403	1.92	0.51
19:A:1788:CLA:H152	22:L:1169:BCR:H361	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:254:LEU:C	5:A:256:ALA:N	2.64	0.51
17:N:38:GLY:C	17:N:39:SER:O	2.47	0.51
17:N:49:CYS:O	17:N:50:GLN:O	2.29	0.51
17:N:59:PRO:O	17:N:61:LEU:O	2.28	0.51
18:R:35:UNK:O	18:R:36:UNK:O	2.29	0.51
20:A:7016:LMU:H71	20:A:7016:LMU:H111	1.92	0.51
19:J:1044:CLA:OBD	19:J:1044:CLA:O2D	2.28	0.51
10:F:50:LYS:C	10:F:52:ARG:N	2.64	0.51
20:A:7039:LMU:O6B	20:A:7039:LMU:O3'	2.29	0.51
8:D:48:ILE:HG12	8:D:49:THR:N	2.23	0.51
8:D:50:TRP:N	8:D:50:TRP:CD1	2.79	0.51
16:L:9:GLN:HG3	16:L:10:VAL:H	1.76	0.51
5:A:464:ASN:O	5:A:468:SER:N	2.39	0.51
4:4:177:PRO:HB2	4:4:178:PHE:CD1	2.46	0.51
4:4:104:ARG:HD2	19:4:1208:CLA:C3C	2.35	0.50
19:4:1196:CLA:HAA1	19:4:1196:CLA:HBD	1.92	0.50
4:4:83:TYR:O	4:4:87:SER:OG	2.30	0.50
4:4:95:PHE:O	4:4:98:SER:OG	2.29	0.50
5:A:747:TRP:HB2	19:A:1783:CLA:HBB1	1.92	0.50
19:A:1784:CLA:H52	19:A:1784:CLA:CMD	2.41	0.50
19:A:1788:CLA:H11	19:A:1799:CLA:H43	1.93	0.50
5:A:185:HIS:O	5:A:188:LYS:HG3	2.11	0.50
5:A:379:MET:SD	5:A:511:THR:O	2.69	0.50
5:A:580:PRO:HB3	5:A:727:ILE:HG21	1.92	0.50
5:A:88:ILE:C	5:A:90:PHE:N	2.62	0.50
6:B:58:PHE:CE2	6:B:145:LEU:HD12	2.45	0.50
19:B:1740:CLA:C9	22:B:1782:BCR:H361	2.39	0.50
19:B:1741:CLA:HBC3	19:B:1787:CLA:C14	2.41	0.50
6:B:231:ASN:O	6:B:233:TYR:N	2.44	0.50
6:B:290:MET:HG2	6:B:290:MET:O	2.10	0.50
6:B:382:ILE:O	6:B:385:GLY:N	2.41	0.50
6:B:17:THR:HA	6:B:696:LYS:N	2.26	0.50
7:C:72:GLU:C	7:C:73:THR:O	2.45	0.50
8:D:46:TYR:HD1	8:D:80:LYS:HB3	1.75	0.50
19:G:1099:CLA:O2A	19:G:1099:CLA:CMA	2.59	0.50
11:G:32:ALA:C	11:G:34:GLN:N	2.64	0.50
4:4:68:GLY:O	4:4:69:ILE:O	2.29	0.50
1:1:29:LEU:O	1:1:33:PRO:HD3	2.11	0.50
17:N:51:ASP:N	17:N:51:ASP:OD2	2.30	0.50
17:N:47:THR:OG1	17:N:52:LEU:O	2.28	0.50
19:1:1148:CLA:C7	19:1:1148:CLA:H2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:38:UNK:O	18:R:42:UNK:O	2.29	0.50
5:A:25:ASP:O	5:A:26:PRO:O	2.29	0.50
10:F:28:SER:O	10:F:30:LYS:O	2.27	0.50
10:F:53:PHE:C	10:F:55:ASN:N	2.63	0.50
19:1:1145:CLA:H2A	19:1:1145:CLA:O1A	2.08	0.50
3:3:74:ALA:CB	3:3:75:PRO:HD3	2.26	0.50
15:K:24:PHE:CG	15:K:52:PRO:HG2	2.43	0.50
2:2:37:ASP:OD2	3:3:41:ASP:OD1	2.29	0.50
19:A:1768:CLA:C4D	19:A:1769:CLA:HMC3	2.41	0.50
5:A:375:HIS:HE1	19:A:1782:CLA:NC	2.07	0.50
5:A:90:PHE:HE2	5:A:178:MET:SD	2.33	0.50
6:B:311:PRO:HD3	19:B:1773:CLA:C3C	2.41	0.50
19:B:1744:CLA:H11	22:B:1776:BCR:C10	2.41	0.50
6:B:305:LEU:O	6:B:308:HIS:N	2.25	0.50
6:B:420:SER:O	6:B:424:TRP:N	2.35	0.50
6:B:458:ILE:HD11	19:F:1156:CLA:HED1	1.92	0.50
20:A:7042:LMU:H5'	20:A:7042:LMU:C2B	2.40	0.50
17:N:62:SER:O	17:N:63:ASP:OD1	2.29	0.50
15:K:44:GLU:O	15:K:45:SER:CB	2.59	0.50
10:F:28:SER:O	10:F:29:LEU:O	2.29	0.50
20:A:7021:LMU:C2	20:A:7021:LMU:C6	2.71	0.50
19:A:1798:CLA:CED	19:A:1798:CLA:HBA1	2.41	0.50
19:1:1149:CLA:CGD	19:1:1149:CLA:HAA1	2.42	0.50
5:A:274:TRP:NE1	5:A:277:TYR:CE2	2.79	0.50
1:1:42:SER:HA	1:1:45:ILE:HG12	1.92	0.50
10:F:116:GLN:O	10:F:118:GLU:N	2.44	0.50
5:A:68:THR:O	5:A:70:ASP:N	2.42	0.50
5:A:529:LEU:H	5:A:529:LEU:HD12	1.76	0.50
2:2:106:GLU:O	19:2:1222:CLA:CMA	2.60	0.50
19:A:1759:CLA:H42	19:A:1796:CLA:H8	1.91	0.50
19:A:1765:CLA:CBA	19:A:1765:CLA:CHA	2.88	0.50
19:A:1781:CLA:HAA1	19:A:1781:CLA:HBD	1.93	0.50
19:A:1782:CLA:C10	19:A:1782:CLA:H143	2.40	0.50
19:A:1799:CLA:HMB2	19:L:1167:CLA:CBC	2.38	0.50
5:A:329:ASP:O	5:A:332:GLU:O	2.29	0.50
5:A:72:GLU:HB3	5:A:76:ARG:NH2	2.26	0.50
5:A:750:PHE:O	5:A:752:ALA:N	2.45	0.50
19:B:1752:CLA:HMA3	19:B:1753:CLA:C3D	2.41	0.50
19:B:1754:CLA:H43	19:B:1754:CLA:C2A	2.39	0.50
6:B:310:PRO:O	19:B:1773:CLA:CHD	2.60	0.50
6:B:626:LEU:HD12	6:B:627:ASN:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:726:ILE:C	6:B:728:SER:H	2.13	0.50
4:4:75:TRP:CH2	4:4:76:TYR:HB3	2.46	0.50
3:3:92:TRP:O	3:3:95:THR:HG23	2.11	0.50
17:N:45:ASN:O	17:N:45:ASN:ND2	2.45	0.50
17:N:45:ASN:CA	17:N:57:LYS:HZ2	2.24	0.50
17:N:82:PHE:HD2	17:N:82:PHE:N	2.08	0.50
7:C:15:THR:N	7:C:17:CYS:SG	2.84	0.50
20:A:7050:LMU:O3'	20:A:7050:LMU:O5B	2.29	0.50
20:A:7026:LMU:O3B	21:B:8062:SUC:C6'	2.56	0.50
21:B:8062:SUC:O1	21:B:8062:SUC:O6	2.30	0.50
3:3:109:ASP:O	3:3:110:SER:O	2.28	0.50
3:3:157:ALA:O	3:3:158:TYR:CB	2.59	0.50
5:A:141:ARG:NH2	5:A:141:ARG:HG3	2.15	0.50
6:B:136:TYR:O	6:B:140:ILE:HD11	2.12	0.50
4:4:118:ASP:C	4:4:122:LYS:HA	2.32	0.50
4:4:40:PHE:C	4:4:43:ALA:CB	2.79	0.50
5:A:365:LEU:CD2	19:A:1761:CLA:CED	2.67	0.50
19:A:1764:CLA:HBC3	19:A:1764:CLA:HHD	1.93	0.50
5:A:126:ILE:CG1	19:A:1765:CLA:HMA3	2.40	0.50
19:A:1776:CLA:H18	22:A:1804:BCR:H383	1.94	0.50
5:A:242:ILE:HD13	5:A:242:ILE:N	2.27	0.50
5:A:283:PHE:O	5:A:284:ARG:NH1	2.44	0.50
5:A:327:ILE:HG13	5:A:328:LYS:H	1.76	0.50
5:A:430:ASP:O	5:A:434:ARG:HB2	2.12	0.50
5:A:547:PHE:CE2	19:B:1788:CLA:O1A	2.63	0.50
5:A:685:VAL:HG12	5:A:741:GLY:CA	2.40	0.50
6:B:29:HIS:CE1	19:B:1760:CLA:H43	2.46	0.50
6:B:631:LEU:HG	6:B:632:ILE:HG23	1.94	0.50
7:C:73:THR:O	7:C:76:SER:OG	2.29	0.50
11:G:8:ILE:CG1	11:G:8:ILE:O	2.56	0.50
16:L:163:LEU:HD13	16:L:164:PRO:CG	2.41	0.50
3:3:205:GLY:CA	5:A:252:ARG:HH12	2.24	0.50
20:B:1783:LMU:O3'	20:B:1783:LMU:O6B	2.30	0.50
20:A:7016:LMU:H112	20:A:7016:LMU:H72	1.90	0.50
21:B:8055:SUC:O1'	21:B:8055:SUC:O6'	2.30	0.50
5:A:27:ILE:C	5:A:28:LYS:HG3	2.25	0.50
18:R:44:UNK:O	18:R:45:UNK:O	2.30	0.50
5:A:176:GLY:O	5:A:180:PHE:HB2	2.12	0.50
2:2:54:TRP:HZ2	2:2:109:ARG:CB	2.24	0.50
5:A:169:ILE:O	5:A:173:VAL:HG13	2.11	0.50
19:A:1771:CLA:O1D	19:A:1771:CLA:OBD	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1810:CLA:HBB2	19:A:1811:CLA:HED1	1.94	0.50
5:A:394:SER:OG	5:A:395:LEU:N	2.44	0.50
5:A:620:MET:SD	5:A:624:VAL:HG21	2.52	0.50
5:A:672:LEU:C	5:A:674:ALA:H	2.08	0.50
5:A:93:LEU:O	5:A:97:TYR:HD2	1.94	0.50
6:B:124:TRP:HZ2	6:B:135:LEU:HB2	1.76	0.50
19:B:1760:CLA:C9	24:B:1784:LMG:H311	2.42	0.50
19:B:1756:CLA:OBD	19:B:1768:CLA:HBB1	2.12	0.50
22:B:1776:BCR:H331	22:B:1776:BCR:C8	2.41	0.50
19:B:1787:CLA:H71	19:B:1787:CLA:H122	1.94	0.50
6:B:331:HIS:CE1	6:B:392:ILE:CG2	2.91	0.50
6:B:551:LYS:HE2	8:D:143:PRO:CA	2.42	0.50
17:N:58:VAL:HG12	17:N:59:PRO:HD3	1.94	0.50
17:N:82:PHE:CD2	17:N:82:PHE:N	2.78	0.50
18:R:38:UNK:O	18:R:39:UNK:O	2.30	0.50
5:A:24:ARG:O	5:A:25:ASP:O	2.30	0.50
19:4:4014:CLA:HAA2	19:4:4014:CLA:HBD	1.94	0.50
3:3:86:GLN:HB2	3:3:88:THR:N	2.26	0.50
6:B:406:ASN:ND2	6:B:406:ASN:C	2.65	0.50
19:1:1196:CLA:OBD	19:1:1196:CLA:CMD	2.53	0.50
3:3:106:TYR:CD2	3:3:107:TRP:CG	2.99	0.50
1:1:185:TRP:O	1:1:186:HIS:O	2.30	0.50
4:4:115:VAL:C	4:4:117:GLN:HG3	2.32	0.50
5:A:188:LYS:O	5:A:190:ALA:N	2.45	0.50
5:A:354:TRP:O	5:A:358:LEU:N	2.44	0.50
5:A:409:GLY:C	5:A:411:ALA:N	2.65	0.50
5:A:538:ASP:O	5:A:542:HIS:HB2	2.10	0.50
5:A:618:TRP:CZ2	5:A:655:ASP:HB3	2.46	0.50
5:A:685:VAL:CG1	5:A:741:GLY:HA2	2.42	0.50
19:B:1742:CLA:HBD	19:B:1742:CLA:C1	2.41	0.50
19:B:1756:CLA:HED1	19:B:1757:CLA:HMD2	1.87	0.50
6:B:521:HIS:CE1	19:B:1769:CLA:C4A	2.91	0.50
6:B:420:SER:H	6:B:422:LEU:H	1.60	0.50
5:A:558:LYS:HZ1	6:B:674:LEU:HD23	1.77	0.50
9:E:85:ASP:OD1	9:E:85:ASP:O	2.30	0.50
11:G:16:LEU:CD1	11:G:17:PHE:CE2	2.91	0.50
19:A:1797:CLA:C9	15:K:61:LEU:HD13	2.35	0.50
16:L:101:MET:SD	16:L:104:ILE:HG12	2.52	0.50
16:L:56:VAL:HG22	19:L:1167:CLA:HED2	1.94	0.50
17:N:52:LEU:CB	17:N:53:ALA:CA	2.90	0.50
18:R:34:UNK:O	18:R:36:UNK:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:38:UNK:C	18:R:42:UNK:C	2.89	0.50
11:G:92:GLY:O	11:G:93:TYR:O	2.30	0.50
19:1:1146:CLA:CMC	19:1:1146:CLA:HBC2	2.20	0.50
19:1:1145:CLA:C6	19:1:1145:CLA:HMA1	2.42	0.50
17:N:5:GLU:OE2	17:N:6:TYR:N	2.45	0.50
6:B:31:PHE:O	6:B:32:GLU:C	2.49	0.50
4:4:33:ASP:O	4:4:34:PRO:O	2.29	0.50
6:B:429:LEU:HD11	19:B:1769:CLA:CMB	2.42	0.50
6:B:447:GLY:O	6:B:449:PRO:CD	2.60	0.50
6:B:50:HIS:CA	6:B:53:GLN:HB2	2.41	0.50
9:E:88:GLU:O	9:E:90:VAL:N	2.44	0.50
17:N:38:GLY:O	17:N:39:SER:O	2.29	0.50
19:1:1308:CLA:H2	19:J:1044:CLA:CED	2.42	0.50
15:K:17:LEU:HD22	15:K:18:MET:N	2.26	0.50
15:K:55:PHE:N	15:K:55:PHE:CD1	2.77	0.50
7:C:31:TRP:CD1	7:C:31:TRP:C	2.85	0.50
9:E:69:PHE:CG	9:E:70:ALA:N	2.79	0.50
8:D:120:PRO:O	8:D:121:GLU:HB3	2.11	0.50
2:2:128:ASN:ND2	14:J:3:ASP:HB3	2.27	0.50
3:3:84:ILE:HD13	3:3:84:ILE:O	2.12	0.50
4:4:144:ALA:O	4:4:147:LEU:O	2.29	0.50
4:4:34:PRO:CA	4:4:35:GLU:CD	2.78	0.50
4:4:38:ARG:O	4:4:39:TRP:O	2.30	0.50
19:A:1781:CLA:HAA1	19:A:1781:CLA:HED2	1.92	0.50
5:A:382:TYR:HE2	19:A:1784:CLA:HED3	1.74	0.50
5:A:208:ALA:HA	5:A:310:PHE:C	2.28	0.50
5:A:364:MET:O	5:A:368:LEU:HB2	2.11	0.50
6:B:141:PHE:O	6:B:144:PHE:N	2.45	0.50
6:B:290:MET:HB2	19:B:1752:CLA:HMC3	1.94	0.50
19:B:1759:CLA:H171	22:B:1776:BCR:H363	1.92	0.50
24:B:1784:LMG:HC91	24:B:1784:LMG:C11	2.40	0.50
6:B:22:TRP:HA	6:B:25:ILE:HD11	1.92	0.50
6:B:320:LYS:O	6:B:322:LEU:N	2.44	0.50
6:B:346:SER:O	6:B:350:GLN:N	2.43	0.50
6:B:718:ILE:HD11	19:B:1758:CLA:HHC	1.94	0.50
9:E:41:ARG:NE	9:E:46:PHE:CZ	2.80	0.50
5:A:249:ILE:HD13	5:A:250:LEU:HB2	1.93	0.50
5:A:249:ILE:N	5:A:251:ASN:OD1	2.45	0.50
17:N:47:THR:O	17:N:52:LEU:O	2.30	0.50
17:N:61:LEU:O	17:N:66:ASP:OD1	2.28	0.50
20:A:7048:LMU:O4'	20:A:7048:LMU:O6B	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:8055:SUC:O3'	21:B:8055:SUC:O6'	2.29	0.50
19:2:1212:CLA:H43	19:2:1212:CLA:CGA	2.34	0.50
7:C:34:CYS:SG	7:C:39:ILE:HD12	2.52	0.50
6:B:67:HIS:O	6:B:88:ALA:O	2.30	0.50
12:H:47:PHE:CD2	16:L:141:GLY:HA2	2.46	0.50
3:3:80:LYS:HD3	3:3:105:ASN:HB3	1.91	0.50
19:L:1166:CLA:HBC2	19:L:1166:CLA:HHD	1.94	0.50
6:B:509:PHE:N	6:B:509:PHE:CD2	2.80	0.50
19:2:1213:CLA:CBC	19:2:1213:CLA:CHD	2.88	0.50
19:A:1774:CLA:CBB	19:A:1774:CLA:H8	2.42	0.50
5:A:546:ALA:HB1	19:A:1793:CLA:HMB3	1.94	0.50
5:A:553:VAL:O	5:A:557:LEU:HB2	2.11	0.50
5:A:89:ILE:O	5:A:93:LEU:HG	2.12	0.50
6:B:125:TYR:CE1	6:B:130:ARG:NH1	2.80	0.50
19:B:1756:CLA:O2D	19:B:1757:CLA:OBD	2.29	0.50
19:B:1759:CLA:H62	22:B:1777:BCR:C32	2.42	0.50
19:B:1760:CLA:HBC3	19:B:1760:CLA:CMC	2.36	0.50
6:B:178:HIS:C	6:B:180:SER:N	2.64	0.50
6:B:586:THR:O	6:B:589:TRP:N	2.44	0.50
6:B:441:ASP:OD1	6:B:617:MET:HB3	2.11	0.50
6:B:707:LEU:HD12	6:B:711:VAL:CG2	2.42	0.50
6:B:11:GLY:CA	7:C:71:HIS:CD2	2.86	0.50
16:L:136:TRP:O	16:L:140:THR:HG23	2.12	0.50
20:A:7036:LMU:O5B	20:A:7036:LMU:O6'	2.29	0.50
19:1:1142:CLA:O1D	19:1:1142:CLA:H2A	2.12	0.50
20:A:7032:LMU:O1'	20:A:7032:LMU:O5B	2.29	0.50
3:3:114:PHE:CE1	19:3:1220:CLA:C3D	2.94	0.50
6:B:503:GLU:CB	6:B:507:SER:HB2	2.41	0.50
5:A:630:ASP:O	5:A:632:GLY:N	2.45	0.50
15:K:59:ASP:O	15:K:59:ASP:OD1	2.30	0.50
15:K:40:LEU:O	15:K:41:GLU:HG3	2.12	0.50
4:4:163:PHE:O	4:4:166:PHE:CB	2.56	0.49
5:A:131:ILE:HG23	5:A:132:LEU:N	2.27	0.49
5:A:301:HIS:NE2	19:A:1772:CLA:C1A	2.75	0.49
19:A:1810:CLA:HMB3	19:A:1811:CLA:HMD1	1.94	0.49
5:A:218:TRP:CZ3	19:A:1770:CLA:HMB3	2.47	0.49
5:A:332:GLU:HA	5:A:344:LYS:HG2	1.93	0.49
5:A:347:TYR:HE1	5:A:417:PHE:HZ	1.59	0.49
6:B:141:PHE:CG	19:B:1745:CLA:H12	2.47	0.49
19:B:1737:CLA:HAC1	19:B:1760:CLA:HMA1	1.92	0.49
6:B:492:ILE:O	6:B:493:TRP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:595:HIS:CE1	6:B:599:ILE:HD11	2.46	0.49
6:B:667:TRP:O	6:B:669:GLY:N	2.45	0.49
6:B:11:GLY:CA	7:C:71:HIS:HD2	2.07	0.49
11:G:37:GLU:O	11:G:38:GLN:O	2.29	0.49
11:G:44:PHE:C	11:G:46:ALA:HB2	2.32	0.49
16:L:123:ARG:HB3	16:L:126:GLN:CG	2.41	0.49
4:4:75:TRP:CE3	4:4:76:TYR:HB3	2.47	0.49
10:F:19:LYS:O	10:F:23:LYS:HB2	2.11	0.49
3:3:87:GLU:CA	22:3:1225:BCR:C38	2.90	0.49
3:3:87:GLU:CB	22:3:1225:BCR:C38	2.90	0.49
1:1:64:GLY:O	1:1:66:GLY:O	2.30	0.49
21:B:8062:SUC:O3'	21:B:8062:SUC:C1	2.60	0.49
12:H:45:ALA:C	12:H:48:THR:H	2.08	0.49
2:2:137:TYR:HD1	2:2:138:PRO:CD	2.25	0.49
6:B:160:LYS:O	6:B:162:LYS:N	2.44	0.49
12:H:70:ALA:O	12:H:71:ASN:CB	2.59	0.49
6:B:681:ALA:O	6:B:682:HIS:C	2.50	0.49
15:K:23:ARG:O	15:K:23:ARG:HG2	2.12	0.49
2:2:120:ASN:CB	14:J:5:LYS:HD2	2.43	0.49
2:2:60:ALA:HA	2:2:63:PHE:CD2	2.48	0.49
5:A:44:ILE:O	5:A:46:LYS:CA	2.60	0.49
5:A:697:ARG:NH1	5:A:724:ALA:HB3	2.26	0.49
5:A:744:ALA:HA	5:A:747:TRP:HB3	1.93	0.49
6:B:183:PHE:CE1	19:B:1744:CLA:H51	2.48	0.49
6:B:190:TRP:CD2	19:B:1749:CLA:HMD3	2.47	0.49
14:J:22:LEU:O	14:J:23:ALA:C	2.51	0.49
1:1:32:VAL:CG2	19:1:1197:CLA:C1D	2.90	0.49
21:B:8052:SUC:O1	21:B:8052:SUC:O4	2.28	0.49
7:C:9:ASP:HB3	25:C:1083:SF4:S2	2.52	0.49
10:F:25:LEU:O	10:F:26:GLN:O	2.30	0.49
3:3:86:GLN:HB2	3:3:88:THR:H	1.76	0.49
20:A:7050:LMU:O3'	20:A:7050:LMU:O6B	2.29	0.49
5:A:29:THR:OG1	5:A:31:PHE:CB	2.57	0.49
20:A:7013:LMU:O3'	20:A:7013:LMU:O5B	2.29	0.49
16:L:115:ALA:N	16:L:116:PRO:CD	2.70	0.49
2:2:188:PRO:O	2:2:189:ILE:C	2.50	0.49
6:B:232:LEU:HD21	6:B:235:GLN:OE1	2.12	0.49
2:2:165:LYS:C	2:2:167:GLY:N	2.65	0.49
19:A:1776:CLA:H101	19:A:1779:CLA:H93	1.94	0.49
19:A:1793:CLA:H171	19:A:1800:CLA:CBB	2.42	0.49
5:A:197:GLN:NE2	5:A:351:THR:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:648:THR:O	5:A:649:ILE:HG22	2.11	0.49
19:B:1752:CLA:HMD2	22:B:1775:BCR:C32	2.42	0.49
19:G:1099:CLA:H3A	19:G:1099:CLA:CGA	2.39	0.49
11:G:34:GLN:O	11:G:36:PRO:HD3	2.11	0.49
11:G:7:VAL:HG23	11:G:8:ILE:H	1.65	0.49
16:L:95:LEU:O	16:L:99:LEU:HD13	2.11	0.49
4:4:69:ILE:C	4:4:71:ASN:N	2.60	0.49
17:N:42:PHE:O	17:N:43:PRO:O	2.29	0.49
17:N:60:PHE:N	17:N:61:LEU:O	2.45	0.49
4:4:191:ASN:C	4:4:192:THR:O	2.50	0.49
20:A:7022:LMU:H2O2	20:A:7022:LMU:H5'	1.76	0.49
3:3:157:ALA:O	3:3:158:TYR:HD2	1.95	0.49
20:A:7013:LMU:H22	20:A:7013:LMU:O5'	2.11	0.49
21:2:1225:SUC:O2	21:2:1225:SUC:O4'	2.30	0.49
16:L:11:ILE:O	16:L:12:GLN:HG3	2.12	0.49
16:L:112:PRO:O	16:L:113:SER:HB3	2.12	0.49
16:L:48:ASN:CB	16:L:49:PRO:HD2	2.35	0.49
2:2:96:ILE:O	2:2:100:VAL:CG1	2.60	0.49
19:4:1200:CLA:HED2	19:4:1200:CLA:CAD	2.43	0.49
5:A:144:GLN:C	5:A:145:ILE:HG12	2.33	0.49
5:A:163:GLN:C	5:A:165:TYR:N	2.63	0.49
5:A:678:PHE:CZ	19:A:1783:CLA:H142	2.46	0.49
5:A:594:ALA:O	5:A:598:VAL:HG23	2.11	0.49
5:A:733:VAL:CG1	19:A:1796:CLA:C4D	2.90	0.49
19:B:1763:CLA:HMD2	19:B:1763:CLA:H13	1.94	0.49
19:B:1756:CLA:C4A	19:B:1770:CLA:HAA2	2.43	0.49
6:B:339:ALA:O	6:B:340:SER:CB	2.60	0.49
6:B:377:TYR:O	6:B:378:ILE:HB	2.13	0.49
6:B:580:VAL:HG11	6:B:710:LEU:HD21	1.94	0.49
6:B:577:TYR:CD1	6:B:706:ARG:HB3	2.47	0.49
5:A:567:ARG:HH11	8:D:35:GLY:N	2.11	0.49
9:E:43:SER:CB	9:E:82:TYR:HE1	2.21	0.49
11:G:57:LEU:O	11:G:61:ASN:OD1	2.30	0.49
13:I:24:LEU:HD21	22:L:1169:BCR:H271	1.95	0.49
19:1:1188:CLA:CBB	19:1:1192:CLA:CHC	2.90	0.49
17:N:59:PRO:O	17:N:66:ASP:OD1	2.30	0.49
4:4:191:ASN:OD1	4:4:192:THR:O	2.29	0.49
6:B:517:PHE:O	6:B:517:PHE:CG	2.61	0.49
20:A:7038:LMU:C6'	20:A:7038:LMU:C1B	2.90	0.49
2:2:179:PHE:O	2:2:183:TYR:CD2	2.66	0.49
4:4:104:ARG:HA	4:4:107:GLN:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:147:LEU:O	4:4:148:GLU:O	2.29	0.49
5:A:385:LEU:O	5:A:386:ALA:HB3	2.12	0.49
19:B:1735:CLA:H52	19:B:1735:CLA:C1C	2.43	0.49
19:B:1759:CLA:H172	22:B:1776:BCR:H363	1.93	0.49
23:B:1774:PQN:H141	22:B:1781:BCR:H331	1.94	0.49
6:B:392:ILE:HD13	19:B:1760:CLA:HED1	1.93	0.49
6:B:724:PHE:CD1	19:B:1786:CLA:HMD1	2.48	0.49
7:C:63:LEU:CG	7:C:64:SER:N	2.49	0.49
6:B:564:ARG:NE	7:C:64:SER:OG	2.46	0.49
9:E:55:VAL:CG2	9:E:65:VAL:HB	2.40	0.49
22:B:1780:BCR:C33	19:F:1156:CLA:HMA1	2.42	0.49
19:L:1167:CLA:CAC	22:L:1169:BCR:HC42	2.42	0.49
5:A:23:ASP:CA	5:A:24:ARG:HD3	2.42	0.49
20:A:7037:LMU:O1B	20:A:7037:LMU:O2'	2.30	0.49
10:F:22:LEU:HB3	10:F:25:LEU:HD13	1.94	0.49
15:K:11:MET:O	15:K:15:THR:OG1	2.30	0.49
20:A:7021:LMU:H6'1	20:A:7021:LMU:O3B	2.10	0.49
21:B:8059:SUC:O2	21:B:8059:SUC:O2'	2.29	0.49
6:B:247:THR:HB	6:B:248:GLN:OE1	2.11	0.49
8:D:124:ASN:HB3	8:D:125:PRO:CD	2.29	0.49
5:A:568:LEU:O	5:A:586:ARG:HD3	2.12	0.49
1:1:18:ALA:N	1:1:19:PRO:HD2	2.26	0.49
2:2:36:SER:O	2:2:37:ASP:HB2	2.11	0.49
5:A:104:SER:OG	5:A:161:GLU:OE1	2.31	0.49
5:A:109:TRP:HA	5:A:116:ILE:CG1	2.41	0.49
19:A:1762:CLA:HAA2	19:A:1762:CLA:HBD	1.94	0.49
19:A:1787:CLA:O1A	6:B:686:PRO:HD3	2.12	0.49
5:A:79:PHE:HZ	5:A:185:HIS:HE2	1.57	0.49
6:B:724:PHE:CE2	19:B:1786:CLA:CMD	2.96	0.49
6:B:502:ASN:OD1	6:B:511:THR:HG21	2.12	0.49
6:B:646:TRP:CZ3	6:B:726:ILE:CD1	2.95	0.49
7:C:6:LYS:O	7:C:63:LEU:HD21	2.12	0.49
10:F:23:LYS:O	10:F:24:LYS:CE	2.60	0.49
21:B:8053:SUC:C5	21:B:8053:SUC:HO4'	2.25	0.49
21:B:8053:SUC:O4'	21:B:8053:SUC:O2	2.30	0.49
10:F:151:ASP:HA	10:F:154:PHE:CB	2.43	0.49
5:A:589:THR:HG22	5:A:589:THR:O	2.13	0.49
12:H:57:LEU:HD13	12:H:57:LEU:C	2.33	0.49
3:3:133:ALA:O	3:3:134:LYS:HB2	2.12	0.49
7:C:42:ALA:O	8:D:129:GLY:HA3	2.13	0.49
5:A:185:HIS:O	5:A:187:HIS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:364:MET:CE	19:A:1782:CLA:H2	2.43	0.49
5:A:435:VAL:HA	5:A:438:HIS:HE1	1.76	0.49
5:A:508:THR:O	5:A:509:ALA:HB3	2.12	0.49
5:A:549:ILE:O	5:A:552:THR:O	2.30	0.49
19:B:1754:CLA:H43	19:B:1754:CLA:CHA	2.38	0.49
19:B:1748:CLA:H8	19:B:1766:CLA:HMA1	1.93	0.49
6:B:323:TYR:CD1	19:B:1755:CLA:CBC	2.95	0.49
6:B:419:ILE:C	6:B:420:SER:OG	2.47	0.49
6:B:647:ALA:O	6:B:651:LEU:HD22	2.12	0.49
7:C:7:ILE:HA	7:C:60:THR:OG1	2.13	0.49
10:F:123:VAL:O	10:F:126:ALA:N	2.45	0.49
11:G:17:PHE:O	11:G:20:ARG:CB	2.57	0.49
17:N:61:LEU:HD21	17:N:64:ASP:N	2.28	0.49
17:N:77:CYS:O	17:N:79:SER:O	2.29	0.49
20:A:7048:LMU:H11	20:A:7048:LMU:H51	1.90	0.49
10:F:17:ARG:O	10:F:18:GLU:C	2.51	0.49
21:B:8062:SUC:O6'	21:B:8062:SUC:O1'	2.30	0.49
6:B:247:THR:O	6:B:248:GLN:C	2.51	0.49
6:B:475:ASP:HA	6:B:480:SER:CA	2.43	0.49
6:B:317:ARG:HD3	6:B:410:ARG:HG2	1.95	0.49
13:I:4:LEU:O	13:I:4:LEU:HG	2.13	0.49
19:A:1762:CLA:H51	19:A:1785:CLA:NC	2.28	0.49
19:A:1779:CLA:NC	22:A:1804:BCR:C17	2.75	0.49
19:A:1781:CLA:C3B	22:A:1805:BCR:C37	2.90	0.49
5:A:733:VAL:HG21	19:A:1796:CLA:HMD3	1.95	0.49
19:A:1761:CLA:C4	22:A:1803:BCR:C31	2.90	0.49
22:A:1806:BCR:C15	19:A:1811:CLA:H151	2.43	0.49
5:A:747:TRP:CE3	22:A:1806:BCR:H402	2.44	0.49
5:A:331:LEU:CD2	5:A:343:HIS:C	2.61	0.49
6:B:396:ARG:HH11	19:B:1760:CLA:HED2	1.78	0.49
21:B:8054:SUC:O1'	21:B:8054:SUC:O2	2.29	0.49
8:D:41:GLN:HG3	16:L:125:LYS:HZ2	1.78	0.49
11:G:16:LEU:HB2	11:G:17:PHE:CD2	2.48	0.49
11:G:42:SER:OG	11:G:43:HIS:O	2.30	0.49
4:4:70:ILE:O	4:4:71:ASN:C	2.47	0.49
4:4:73:PRO:CB	4:4:75:TRP:HA	2.43	0.49
1:1:27:LEU:H	6:B:314:ARG:NH1	2.09	0.49
17:N:45:ASN:O	17:N:46:PHE:O	2.30	0.49
20:A:7016:LMU:O6'	20:A:7016:LMU:H1'	1.88	0.49
19:K:1085:CLA:HAA2	19:K:1085:CLA:HBD	1.93	0.49
15:K:5:SER:O	15:K:9:LEU:HD21	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:1221:CLA:C2A	19:3:3011:CLA:HHD	2.43	0.49
3:3:158:TYR:CB	3:3:159:PRO:HD2	2.22	0.49
8:D:101:TYR:CD1	8:D:114:PRO:CD	2.95	0.49
7:C:12:ILE:N	7:C:12:ILE:CD1	2.71	0.49
21:2:1225:SUC:O2	21:2:1225:SUC:O2'	2.28	0.49
4:4:60:LEU:HG	4:4:61:PRO:CD	2.34	0.49
5:A:258:LEU:HG	5:A:280:PHE:CD1	2.48	0.49
8:D:28:ILE:O	8:D:66:ALA:CB	2.61	0.49
6:B:48:ALA:HB3	6:B:157:LEU:HD22	1.93	0.49
1:1:184:PRO:O	1:1:185:TRP:CZ3	2.64	0.49
2:2:51:HIS:CA	2:2:54:TRP:HB2	2.42	0.49
4:4:94:GLU:C	4:4:95:PHE:HD1	2.15	0.49
19:A:1761:CLA:HMB3	19:A:1762:CLA:HAA1	1.95	0.49
5:A:158:ILE:HG21	19:A:1770:CLA:O1D	2.13	0.49
19:A:1764:CLA:HAA2	19:A:1783:CLA:HED3	1.94	0.49
19:A:1781:CLA:CBA	19:A:1794:CLA:CED	2.87	0.49
19:A:1779:CLA:CAB	22:A:1804:BCR:H353	2.33	0.49
5:A:452:PHE:CD2	5:A:456:HIS:CE1	3.00	0.49
5:A:473:PRO:C	5:A:475:ASP:H	2.16	0.49
5:A:497:ALA:HA	5:A:510:SER:OG	2.13	0.49
5:A:53:TRP:CA	5:A:56:ASN:HB2	2.37	0.49
19:B:1738:CLA:H161	19:B:1738:CLA:H91	1.94	0.49
19:B:1760:CLA:HMD2	24:B:1784:LMG:H341	1.95	0.49
6:B:724:PHE:CE1	19:B:1786:CLA:HMD1	2.47	0.49
6:B:255:LEU:N	6:B:255:LEU:HD23	2.28	0.49
6:B:292:ARG:CZ	6:B:297:ILE:H	2.26	0.49
6:B:535:VAL:CG2	6:B:539:LEU:HD23	2.42	0.49
10:F:80:TRP:CH2	19:F:1156:CLA:CAC	2.95	0.49
11:G:46:ALA:N	11:G:48:ASP:CG	2.60	0.49
14:J:21:SER:O	14:J:22:LEU:C	2.51	0.49
16:L:63:LEU:HD13	16:L:64:LEU:HG	1.94	0.49
16:L:162:ASP:HB2	16:L:163:LEU:CA	2.43	0.49
17:N:81:VAL:C	17:N:83:TRP:N	2.66	0.49
10:F:22:LEU:HB2	10:F:23:LYS:HD3	1.94	0.49
3:3:74:ALA:CB	19:3:1217:CLA:C1D	2.91	0.49
16:L:5:LYS:N	16:L:6:PRO:HD3	2.28	0.49
12:H:42:THR:O	12:H:45:ALA:N	2.46	0.49
6:B:110:LEU:CD1	6:B:111:GLY:H	2.18	0.49
5:A:484:LEU:N	5:A:485:GLN:OE1	2.40	0.49
10:F:113:LYS:NZ	10:F:115:THR:HG21	2.27	0.49
6:B:488:ALA:HB2	19:B:1767:CLA:C3C	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:129:PHE:O	3:3:129:PHE:CD1	2.66	0.49
16:L:78:GLU:O	16:L:78:GLU:HG3	2.13	0.49
6:B:238:SER:OG	6:B:239:SER:N	2.45	0.49
2:2:54:TRP:O	2:2:55:ALA:C	2.49	0.49
5:A:462:ILE:HG21	19:A:1789:CLA:HMC3	1.95	0.49
5:A:396:PHE:O	5:A:396:PHE:CD1	2.65	0.49
5:A:40:PHE:N	5:A:44:ILE:CG2	2.76	0.49
5:A:453:LEU:CD2	19:A:1793:CLA:CBB	2.90	0.49
19:B:1738:CLA:C2A	19:B:1738:CLA:O1D	2.53	0.49
6:B:343:VAL:HG11	19:B:1757:CLA:H2	1.95	0.49
6:B:50:HIS:HB2	6:B:53:GLN:HB2	1.95	0.49
6:B:556:SER:CA	6:B:558:PRO:HD2	2.43	0.49
6:B:691:ILE:HA	16:L:102:TYR:OH	2.11	0.49
19:1:1188:CLA:HED1	19:1:1188:CLA:CGA	2.41	0.49
17:N:61:LEU:O	17:N:62:SER:O	2.30	0.49
17:N:62:SER:OG	17:N:66:ASP:HB3	2.13	0.49
18:R:34:UNK:CB	18:R:35:UNK:CA	2.79	0.49
19:1:1142:CLA:OBD	19:K:1085:CLA:C1B	2.61	0.49
19:K:1085:CLA:CMC	19:K:1085:CLA:HBC2	2.38	0.49
8:D:132:LEU:O	8:D:135:ARG:O	2.31	0.49
21:B:8053:SUC:O4'	21:B:8053:SUC:O5	2.29	0.49
20:A:7030:LMU:C2'	20:A:7030:LMU:H6E	2.36	0.49
1:1:89:VAL:HB	1:1:90:PRO:CD	2.33	0.49
2:2:43:TRP:CD2	2:2:125:PHE:CD1	3.01	0.48
4:4:90:LEU:CA	4:4:91:PHE:HB3	2.42	0.48
5:A:126:ILE:CD1	19:A:1765:CLA:HMA3	2.43	0.48
5:A:172:LEU:O	5:A:175:ALA:O	2.31	0.48
19:A:1771:CLA:CGA	19:A:1771:CLA:C4A	2.91	0.48
19:A:1776:CLA:HMC2	19:A:1782:CLA:H193	1.94	0.48
5:A:455:PHE:CD1	19:A:1788:CLA:HMA2	2.47	0.48
22:A:1806:BCR:C35	19:A:1811:CLA:H41	2.43	0.48
5:A:411:ALA:O	5:A:412:ALA:C	2.52	0.48
19:B:1765:CLA:H2A	19:B:1765:CLA:O1D	2.13	0.48
6:B:304:ILE:HG22	19:B:1753:CLA:O1D	2.11	0.48
6:B:577:TYR:CE1	6:B:706:ARG:HB3	2.48	0.48
9:E:43:SER:HB2	9:E:82:TYR:CE1	2.34	0.48
9:E:52:VAL:HA	9:E:67:VAL:HA	1.96	0.48
1:1:181:LEU:HD12	1:1:182:ALA:H	1.78	0.48
2:2:208:PHE:O	2:2:209:THR:HB	2.13	0.48
19:3:1212:CLA:HMA3	5:A:246:HIS:CE1	2.48	0.48
5:A:151:GLN:HA	5:A:154:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1774:CLA:H203	19:A:1782:CLA:HAA1	1.95	0.48
5:A:229:ILE:O	5:A:229:ILE:HG22	2.13	0.48
5:A:86:LEU:H	5:A:86:LEU:HD22	1.79	0.48
19:B:1763:CLA:C5	22:B:1780:BCR:C40	2.91	0.48
9:E:41:ARG:CD	9:E:46:PHE:CZ	2.96	0.48
11:G:19:GLY:N	11:G:21:PHE:H	2.11	0.48
11:G:50:ARG:HB2	11:G:51:ALA:HB2	1.94	0.48
20:A:7032:LMU:H2B	20:A:7032:LMU:C4	2.43	0.48
18:R:46:UNK:CB	18:R:47:UNK:CA	2.90	0.48
21:2:1225:SUC:H2	21:2:1225:SUC:O2'	2.13	0.48
15:K:74:ILE:CG2	15:K:75:VAL:HG22	2.35	0.48
5:A:220:ARG:O	5:A:221:HIS:CB	2.60	0.48
5:A:720:THR:O	5:A:720:THR:CG2	2.61	0.48
2:2:117:GLY:HA3	2:2:131:THR:HA	1.94	0.48
2:2:166:ASN:O	2:2:166:ASN:ND2	2.46	0.48
4:4:108:ASP:OD2	4:4:108:ASP:O	2.30	0.48
5:A:747:TRP:HB2	19:A:1783:CLA:CBB	2.43	0.48
5:A:299:ILE:HD11	19:A:1774:CLA:HMA3	1.94	0.48
5:A:312:ILE:O	5:A:313:ALA:HB2	2.13	0.48
5:A:382:TYR:HB2	5:A:385:LEU:HD11	1.95	0.48
5:A:392:GLN:O	5:A:392:GLN:CG	2.62	0.48
6:B:96:PHE:HZ	6:B:104:PHE:CE2	2.31	0.48
19:B:1735:CLA:CBC	22:B:1779:BCR:C33	2.91	0.48
19:B:1748:CLA:O1D	19:B:1749:CLA:HMA1	2.13	0.48
6:B:293:THR:C	6:B:294:ASN:ND2	2.50	0.48
6:B:356:PRO:HB2	6:B:361:ILE:CG2	2.43	0.48
6:B:531:THR:O	6:B:535:VAL:CG1	2.54	0.48
6:B:546:LEU:HD11	6:B:567:THR:CG2	2.37	0.48
6:B:568:CYS:O	6:B:570:ILE:HG23	2.12	0.48
5:A:694:PHE:CZ	6:B:661:PHE:CD1	3.01	0.48
9:E:60:LYS:CG	9:E:61:THR:N	2.70	0.48
11:G:34:GLN:O	11:G:36:PRO:N	2.45	0.48
13:I:9:VAL:H	13:I:10:PRO:CD	2.26	0.48
16:L:126:GLN:O	16:L:127:PRO:O	2.31	0.48
17:N:80:ASN:OD1	17:N:80:ASN:C	2.52	0.48
21:B:8055:SUC:C2	21:B:8055:SUC:O2'	2.56	0.48
1:1:59:VAL:CG1	1:1:60:PRO:CD	2.91	0.48
20:A:7020:LMU:O2B	20:A:7020:LMU:O6'	2.31	0.48
3:3:114:PHE:HE1	19:3:1220:CLA:C3D	2.26	0.48
21:3:1226:SUC:O1'	21:3:1226:SUC:O6'	2.29	0.48
8:D:67:ILE:O	8:D:68:MET:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:36:ALA:O	14:J:37:LEU:HB2	2.12	0.48
16:L:57:GLY:HA3	16:L:146:GLY:HA3	1.96	0.48
2:2:115:ASN:ND2	2:2:115:ASN:N	2.60	0.48
5:A:165:TYR:HD2	5:A:165:TYR:O	1.95	0.48
19:A:1774:CLA:HAC2	22:A:1803:BCR:H352	1.96	0.48
5:A:312:ILE:O	5:A:313:ALA:CB	2.61	0.48
5:A:506:GLY:O	5:A:507:ALA:HB3	2.13	0.48
5:A:681:GLY:C	5:A:683:HIS:H	2.16	0.48
5:A:693:LEU:HD23	5:A:734:GLY:HA3	1.96	0.48
6:B:145:LEU:HD22	6:B:148:ILE:HD12	1.94	0.48
19:B:1736:CLA:HBC3	19:B:1760:CLA:H41	1.95	0.48
19:B:1772:CLA:H51	23:B:1774:PQN:H251	1.94	0.48
5:A:462:ILE:HD13	19:B:1787:CLA:H72	1.95	0.48
6:B:21:ILE:HD12	6:B:21:ILE:N	2.29	0.48
6:B:415:LYS:HG2	6:B:416:GLU:OE2	2.12	0.48
6:B:662:MET:HE2	23:B:1774:PQN:H2M3	1.96	0.48
7:C:81:TYR:CD1	7:C:81:TYR:N	2.81	0.48
9:E:38:ILE:HB	9:E:46:PHE:O	2.14	0.48
10:F:123:VAL:HG13	14:J:7:TYR:N	2.28	0.48
11:G:43:HIS:C	11:G:45:GLU:CB	2.61	0.48
16:L:99:LEU:O	16:L:136:TRP:HZ3	1.96	0.48
16:L:65:VAL:C	16:L:67:PRO:CD	2.82	0.48
16:L:164:PRO:CG	16:L:165:TYR:CD2	2.79	0.48
3:3:74:ALA:HB2	19:3:1217:CLA:C1D	2.43	0.48
8:D:118:VAL:HG13	8:D:119:TYR:H	1.76	0.48
5:A:338:PHE:O	5:A:339:THR:O	2.30	0.48
7:C:29:ILE:CG2	8:D:126:GLY:CA	2.91	0.48
20:A:7005:LMU:O3'	20:A:7005:LMU:O2B	2.29	0.48
20:A:7040:LMU:O6B	20:A:7040:LMU:O4'	2.29	0.48
11:G:80:ILE:O	11:G:81:VAL:O	2.30	0.48
5:A:569:ILE:HB	5:A:572:LYS:HG3	1.95	0.48
6:B:154:TRP:O	6:B:155:LEU:C	2.51	0.48
19:3:3008:CLA:HAA2	19:3:3008:CLA:HBD	1.95	0.48
2:2:42:ARG:CB	2:2:45:VAL:CB	2.91	0.48
4:4:128:ALA:C	4:4:130:GLU:H	2.14	0.48
5:A:159:THR:O	5:A:163:GLN:OE1	2.31	0.48
19:A:1782:CLA:O2D	19:A:1782:CLA:OBD	2.31	0.48
19:A:1797:CLA:HBA1	19:A:1797:CLA:HMA3	1.74	0.48
5:A:430:ASP:HA	5:A:434:ARG:HH21	1.78	0.48
5:A:499:ALA:N	5:A:500:PRO:CD	2.76	0.48
5:A:679:PHE:CE2	5:A:683:HIS:CD2	2.99	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:679:PHE:O	5:A:683:HIS:CB	2.62	0.48
5:A:710:ALA:HB1	19:B:1735:CLA:HED2	1.93	0.48
6:B:279:ALA:HA	19:B:1747:CLA:HMA1	1.94	0.48
6:B:304:ILE:CD1	19:B:1750:CLA:CED	2.89	0.48
19:B:1788:CLA:C3A	19:B:1788:CLA:O2A	2.57	0.48
6:B:292:ARG:NH1	6:B:293:THR:H	2.12	0.48
6:B:354:SER:OG	19:B:1757:CLA:HBC3	2.13	0.48
6:B:471:THR:HB	6:B:472:TYR:CE1	2.49	0.48
6:B:560:ASP:HB2	7:C:66:ARG:CZ	2.41	0.48
6:B:720:THR:O	6:B:724:PHE:N	2.46	0.48
19:B:1740:CLA:HED1	19:I:1031:CLA:HMA2	1.95	0.48
3:3:94:ARG:CB	3:3:97:PHE:HE1	2.26	0.48
20:A:7037:LMU:O4'	20:A:7037:LMU:O6B	2.29	0.48
15:K:4:GLY:HA2	15:K:7:THR:CB	2.42	0.48
8:D:58:PHE:HE2	8:D:60:MET:HA	1.78	0.48
6:B:63:GLY:HA2	6:B:66:PHE:HB3	1.96	0.48
6:B:601:LEU:O	6:B:601:LEU:HD22	2.12	0.48
2:2:62:ILE:HG13	2:2:66:GLU:OE2	2.13	0.48
4:4:123:GLN:O	4:4:124:TYR:CB	2.62	0.48
19:A:1774:CLA:HBB2	19:A:1774:CLA:H8	1.96	0.48
19:A:1790:CLA:C2B	22:A:1805:BCR:H333	2.44	0.48
5:A:578:ARG:O	5:A:593:SER:OG	2.27	0.48
5:A:665:ILE:CD1	5:A:665:ILE:C	2.82	0.48
5:A:64:PHE:CE1	5:A:74:ILE:HG22	2.49	0.48
19:B:1739:CLA:C9	19:B:1739:CLA:CBB	2.67	0.48
6:B:190:TRP:HE3	19:B:1745:CLA:CAB	2.26	0.48
19:B:1763:CLA:CBB	22:B:1779:BCR:C26	2.92	0.48
24:B:1784:LMG:O8	24:B:1784:LMG:H111	2.13	0.48
6:B:272:ASP:C	6:B:274:ALA:H	2.17	0.48
6:B:81:PRO:HG2	6:B:360:PHE:CE1	2.48	0.48
6:B:461:GLN:N	6:B:512:ILE:HD12	2.29	0.48
11:G:20:ARG:NH1	11:G:64:VAL:C	2.67	0.48
17:N:84:LYS:HZ2	17:N:84:LYS:HG2	1.43	0.48
19:1:1187:CLA:CMA	19:1:1187:CLA:HBA1	2.17	0.48
12:H:19:GLY:O	12:H:20:GLN:HB2	2.14	0.48
15:K:5:SER:O	15:K:9:LEU:HG	2.14	0.48
15:K:9:LEU:HA	15:K:12:VAL:CG2	2.44	0.48
21:B:8053:SUC:C2	21:B:8053:SUC:H5'	2.38	0.48
6:B:224:PRO:HB3	6:B:227:THR:CB	2.43	0.48
17:N:28:ASN:CA	17:N:30:ALA:H	2.26	0.48
2:2:98:GLU:C	2:2:99:LEU:HG	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:154:ARG:O	5:A:155:ALA:C	2.52	0.48
22:A:1806:BCR:H17C	19:A:1811:CLA:C17	2.44	0.48
5:A:284:ARG:HB2	5:A:298:ASP:OD1	2.12	0.48
5:A:415:ALA:HB2	5:A:560:VAL:HG12	1.95	0.48
5:A:705:GLU:O	5:A:708:VAL:N	2.46	0.48
19:B:1739:CLA:H162	19:B:1758:CLA:H192	1.95	0.48
22:B:1776:BCR:H15C	22:B:1776:BCR:H351	1.69	0.48
6:B:196:HIS:CE1	19:B:1746:CLA:C4D	2.96	0.48
6:B:36:ASP:O	6:B:41:ARG:CZ	2.62	0.48
6:B:471:THR:CG2	6:B:502:ASN:ND2	2.76	0.48
19:4:1199:CLA:CBA	19:F:1157:CLA:H42	2.44	0.48
19:1:1188:CLA:HAA2	19:1:1188:CLA:O2D	2.14	0.48
19:1:1190:CLA:CMC	19:1:1195:CLA:CAC	2.91	0.48
19:3:1224:CLA:OBD	19:3:1224:CLA:O1D	2.30	0.48
15:K:9:LEU:O	15:K:13:THR:HG22	2.13	0.48
1:1:40:LYS:O	1:1:44:LEU:HG	2.13	0.48
11:G:80:ILE:O	11:G:80:ILE:HD12	2.14	0.48
5:A:539:PHE:HE2	5:A:543:HIS:CE1	2.31	0.48
2:2:41:LEU:CD2	2:2:42:ARG:HD3	2.44	0.48
19:3:1212:CLA:HMA2	19:3:1212:CLA:CBA	2.39	0.48
4:4:124:TYR:HD1	4:4:127:PRO:HG2	1.78	0.48
4:4:147:LEU:CD2	4:4:148:GLU:HG2	2.33	0.48
5:A:103:PHE:H	5:A:103:PHE:HD2	1.60	0.48
5:A:159:THR:O	5:A:160:SER:CB	2.62	0.48
19:A:1774:CLA:CAB	19:A:1774:CLA:H71	2.44	0.48
5:A:417:PHE:CD1	5:A:417:PHE:C	2.87	0.48
19:B:1786:CLA:H193	19:B:1786:CLA:H161	1.53	0.48
6:B:180:SER:CB	6:B:288:GLY:HA3	2.41	0.48
16:L:163:LEU:CD2	16:L:165:TYR:HA	2.38	0.48
17:N:83:TRP:O	17:N:83:TRP:CE3	2.64	0.48
4:4:192:THR:HG23	4:4:193:ILE:HB	1.96	0.48
3:3:86:GLN:CB	3:3:88:THR:HB	2.37	0.48
12:H:20:GLN:HB2	12:H:22:ASP:CB	2.39	0.48
2:2:183:TYR:CD2	2:2:184:THR:N	2.81	0.48
18:R:7:UNK:O	18:R:10:UNK:CB	2.62	0.48
2:2:57:LEU:O	2:2:60:ALA:HB2	2.14	0.48
19:A:1781:CLA:H93	22:A:1805:BCR:C10	2.44	0.48
19:A:1771:CLA:HBB1	22:A:1802:BCR:C12	2.44	0.48
22:A:1803:BCR:C8	22:A:1803:BCR:H311	2.43	0.48
5:A:218:TRP:HZ3	19:A:1770:CLA:HMB3	1.78	0.48
5:A:229:ILE:HG12	5:A:243:PRO:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:330:ILE:O	5:A:330:ILE:CG2	2.62	0.48
5:A:434:ARG:O	5:A:437:ARG:N	2.46	0.48
5:A:740:LEU:CD1	19:A:1796:CLA:HMA1	2.43	0.48
19:B:1740:CLA:H192	22:B:1782:BCR:H19C	1.96	0.48
19:B:1765:CLA:CMD	19:B:1766:CLA:C1C	2.91	0.48
6:B:309:ILE:HG22	6:B:319:HIS:CD2	2.48	0.48
10:F:124:PRO:O	10:F:125:LEU:HB2	2.13	0.48
10:F:131:PHE:C	10:F:133:GLY:N	2.66	0.48
5:A:22:VAL:CA	5:A:23:ASP:O	2.62	0.48
10:F:22:LEU:N	10:F:22:LEU:CD1	2.32	0.48
15:K:16:THR:O	15:K:17:LEU:C	2.50	0.48
3:3:195:LEU:HA	3:3:198:PHE:HB2	1.96	0.48
5:A:258:LEU:HG	5:A:280:PHE:CE1	2.48	0.48
2:2:189:ILE:HD13	2:2:189:ILE:N	2.28	0.48
19:2:1213:CLA:HAA2	19:2:1218:CLA:HED2	1.94	0.48
2:2:96:ILE:O	2:2:100:VAL:HG12	2.14	0.48
4:4:161:LEU:O	4:4:162:ALA:CB	2.61	0.48
19:A:1783:CLA:C10	22:A:1806:BCR:C37	2.87	0.48
5:A:462:ILE:CG2	19:A:1789:CLA:HMC3	2.43	0.48
19:A:1790:CLA:C3D	19:A:1791:CLA:CAC	2.91	0.48
5:A:313:ALA:C	5:A:315:HIS:H	2.17	0.48
5:A:650:ASN:O	5:A:654:ARG:N	2.36	0.48
5:A:700:TRP:HZ3	19:A:1812:CLA:O1D	1.97	0.48
5:A:73:GLU:HA	5:A:76:ARG:HB2	1.95	0.48
6:B:135:LEU:HD12	6:B:135:LEU:O	2.14	0.48
6:B:91:ILE:CG2	19:B:1740:CLA:HMD1	2.36	0.48
6:B:593:TYR:CZ	19:B:1768:CLA:HBC2	2.48	0.48
6:B:292:ARG:HH22	19:B:1751:CLA:HED1	1.77	0.48
6:B:382:ILE:CG2	6:B:383:MET:N	2.51	0.48
8:D:34:GLY:HA3	8:D:62:THR:HB	1.95	0.48
11:G:30:ASN:ND2	11:G:34:GLN:H	2.12	0.48
11:G:20:ARG:NH2	11:G:61:ASN:CA	2.77	0.48
16:L:99:LEU:HD11	22:L:1169:BCR:C7	2.42	0.48
1:1:27:LEU:O	1:1:31:GLU:HB2	2.14	0.48
19:4:1201:CLA:CMA	19:4:1201:CLA:O2A	2.62	0.48
7:C:28:MET:HA	7:C:38:GLN:HB2	1.95	0.48
7:C:25:VAL:HA	7:C:43:PRO:CD	2.44	0.48
2:2:171:MET:HE1	2:2:175:MET:CB	2.41	0.47
4:4:37:LEU:O	4:4:38:ARG:C	2.52	0.47
4:4:89:THR:H	4:4:90:LEU:HD22	1.71	0.47
19:A:1797:CLA:H93	19:A:1797:CLA:H51	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:110:LEU:CD1	5:A:239:PRO:HG2	2.36	0.47
5:A:329:ASP:OD2	19:A:1778:CLA:HED1	2.14	0.47
6:B:125:TYR:HE1	6:B:130:ARG:NH1	2.12	0.47
6:B:167:TRP:O	6:B:167:TRP:CG	2.66	0.47
6:B:50:HIS:HB3	19:B:1737:CLA:CHB	2.44	0.47
19:B:1756:CLA:CAD	19:B:1768:CLA:CBB	2.91	0.47
19:B:1771:CLA:H191	13:I:21:MET:CE	2.44	0.47
22:B:1779:BCR:C8	22:B:1779:BCR:C33	2.91	0.47
6:B:464:GLN:CG	6:B:469:LYS:HD3	2.43	0.47
6:B:535:VAL:CG1	6:B:536:LYS:N	2.76	0.47
6:B:594:TRP:CD1	6:B:595:HIS:N	2.82	0.47
6:B:672:GLN:NE2	6:B:672:GLN:CA	2.59	0.47
8:D:138:GLY:O	8:D:140:ASN:N	2.47	0.47
16:L:36:TYR:O	16:L:37:LEU:CB	2.59	0.47
20:A:7042:LMU:H121	20:A:7042:LMU:H91	1.48	0.47
17:N:61:LEU:HG	17:N:64:ASP:HB2	1.95	0.47
7:C:17:CYS:SG	7:C:18:VAL:N	2.87	0.47
19:1:1142:CLA:CHD	19:1:1142:CLA:HBC3	2.44	0.47
12:H:23:VAL:O	12:H:23:VAL:HG13	2.13	0.47
19:3:1222:CLA:HBC2	19:3:1222:CLA:CHD	2.43	0.47
6:B:479:SER:C	6:B:481:THR:H	2.16	0.47
11:G:66:PHE:O	11:G:69:VAL:HG12	2.14	0.47
2:2:159:LEU:HD12	2:2:160:ARG:HG3	1.95	0.47
4:4:106:TRP:CZ3	19:4:1198:CLA:HBC1	2.48	0.47
4:4:36:ASN:CB	4:4:39:TRP:CH2	2.88	0.47
19:A:1781:CLA:HMB3	22:A:1805:BCR:C17	2.44	0.47
5:A:678:PHE:HZ	19:A:1783:CLA:H142	1.79	0.47
19:A:1793:CLA:H71	19:A:1793:CLA:H112	1.37	0.47
5:A:733:VAL:HG11	19:A:1796:CLA:C4D	2.44	0.47
5:A:374:GLN:O	5:A:377:TYR:CD2	2.62	0.47
5:A:377:TYR:HD1	5:A:616:PHE:HE1	1.58	0.47
5:A:679:PHE:O	5:A:679:PHE:CD2	2.67	0.47
5:A:99:HIS:C	5:A:101:ALA:H	2.16	0.47
6:B:167:TRP:HD1	11:G:41:MET:HE1	1.80	0.47
19:B:1749:CLA:C4A	19:B:1749:CLA:CGA	2.92	0.47
6:B:527:LEU:O	19:B:1770:CLA:HMA3	2.13	0.47
22:B:1780:BCR:HC8	22:B:1780:BCR:H311	1.96	0.47
22:B:1781:BCR:H331	22:B:1781:BCR:C8	2.44	0.47
19:B:1786:CLA:H3A	19:B:1786:CLA:HBA2	1.40	0.47
6:B:255:LEU:HA	6:B:271:THR:HB	1.96	0.47
5:A:131:ILE:HD13	6:B:447:GLY:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:573:TRP:O	6:B:576:PHE:HB3	2.14	0.47
6:B:628:SER:O	6:B:629:SER:C	2.52	0.47
6:B:732:LYS:CD	6:B:734:GLY:CA	2.92	0.47
9:E:37:LYS:N	9:E:49:VAL:HG13	2.28	0.47
9:E:36:VAL:HG23	9:E:52:VAL:HG22	1.96	0.47
9:E:83:ALA:O	9:E:85:ASP:N	2.46	0.47
9:E:88:GLU:O	9:E:89:GLU:C	2.52	0.47
19:1:1148:CLA:CAA	19:1:1148:CLA:CED	2.91	0.47
4:4:192:THR:CG2	4:4:193:ILE:CA	2.93	0.47
5:A:21:LEU:CA	5:A:22:VAL:HB	2.39	0.47
20:A:7037:LMU:H102	20:A:7051:LMU:H92	1.43	0.47
19:4:4014:CLA:H2A	19:4:4014:CLA:O1A	2.14	0.47
21:B:8059:SUC:HO6	21:B:8059:SUC:H1	1.73	0.47
21:B:8059:SUC:O2'	21:B:8059:SUC:O5	2.30	0.47
2:2:85:GLN:O	2:2:86:GLU:OE2	2.31	0.47
1:1:160:GLY:C	1:1:162:CYS:H	2.17	0.47
2:2:110:TRP:CE3	19:2:1222:CLA:HED1	2.49	0.47
4:4:166:PHE:CD2	4:4:167:ILE:N	2.82	0.47
4:4:36:ASN:CG	4:4:39:TRP:CZ2	2.75	0.47
19:A:1782:CLA:H151	19:A:1782:CLA:H111	1.56	0.47
5:A:302:HIS:CD2	19:A:1773:CLA:NB	2.81	0.47
5:A:385:LEU:O	5:A:386:ALA:HB2	2.12	0.47
5:A:462:ILE:HG21	19:A:1789:CLA:CMC	2.44	0.47
5:A:502:THR:C	5:A:504:ALA:N	2.68	0.47
5:A:63:ASP:HA	19:A:1785:CLA:HED2	1.96	0.47
5:A:703:LEU:HD13	5:A:707:ILE:HD11	1.96	0.47
5:A:78:VAL:O	5:A:82:HIS:CD2	2.66	0.47
19:B:1763:CLA:HBB2	22:B:1779:BCR:C25	2.44	0.47
19:B:1771:CLA:H91	22:B:1782:BCR:H333	1.95	0.47
6:B:309:ILE:HD11	6:B:313:GLY:H	1.80	0.47
20:A:7048:LMU:H92	20:A:7048:LMU:H122	1.44	0.47
21:B:8052:SUC:O3'	21:B:8052:SUC:O1'	2.30	0.47
19:3:1217:CLA:C3A	19:3:1222:CLA:HBB2	2.44	0.47
20:A:7039:LMU:O2'	20:A:7039:LMU:O1B	2.29	0.47
19:3:3011:CLA:H93	19:3:3011:CLA:H52	1.96	0.47
20:A:7027:LMU:H31	20:A:7027:LMU:H62	1.60	0.47
5:A:629:ASN:CG	5:A:630:ASP:N	2.67	0.47
6:B:31:PHE:O	6:B:37:ILE:HG21	2.13	0.47
12:H:75:ASP:CB	12:H:77:LEU:HG	2.43	0.47
6:B:600:THR:O	6:B:605:ASN:O	2.33	0.47
2:2:102:ILE:O	2:2:103:GLY:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1762:CLA:H12	19:A:1762:CLA:HED2	1.95	0.47
23:A:1801:PQN:H221	19:B:1735:CLA:HAC2	1.96	0.47
5:A:302:HIS:HD2	19:A:1773:CLA:NB	2.11	0.47
5:A:327:ILE:HG13	5:A:328:LYS:N	2.29	0.47
5:A:53:TRP:HA	5:A:56:ASN:CG	2.35	0.47
5:A:603:PHE:CZ	5:A:693:LEU:CD2	2.97	0.47
5:A:400:MET:HE3	5:A:612:VAL:HG11	1.96	0.47
19:B:1745:CLA:H111	19:B:1745:CLA:H71	1.41	0.47
19:B:1772:CLA:H191	13:I:21:MET:CB	2.40	0.47
19:B:1741:CLA:HHD	22:B:1782:BCR:H342	1.95	0.47
6:B:198:ALA:H	6:B:200:PRO:HG2	1.79	0.47
6:B:280:ILE:HD13	19:B:1749:CLA:HBB2	1.95	0.47
17:N:72:LYS:HB2	17:N:73:ASP:HA	1.86	0.47
15:K:20:PHE:CD2	15:K:21:ALA:CA	2.93	0.47
5:A:426:THR:HG23	5:A:428:TYR:OH	2.14	0.47
2:2:137:TYR:O	2:2:143:PHE:HE2	1.96	0.47
10:F:136:TRP:HB2	10:F:139:ALA:CB	2.44	0.47
2:2:54:TRP:CE2	2:2:109:ARG:CD	2.86	0.47
4:4:106:TRP:CH2	19:4:1198:CLA:HBC1	2.50	0.47
5:A:197:GLN:HE22	5:A:351:THR:CB	2.22	0.47
5:A:452:PHE:O	5:A:456:HIS:ND1	2.28	0.47
19:B:1772:CLA:H2	23:B:1774:PQN:H251	1.96	0.47
10:F:96:TRP:HZ2	19:F:1155:CLA:CAB	2.27	0.47
16:L:63:LEU:O	16:L:65:VAL:N	2.48	0.47
16:L:164:PRO:N	16:L:165:TYR:CD2	2.81	0.47
17:N:44:GLU:HB3	17:N:45:ASN:H	1.41	0.47
20:R:1056:LMU:H102	20:R:1056:LMU:H71	1.65	0.47
21:3:1226:SUC:O5	21:3:1226:SUC:O2'	2.30	0.47
21:B:8059:SUC:C1'	21:B:8059:SUC:C6'	2.55	0.47
10:F:43:LYS:HE3	10:F:43:LYS:N	2.29	0.47
6:B:244:PHE:CD2	6:B:244:PHE:C	2.87	0.47
6:B:211:ASN:ND2	6:B:214:ASP:OD1	2.48	0.47
7:C:30:PRO:HB3	7:C:37:LYS:O	2.14	0.47
8:D:96:ILE:O	8:D:97:LYS:HB2	2.13	0.47
2:2:163:GLU:HG2	19:2:1218:CLA:C3C	2.43	0.47
5:A:217:SER:CA	22:A:1802:BCR:C35	2.84	0.47
5:A:302:HIS:HE1	19:A:1774:CLA:C1B	2.27	0.47
5:A:402:ILE:HD11	19:A:1784:CLA:CBB	2.43	0.47
5:A:347:TYR:HE1	5:A:417:PHE:CZ	2.32	0.47
5:A:41:SER:O	5:A:44:ILE:CA	2.61	0.47
5:A:541:VAL:HG12	5:A:545:HIS:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:553:VAL:N	5:A:556:LEU:HD12	2.26	0.47
5:A:605:MET:O	5:A:608:SER:N	2.48	0.47
5:A:64:PHE:CD1	5:A:74:ILE:HG22	2.50	0.47
6:B:290:MET:HA	19:B:1752:CLA:C3C	2.44	0.47
19:B:1757:CLA:CED	19:B:1765:CLA:CBB	2.90	0.47
6:B:421:HIS:O	19:B:1770:CLA:HMC3	2.14	0.47
19:B:1759:CLA:H62	22:B:1777:BCR:HC7	1.96	0.47
6:B:269:TRP:CD1	6:B:497:TRP:HH2	2.32	0.47
6:B:335:GLY:HA2	6:B:338:LEU:HB2	1.96	0.47
6:B:387:PHE:HE2	19:B:1756:CLA:HHC	1.78	0.47
6:B:395:ILE:HG22	6:B:551:LYS:HG3	1.96	0.47
6:B:448:THR:O	6:B:448:THR:OG1	2.31	0.47
8:D:139:LYS:HZ3	9:E:41:ARG:NH1	2.12	0.47
10:F:130:LEU:CD1	21:F:1158:SUC:O3'	2.63	0.47
16:L:63:LEU:CD2	16:L:64:LEU:N	2.73	0.47
17:N:53:ALA:O	17:N:54:LYS:CB	2.61	0.47
17:N:58:VAL:CG1	17:N:59:PRO:HD3	2.44	0.47
20:A:7033:LMU:H6E	20:A:7033:LMU:H2B	1.96	0.47
3:3:73:ILE:C	19:3:1217:CLA:C2D	2.83	0.47
4:4:53:LEU:O	4:4:56:ALA:N	2.47	0.47
16:L:23:LEU:O	16:L:25:THR:N	2.48	0.47
6:B:216:LEU:O	6:B:218:TYR:O	2.33	0.47
5:A:68:THR:C	5:A:70:ASP:N	2.67	0.47
20:A:7031:LMU:H4'	20:A:7031:LMU:H3B	1.95	0.47
5:A:350:LEU:HA	5:A:350:LEU:HD23	1.50	0.47
2:2:179:PHE:CE1	2:2:183:TYR:CZ	3.02	0.47
2:2:128:ASN:CG	14:J:3:ASP:HB3	2.35	0.47
19:A:1767:CLA:H152	19:A:1767:CLA:H202	1.96	0.47
19:A:1776:CLA:HBC3	19:A:1776:CLA:HMC1	1.94	0.47
5:A:692:PHE:HE2	19:A:1796:CLA:HBC3	1.71	0.47
5:A:248:PHE:HD2	5:A:248:PHE:N	1.93	0.47
5:A:457:SER:OG	5:A:544:ILE:HA	2.15	0.47
5:A:660:GLN:HE21	5:A:660:GLN:H	1.62	0.47
5:A:599:PHE:CZ	5:A:731:ARG:HB3	2.47	0.47
19:B:1749:CLA:C15	19:B:1750:CLA:H71	2.45	0.47
19:B:1756:CLA:O1A	19:B:1770:CLA:HAA1	2.15	0.47
6:B:361:ILE:HG22	6:B:361:ILE:O	2.15	0.47
6:B:693:TRP:HE1	19:B:1771:CLA:HHD	1.79	0.47
6:B:653:GLY:HA3	6:B:720:THR:OG1	2.13	0.47
11:G:30:ASN:ND2	11:G:31:MET:O	2.48	0.47
11:G:64:VAL:HG13	11:G:67:ASN:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:15:SER:HA	14:J:18:TRP:HB3	1.96	0.47
2:2:127:ASN:OD1	14:J:2:ARG:CG	2.63	0.47
4:4:119:PRO:C	4:4:121:PHE:H	2.17	0.47
4:4:154:ILE:O	4:4:157:GLY:CA	2.63	0.47
4:4:158:ARG:O	4:4:161:LEU:O	2.33	0.47
19:A:1786:CLA:HMB2	19:A:1787:CLA:C3D	2.45	0.47
19:A:1799:CLA:HMC3	19:B:1771:CLA:ND	2.30	0.47
19:A:1812:CLA:CMA	19:A:1812:CLA:H2	2.44	0.47
5:A:347:TYR:CE1	5:A:417:PHE:HZ	2.32	0.47
5:A:420:ARG:HB3	5:A:420:ARG:CZ	2.45	0.47
5:A:680:LEU:HD22	5:A:680:LEU:N	2.29	0.47
5:A:711:HIS:CB	5:A:717:ALA:HB2	2.38	0.47
5:A:603:PHE:CE1	5:A:735:VAL:HA	2.50	0.47
19:B:1743:CLA:H61	19:B:1743:CLA:C1	2.44	0.47
19:B:1750:CLA:HBA1	19:B:1750:CLA:CHA	2.44	0.47
23:B:1774:PQN:H143	22:B:1781:BCR:H322	1.95	0.47
6:B:334:LEU:HB2	19:B:1737:CLA:CMD	2.41	0.47
6:B:396:ARG:NH1	19:B:1760:CLA:HED2	2.30	0.47
6:B:652:PHE:CZ	6:B:656:VAL:HG21	2.50	0.47
8:D:36:LEU:HB2	16:L:19:PHE:O	2.15	0.47
10:F:95:GLY:O	10:F:99:TRP:CB	2.62	0.47
11:G:28:ARG:HG2	11:G:29:GLU:HB2	1.96	0.47
17:N:59:PRO:CA	17:N:66:ASP:OD1	2.63	0.47
17:N:68:GLU:O	17:N:69:CYS:HB2	2.13	0.47
3:3:59:ILE:HB	3:3:63:ARG:HH21	1.79	0.47
20:A:7033:LMU:O3'	20:A:7033:LMU:O6B	2.29	0.47
15:K:13:THR:OG1	15:K:14:THR:N	2.48	0.47
20:A:7050:LMU:O2B	20:A:7050:LMU:O4'	2.29	0.47
20:A:7010:LMU:O3'	20:A:7010:LMU:C2B	2.63	0.47
9:E:69:PHE:CE2	9:E:70:ALA:HB3	2.50	0.47
4:4:63:VAL:O	4:4:65:THR:HG23	2.14	0.47
16:L:5:LYS:HE2	16:L:5:LYS:CA	2.36	0.47
1:1:44:LEU:CD1	1:1:151:GLY:HA2	2.45	0.47
2:2:188:PRO:C	2:2:190:ASP:H	2.17	0.47
2:2:85:GLN:CA	2:2:85:GLN:OE1	2.59	0.47
5:A:628:ILE:HG13	5:A:632:GLY:CA	2.42	0.47
10:F:116:GLN:C	10:F:118:GLU:N	2.57	0.47
19:3:3008:CLA:HBC2	19:3:3008:CLA:HMC1	1.96	0.47
3:3:171:LYS:HE3	3:3:171:LYS:N	2.29	0.47
5:A:241:GLU:O	5:A:241:GLU:OE1	2.32	0.47
19:2:1218:CLA:CGA	19:2:1218:CLA:C1A	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1783:CLA:H191	19:A:1811:CLA:H13	1.97	0.47
5:A:83:PHE:CE2	5:A:185:HIS:CD2	3.03	0.47
19:B:1768:CLA:HMC1	19:B:1768:CLA:CBC	2.24	0.47
6:B:29:HIS:HB2	19:B:1760:CLA:HBA1	1.97	0.47
7:C:66:ARG:NH2	7:C:66:ARG:CG	2.70	0.47
11:G:43:HIS:CA	11:G:44:PHE:CB	2.60	0.47
17:N:59:PRO:HG2	17:N:73:ASP:O	2.15	0.47
20:A:7016:LMU:O6'	20:A:7016:LMU:H31	2.13	0.47
5:A:21:LEU:HA	5:A:21:LEU:HD13	1.39	0.47
10:F:44:ALA:C	10:F:46:MET:N	2.68	0.47
21:B:8053:SUC:O4'	21:B:8053:SUC:C5	2.63	0.47
17:N:2:VAL:CG2	17:N:2:VAL:O	2.62	0.47
5:A:265:GLY:HA3	5:A:272:LEU:HD21	1.97	0.47
2:2:148:TRP:O	2:2:150:SER:N	2.48	0.47
3:3:127:ARG:C	3:3:129:PHE:H	2.18	0.47
3:3:166:PRO:HB2	3:3:167:LEU:H	1.54	0.47
4:4:140:PRO:O	4:4:141:LEU:HB2	2.13	0.47
19:A:1759:CLA:HHD	19:A:1759:CLA:HBC3	1.97	0.47
19:A:1767:CLA:C4A	19:A:1767:CLA:CBA	2.92	0.47
5:A:372:VAL:HG22	19:A:1774:CLA:C4	2.45	0.47
19:A:1787:CLA:C9	19:A:1800:CLA:H2	2.44	0.47
19:A:1783:CLA:H202	22:A:1807:BCR:C16	2.45	0.47
5:A:185:HIS:O	5:A:186:TYR:C	2.53	0.47
5:A:281:LEU:C	5:A:283:PHE:N	2.68	0.47
5:A:354:TRP:O	5:A:357:GLN:N	2.48	0.47
5:A:409:GLY:O	5:A:411:ALA:N	2.48	0.47
5:A:584:PRO:HG2	7:C:66:ARG:HB2	1.97	0.47
5:A:663:GLN:OE1	5:A:753:ARG:NE	2.48	0.47
20:A:7006:LMU:H5B	20:A:7006:LMU:H3'	1.95	0.47
5:A:701:GLN:O	5:A:703:LEU:N	2.48	0.47
5:A:709:TRP:CE3	5:A:710:ALA:N	2.83	0.47
19:B:1754:CLA:O1D	19:B:1754:CLA:OBD	2.31	0.47
19:B:1756:CLA:C2B	22:B:1778:BCR:H352	2.45	0.47
6:B:353:TYR:C	6:B:355:LEU:N	2.68	0.47
6:B:552:ASP:OD1	6:B:553:PHE:HD2	1.98	0.47
7:C:70:TRP:O	7:C:71:HIS:C	2.53	0.47
11:G:34:GLN:O	11:G:36:PRO:CD	2.63	0.47
16:L:154:ALA:O	16:L:155:CYS:C	2.53	0.47
16:L:46:ALA:CB	16:L:52:ARG:NH2	2.78	0.47
20:1:1199:LMU:O5B	20:1:1199:LMU:H5'	2.13	0.47
17:N:47:THR:O	17:N:48:GLY:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:189:LEU:C	3:3:191:MET:H	2.18	0.47
7:C:14:CYS:SG	7:C:17:CYS:SG	3.13	0.47
20:A:7050:LMU:H6B	20:A:7050:LMU:H3O2	1.63	0.47
20:A:7039:LMU:H6'2	20:A:7039:LMU:H1B	1.41	0.47
20:A:7039:LMU:O5'	20:A:7039:LMU:O3'	2.29	0.47
5:A:258:LEU:O	5:A:259:TYR:HB2	2.14	0.47
8:D:89:ARG:O	8:D:92:SER:N	2.48	0.47
5:A:70:ASP:O	5:A:71:LEU:O	2.33	0.47
6:B:31:PHE:HB2	6:B:42:LEU:HD12	1.96	0.47
3:3:141:GLN:O	3:3:142:TYR:HB2	2.14	0.47
8:D:26:SER:N	8:D:27:PRO:HD3	2.29	0.47
2:2:96:ILE:O	2:2:100:VAL:N	2.47	0.47
5:A:733:VAL:HG13	19:A:1796:CLA:C3D	2.44	0.47
19:A:1799:CLA:HMC3	19:B:1771:CLA:C1D	2.45	0.47
5:A:434:ARG:O	5:A:435:VAL:C	2.53	0.47
5:A:581:CYS:HB3	5:A:590:CYS:O	2.14	0.47
6:B:127:ILE:O	6:B:128:GLY:C	2.53	0.47
6:B:212:PHE:CE1	19:B:1745:CLA:HHD	2.34	0.47
19:B:1750:CLA:H61	19:B:1750:CLA:H41	1.66	0.47
19:B:1756:CLA:H11	19:B:1770:CLA:CAD	2.44	0.47
6:B:183:PHE:HB3	6:B:284:PHE:HD2	1.80	0.47
5:A:705:GLU:CG	6:B:545:LYS:HZ2	2.26	0.47
6:B:558:PRO:HB3	6:B:706:ARG:HH21	1.79	0.47
19:G:1099:CLA:H3A	19:G:1099:CLA:C2	2.44	0.47
11:G:16:LEU:CD1	11:G:17:PHE:CZ	2.98	0.47
13:I:8:PHE:CD1	19:I:1031:CLA:H12	2.49	0.47
4:4:175:LYS:O	4:4:175:LYS:HD2	2.15	0.47
17:N:70:GLU:HB3	17:N:72:LYS:HA	1.95	0.47
7:C:17:CYS:O	7:C:58:CYS:HB2	2.14	0.47
20:A:7043:LMU:H62	20:A:7043:LMU:H92	1.51	0.47
21:B:8059:SUC:H1'2	21:B:8059:SUC:H6'2	1.82	0.47
8:D:48:ILE:CG1	8:D:49:THR:N	2.77	0.47
9:E:44:TYR:HB3	9:E:45:TRP:CZ3	2.51	0.47
20:1:1200:LMU:O1B	20:1:1200:LMU:O4'	2.30	0.47
19:2:1217:CLA:HMA2	19:2:1217:CLA:C5	2.43	0.47
6:B:470:THR:OG1	6:B:501:ILE:HG23	2.15	0.47
3:3:164:PHE:O	3:3:165:ASN:C	2.53	0.47
11:G:79:HIS:NE2	11:G:82:ALA:HB2	2.30	0.47
10:F:137:PRO:O	10:F:139:ALA:N	2.47	0.47
12:H:76:VAL:O	12:H:76:VAL:HG22	2.15	0.47
5:A:132:LEU:HD13	5:A:671:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:132:LEU:O	5:A:143:ILE:HB	2.15	0.46
5:A:193:LEU:O	5:A:195:TRP:N	2.49	0.46
5:A:210:LEU:CD1	19:A:1769:CLA:HHB	2.45	0.46
5:A:463:HIS:NE2	5:A:467:MET:SD	2.88	0.46
5:A:709:TRP:O	5:A:712:ASN:N	2.48	0.46
5:A:733:VAL:HG12	5:A:737:HIS:CE1	2.50	0.46
6:B:289:LEU:O	19:B:1752:CLA:HMC1	2.15	0.46
19:B:1768:CLA:O2D	19:B:1768:CLA:OBD	2.33	0.46
19:B:1786:CLA:HMB3	19:B:1787:CLA:CAD	2.45	0.46
6:B:230:TRP:O	6:B:231:ASN:C	2.52	0.46
6:B:290:MET:SD	6:B:291:TYR:CE1	3.08	0.46
6:B:9:SER:HA	6:B:35:ASP:OD1	2.15	0.46
6:B:540:ASP:OD1	6:B:540:ASP:N	2.47	0.46
6:B:693:TRP:CD1	19:B:1771:CLA:HMD3	2.49	0.46
6:B:708:VAL:C	6:B:710:LEU:O	2.53	0.46
21:B:8054:SUC:H3'	21:B:8054:SUC:H1	1.50	0.46
6:B:294:ASN:O	11:G:36:PRO:HG2	2.15	0.46
11:G:37:GLU:O	11:G:38:GLN:C	2.52	0.46
16:L:123:ARG:HB3	16:L:126:GLN:HG3	1.96	0.46
16:L:162:ASP:OD2	16:L:162:ASP:O	2.33	0.46
20:A:7036:LMU:O5B	20:A:7036:LMU:C5'	2.62	0.46
3:3:63:ARG:NH1	3:3:189:LEU:H	2.13	0.46
6:B:120:VAL:HG22	6:B:123:TRP:HE1	1.80	0.46
16:L:108:LYS:HD3	16:L:132:SER:HB3	1.97	0.46
20:A:7017:LMU:H1B	20:A:7017:LMU:H6'2	1.43	0.46
5:A:539:PHE:CD2	5:A:539:PHE:C	2.89	0.46
2:2:102:ILE:HG22	2:2:106:GLU:HG3	1.98	0.46
2:2:73:ILE:HG22	2:2:73:ILE:O	2.15	0.46
4:4:93:ILE:C	4:4:95:PHE:H	2.17	0.46
19:A:1768:CLA:O1D	19:A:1769:CLA:HMC1	2.16	0.46
5:A:355:HIS:ND1	5:A:416:ILE:HG22	2.24	0.46
5:A:400:MET:CE	5:A:612:VAL:HG11	2.46	0.46
5:A:680:LEU:HB3	19:A:1811:CLA:C2	2.45	0.46
5:A:98:PHE:HD1	5:A:99:HIS:CD2	2.32	0.46
6:B:334:LEU:HA	19:B:1737:CLA:HMD3	1.97	0.46
6:B:30:ASP:O	6:B:34:HIS:HD2	1.98	0.46
6:B:350:GLN:O	6:B:353:TYR:CD1	2.69	0.46
6:B:494:LEU:HD12	19:B:1766:CLA:CED	2.44	0.46
7:C:77:MET:C	7:C:79:LEU:H	2.13	0.46
7:C:81:TYR:HD1	7:C:81:TYR:N	2.14	0.46
11:G:39:ASN:HA	11:G:40:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:1032:BCR:H11C	22:I:1032:BCR:H34I	1.71	0.46
16:L:40:LEU:HD12	16:L:40:LEU:H	1.80	0.46
17:N:70:GLU:CA	17:N:72:LYS:H	2.26	0.46
19:3:1217:CLA:C3B	19:3:1222:CLA:H11	2.46	0.46
6:B:478:LEU:O	6:B:479:SER:HB3	2.15	0.46
17:N:6:TYR:HA	17:N:6:TYR:HD2	1.69	0.46
5:A:476:MET:O	5:A:477:PHE:HB2	2.16	0.46
18:R:1:UNK:O	18:R:2:UNK:O	2.34	0.46
5:A:493:GLN:OE1	5:A:534:LEU:HD11	2.15	0.46
4:4:104:ARG:CG	4:4:105:ARG:N	2.74	0.46
4:4:107:GLN:HA	19:4:1196:CLA:C2A	2.45	0.46
4:4:88:SER:O	4:4:90:LEU:CA	2.53	0.46
4:4:99:HIS:HD1	4:4:103:ILE:HD13	1.81	0.46
19:A:1780:CLA:HMC1	19:A:1780:CLA:HBC2	1.96	0.46
19:A:1781:CLA:CED	19:A:1782:CLA:HMD2	2.37	0.46
19:A:1790:CLA:H3A	19:A:1790:CLA:HBA2	1.51	0.46
22:A:1806:BCR:C8	19:A:1812:CLA:H142	2.45	0.46
5:A:298:ASP:O	5:A:300:ALA:N	2.49	0.46
5:A:458:PHE:C	5:A:458:PHE:CD1	2.89	0.46
5:A:514:THR:HA	5:A:530:LEU:O	2.15	0.46
5:A:550:HIS:C	5:A:552:THR:O	2.53	0.46
5:A:616:PHE:O	5:A:620:MET:HB2	2.16	0.46
5:A:73:GLU:O	5:A:76:ARG:HB2	2.15	0.46
6:B:590:VAL:HG21	19:B:1768:CLA:HBB2	1.98	0.46
19:B:1757:CLA:H122	22:B:1778:BCR:C12	2.46	0.46
6:B:589:TRP:CD1	19:B:1786:CLA:H152	2.51	0.46
6:B:322:LEU:O	6:B:326:ILE:HG22	2.16	0.46
6:B:527:LEU:CD1	6:B:586:THR:HG21	2.43	0.46
6:B:596:TRP:HZ3	6:B:613:SER:CB	2.28	0.46
6:B:732:LYS:C	6:B:733:PHE:O	2.53	0.46
8:D:137:ILE:HG13	8:D:137:ILE:H	1.41	0.46
10:F:145:LEU:C	10:F:146:ASN:ND2	2.69	0.46
11:G:16:LEU:HD12	11:G:17:PHE:CZ	2.48	0.46
11:G:48:ASP:CB	11:G:49:THR:CB	2.91	0.46
2:2:120:ASN:ND2	14:J:5:LYS:HD2	2.30	0.46
16:L:62:PHE:HE2	19:L:1168:CLA:H2A	1.81	0.46
16:L:40:LEU:CB	16:L:41:PRO:HD3	2.37	0.46
17:N:42:PHE:CG	17:N:43:PRO:N	2.79	0.46
10:F:41:ALA:O	10:F:44:ALA:O	2.33	0.46
12:H:29:PRO:O	12:H:30:SER:OG	2.28	0.46
20:A:7020:LMU:C6'	20:A:7020:LMU:C1B	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7022:LMU:O3B	20:A:7022:LMU:H6'2	2.12	0.46
1:1:160:GLY:HA3	19:1:1189:CLA:CBB	2.45	0.46
10:F:34:ASP:O	10:F:34:ASP:OD2	2.33	0.46
2:2:102:ILE:HD13	2:2:102:ILE:N	2.31	0.46
2:2:120:ASN:HB3	14:J:5:LYS:HD2	1.97	0.46
4:4:129:GLY:C	4:4:131:VAL:N	2.68	0.46
5:A:107:GLU:O	5:A:110:LEU:HG	2.15	0.46
19:A:1767:CLA:H171	19:A:1767:CLA:H141	1.97	0.46
19:A:1768:CLA:HBD	19:A:1768:CLA:HAA1	1.95	0.46
19:A:1779:CLA:CBB	22:A:1804:BCR:H352	2.29	0.46
19:A:1812:CLA:H93	6:B:431:PHE:CD1	2.51	0.46
5:A:684:PHE:HD2	5:A:685:VAL:CA	2.27	0.46
19:B:1737:CLA:H92	19:B:1755:CLA:O1A	2.16	0.46
6:B:431:PHE:CD2	19:B:1763:CLA:HMA3	2.50	0.46
6:B:176:ASN:ND2	6:B:293:THR:OG1	2.47	0.46
7:C:52:LYS:C	7:C:54:CYS:H	2.17	0.46
14:J:2:ARG:HH11	14:J:2:ARG:CG	2.29	0.46
16:L:56:VAL:CG1	19:L:1167:CLA:CED	2.87	0.46
16:L:151:VAL:O	16:L:154:ALA:HB3	2.15	0.46
3:3:205:GLY:HA3	5:A:252:ARG:HH12	1.79	0.46
17:N:59:PRO:CB	17:N:75:TYR:CE1	2.95	0.46
19:1:1142:CLA:HAA2	19:1:1142:CLA:HBD	1.96	0.46
20:A:7033:LMU:O2'	20:A:7033:LMU:O6B	2.29	0.46
1:1:63:LEU:CD2	1:1:64:GLY:CA	2.84	0.46
5:A:27:ILE:C	5:A:28:LYS:CG	2.83	0.46
6:B:514:PRO:HG2	10:F:70:HIS:CE1	2.49	0.46
5:A:265:GLY:HA2	5:A:272:LEU:CD2	2.46	0.46
1:1:185:TRP:HB3	1:1:186:HIS:NE2	2.31	0.46
4:4:83:TYR:HB3	4:4:84:PHE:H	1.72	0.46
19:A:1776:CLA:H43	19:A:1779:CLA:C2	2.45	0.46
5:A:680:LEU:HD12	19:A:1811:CLA:O2A	2.16	0.46
5:A:223:VAL:HG12	5:A:224:HIS:H	1.80	0.46
5:A:499:ALA:HB3	19:A:1790:CLA:CED	2.45	0.46
5:A:636:HIS:O	5:A:637:ILE:C	2.53	0.46
6:B:377:TYR:O	6:B:378:ILE:CB	2.62	0.46
6:B:461:GLN:HE21	6:B:461:GLN:HB3	1.61	0.46
9:E:83:ALA:O	9:E:86:GLU:CG	2.49	0.46
11:G:57:LEU:O	11:G:57:LEU:HD22	2.16	0.46
14:J:21:SER:O	14:J:23:ALA:N	2.48	0.46
4:4:72:VAL:O	4:4:72:VAL:HG22	2.15	0.46
16:L:163:LEU:CD1	16:L:164:PRO:CB	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:249:ILE:CG2	5:A:251:ASN:OD1	2.64	0.46
3:3:56:TYR:HD1	3:3:185:LYS:CE	2.29	0.46
19:3:1222:CLA:H162	19:3:1222:CLA:H141	1.59	0.46
6:B:454:LEU:H	6:B:454:LEU:HD12	1.80	0.46
5:A:425:THR:O	5:A:427:ARG:CD	2.64	0.46
2:2:191:ASN:HD21	2:2:194:ALA:HA	1.80	0.46
19:2:1217:CLA:H2	19:2:1217:CLA:H2A	1.97	0.46
6:B:500:ALA:C	6:B:501:ILE:HG12	2.36	0.46
2:2:42:ARG:CA	2:2:45:VAL:CB	2.84	0.46
2:2:73:ILE:CD1	2:2:75:ASN:HB2	2.46	0.46
3:3:84:ILE:HG23	3:3:84:ILE:O	2.16	0.46
4:4:103:ILE:HB	19:4:1197:CLA:HMD1	1.96	0.46
19:A:1759:CLA:HBC3	19:A:1759:CLA:CHD	2.46	0.46
19:A:1760:CLA:HBA2	19:A:1767:CLA:C6	2.44	0.46
5:A:308:ILE:HD13	19:A:1772:CLA:C9	2.38	0.46
19:A:1781:CLA:CMA	19:A:1782:CLA:CGA	2.93	0.46
19:A:1787:CLA:HBB2	19:A:1793:CLA:H203	1.98	0.46
22:A:1802:BCR:C12	22:A:1802:BCR:C34	2.86	0.46
5:A:208:ALA:HB2	5:A:314:GLY:CA	2.38	0.46
5:A:361:ASN:ND2	5:A:361:ASN:C	2.69	0.46
19:B:1735:CLA:H71	19:B:1735:CLA:C2C	2.45	0.46
6:B:172:GLU:O	6:B:173:SER:C	2.54	0.46
19:B:1759:CLA:H101	22:B:1777:BCR:C34	2.44	0.46
6:B:429:LEU:HD11	19:B:1769:CLA:HMB3	1.96	0.46
6:B:53:GLN:NE2	19:B:1736:CLA:HBB1	2.30	0.46
6:B:580:VAL:HG11	6:B:710:LEU:HD11	1.97	0.46
16:L:126:GLN:N	16:L:127:PRO:CD	2.78	0.46
19:3:1222:CLA:H71	19:3:1222:CLA:H112	1.47	0.46
20:A:7050:LMU:C2	20:A:7050:LMU:H81	2.40	0.46
17:N:27:ALA:O	17:N:28:ASN:C	2.54	0.46
5:A:334:HIS:CD2	19:A:1777:CLA:NB	2.84	0.46
5:A:334:HIS:HD2	19:A:1777:CLA:NB	2.14	0.46
5:A:76:ARG:C	5:A:186:TYR:HD2	2.19	0.46
5:A:358:LEU:HD11	5:A:413:HIS:HB2	1.90	0.46
5:A:369:THR:O	5:A:372:VAL:HG23	2.16	0.46
5:A:397:THR:HB	5:A:613:ILE:HG13	1.96	0.46
5:A:613:ILE:HG22	5:A:614:PHE:N	2.29	0.46
6:B:278:LEU:CD1	19:B:1747:CLA:HMA2	2.39	0.46
6:B:292:ARG:NH2	19:B:1751:CLA:HED1	2.31	0.46
19:B:1765:CLA:HBA2	19:B:1765:CLA:H3A	1.47	0.46
22:B:1776:BCR:H11C	22:B:1776:BCR:H341	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:486:LEU:CD1	19:B:1766:CLA:HMD3	2.45	0.46
6:B:57:ILE:HG22	6:B:58:PHE:CD1	2.50	0.46
6:B:596:TRP:CZ3	6:B:613:SER:CB	2.98	0.46
6:B:629:SER:O	6:B:630:GLN:C	2.53	0.46
20:A:7048:LMU:O1B	20:A:7048:LMU:O6'	2.30	0.46
4:4:191:ASN:CG	4:4:191:ASN:O	2.52	0.46
5:A:24:ARG:N	5:A:24:ARG:CD	2.76	0.46
1:1:59:VAL:HG12	1:1:60:PRO:N	2.26	0.46
20:A:7021:LMU:C4	20:A:7021:LMU:H1'	2.43	0.46
7:C:28:MET:SD	8:D:122:LYS:O	2.74	0.46
12:H:53:LEU:HG	12:H:54:LEU:N	2.22	0.46
7:C:26:LEU:O	7:C:43:PRO:HB3	2.16	0.46
20:A:7031:LMU:H21	20:A:7031:LMU:H52	1.68	0.46
2:2:157:LYS:HA	2:2:159:LEU:CD2	2.46	0.46
4:4:51:ALA:O	4:4:55:VAL:HG13	2.16	0.46
2:2:171:MET:SD	2:2:172:LEU:CG	3.00	0.46
19:A:1762:CLA:C2	19:A:1762:CLA:C7	2.94	0.46
19:A:1781:CLA:H93	22:A:1805:BCR:H10C	1.97	0.46
5:A:462:ILE:O	5:A:466:THR:OG1	2.32	0.46
5:A:746:THR:HG1	19:A:1810:CLA:CGD	2.24	0.46
5:A:73:GLU:O	5:A:74:ILE:C	2.54	0.46
6:B:164:SER:HB2	6:B:167:TRP:CE3	2.51	0.46
6:B:167:TRP:HB2	11:G:41:MET:HE3	1.97	0.46
19:B:1741:CLA:O1D	19:B:1741:CLA:H2A	2.16	0.46
22:B:1780:BCR:H24C	22:B:1780:BCR:H371	1.51	0.46
6:B:415:LYS:HG3	6:B:416:GLU:OE2	2.15	0.46
6:B:442:VAL:O	6:B:446:PHE:HB2	2.16	0.46
6:B:721:TYR:HA	6:B:724:PHE:HB3	1.97	0.46
9:E:58:ASP:N	9:E:58:ASP:OD1	2.29	0.46
11:G:10:LEU:HD23	11:G:13:GLY:HA3	1.98	0.46
11:G:24:PHE:C	11:G:26:PHE:N	2.69	0.46
4:4:72:VAL:N	4:4:73:PRO:CD	2.78	0.46
19:4:1206:CLA:H111	19:4:1206:CLA:H71	1.58	0.46
2:2:196:HIS:HB3	2:2:197:LEU:H	1.50	0.46
6:B:318:GLY:HA3	6:B:405:ASP:OD2	2.15	0.46
16:L:158:MET:CG	16:L:159:TYR:N	2.75	0.46
2:2:44:ASN:HD21	14:J:1:MET:CB	2.09	0.46
4:4:116:ASN:HB3	4:4:118:ASP:OD1	2.16	0.46
19:A:1779:CLA:NB	22:A:1804:BCR:C15	2.78	0.46
19:A:1762:CLA:H11	19:A:1785:CLA:O2A	2.16	0.46
22:A:1802:BCR:C31	22:A:1802:BCR:C8	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:531:PRO:O	5:A:532:ILE:HG23	2.16	0.46
5:A:457:SER:HG	5:A:544:ILE:HA	1.80	0.46
5:A:593:SER:O	5:A:594:ALA:HB2	2.15	0.46
5:A:656:PHE:O	5:A:658:TRP:N	2.49	0.46
5:A:660:GLN:O	5:A:661:ALA:HB2	2.14	0.46
6:B:389:HIS:HE1	19:B:1760:CLA:NC	2.14	0.46
5:A:709:TRP:CZ3	6:B:417:ALA:HA	2.50	0.46
6:B:544:SER:O	6:B:547:MET:C	2.55	0.46
6:B:568:CYS:C	6:B:570:ILE:HG23	2.36	0.46
6:B:700:LEU:H	6:B:700:LEU:HD23	1.80	0.46
10:F:149:LEU:CD2	10:F:153:ASN:HD21	2.28	0.46
10:F:72:ILE:O	10:F:73:VAL:HG12	2.16	0.46
19:G:1099:CLA:H2	19:G:1099:CLA:H3A	1.98	0.46
12:H:66:THR:N	12:H:69:SER:HB3	2.29	0.46
16:L:61:GLY:O	16:L:63:LEU:N	2.49	0.46
17:N:45:ASN:CG	17:N:57:LYS:NZ	2.69	0.46
19:4:1201:CLA:HAA2	19:4:1201:CLA:O2D	2.14	0.46
20:A:7005:LMU:C7	20:A:7005:LMU:H32	2.23	0.46
26:B:8057:UNL:O1'	26:B:8057:UNL:O3'	2.28	0.46
6:B:224:PRO:CA	6:B:227:THR:OG1	2.63	0.46
6:B:399:ASN:O	6:B:399:ASN:OD1	2.34	0.46
2:2:125:PHE:O	2:2:127:ASN:HA	2.15	0.46
4:4:101:VAL:O	4:4:104:ARG:HD3	2.15	0.46
4:4:103:ILE:CB	19:4:1197:CLA:HMD1	2.46	0.46
4:4:142:ASN:C	4:4:143:PHE:CG	2.89	0.46
19:A:1774:CLA:ND	19:A:1784:CLA:H72	2.31	0.46
19:A:1776:CLA:H121	22:A:1805:BCR:H23C	1.97	0.46
5:A:296:LEU:C	5:A:298:ASP:N	2.68	0.46
5:A:374:GLN:C	5:A:376:MET:N	2.68	0.46
5:A:405:PHE:O	19:A:1785:CLA:HMC1	2.15	0.46
5:A:584:PRO:HG3	6:B:559:CYS:SG	2.56	0.46
5:A:645:SER:O	5:A:651:GLY:HA3	2.15	0.46
6:B:275:HIS:HD2	19:B:1747:CLA:HMA3	1.81	0.46
6:B:435:GLY:HA3	19:B:1764:CLA:CBB	2.46	0.46
19:B:1746:CLA:HMA1	22:B:1777:BCR:H372	1.98	0.46
6:B:256:THR:HG22	6:B:271:THR:OG1	2.16	0.46
6:B:336:LEU:HD13	19:B:1755:CLA:CBB	2.45	0.46
6:B:518:LEU:O	6:B:521:HIS:N	2.41	0.46
6:B:714:SER:O	6:B:718:ILE:HG22	2.16	0.46
19:4:1199:CLA:HAA1	19:F:1157:CLA:H12	1.97	0.46
10:F:78:ARG:O	10:F:80:TRP:CD1	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:28:ARG:CG	11:G:29:GLU:CB	2.94	0.46
13:I:15:LEU:HD12	13:I:18:ALA:HB3	1.98	0.46
4:4:69:ILE:O	4:4:71:ASN:HB2	2.16	0.46
3:3:56:TYR:HD1	3:3:185:LYS:NZ	2.12	0.46
20:A:7048:LMU:O2B	20:A:7048:LMU:O6'	2.30	0.46
5:A:22:VAL:H	5:A:23:ASP:C	2.19	0.46
10:F:22:LEU:CB	10:F:25:LEU:HD13	2.46	0.46
3:3:112:THR:C	3:3:114:PHE:N	2.69	0.46
15:K:24:PHE:CG	15:K:52:PRO:CG	2.99	0.46
3:3:66:MET:CE	3:3:69:ALA:HB3	2.46	0.46
10:F:63:CYS:CA	10:F:69:PRO:HA	2.43	0.46
2:2:191:ASN:CG	2:2:191:ASN:O	2.53	0.46
3:3:162:PRO:HG2	3:3:164:PHE:CG	2.51	0.46
3:3:165:ASN:HA	3:3:165:ASN:HD22	1.59	0.46
5:A:49:ASP:HB2	5:A:720:THR:HA	1.97	0.46
10:F:37:ALA:N	10:F:38:PRO:HD3	2.31	0.46
2:2:102:ILE:CG2	2:2:106:GLU:HG3	2.46	0.45
2:2:128:ASN:O	2:2:129:LYS:C	2.54	0.45
5:A:126:ILE:O	5:A:129:GLN:HB2	2.16	0.45
22:A:1803:BCR:C31	22:A:1803:BCR:C8	2.94	0.45
5:A:302:HIS:O	5:A:306:ILE:CG1	2.51	0.45
5:A:552:THR:O	5:A:553:VAL:HB	2.16	0.45
5:A:707:ILE:H	5:A:707:ILE:HG12	1.54	0.45
5:A:708:VAL:N	5:A:711:HIS:HD2	2.14	0.45
5:A:72:GLU:HB2	5:A:73:GLU:H	1.55	0.45
5:A:685:VAL:CG1	5:A:741:GLY:CA	2.94	0.45
6:B:193:HIS:CD2	19:B:1745:CLA:NB	2.84	0.45
22:B:1776:BCR:H331	22:B:1776:BCR:HC8	1.95	0.45
19:B:1786:CLA:HMB3	19:B:1787:CLA:OBD	2.16	0.45
6:B:721:TYR:N	19:B:1786:CLA:O1D	2.49	0.45
6:B:354:SER:OG	19:B:1757:CLA:CBC	2.64	0.45
6:B:260:GLY:HA2	6:B:497:TRP:CE2	2.51	0.45
6:B:556:SER:HA	6:B:558:PRO:HD3	1.98	0.45
6:B:60:TRP:CD1	19:B:1738:CLA:HBC1	2.51	0.45
8:D:102:ARG:NH2	8:D:110:GLN:HB2	2.30	0.45
10:F:123:VAL:CB	10:F:126:ALA:O	2.64	0.45
19:L:1168:CLA:HHD	19:L:1168:CLA:HBC2	1.88	0.45
16:L:123:ARG:CA	16:L:123:ARG:NE	2.71	0.45
3:3:132:TRP:HZ3	3:3:155:GLU:CD	1.82	0.45
20:B:1783:LMU:O6B	20:B:1783:LMU:O2'	2.30	0.45
3:3:188:ARG:HA	3:3:191:MET:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:64:GLY:C	1:1:66:GLY:N	2.69	0.45
3:3:106:TYR:O	3:3:107:TRP:C	2.54	0.45
21:2:1225:SUC:C2	21:2:1225:SUC:C6	2.87	0.45
17:N:7:LEU:O	17:N:8:GLU:HB2	2.16	0.45
16:L:59:ALA:HB2	19:L:1166:CLA:HMA1	1.97	0.45
10:F:115:THR:O	10:F:116:GLN:CB	2.63	0.45
10:F:116:GLN:HA	10:F:118:GLU:OE1	2.16	0.45
1:1:34:ALA:O	1:1:35:ASN:C	2.55	0.45
12:H:77:LEU:HD23	12:H:78:PRO:CD	2.46	0.45
8:D:146:VAL:HG21	8:D:152:GLN:HG3	1.98	0.45
2:2:39:GLU:CA	2:2:40:SER:CB	2.71	0.45
5:A:122:VAL:HG22	5:A:142:GLY:CA	2.46	0.45
19:A:1761:CLA:H202	19:A:1761:CLA:H161	1.61	0.45
5:A:368:LEU:HD12	19:A:1782:CLA:H62	1.98	0.45
5:A:637:ILE:HG12	5:A:637:ILE:H	1.52	0.45
5:A:660:GLN:O	5:A:661:ALA:HB3	2.15	0.45
5:A:669:GLY:H	6:B:445:ALA:CA	2.24	0.45
6:B:103:ALA:HA	6:B:105:THR:O	2.17	0.45
6:B:428:PHE:HE1	19:B:1763:CLA:HMD3	1.80	0.45
23:B:1774:PQN:H192	22:B:1781:BCR:HC8	1.95	0.45
6:B:439:HIS:NE2	6:B:443:MET:SD	2.89	0.45
11:G:57:LEU:CD2	11:G:57:LEU:O	2.64	0.45
17:N:42:PHE:N	17:N:43:PRO:CD	2.58	0.45
14:J:31:ARG:O	14:J:34:PRO:HG3	2.17	0.45
10:F:26:GLN:O	10:F:28:SER:N	2.49	0.45
20:A:7050:LMU:H6'2	20:A:7050:LMU:H1B	1.08	0.45
20:A:7050:LMU:H71	20:A:7050:LMU:H41	1.78	0.45
21:B:8056:SUC:H3'	21:B:8056:SUC:HO2	1.67	0.45
3:3:114:PHE:HD1	19:3:1220:CLA:CHA	2.27	0.45
8:D:132:LEU:HD12	8:D:136:SER:OG	2.17	0.45
19:A:1798:CLA:CED	19:A:1798:CLA:HBA2	2.46	0.45
10:F:102:ARG:NH1	10:F:106:ILE:HD12	2.31	0.45
8:D:31:GLY:CA	16:L:13:PRO:HB3	2.44	0.45
16:L:50:LEU:HD23	16:L:51:LEU:H	1.81	0.45
6:B:221:GLY:C	6:B:223:GLY:N	2.69	0.45
1:1:34:ALA:O	1:1:38:ARG:N	2.40	0.45
2:2:41:LEU:C	2:2:42:ARG:HD3	2.36	0.45
5:A:128:GLY:HA3	6:B:446:PHE:HD2	1.79	0.45
5:A:657:LEU:HD13	19:A:1810:CLA:H93	1.99	0.45
5:A:606:TYR:OH	19:A:1810:CLA:HED3	2.17	0.45
5:A:284:ARG:HG3	5:A:295:TRP:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:377:TYR:CD1	5:A:616:PHE:CE1	3.02	0.45
5:A:551:VAL:HG21	5:A:604:TRP:CZ2	2.51	0.45
23:B:1774:PQN:H2M1	23:B:1774:PQN:H111	1.67	0.45
6:B:319:HIS:O	6:B:320:LYS:O	2.34	0.45
6:B:551:LYS:HG2	6:B:552:ASP:H	1.79	0.45
6:B:561:GLY:HA3	7:C:52:LYS:CB	2.46	0.45
19:4:1205:CLA:CBD	19:4:1205:CLA:HBA2	2.47	0.45
4:4:75:TRP:CD1	19:4:1205:CLA:CHD	2.99	0.45
10:F:24:LYS:HE3	10:F:24:LYS:N	2.24	0.45
12:H:24:TYR:HB3	12:H:25:GLY:H	1.60	0.45
20:A:7009:LMU:O6B	20:A:7009:LMU:H3'	2.17	0.45
6:B:138:GLY:H	6:B:140:ILE:HG12	1.80	0.45
3:3:90:LEU:HD12	3:3:90:LEU:N	2.31	0.45
6:B:15:ASP:OD2	6:B:15:ASP:C	2.55	0.45
19:1:1505:CLA:HAA2	19:1:1505:CLA:HBD	1.97	0.45
6:B:638:LEU:N	6:B:638:LEU:HD22	2.31	0.45
4:4:169:GLN:HE22	19:4:1199:CLA:HHD	1.73	0.45
19:A:1760:CLA:HMC3	19:A:1762:CLA:CED	2.47	0.45
19:A:1795:CLA:HBA1	19:A:1795:CLA:H3A	1.66	0.45
5:A:207:LEU:HD11	5:A:313:ALA:HB1	1.98	0.45
5:A:57:LEU:HD22	5:A:58:HIS:CD2	2.51	0.45
5:A:707:ILE:HG22	5:A:711:HIS:CD2	2.50	0.45
5:A:73:GLU:O	5:A:76:ARG:CA	2.64	0.45
6:B:290:MET:CA	19:B:1752:CLA:HAC2	2.44	0.45
19:B:1738:CLA:CBC	19:B:1758:CLA:CMD	2.95	0.45
19:B:1764:CLA:H3A	19:B:1764:CLA:HBA1	1.66	0.45
19:B:1772:CLA:HHD	23:B:1774:PQN:H18	1.98	0.45
6:B:180:SER:O	6:B:181:GLY:C	2.54	0.45
6:B:336:LEU:CD1	19:B:1755:CLA:CBB	2.95	0.45
6:B:626:LEU:O	6:B:627:ASN:CB	2.64	0.45
8:D:46:TYR:HD2	8:D:46:TYR:N	2.11	0.45
10:F:104:TYR:OH	10:F:121:ILE:HA	2.17	0.45
8:D:75:LEU:HD21	16:L:19:PHE:CE1	2.51	0.45
16:L:161:LEU:CD1	16:L:162:ASP:O	2.63	0.45
10:F:22:LEU:HA	10:F:25:LEU:CD1	2.47	0.45
19:3:1222:CLA:O2D	19:3:1222:CLA:OBD	2.29	0.45
20:R:1056:LMU:H22	20:R:1056:LMU:O2'	2.17	0.45
5:A:260:PRO:HG3	5:A:277:TYR:CZ	2.51	0.45
6:B:513:GLY:O	6:B:516:ASP:OD1	2.34	0.45
14:J:32:PHE:HE2	14:J:33:PHE:CE1	2.35	0.45
2:2:54:TRP:CZ2	2:2:109:ARG:CB	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:84:ILE:HG13	19:3:1212:CLA:O1A	2.15	0.45
19:4:1200:CLA:HAA2	19:4:1200:CLA:CBD	2.46	0.45
19:A:1764:CLA:H111	22:A:1807:BCR:C10	2.46	0.45
19:A:1764:CLA:ND	19:A:1783:CLA:C4	2.79	0.45
19:A:1766:CLA:HBB2	19:A:1769:CLA:HMA3	1.97	0.45
5:A:351:THR:O	19:A:1780:CLA:H201	2.17	0.45
22:A:1804:BCR:C8	22:A:1804:BCR:H321	2.47	0.45
5:A:372:VAL:HG22	19:A:1774:CLA:H41	1.96	0.45
5:A:499:ALA:O	5:A:501:GLY:N	2.38	0.45
5:A:575:LEU:HD12	5:A:575:LEU:H	1.81	0.45
5:A:705:GLU:O	5:A:706:SER:C	2.55	0.45
5:A:693:LEU:HD11	5:A:738:TYR:HD1	1.78	0.45
19:B:1750:CLA:C2	19:B:1755:CLA:H92	2.45	0.45
22:B:1775:BCR:H15C	22:B:1775:BCR:H351	1.77	0.45
6:B:535:VAL:O	6:B:539:LEU:HB2	2.17	0.45
6:B:557:PHE:O	6:B:557:PHE:CD2	2.69	0.45
6:B:353:TYR:CB	6:B:594:TRP:CH2	2.99	0.45
5:A:680:LEU:CD2	6:B:617:MET:HB2	2.46	0.45
6:B:668:ARG:NH1	6:B:672:GLN:HG2	2.31	0.45
10:F:99:TRP:CZ3	10:F:140:ALA:HB2	2.52	0.45
11:G:16:LEU:CA	11:G:68:ILE:HG13	2.45	0.45
22:I:1032:BCR:C39	22:L:1169:BCR:C40	2.94	0.45
22:L:1169:BCR:H341	22:L:1169:BCR:H11C	1.83	0.45
16:L:56:VAL:HG13	19:L:1167:CLA:HED2	1.96	0.45
1:1:57:ILE:C	1:1:57:ILE:CD1	2.29	0.45
19:1:1196:CLA:CBD	19:1:1196:CLA:HAA2	2.44	0.45
20:A:7021:LMU:H6'	20:A:7021:LMU:H12	1.80	0.45
20:A:7004:LMU:H2O2	20:A:7004:LMU:H11	1.74	0.45
8:D:113:HIS:O	8:D:113:HIS:HD2	2.00	0.45
8:D:99:GLN:HG2	8:D:101:TYR:CE2	2.52	0.45
5:A:257:GLN:O	5:A:258:LEU:CB	2.65	0.45
2:2:108:ARG:HD3	2:2:108:ARG:HA	1.75	0.45
19:2:1213:CLA:OBD	19:2:1213:CLA:O2D	2.35	0.45
5:A:401:TRP:CB	19:A:1783:CLA:HMC3	2.47	0.45
19:A:1797:CLA:H41	19:A:1797:CLA:H62	1.45	0.45
5:A:683:HIS:O	19:A:1811:CLA:HAA2	2.17	0.45
5:A:347:TYR:CE1	5:A:417:PHE:CZ	3.04	0.45
5:A:499:ALA:CB	19:A:1790:CLA:O2D	2.64	0.45
5:A:555:ILE:HG12	5:A:555:ILE:H	1.46	0.45
5:A:672:LEU:HD23	5:A:673:SER:H	1.81	0.45
6:B:141:PHE:O	6:B:142:LEU:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:167:TRP:O	6:B:167:TRP:CD2	2.70	0.45
19:B:1757:CLA:H162	19:B:1757:CLA:H202	1.64	0.45
19:B:1759:CLA:H3A	19:B:1759:CLA:HBA2	1.54	0.45
6:B:424:TRP:CH2	19:B:1762:CLA:HAC1	2.52	0.45
6:B:176:ASN:ND2	6:B:291:TYR:O	2.48	0.45
6:B:393:PHE:CE2	6:B:398:TYR:HB2	2.52	0.45
6:B:395:ILE:HG13	6:B:395:ILE:H	1.72	0.45
6:B:535:VAL:CG1	6:B:536:LYS:H	2.30	0.45
8:D:40:ALA:O	8:D:45:PHE:CD2	2.69	0.45
10:F:131:PHE:CE1	21:F:1158:SUC:O3'	2.66	0.45
16:L:162:ASP:C	16:L:162:ASP:OD2	2.54	0.45
17:N:40:CYS:N	17:N:41:LYS:CA	2.79	0.45
17:N:59:PRO:HA	17:N:66:ASP:OD1	2.15	0.45
19:J:1044:CLA:C8	19:J:1044:CLA:C4	2.75	0.45
6:B:369:ALA:C	6:B:725:LEU:HD11	2.36	0.45
12:H:42:THR:HG22	12:H:45:ALA:CB	2.43	0.45
6:B:216:LEU:O	6:B:217:PRO:C	2.54	0.45
3:3:164:PHE:HA	3:3:164:PHE:HD1	1.71	0.45
2:2:209:THR:CG2	2:2:209:THR:O	2.64	0.45
5:A:34:TRP:O	5:A:35:ALA:CB	2.65	0.45
4:4:101:VAL:O	4:4:104:ARG:CD	2.64	0.45
19:4:1200:CLA:HBC2	19:4:1200:CLA:HMC1	0.67	0.45
4:4:30:LEU:CD1	20:4:1212:LMU:C12	2.94	0.45
4:4:164:LEU:O	4:4:166:PHE:N	2.50	0.45
19:A:1771:CLA:O1A	19:A:1771:CLA:C1A	2.63	0.45
19:A:1783:CLA:H18	19:A:1783:CLA:H122	1.98	0.45
19:A:1781:CLA:C4	19:A:1793:CLA:HBA1	2.46	0.45
22:A:1804:BCR:H341	22:A:1804:BCR:H11C	1.71	0.45
19:A:1783:CLA:C20	22:A:1807:BCR:C15	2.93	0.45
5:A:430:ASP:C	5:A:432:LEU:H	2.19	0.45
5:A:472:ARG:O	5:A:474:GLN:CB	2.65	0.45
6:B:199:ILE:N	6:B:200:PRO:HD2	2.31	0.45
6:B:347:LEU:HD21	6:B:351:HIS:CE1	2.40	0.45
6:B:57:ILE:HG12	19:B:1738:CLA:HMC2	1.98	0.45
8:D:139:LYS:HG2	8:D:141:VAL:HG22	1.97	0.45
11:G:33:LYS:O	11:G:34:GLN:HG2	2.15	0.45
17:N:62:SER:HB3	17:N:66:ASP:N	2.31	0.45
17:N:78:GLY:O	17:N:82:PHE:CE2	2.70	0.45
10:F:23:LYS:HB3	10:F:24:LYS:NZ	2.19	0.45
20:A:7039:LMU:H4B	20:A:7039:LMU:H1B	1.57	0.45
21:B:8062:SUC:O2	21:B:8062:SUC:O4	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:102:ILE:HG13	19:2:1223:CLA:CMD	2.43	0.45
2:2:127:ASN:HD21	14:J:7:TYR:CA	2.18	0.45
2:2:169:LEU:HD11	19:2:1215:CLA:C1C	2.47	0.45
19:4:1196:CLA:H41	19:4:1196:CLA:H62	1.58	0.45
19:4:1198:CLA:HBC3	19:4:1198:CLA:CMC	2.46	0.45
4:4:169:GLN:CA	4:4:169:GLN:NE2	2.68	0.45
5:A:163:GLN:C	5:A:165:TYR:H	2.19	0.45
5:A:436:LEU:C	5:A:438:HIS:O	2.55	0.45
5:A:438:HIS:NE2	19:A:1786:CLA:ND	2.65	0.45
5:A:461:TYR:CD2	5:A:649:ILE:HD12	2.51	0.45
5:A:83:PHE:HA	5:A:86:LEU:CD2	2.47	0.45
19:B:1748:CLA:NA	19:B:1748:CLA:H12	2.31	0.45
19:B:1761:CLA:CAA	19:B:1761:CLA:CED	2.89	0.45
6:B:355:LEU:CD2	19:B:1757:CLA:HMC2	2.46	0.45
6:B:603:ARG:HB3	6:B:734:GLY:H	1.81	0.45
6:B:77:TRP:O	6:B:81:PRO:HG3	2.17	0.45
6:B:564:ARG:NH2	7:C:66:ARG:HH12	2.15	0.45
9:E:46:PHE:CD2	9:E:47:LYS:N	2.85	0.45
9:E:62:ARG:O	9:E:83:ALA:CB	2.65	0.45
10:F:84:ILE:HD13	10:F:84:ILE:N	2.32	0.45
1:1:24:PHE:CB	6:B:314:ARG:NH2	2.70	0.45
3:3:94:ARG:HG2	3:3:97:PHE:CD1	2.52	0.45
17:N:38:GLY:HA3	17:N:46:PHE:HD1	1.80	0.45
10:F:51:LYS:O	10:F:53:PHE:N	2.45	0.45
19:4:4014:CLA:HBC3	19:4:4014:CLA:CMC	2.12	0.45
15:K:52:PRO:HB2	15:K:53:ALA:H	1.52	0.45
19:1:1149:CLA:HAA1	19:1:1149:CLA:O1D	2.14	0.45
12:H:58:ILE:CD1	16:L:97:MET:SD	2.89	0.45
5:A:70:ASP:O	5:A:71:LEU:C	2.54	0.45
2:2:103:GLY:O	2:2:104:TRP:O	2.35	0.45
4:4:103:ILE:HB	19:4:1197:CLA:CMD	2.46	0.45
19:4:1204:CLA:C2D	19:4:1207:CLA:C2A	2.95	0.45
4:4:89:THR:OG1	4:4:92:VAL:HB	2.16	0.45
5:A:164:LEU:HA	5:A:167:THR:CG2	2.43	0.45
5:A:515:TRP:CZ2	19:A:1782:CLA:HMC3	2.52	0.45
19:A:1787:CLA:H72	19:A:1800:CLA:CBA	2.47	0.45
19:A:1789:CLA:H41	19:A:1789:CLA:H61	1.62	0.45
22:A:1806:BCR:H11C	22:A:1806:BCR:H341	1.71	0.45
5:A:308:ILE:HG21	19:A:1772:CLA:CMC	2.47	0.45
5:A:665:ILE:HD12	5:A:666:GLN:N	2.31	0.45
19:B:1744:CLA:CMC	19:B:1744:CLA:HBC3	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1756:CLA:CAB	19:B:1770:CLA:HMA1	2.47	0.45
6:B:700:LEU:N	23:B:1774:PQN:O4	2.43	0.45
6:B:323:TYR:O	6:B:327:ASN:HB2	2.17	0.45
6:B:460:ALA:O	6:B:463:ILE:N	2.50	0.45
9:E:60:LYS:HG3	9:E:61:THR:OG1	2.17	0.45
14:J:26:LEU:H	14:J:28:GLU:H	1.65	0.45
16:L:65:VAL:C	16:L:69:VAL:HG22	2.36	0.45
1:1:25:ASP:O	1:1:26:PRO:C	2.54	0.45
19:1:1188:CLA:H8	19:1:1188:CLA:H42	1.70	0.45
17:N:62:SER:OG	17:N:66:ASP:HA	2.17	0.45
19:1:1146:CLA:CGA	19:1:1146:CLA:C3A	2.93	0.45
15:K:51:ASP:OD1	15:K:55:PHE:CB	2.65	0.45
6:B:218:TYR:HB3	6:B:219:PRO:HD2	1.99	0.45
5:A:539:PHE:CD2	5:A:539:PHE:O	2.65	0.45
6:B:42:LEU:O	6:B:43:TYR:O	2.35	0.45
20:L:1171:LMU:H52	20:L:1171:LMU:H82	1.78	0.45
20:L:1171:LMU:O6'	20:L:1171:LMU:H81	2.16	0.45
10:F:152:ASN:N	10:F:152:ASN:HD22	2.12	0.45
2:2:72:GLY:C	2:2:74:LEU:N	2.67	0.45
4:4:93:ILE:HG22	4:4:94:GLU:CA	2.45	0.45
5:A:113:PRO:O	5:A:115:HIS:CD2	2.70	0.45
5:A:163:GLN:O	5:A:165:TYR:N	2.50	0.45
19:A:1764:CLA:HBB2	19:A:1765:CLA:C3D	2.47	0.45
19:A:1774:CLA:HBA2	19:A:1774:CLA:H3A	1.70	0.45
5:A:488:PHE:CZ	5:A:533:PRO:HB3	2.52	0.45
5:A:53:TRP:HA	5:A:56:ASN:ND2	2.32	0.45
5:A:98:PHE:O	5:A:99:HIS:CD2	2.70	0.45
19:B:1738:CLA:CBC	19:B:1758:CLA:HMD3	2.47	0.45
6:B:462:TRP:CZ3	19:B:1765:CLA:HBC1	2.51	0.45
22:B:1781:BCR:C38	22:B:1781:BCR:C23	2.74	0.45
6:B:199:ILE:HG22	6:B:203:ARG:CZ	2.47	0.45
6:B:47:PHE:CZ	6:B:51:PHE:HE1	2.35	0.45
6:B:710:LEU:O	6:B:712:HIS:N	2.50	0.45
6:B:718:ILE:HD11	19:B:1758:CLA:CHC	2.46	0.45
6:B:719:PHE:CE2	19:B:1758:CLA:H72	2.52	0.45
6:B:80:ASP:HA	6:B:81:PRO:HD3	1.57	0.45
5:A:584:PRO:CB	7:C:67:VAL:HB	2.47	0.45
8:D:139:LYS:NZ	9:E:41:ARG:NH1	2.64	0.45
4:4:193:ILE:CG2	14:J:42:PHE:HD1	2.30	0.45
20:A:7010:LMU:H22	20:A:7010:LMU:H51	1.40	0.45
19:3:3011:CLA:H62	19:3:3011:CLA:H41	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:12:ILE:HD12	7:C:12:ILE:H	1.80	0.45
2:2:153:PRO:HB2	2:2:157:LYS:NZ	2.32	0.45
6:B:679:ALA:O	6:B:683:GLU:OE2	2.35	0.45
6:B:509:PHE:N	6:B:509:PHE:HD2	2.15	0.45
2:2:115:ASN:HD22	2:2:115:ASN:N	2.13	0.45
2:2:168:ARG:NH2	2:2:171:MET:CB	2.63	0.44
2:2:91:THR:C	2:2:94:LEU:CB	2.86	0.44
2:2:93:THR:HA	2:2:96:ILE:HG12	1.98	0.44
5:A:173:VAL:O	5:A:175:ALA:O	2.35	0.44
5:A:365:LEU:HD22	19:A:1761:CLA:HED3	1.93	0.44
19:A:1778:CLA:HAA2	19:A:1778:CLA:CGD	2.48	0.44
5:A:451:ILE:HD13	19:A:1788:CLA:HED1	1.97	0.44
5:A:615:HIS:CE1	19:A:1792:CLA:CBC	2.98	0.44
22:A:1803:BCR:H351	22:A:1803:BCR:H15C	1.78	0.44
5:A:363:ALA:O	5:A:367:SER:CB	2.65	0.44
5:A:396:PHE:CE2	5:A:616:PHE:CB	2.93	0.44
19:B:1736:CLA:H2A	19:B:1736:CLA:O1D	2.17	0.44
19:B:1738:CLA:H3A	19:B:1738:CLA:HBA1	1.70	0.44
6:B:326:ILE:HG23	19:B:1755:CLA:HBC3	1.99	0.44
6:B:355:LEU:HD21	19:B:1757:CLA:HMC2	1.99	0.44
6:B:719:PHE:CE2	19:B:1758:CLA:C7	3.01	0.44
19:B:1772:CLA:C2	23:B:1774:PQN:H251	2.47	0.44
19:B:1788:CLA:H162	19:B:1788:CLA:H202	1.71	0.44
6:B:17:THR:OG1	6:B:18:THR:N	2.50	0.44
6:B:288:GLY:O	6:B:289:LEU:HB2	2.17	0.44
6:B:347:LEU:HD13	6:B:351:HIS:ND1	2.30	0.44
6:B:544:SER:N	6:B:547:MET:O	2.47	0.44
7:C:5:VAL:CA	7:C:65:VAL:HG22	2.45	0.44
9:E:36:VAL:CG2	9:E:52:VAL:CG2	2.94	0.44
3:3:93:PHE:HD2	3:3:95:THR:N	2.12	0.44
17:N:53:ALA:O	17:N:54:LYS:CG	2.65	0.44
19:1:1148:CLA:H72	19:1:1148:CLA:HED3	1.98	0.44
19:1:1014:CLA:H12	19:1:1014:CLA:HBA2	1.60	0.44
19:4:1201:CLA:HBC3	19:4:1201:CLA:CHD	2.47	0.44
3:3:194:ILE:HG13	19:3:1214:CLA:HMC1	1.90	0.44
20:A:7033:LMU:H61	20:A:7033:LMU:H31	1.59	0.44
15:K:8:ASN:C	15:K:9:LEU:HD23	2.30	0.44
3:3:111:TYR:HB2	3:3:112:THR:H	1.68	0.44
10:F:151:ASP:O	10:F:154:PHE:N	2.51	0.44
4:4:61:PRO:HA	4:4:65:THR:O	2.17	0.44
16:L:107:PHE:CB	16:L:109:GLU:OE1	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:ARG:NH2	1:1:139:LYS:HB2	2.31	0.44
10:F:152:ASN:N	10:F:152:ASN:ND2	2.64	0.44
10:F:89:LEU:HA	10:F:89:LEU:HD12	1.87	0.44
4:4:101:VAL:HG13	4:4:101:VAL:O	2.12	0.44
19:A:1763:CLA:HHD	19:A:1763:CLA:HBC2	1.98	0.44
5:A:187:HIS:CE1	19:A:1767:CLA:CHA	2.97	0.44
19:A:1781:CLA:HMB3	22:A:1805:BCR:C19	2.47	0.44
19:A:1788:CLA:H192	19:B:1771:CLA:HMB2	1.99	0.44
19:A:1788:CLA:HED1	19:A:1799:CLA:O1A	2.16	0.44
19:A:1810:CLA:H122	19:A:1810:CLA:H162	1.68	0.44
5:A:370:ILE:CG2	5:A:400:MET:CA	2.85	0.44
5:A:567:ARG:HH11	8:D:34:GLY:C	2.20	0.44
5:A:596:ASP:HA	5:A:599:PHE:CB	2.39	0.44
19:B:1742:CLA:H8	19:B:1742:CLA:H51	1.58	0.44
19:B:1745:CLA:H143	19:B:1745:CLA:H162	1.72	0.44
6:B:467:HIS:CD2	19:B:1765:CLA:CGD	3.00	0.44
6:B:414:HIS:O	6:B:414:HIS:CD2	2.69	0.44
6:B:661:PHE:HB3	19:B:1788:CLA:HMC1	1.97	0.44
6:B:672:GLN:HE22	6:B:698:VAL:HA	1.83	0.44
11:G:62:ASP:CB	11:G:63:PRO:HD3	2.42	0.44
14:J:2:ARG:HB3	14:J:7:TYR:CE1	2.53	0.44
16:L:127:PRO:O	16:L:128:ASP:O	2.36	0.44
20:A:7042:LMU:H61	20:A:7042:LMU:H31	1.49	0.44
19:1:1188:CLA:HHD	19:1:1188:CLA:HBC2	1.98	0.44
20:N:1086:LMU:H91	20:N:1086:LMU:C5	2.33	0.44
17:N:45:ASN:O	17:N:46:PHE:C	2.50	0.44
20:A:7048:LMU:C2B	20:A:7048:LMU:O6'	2.65	0.44
7:C:9:ASP:HB2	25:C:1083:SF4:S2	2.57	0.44
19:1:1308:CLA:O1A	19:1:1308:CLA:CGD	2.65	0.44
8:D:74:LEU:O	8:D:74:LEU:HG	2.16	0.44
5:A:336:GLY:HA3	19:A:1798:CLA:CMC	2.48	0.44
5:A:349:ILE:HD13	5:A:422:TYR:HB3	1.99	0.44
1:1:181:LEU:HD13	19:1:1189:CLA:HAC1	1.99	0.44
19:L:1166:CLA:HBA2	19:L:1166:CLA:H3A	1.54	0.44
14:J:32:PHE:CE2	14:J:33:PHE:CZ	3.03	0.44
19:2:1213:CLA:H42	19:2:1213:CLA:CHD	2.48	0.44
4:4:152:LYS:HA	4:4:154:ILE:CG1	2.48	0.44
5:A:144:GLN:HG3	5:A:145:ILE:H	1.81	0.44
5:A:550:HIS:CD2	19:A:1794:CLA:HMA3	2.52	0.44
5:A:202:MET:HB3	19:A:1780:CLA:HMD3	1.99	0.44
19:3:1212:CLA:HMA3	5:A:246:HIS:HE1	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:581:CYS:HB2	5:A:590:CYS:O	2.16	0.44
5:A:729:GLN:O	5:A:732:ALA:HB3	2.17	0.44
6:B:145:LEU:HA	6:B:145:LEU:HD22	1.82	0.44
19:B:1756:CLA:C2	19:B:1769:CLA:HBA2	2.47	0.44
22:B:1778:BCR:H15C	22:B:1778:BCR:H351	1.80	0.44
6:B:179:LEU:O	6:B:284:PHE:O	2.35	0.44
6:B:190:TRP:O	6:B:191:ALA:C	2.56	0.44
6:B:353:TYR:CD1	6:B:594:TRP:HZ3	2.29	0.44
6:B:623:TYR:H	6:B:626:LEU:HB3	1.81	0.44
8:D:41:GLN:CD	8:D:41:GLN:C	2.76	0.44
9:E:65:VAL:HG23	9:E:66:VAL:O	2.17	0.44
3:3:49:ILE:CG1	3:3:52:LYS:CB	2.94	0.44
20:A:7032:LMU:H81	20:A:7032:LMU:H52	1.36	0.44
3:3:86:GLN:HB2	3:3:88:THR:CA	2.48	0.44
19:3:1222:CLA:H12	19:3:1222:CLA:H51	1.75	0.44
20:A:7039:LMU:H82	20:A:7039:LMU:H112	1.37	0.44
17:N:22:LEU:HD23	17:N:22:LEU:O	2.17	0.44
12:H:40:PHE:O	12:H:41:GLU:C	2.56	0.44
10:F:33:ALA:C	10:F:35:ASP:H	2.20	0.44
5:A:586:ARG:H	7:C:49:VAL:HG22	1.83	0.44
5:A:479:ASP:HA	5:A:536:THR:CG2	2.45	0.44
1:1:54:VAL:C	1:1:56:GLY:N	2.71	0.44
15:K:35:THR:HG23	15:K:36:ALA:H	1.82	0.44
1:1:183:ASP:CB	1:1:184:PRO:HD2	2.47	0.44
2:2:97:VAL:C	2:2:100:VAL:HG13	2.37	0.44
2:2:116:PRO:O	2:2:135:VAL:O	2.36	0.44
2:2:54:TRP:CZ2	2:2:109:ARG:HD3	2.44	0.44
2:2:98:GLU:OE1	19:2:1223:CLA:C4C	2.65	0.44
4:4:104:ARG:HD2	19:4:1208:CLA:C1C	2.36	0.44
4:4:139:ASN:HA	4:4:139:ASN:HD22	1.64	0.44
4:4:146:THR:HA	4:4:147:LEU:HA	1.62	0.44
19:A:1780:CLA:HMD2	19:A:1780:CLA:C14	2.34	0.44
5:A:500:PRO:HA	5:A:504:ALA:HB1	1.98	0.44
5:A:665:ILE:HD13	6:B:621:ARG:HG3	1.99	0.44
5:A:76:ARG:CZ	5:A:192:LYS:CG	2.71	0.44
19:B:1739:CLA:HMB3	19:I:1031:CLA:HMA1	1.98	0.44
6:B:343:VAL:HG12	19:B:1757:CLA:H2	2.00	0.44
19:B:1738:CLA:CBB	19:B:1759:CLA:HHC	2.47	0.44
6:B:194:LEU:O	6:B:199:ILE:HG13	2.17	0.44
6:B:290:MET:HG3	19:B:1752:CLA:CMC	2.47	0.44
6:B:662:MET:O	6:B:664:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:726:ILE:C	6:B:728:SER:N	2.70	0.44
9:E:65:VAL:CG2	9:E:66:VAL:O	2.65	0.44
5:A:130:GLU:HG3	10:F:45:THR:HG21	1.99	0.44
10:F:62:LEU:HG	10:F:72:ILE:HD11	1.96	0.44
14:J:2:ARG:HH22	14:J:8:LEU:HD22	1.81	0.44
19:A:1799:CLA:H93	22:L:1169:BCR:H321	1.98	0.44
18:R:34:UNK:C	18:R:36:UNK:O	2.66	0.44
3:3:50:GLU:OE1	3:3:54:LEU:HB2	2.17	0.44
7:C:18:VAL:HB	7:C:58:CYS:HB2	2.00	0.44
20:A:7032:LMU:C1B	20:A:7032:LMU:C1	2.95	0.44
20:A:7014:LMU:H1B	20:A:7014:LMU:H3'	1.30	0.44
15:K:51:ASP:OD1	15:K:55:PHE:HB2	2.17	0.44
20:A:7030:LMU:H42	20:A:7030:LMU:H11	1.76	0.44
6:B:67:HIS:CD2	6:B:71:GLN:HE22	2.35	0.44
12:H:45:ALA:CB	12:H:46:PRO:CD	2.88	0.44
6:B:158:GLN:O	6:B:159:PRO:O	2.36	0.44
12:H:75:ASP:HB3	12:H:77:LEU:HG	2.00	0.44
8:D:152:GLN:HA	8:D:153:PRO:HD2	1.72	0.44
19:3:1212:CLA:CBC	19:A:1770:CLA:C1D	2.95	0.44
5:A:105:ASN:HB3	5:A:150:PHE:HZ	1.83	0.44
19:A:1773:CLA:C4C	19:A:1773:CLA:H62	2.47	0.44
19:A:1793:CLA:C1B	19:A:1794:CLA:HMD3	2.47	0.44
5:A:363:ALA:N	5:A:410:ALA:CB	2.81	0.44
5:A:432:LEU:O	5:A:435:VAL:N	2.50	0.44
5:A:467:MET:HE1	5:A:475:ASP:C	2.38	0.44
5:A:655:ASP:O	5:A:659:ALA:HB3	2.17	0.44
5:A:664:VAL:HG11	5:A:749:PHE:HA	1.99	0.44
5:A:681:GLY:O	5:A:682:ALA:HB3	2.17	0.44
19:B:1736:CLA:H3A	19:B:1736:CLA:HBA2	1.53	0.44
6:B:493:TRP:HH2	19:B:1748:CLA:H122	1.82	0.44
23:B:1774:PQN:C2M	23:B:1774:PQN:H142	2.47	0.44
6:B:693:TRP:CZ2	6:B:697:PRO:HG3	2.52	0.44
7:C:53:ARG:O	7:C:55:GLU:O	2.36	0.44
22:B:1780:BCR:C5	19:F:1156:CLA:HMA1	2.47	0.44
19:F:1157:CLA:OBD	19:F:1157:CLA:O2D	2.31	0.44
5:A:251:ASN:O	5:A:253:ASP:HB3	2.17	0.44
17:N:45:ASN:HD21	17:N:53:ALA:C	2.02	0.44
18:R:50:UNK:HA	18:R:51:UNK:HA	1.69	0.44
20:A:7038:LMU:O6'	20:A:7038:LMU:O1B	2.30	0.44
2:2:188:PRO:HB2	2:2:189:ILE:HD13	1.98	0.44
5:A:631:GLN:HG2	5:A:633:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:63:SER:O	12:H:67:TYR:HB3	2.16	0.44
6:B:32:GLU:N	6:B:42:LEU:HD13	2.33	0.44
12:H:11:LEU:HA	12:H:11:LEU:HD22	1.86	0.44
8:D:21:ASP:HB3	8:D:22:PRO:HD3	1.99	0.44
2:2:63:PHE:CD1	2:2:64:ILE:N	2.86	0.44
2:2:95:PHE:O	2:2:99:LEU:HD12	2.17	0.44
4:4:142:ASN:O	4:4:143:PHE:CD2	2.70	0.44
5:A:179:LEU:HD13	5:A:179:LEU:O	2.17	0.44
5:A:700:TRP:CE2	23:A:1801:PQN:H2M3	2.52	0.44
5:A:223:VAL:CG1	5:A:224:HIS:H	2.30	0.44
5:A:154:ARG:NH2	5:A:233:LEU:CD1	2.80	0.44
5:A:334:HIS:HD2	19:A:1777:CLA:C1B	2.30	0.44
19:B:1768:CLA:HAA1	19:B:1769:CLA:HAA2	1.99	0.44
19:B:1769:CLA:C8	19:B:1769:CLA:HBB2	2.42	0.44
6:B:182:LEU:HG	6:B:183:PHE:N	2.32	0.44
6:B:309:ILE:HA	6:B:310:PRO:HD3	1.81	0.44
6:B:385:GLY:N	19:B:1760:CLA:HBC3	2.33	0.44
6:B:707:LEU:CD1	24:B:1784:LMG:H301	2.48	0.44
7:C:60:THR:HG21	7:C:64:SER:HB3	1.99	0.44
16:L:95:LEU:HA	16:L:98:CYS:CB	2.42	0.44
17:N:72:LYS:HA	17:N:72:LYS:HD2	1.57	0.44
2:2:178:TRP:N	2:2:178:TRP:CD1	2.84	0.44
18:R:38:UNK:O	18:R:39:UNK:C	2.61	0.44
3:3:86:GLN:CB	3:3:88:THR:H	2.31	0.44
19:3:1222:CLA:H3A	19:3:1222:CLA:HBA2	1.61	0.44
6:B:247:THR:HG22	6:B:250:ALA:HB3	2.00	0.44
19:2:1217:CLA:HAC2	19:2:1217:CLA:HHD	1.82	0.44
18:R:5:UNK:O	18:R:6:UNK:CB	2.65	0.44
6:B:332:PHE:HE1	6:B:408:LEU:CD2	2.30	0.44
5:A:569:ILE:HG12	5:A:586:ARG:NH1	2.33	0.44
5:A:539:PHE:HE2	5:A:543:HIS:HE1	1.66	0.44
15:K:47:ILE:HG23	15:K:48:GLN:N	2.28	0.44
2:2:70:LYS:CG	2:2:73:ILE:HG13	2.33	0.44
3:3:84:ILE:N	19:3:1212:CLA:C3	2.65	0.44
4:4:107:GLN:HA	19:4:1196:CLA:C3A	2.40	0.44
4:4:122:LYS:HG2	4:4:150:LYS:HE2	1.36	0.44
4:4:94:GLU:C	4:4:95:PHE:CD1	2.91	0.44
19:A:1765:CLA:HBC3	19:A:1765:CLA:CMC	2.48	0.44
19:A:1786:CLA:HMB2	19:A:1787:CLA:C4D	2.48	0.44
5:A:79:PHE:CD2	5:A:185:HIS:CD2	2.98	0.44
5:A:306:ILE:O	5:A:309:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:400:MET:HG3	5:A:609:ILE:HG23	2.00	0.44
5:A:541:VAL:O	5:A:544:ILE:HG22	2.17	0.44
5:A:650:ASN:C	5:A:652:TRP:N	2.69	0.44
6:B:167:TRP:CD1	11:G:41:MET:CE	3.01	0.44
6:B:378:ILE:H	6:B:381:PHE:HD1	1.66	0.44
6:B:447:GLY:C	6:B:449:PRO:HD3	2.37	0.44
11:G:28:ARG:NH2	11:G:28:ARG:CG	2.72	0.44
6:B:167:TRP:CB	11:G:41:MET:CE	2.90	0.44
16:L:66:GLY:HA3	19:L:1168:CLA:C4B	2.45	0.44
1:1:27:LEU:HD13	1:1:28:GLY:H	1.83	0.44
19:1:1188:CLA:C2	19:1:1188:CLA:HBA2	2.47	0.44
17:N:84:LYS:HA	17:N:85:TRP:HA	1.46	0.44
20:A:7016:LMU:H42	20:A:7016:LMU:H72	1.51	0.44
11:G:88:THR:HG23	11:G:91:ASN:O	2.17	0.44
1:1:63:LEU:HB2	1:1:65:TYR:N	2.32	0.44
3:3:111:TYR:HB2	3:3:112:THR:HG22	2.00	0.44
3:3:112:THR:HG1	3:3:113:LEU:H	1.57	0.44
14:J:10:VAL:CG2	14:J:14:LEU:HD12	2.48	0.44
10:F:61:LEU:HD23	10:F:69:PRO:HB3	1.96	0.44
9:E:73:ASN:ND2	9:E:78:SER:HB2	2.33	0.44
9:E:69:PHE:HD2	9:E:71:LYS:H	1.61	0.44
8:D:94:TYR:O	8:D:95:LYS:NZ	2.33	0.44
10:F:13:GLN:HG3	10:F:66:ASP:H	1.83	0.44
15:K:27:ALA:HB1	15:K:28:PRO:HD3	1.96	0.44
5:A:570:PRO:C	5:A:572:LYS:H	2.21	0.44
6:B:341:LEU:O	6:B:345:THR:OG1	2.17	0.44
4:4:149:ALA:C	4:4:151:GLU:HG3	2.38	0.44
4:4:151:GLU:CA	4:4:154:ILE:H	2.27	0.44
5:A:131:ILE:HG21	6:B:446:PHE:HA	1.99	0.44
5:A:143:ILE:HG12	19:A:1764:CLA:HBC2	2.00	0.44
22:A:1805:BCR:H341	22:A:1805:BCR:H11C	1.70	0.44
5:A:212:GLY:O	5:A:214:GLY:N	2.51	0.44
5:A:390:ALA:HA	5:A:393:LEU:HD21	1.97	0.44
5:A:547:PHE:CD1	5:A:547:PHE:C	2.88	0.44
5:A:591:GLN:HA	5:A:591:GLN:NE2	2.25	0.44
6:B:375:HIS:CE1	19:B:1759:CLA:NC	2.77	0.44
6:B:289:LEU:CD2	22:B:1775:BCR:H352	2.45	0.44
6:B:590:VAL:O	6:B:593:TYR:HB3	2.18	0.44
6:B:594:TRP:HD1	6:B:595:HIS:N	2.15	0.44
7:C:62:PHE:CE2	9:E:42:GLU:CD	2.83	0.44
7:C:77:MET:C	7:C:79:LEU:N	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1743:CLA:O2D	11:G:39:ASN:ND2	2.50	0.44
4:4:75:TRP:HB2	19:4:1205:CLA:CMD	2.44	0.44
20:N:1086:LMU:C3	20:N:1086:LMU:C6'	2.95	0.44
17:N:62:SER:CB	17:N:66:ASP:HA	2.48	0.44
19:1:1148:CLA:C2A	19:1:1148:CLA:CGD	2.86	0.44
7:C:58:CYS:HA	7:C:59:PRO:HD2	1.66	0.44
5:A:316:MET:CA	5:A:317:TYR:CB	2.94	0.44
19:1:1149:CLA:CBC	19:1:1149:CLA:CMC	2.80	0.44
17:N:32:ALA:CB	17:N:35:VAL:HA	2.47	0.44
8:D:29:PHE:HA	8:D:66:ALA:HB2	1.99	0.44
6:B:5:ILE:CB	6:B:6:PRO:CD	2.85	0.44
6:B:242:HIS:CE1	6:B:244:PHE:HA	2.53	0.44
6:B:680:TRP:O	6:B:681:ALA:O	2.36	0.44
2:2:168:ARG:HH21	2:2:171:MET:CG	2.31	0.44
4:4:156:ASN:N	4:4:156:ASN:OD1	2.51	0.44
4:4:82:GLU:O	4:4:83:TYR:HD1	2.01	0.44
19:A:1776:CLA:HMB2	19:A:1780:CLA:HMA3	1.99	0.44
19:A:1764:CLA:H161	19:A:1785:CLA:C20	2.48	0.44
5:A:462:ILE:HD13	19:B:1787:CLA:H93	2.00	0.44
5:A:682:ALA:HA	5:A:685:VAL:HG12	1.99	0.44
5:A:714:LEU:HB2	5:A:716:VAL:HG13	1.99	0.44
5:A:86:LEU:HA	5:A:89:ILE:HD12	1.99	0.44
6:B:365:PHE:HB3	6:B:602:TRP:CZ2	2.52	0.44
6:B:434:LEU:O	6:B:438:VAL:HG13	2.18	0.44
6:B:74:PHE:C	6:B:76:ALA:N	2.70	0.44
8:D:79:ARG:H	8:D:82:GLN:HE21	1.63	0.44
11:G:46:ALA:C	11:G:48:ASP:CB	2.80	0.44
11:G:60:SER:O	11:G:62:ASP:N	2.50	0.44
16:L:64:LEU:CD2	16:L:91:LEU:HD22	2.48	0.44
17:N:42:PHE:CD1	17:N:43:PRO:CD	3.01	0.44
21:B:8055:SUC:O2'	21:B:8055:SUC:O5	2.30	0.44
10:F:47:GLU:N	10:F:50:LYS:HB2	2.33	0.44
20:A:7032:LMU:C6B	20:A:7032:LMU:H22	2.43	0.44
6:B:120:VAL:C	6:B:123:TRP:HD1	2.20	0.44
8:D:113:HIS:O	8:D:113:HIS:CD2	2.70	0.44
6:B:454:LEU:HD13	10:F:69:PRO:O	2.14	0.44
8:D:126:GLY:C	8:D:127:ARG:CG	2.85	0.44
5:A:568:LEU:HD21	5:A:586:ARG:HB3	1.99	0.44
16:L:159:TYR:O	16:L:159:TYR:CG	2.71	0.44
6:B:154:TRP:CD1	6:B:154:TRP:C	2.91	0.44
19:3:3008:CLA:CBD	19:3:3008:CLA:HAA2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:673:GLU:O	6:B:676:GLU:HB2	2.18	0.44
2:2:69:THR:O	2:2:70:LYS:CD	2.66	0.43
5:A:113:PRO:C	5:A:115:HIS:N	2.69	0.43
19:A:1796:CLA:NC	19:A:1796:CLA:H41	2.33	0.43
5:A:222:GLN:O	5:A:227:LEU:HD12	2.18	0.43
5:A:343:HIS:O	5:A:346:LEU:HB2	2.18	0.43
5:A:379:MET:HE3	19:A:1773:CLA:HED2	2.00	0.43
5:A:42:ARG:O	5:A:44:ILE:HG13	2.18	0.43
5:A:458:PHE:C	5:A:460:LEU:N	2.71	0.43
19:B:1737:CLA:HMC3	19:B:1760:CLA:H3A	1.99	0.43
19:B:1769:CLA:HAA1	19:B:1769:CLA:HBD	1.99	0.43
6:B:289:LEU:CD2	19:B:1751:CLA:C1A	2.96	0.43
6:B:583:MET:CE	6:B:583:MET:O	2.66	0.43
7:C:55:GLU:HG3	7:C:60:THR:HG22	2.00	0.43
9:E:37:LYS:CB	9:E:49:VAL:HG22	2.47	0.43
3:3:132:TRP:CE3	3:3:155:GLU:HG2	2.26	0.43
17:N:69:CYS:O	17:N:72:LYS:HD2	2.17	0.43
20:A:7051:LMU:C1B	20:A:7051:LMU:O6B	2.66	0.43
8:D:48:ILE:HA	8:D:100:PHE:HB3	1.99	0.43
2:2:186:THR:O	2:2:188:PRO:O	2.36	0.43
3:3:199:VAL:HG22	19:3:1216:CLA:C4C	2.48	0.43
17:N:25:THR:HG22	17:N:26:GLY:N	2.33	0.43
4:4:107:GLN:HA	19:4:1196:CLA:H2A	2.00	0.43
4:4:169:GLN:CG	19:4:1199:CLA:CAC	2.89	0.43
19:A:1773:CLA:HBA2	19:A:1773:CLA:H3A	1.24	0.43
19:A:1776:CLA:HBA1	19:A:1780:CLA:CBB	2.48	0.43
5:A:203:LEU:O	5:A:207:LEU:HD23	2.17	0.43
5:A:219:ALA:O	5:A:222:GLN:N	2.47	0.43
5:A:310:PHE:H	5:A:313:ALA:CB	2.31	0.43
5:A:588:GLY:N	6:B:668:ARG:CD	2.77	0.43
5:A:412:ALA:CB	5:A:598:VAL:HG11	2.30	0.43
5:A:651:GLY:O	5:A:655:ASP:HB2	2.18	0.43
5:A:680:LEU:HB3	19:A:1811:CLA:C1	2.48	0.43
19:B:1741:CLA:CHD	22:B:1782:BCR:C34	2.95	0.43
19:B:1745:CLA:HBA2	19:B:1745:CLA:H3A	1.58	0.43
19:B:1752:CLA:HBA2	19:B:1753:CLA:O1A	2.17	0.43
6:B:693:TRP:NE1	19:B:1771:CLA:CHD	2.81	0.43
6:B:269:TRP:HA	6:B:269:TRP:CE3	2.53	0.43
6:B:457:PRO:O	6:B:460:ALA:HB3	2.19	0.43
5:A:588:GLY:HA3	6:B:668:ARG:HB3	2.00	0.43
11:G:50:ARG:HB2	11:G:51:ALA:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:25:PHE:CE2	13:I:28:VAL:HG21	2.53	0.43
20:A:7037:LMU:H12	20:A:7037:LMU:H41	1.44	0.43
6:B:330:ILE:HA	6:B:333:GLN:NE2	2.33	0.43
20:R:1056:LMU:H62	20:R:1056:LMU:H32	1.69	0.43
8:D:133:ASN:C	8:D:134:MET:SD	2.92	0.43
15:K:24:PHE:CD1	15:K:52:PRO:CG	2.89	0.43
9:E:44:TYR:HD2	9:E:45:TRP:HE3	1.65	0.43
6:B:473:GLY:O	6:B:474:PHE:HB3	2.19	0.43
5:A:536:THR:HA	5:A:539:PHE:HB2	2.00	0.43
16:L:43:TYR:O	16:L:44:ARG:CB	2.62	0.43
17:N:25:THR:HG22	17:N:26:GLY:H	1.83	0.43
1:I:168:TYR:N	1:I:169:PRO:HD3	2.33	0.43
8:D:151:LYS:HB3	8:D:151:LYS:NZ	2.32	0.43
2:2:99:LEU:HB3	2:2:102:ILE:HB	1.99	0.43
2:2:69:THR:O	2:2:70:LYS:CB	2.66	0.43
2:2:90:ASP:HB3	2:2:94:LEU:HB2	1.99	0.43
19:A:1783:CLA:C11	22:A:1807:BCR:C35	2.96	0.43
19:A:1797:CLA:CAA	19:A:1797:CLA:CGD	2.96	0.43
5:A:388:ASP:O	5:A:390:ALA:N	2.51	0.43
5:A:58:HIS:CE1	19:A:1759:CLA:C4D	3.01	0.43
19:B:1758:CLA:H193	19:B:1758:CLA:H161	1.88	0.43
22:B:1778:BCR:C23	22:B:1778:BCR:C38	2.67	0.43
6:B:460:ALA:O	6:B:462:TRP:N	2.51	0.43
6:B:493:TRP:CZ2	19:B:1748:CLA:H122	2.53	0.43
6:B:727:ALA:O	6:B:728:SER:OG	2.29	0.43
9:E:80:ASN:OD1	9:E:81:ASN:N	2.49	0.43
11:G:48:ASP:HB3	11:G:49:THR:CB	2.43	0.43
11:G:60:SER:O	11:G:61:ASN:C	2.56	0.43
19:A:1796:CLA:C19	14:J:19:PHE:CD2	3.01	0.43
2:2:120:ASN:OD1	14:J:5:LYS:HG3	2.18	0.43
16:L:163:LEU:HD13	16:L:165:TYR:HB3	2.00	0.43
17:N:47:THR:CG2	17:N:54:LYS:HZ2	2.15	0.43
3:3:121:MET:O	19:3:1222:CLA:HED1	2.18	0.43
16:L:77:THR:OG1	16:L:82:ALA:HB3	2.19	0.43
17:N:4:GLU:OE2	17:N:5:GLU:N	2.51	0.43
8:D:56:GLN:OE1	8:D:94:TYR:CE2	2.71	0.43
8:D:92:SER:O	8:D:93:LYS:HG3	2.19	0.43
4:4:41:VAL:HG12	4:4:41:VAL:O	2.06	0.43
16:L:92:VAL:HG11	16:L:147:GLY:CA	2.48	0.43
2:2:127:ASN:OD1	14:J:7:TYR:CD2	2.71	0.43
4:4:103:ILE:CG1	19:4:1197:CLA:HMD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:118:ASP:O	4:4:122:LYS:HA	2.18	0.43
5:A:154:ARG:NE	5:A:154:ARG:HA	2.32	0.43
5:A:394:SER:CB	19:A:1783:CLA:HMA1	2.27	0.43
19:A:1784:CLA:H52	19:A:1784:CLA:HMD2	2.00	0.43
5:A:656:PHE:O	5:A:657:LEU:C	2.57	0.43
19:B:1748:CLA:H3A	19:B:1748:CLA:HBA2	1.33	0.43
6:B:60:TRP:HH2	19:B:1759:CLA:CHB	2.31	0.43
19:B:1746:CLA:C4B	22:B:1775:BCR:H291	2.49	0.43
16:L:124:LYS:NZ	16:L:124:LYS:CB	2.67	0.43
19:B:1741:CLA:H41	16:L:87:ALA:HB1	2.00	0.43
17:N:62:SER:HA	17:N:64:ASP:HB3	2.01	0.43
17:N:72:LYS:HZ2	17:N:74:LYS:HG2	1.58	0.43
3:3:50:GLU:OE2	3:3:54:LEU:HD13	2.17	0.43
19:1:1308:CLA:H2	19:J:1044:CLA:HED2	1.99	0.43
11:G:92:GLY:O	11:G:94:ASP:OD1	2.36	0.43
10:F:44:ALA:O	10:F:46:MET:HG2	2.19	0.43
3:3:74:ALA:CA	19:3:1217:CLA:C4D	2.84	0.43
20:A:7043:LMU:H4'	20:A:7043:LMU:H1'	1.55	0.43
19:R:1054:CLA:H62	19:R:1054:CLA:H41	1.87	0.43
5:A:478:SER:HB2	5:A:481:ALA:H	1.84	0.43
12:H:53:LEU:CG	12:H:54:LEU:N	2.77	0.43
1:1:134:SER:HB3	1:1:135:LYS:H	1.60	0.43
6:B:505:SER:O	6:B:506:ASN:HB3	2.18	0.43
1:1:179:THR:CB	4:4:87:SER:CB	2.64	0.43
2:2:169:LEU:HD22	19:2:1215:CLA:C4B	2.48	0.43
5:A:315:HIS:HB2	19:A:1778:CLA:HBC1	2.01	0.43
5:A:388:ASP:OD1	5:A:391:THR:HB	2.18	0.43
5:A:560:VAL:O	5:A:563:ALA:HB2	2.17	0.43
5:A:575:LEU:HD13	5:A:576:GLY:H	1.84	0.43
19:B:1743:CLA:C4C	19:B:1744:CLA:CBB	2.92	0.43
19:B:1766:CLA:CBB	22:B:1778:BCR:C28	2.97	0.43
6:B:22:TRP:HA	6:B:25:ILE:CD1	2.49	0.43
6:B:568:CYS:HB3	6:B:569:ASP:H	1.65	0.43
6:B:365:PHE:HB3	6:B:602:TRP:CH2	2.53	0.43
6:B:659:THR:OG1	19:B:1788:CLA:C3B	2.67	0.43
6:B:715:VAL:O	6:B:719:PHE:HB2	2.18	0.43
6:B:377:TYR:OH	6:B:717:TYR:HE1	2.02	0.43
6:B:564:ARG:CZ	7:C:64:SER:OG	2.66	0.43
8:D:41:GLN:HG3	16:L:125:LYS:NZ	2.33	0.43
10:F:80:TRP:CE3	19:F:1157:CLA:CHC	3.01	0.43
16:L:65:VAL:O	16:L:69:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:1205:CLA:C8	19:4:1205:CLA:H41	2.49	0.43
1:1:149:LYS:CB	19:1:1192:CLA:HMC2	2.44	0.43
3:3:182:LYS:C	3:3:185:LYS:H	2.21	0.43
10:F:44:ALA:O	10:F:46:MET:N	2.50	0.43
1:1:142:GLU:OE1	19:1:1187:CLA:CMD	2.67	0.43
19:2:1212:CLA:CMC	19:2:1212:CLA:CBC	2.63	0.43
19:1:1189:CLA:O1A	19:1:1189:CLA:C2	2.65	0.43
1:1:181:LEU:CD1	19:1:1189:CLA:HAC1	2.48	0.43
20:A:7019:LMU:H72	20:A:7019:LMU:H101	1.65	0.43
6:B:112:PRO:O	6:B:113:VAL:HG13	2.19	0.43
1:1:185:TRP:CA	1:1:186:HIS:CE1	2.93	0.43
2:2:171:MET:SD	2:2:171:MET:O	2.76	0.43
19:A:1763:CLA:HAA1	19:A:1765:CLA:HED1	2.01	0.43
5:A:284:ARG:CZ	5:A:284:ARG:CA	2.91	0.43
5:A:208:ALA:CA	5:A:310:PHE:O	2.43	0.43
5:A:506:GLY:O	5:A:507:ALA:CB	2.66	0.43
6:B:144:PHE:O	6:B:148:ILE:HD11	2.18	0.43
6:B:167:TRP:HD1	11:G:41:MET:CE	2.31	0.43
19:B:1751:CLA:HMA1	11:G:21:PHE:CG	2.54	0.43
19:B:1751:CLA:O2A	19:B:1751:CLA:NA	2.52	0.43
19:B:1753:CLA:HBB1	19:B:1753:CLA:H72	1.97	0.43
6:B:583:MET:HA	19:B:1756:CLA:HBC1	2.00	0.43
6:B:621:ARG:HB3	6:B:621:ARG:HE	1.57	0.43
6:B:632:ILE:C	6:B:634:GLY:N	2.71	0.43
6:B:674:LEU:O	6:B:678:LEU:HB2	2.18	0.43
9:E:42:GLU:CG	9:E:43:SER:N	2.70	0.43
20:N:1086:LMU:H81	20:N:1086:LMU:H112	1.60	0.43
20:A:7037:LMU:H4B	20:A:7037:LMU:H1B	1.51	0.43
21:B:8055:SUC:O4'	21:B:8055:SUC:H5	2.19	0.43
10:F:53:PHE:O	10:F:55:ASN:N	2.52	0.43
19:2:1212:CLA:C4A	19:2:1212:CLA:CGA	2.97	0.43
20:A:7021:LMU:O6'	20:A:7021:LMU:H22	2.13	0.43
20:A:7026:LMU:H1B	20:A:7026:LMU:H4B	1.07	0.43
19:3:3011:CLA:H142	19:3:3011:CLA:H101	2.00	0.43
8:D:125:PRO:HG2	8:D:127:ARG:HH11	1.82	0.43
17:N:29:PHE:O	17:N:33:TYR:N	2.51	0.43
2:2:79:TRP:O	2:2:79:TRP:CD2	2.72	0.43
6:B:488:ALA:CB	19:B:1767:CLA:C1C	2.96	0.43
2:2:112:ASP:C	2:2:114:LEU:N	2.70	0.43
4:4:44:GLU:O	4:4:45:LEU:C	2.56	0.43
19:A:1782:CLA:H91	19:A:1782:CLA:H112	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:224:HIS:HE1	19:A:1771:CLA:C1D	2.31	0.43
5:A:379:MET:HB2	5:A:379:MET:HE2	1.80	0.43
5:A:40:PHE:O	5:A:40:PHE:CD1	2.72	0.43
5:A:530:LEU:HD11	5:A:624:VAL:HA	2.01	0.43
5:A:654:ARG:HG3	5:A:655:ASP:N	2.33	0.43
5:A:705:GLU:HG2	6:B:545:LYS:NZ	2.31	0.43
5:A:74:ILE:O	5:A:78:VAL:HG13	2.19	0.43
6:B:126:THR:HG21	6:B:358:TYR:HD1	1.84	0.43
19:B:1757:CLA:H201	19:B:1770:CLA:C2	2.49	0.43
6:B:535:VAL:HG23	6:B:539:LEU:HD23	1.99	0.43
6:B:555:TYR:HE2	6:B:573:TRP:HD1	1.67	0.43
6:B:661:PHE:O	6:B:665:ILE:N	2.51	0.43
6:B:662:MET:HB3	6:B:663:PHE:H	1.55	0.43
6:B:707:LEU:HD13	24:B:1784:LMG:H331	2.00	0.43
9:E:40:ARG:N	9:E:46:PHE:CE1	2.82	0.43
16:L:99:LEU:HD12	22:L:1169:BCR:HC7	2.00	0.43
16:L:127:PRO:C	16:L:128:ASP:O	2.57	0.43
5:A:249:ILE:C	5:A:251:ASN:N	2.65	0.43
20:A:7048:LMU:H4B	20:A:7048:LMU:H1B	1.56	0.43
11:G:93:TYR:CG	11:G:94:ASP:HB2	2.54	0.43
21:B:8055:SUC:C4'	21:B:8055:SUC:O5	2.65	0.43
20:A:7030:LMU:H6D	20:A:7030:LMU:H1'	1.18	0.43
8:D:83:CYS:O	8:D:83:CYS:SG	2.76	0.43
6:B:475:ASP:CB	6:B:480:SER:HA	2.49	0.43
20:A:7005:LMU:H52	20:A:7005:LMU:H81	1.53	0.43
17:N:6:TYR:H	17:N:8:GLU:HA	1.84	0.43
2:2:153:PRO:HB2	2:2:157:LYS:HZ1	1.84	0.43
5:A:561:LEU:HA	5:A:561:LEU:HD23	1.75	0.43
2:2:47:ALA:HB1	2:2:110:TRP:CZ2	2.54	0.43
19:2:1215:CLA:H2	19:2:1218:CLA:CMD	2.49	0.43
4:4:167:ILE:C	4:4:169:GLN:H	2.22	0.43
5:A:129:GLN:HE22	19:A:1765:CLA:C1A	2.15	0.43
19:A:1767:CLA:CMC	19:A:1767:CLA:HBC3	2.38	0.43
22:A:1806:BCR:C12	19:A:1811:CLA:H122	2.48	0.43
5:A:413:HIS:CG	5:A:416:ILE:HD12	2.54	0.43
5:A:538:ASP:O	5:A:542:HIS:CD2	2.71	0.43
5:A:703:LEU:O	5:A:707:ILE:CG1	2.67	0.43
5:A:706:SER:HB3	6:B:419:ILE:O	2.18	0.43
6:B:175:LEU:HD11	19:B:1750:CLA:CMA	2.49	0.43
19:B:1769:CLA:HBC1	10:F:83:PHE:CE1	2.52	0.43
6:B:393:PHE:CZ	6:B:398:TYR:CD2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:458:ILE:HG13	6:B:459:PHE:CD1	2.54	0.43
6:B:655:LEU:CD2	19:B:1772:CLA:CAB	2.97	0.43
6:B:17:THR:HA	6:B:696:LYS:CB	2.48	0.43
20:N:1086:LMU:H21	20:N:1086:LMU:H1'	1.66	0.43
20:A:7016:LMU:O6'	20:A:7016:LMU:H41	2.17	0.43
19:1:1146:CLA:HMD2	20:K:1086:LMU:H52	2.01	0.43
2:2:191:ASN:O	2:2:192:LEU:C	2.57	0.43
5:A:277:TYR:CD2	5:A:278:ALA:N	2.87	0.43
12:H:54:LEU:O	12:H:54:LEU:HD22	2.19	0.43
11:G:75:GLY:O	11:G:80:ILE:HG23	2.19	0.43
16:L:107:PHE:HA	16:L:133:ALA:HB2	2.00	0.43
2:2:150:SER:HB3	2:2:151:ALA:H	1.50	0.43
4:4:30:LEU:O	4:4:32:GLU:OE1	2.36	0.43
5:A:163:GLN:HA	5:A:166:CYS:SG	2.59	0.43
19:A:1764:CLA:H122	19:A:1764:CLA:H161	1.73	0.43
19:A:1764:CLA:HBC3	19:A:1764:CLA:CHD	2.48	0.43
19:A:1776:CLA:H111	19:A:1776:CLA:C16	2.47	0.43
19:A:1761:CLA:H122	22:A:1802:BCR:C39	2.49	0.43
19:A:1784:CLA:C4C	22:A:1803:BCR:H333	2.48	0.43
5:A:620:MET:C	5:A:623:ASP:O	2.57	0.43
20:A:7006:LMU:H71	20:A:7006:LMU:H41	1.80	0.43
6:B:114:ASN:O	6:B:115:ASN:OD1	2.37	0.43
19:B:1751:CLA:C1C	19:B:1751:CLA:H43	2.49	0.43
6:B:175:LEU:O	6:B:179:LEU:CG	2.66	0.43
19:B:1788:CLA:C3A	19:B:1788:CLA:CGA	2.92	0.43
6:B:182:LEU:HG	6:B:183:PHE:H	1.84	0.43
6:B:183:PHE:HB3	6:B:284:PHE:CD2	2.54	0.43
6:B:361:ILE:O	6:B:362:ALA:O	2.36	0.43
6:B:556:SER:CA	6:B:558:PRO:CD	2.97	0.43
6:B:560:ASP:O	25:B:1785:SF4:S1	2.77	0.43
6:B:625:TRP:C	6:B:625:TRP:CD2	2.91	0.43
10:F:104:TYR:N	10:F:129:LEU:HD13	2.34	0.43
10:F:149:LEU:HD23	10:F:153:ASN:HD21	1.83	0.43
13:I:8:PHE:HB3	19:I:1031:CLA:OBD	2.16	0.43
16:L:161:LEU:HA	16:L:161:LEU:HD13	1.63	0.43
17:N:45:ASN:HA	17:N:57:LYS:HZ3	1.84	0.43
19:3:3011:CLA:H112	19:3:3011:CLA:H71	1.54	0.43
8:D:112:LEU:N	8:D:114:PRO:HG2	2.34	0.43
7:C:27:GLU:OE1	7:C:40:ALA:HB3	2.18	0.43
16:L:49:PRO:HG3	16:L:131:GLN:NE2	2.34	0.43
5:A:422:TYR:N	5:A:422:TYR:HD1	2.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:94:TYR:O	8:D:95:LYS:HB3	2.19	0.43
14:J:38:THR:O	14:J:39:PHE:CB	2.67	0.43
2:2:69:THR:O	2:2:70:LYS:CG	2.66	0.43
2:2:73:ILE:HD13	2:2:75:ASN:CB	2.49	0.43
4:4:158:ARG:HG2	4:4:159:LEU:N	2.31	0.43
5:A:370:ILE:HD11	19:A:1781:CLA:O1D	2.17	0.43
5:A:361:ASN:O	5:A:364:MET:N	2.52	0.43
5:A:553:VAL:CG2	22:A:1805:BCR:C40	2.97	0.43
5:A:575:LEU:HD13	5:A:579:PHE:HB3	2.00	0.43
5:A:78:VAL:O	5:A:82:HIS:CG	2.72	0.43
6:B:190:TRP:CE3	19:B:1745:CLA:HBB2	2.50	0.43
19:B:1759:CLA:H122	22:B:1776:BCR:C14	2.49	0.43
6:B:274:ALA:HA	6:B:277:HIS:HB2	2.00	0.43
5:A:697:ARG:CD	6:B:566:GLY:O	2.66	0.43
6:B:693:TRP:CD1	19:B:1771:CLA:CMD	3.02	0.43
6:B:91:ILE:HD12	19:B:1740:CLA:HMD3	2.00	0.43
7:C:60:THR:HG21	7:C:63:LEU:O	2.16	0.43
19:L:1168:CLA:O1D	19:L:1168:CLA:CAA	2.63	0.43
16:L:33:ILE:HG23	16:L:34:ALA:N	2.34	0.43
19:1:1188:CLA:HAC1	19:1:1188:CLA:HMC1	1.86	0.43
19:1:1148:CLA:HBA2	19:1:1148:CLA:O2D	2.17	0.43
10:F:52:ARG:N	10:F:52:ARG:HD2	2.33	0.43
21:B:8060:SUC:H1'2	21:B:8060:SUC:C5	2.46	0.43
5:A:141:ARG:HE	10:F:40:LEU:H	1.67	0.43
19:4:1211:CLA:C3D	19:4:1211:CLA:O1D	2.57	0.43
6:B:332:PHE:HE1	6:B:408:LEU:HD21	1.84	0.43
8:D:149:THR:O	8:D:151:LYS:N	2.51	0.43
6:B:543:GLY:HA3	6:B:548:PRO:O	2.19	0.43
4:4:147:LEU:HD22	4:4:148:GLU:HA	1.96	0.42
4:4:151:GLU:CA	4:4:154:ILE:HG23	2.45	0.42
4:4:99:HIS:ND1	4:4:103:ILE:HD13	2.29	0.42
19:A:1764:CLA:CGA	19:A:1783:CLA:H11	2.49	0.42
19:A:1796:CLA:H13	19:A:1796:CLA:H193	2.00	0.42
22:A:1805:BCR:H15C	22:A:1805:BCR:H351	1.86	0.42
5:A:299:ILE:HA	5:A:299:ILE:HD12	1.69	0.42
5:A:358:LEU:HD11	5:A:413:HIS:CD2	2.51	0.42
5:A:553:VAL:O	5:A:557:LEU:CB	2.67	0.42
6:B:167:TRP:HZ2	19:B:1744:CLA:HAC1	1.74	0.42
19:B:1758:CLA:H41	19:B:1758:CLA:H71	2.01	0.42
22:B:1782:BCR:HC7	22:B:1782:BCR:H342	1.61	0.42
6:B:192:GLY:HA2	19:B:1746:CLA:CHC	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:348:VAL:HG21	19:B:1759:CLA:HHD	1.99	0.42
6:B:440:ASN:OD1	6:B:452:GLN:NE2	2.52	0.42
6:B:493:TRP:HE1	19:B:1747:CLA:CAC	2.28	0.42
5:A:680:LEU:HD21	6:B:617:MET:HB2	2.00	0.42
6:B:668:ARG:CG	6:B:700:LEU:O	2.67	0.42
6:B:8:PHE:CD2	6:B:34:HIS:ND1	2.87	0.42
19:A:1789:CLA:HMD2	6:B:95:HIS:HD2	1.84	0.42
6:B:398:TYR:O	8:D:143:PRO:HG2	2.18	0.42
5:A:249:ILE:CD1	5:A:250:LEU:HB2	2.48	0.42
17:N:67:LEU:CB	17:N:68:GLU:HB3	2.46	0.42
3:3:49:ILE:O	3:3:49:ILE:HG23	2.18	0.42
20:A:7037:LMU:C6'	20:A:7037:LMU:H3O2	2.20	0.42
19:3:1224:CLA:H3A	19:3:1224:CLA:O1A	2.19	0.42
19:1:1146:CLA:HMA2	19:1:1146:CLA:H43	2.00	0.42
10:F:26:GLN:HB3	10:F:27:ALA:H	1.68	0.42
15:K:10:ILE:HA	15:K:13:THR:HG22	1.85	0.42
3:3:114:PHE:CE1	19:3:1220:CLA:C4D	3.02	0.42
8:D:84:LEU:HD12	8:D:100:PHE:CZ	2.50	0.42
6:B:70:TRP:H	6:B:70:TRP:HD1	1.65	0.42
3:3:127:ARG:HG2	3:3:131:ASP:OD1	2.18	0.42
5:A:419:VAL:HG21	5:A:577:PHE:HB2	2.01	0.42
2:2:99:LEU:HD23	2:2:102:ILE:CG1	2.50	0.42
4:4:104:ARG:CZ	4:4:105:ARG:H	2.32	0.42
4:4:127:PRO:HB2	4:4:143:PHE:HE1	1.83	0.42
4:4:163:PHE:O	4:4:166:PHE:CA	2.68	0.42
5:A:90:PHE:HB3	5:A:175:ALA:HB2	2.01	0.42
19:A:1779:CLA:HBC1	22:A:1804:BCR:H393	2.02	0.42
19:A:1783:CLA:H193	19:A:1783:CLA:H162	1.74	0.42
5:A:588:GLY:H	6:B:668:ARG:HH11	1.63	0.42
5:A:664:VAL:HG22	5:A:665:ILE:HG23	1.99	0.42
6:B:139:ALA:O	6:B:141:PHE:N	2.52	0.42
6:B:172:GLU:O	6:B:176:ASN:N	2.51	0.42
19:B:1744:CLA:C1	22:B:1776:BCR:C10	2.96	0.42
6:B:655:LEU:HD22	19:B:1772:CLA:CAB	2.48	0.42
7:C:63:LEU:CD1	7:C:65:VAL:H	2.33	0.42
11:G:27:GLN:HG2	19:G:1099:CLA:C4D	2.49	0.42
11:G:67:ASN:HA	11:G:70:ASP:CG	2.38	0.42
17:N:72:LYS:CA	17:N:73:ASP:C	2.88	0.42
20:A:7026:LMU:C4	20:A:7026:LMU:H82	2.30	0.42
20:A:7005:LMU:H32	20:A:7005:LMU:H61	1.50	0.42
5:A:277:TYR:HD2	5:A:278:ALA:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:108:ALA:CB	5:A:138:GLY:HA3	2.41	0.42
8:D:20:LEU:O	8:D:21:ASP:C	2.58	0.42
2:2:154:GLN:OE1	2:2:154:GLN:HA	2.19	0.42
2:2:73:ILE:HD13	2:2:75:ASN:CA	2.48	0.42
4:4:149:ALA:CA	4:4:151:GLU:CG	2.96	0.42
5:A:149:PHE:C	5:A:151:GLN:N	2.71	0.42
19:A:1800:CLA:H62	19:A:1800:CLA:H41	1.62	0.42
5:A:159:THR:OG1	5:A:239:PRO:HB3	2.20	0.42
5:A:472:ARG:HG2	6:B:97:GLY:HA3	2.02	0.42
5:A:648:THR:HG23	5:A:650:ASN:H	1.83	0.42
5:A:693:LEU:CD2	5:A:734:GLY:HA3	2.49	0.42
6:B:58:PHE:HE2	6:B:145:LEU:HD12	1.85	0.42
24:B:1784:LMG:H112	24:B:1784:LMG:H292	2.00	0.42
19:B:1760:CLA:HHD	24:B:1784:LMG:H352	2.00	0.42
6:B:203:ARG:CG	6:B:204:GLY:N	2.70	0.42
6:B:531:THR:HG21	19:B:1756:CLA:CHC	2.49	0.42
8:D:41:GLN:NE2	8:D:42:VAL:HA	2.34	0.42
9:E:88:GLU:O	9:E:90:VAL:HA	2.14	0.42
10:F:96:TRP:HZ3	10:F:134:PHE:CB	2.21	0.42
11:G:42:SER:HG	11:G:45:GLU:CB	2.32	0.42
22:L:1170:BCR:HC7	22:L:1170:BCR:H342	1.53	0.42
16:L:99:LEU:HB3	16:L:140:THR:HG21	2.02	0.42
20:A:7042:LMU:H11	20:A:7042:LMU:H71	1.99	0.42
12:H:27:ASP:O	12:H:29:PRO:CD	2.67	0.42
14:J:10:VAL:HG13	14:J:14:LEU:CG	2.43	0.42
10:F:39:ALA:O	10:F:42:ILE:CG2	2.68	0.42
7:C:44:ARG:NH2	8:D:127:ARG:NE	2.64	0.42
9:E:69:PHE:CD2	9:E:71:LYS:N	2.82	0.42
6:B:160:LYS:NZ	6:B:160:LYS:HB2	2.30	0.42
5:A:67:HIS:O	5:A:68:THR:HB	2.20	0.42
1:1:38:ARG:CZ	1:1:139:LYS:CB	2.97	0.42
4:4:179:ASP:H	4:4:184:HIS:CD2	2.37	0.42
20:A:7034:LMU:H1B	20:A:7034:LMU:H5'	1.48	0.42
2:2:54:TRP:CZ2	2:2:109:ARG:HB3	2.49	0.42
19:2:1213:CLA:HBA2	19:2:1213:CLA:H3A	1.79	0.42
4:4:121:PHE:O	4:4:122:LYS:CG	2.66	0.42
4:4:38:ARG:O	4:4:39:TRP:C	2.56	0.42
5:A:173:VAL:HG23	5:A:174:PHE:N	2.34	0.42
22:A:1804:BCR:H351	22:A:1804:BCR:H15C	1.83	0.42
5:A:204:ASN:HA	5:A:314:GLY:O	2.20	0.42
5:A:374:GLN:C	5:A:376:MET:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:579:PHE:HA	5:A:580:PRO:HD2	1.64	0.42
5:A:606:TYR:HB2	5:A:739:LEU:HD22	2.01	0.42
5:A:705:GLU:OE1	5:A:708:VAL:HG12	2.19	0.42
5:A:748:ALA:O	5:A:749:PHE:C	2.58	0.42
5:A:64:PHE:HZ	5:A:77:LYS:CE	2.32	0.42
6:B:144:PHE:CD2	6:B:144:PHE:C	2.92	0.42
19:B:1748:CLA:H141	19:B:1748:CLA:HMC2	2.02	0.42
19:B:1750:CLA:HBB2	19:B:1755:CLA:C4	2.47	0.42
6:B:174:ARG:C	6:B:176:ASN:H	2.22	0.42
23:A:1801:PQN:C15	22:B:1779:BCR:H322	2.50	0.42
19:B:1786:CLA:HAA2	19:B:1786:CLA:H11	2.02	0.42
6:B:176:ASN:ND2	6:B:292:ARG:O	2.52	0.42
6:B:416:GLU:N	6:B:416:GLU:CD	2.73	0.42
6:B:674:LEU:CD1	6:B:674:LEU:C	2.88	0.42
10:F:123:VAL:O	10:F:126:ALA:CA	2.68	0.42
11:G:45:GLU:C	11:G:49:THR:CG2	2.62	0.42
16:L:66:GLY:CA	16:L:69:VAL:HG22	2.48	0.42
20:A:7042:LMU:H4'	20:A:7042:LMU:H1'	1.57	0.42
5:A:254:LEU:HD13	5:A:254:LEU:HA	1.66	0.42
20:A:7016:LMU:H6'	20:A:7016:LMU:H12	1.84	0.42
11:G:93:TYR:CB	11:G:94:ASP:HB2	2.42	0.42
21:B:8055:SUC:O4'	21:B:8055:SUC:C5	2.67	0.42
21:B:8062:SUC:HO6	21:B:8062:SUC:C2'	2.31	0.42
2:2:197:LEU:O	2:2:198:ALA:HB2	2.20	0.42
6:B:684:ARG:HA	6:B:684:ARG:HD3	1.74	0.42
2:2:73:ILE:HD13	2:2:75:ASN:HB2	2.02	0.42
4:4:108:ASP:O	4:4:111:ASN:C	2.57	0.42
4:4:121:PHE:HB2	4:4:128:ALA:CB	2.48	0.42
4:4:122:LYS:HB2	4:4:143:PHE:HD2	0.51	0.42
4:4:166:PHE:O	4:4:169:GLN:N	2.50	0.42
19:A:1811:CLA:H122	19:A:1811:CLA:C9	2.47	0.42
5:A:193:LEU:O	5:A:196:PHE:CD2	2.73	0.42
5:A:227:LEU:O	5:A:231:GLN:HB2	2.18	0.42
5:A:445:HIS:CE1	19:A:1786:CLA:HMB1	2.53	0.42
5:A:620:MET:HG3	5:A:625:TRP:CD2	2.54	0.42
5:A:662:SER:HA	5:A:665:ILE:CD1	2.49	0.42
5:A:82:HIS:CE1	19:A:1761:CLA:HAA1	2.54	0.42
5:A:96:MET:N	5:A:98:PHE:O	2.52	0.42
19:B:1769:CLA:CBB	19:B:1769:CLA:C9	2.55	0.42
6:B:228:GLY:CA	11:G:8:ILE:HB	2.49	0.42
6:B:278:LEU:O	6:B:279:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:518:LEU:O	6:B:519:VAL:C	2.58	0.42
6:B:531:THR:O	6:B:535:VAL:N	2.50	0.42
6:B:685:THR:HA	6:B:686:PRO:HD3	1.92	0.42
6:B:17:THR:CA	6:B:696:LYS:H	2.31	0.42
9:E:36:VAL:CG1	9:E:87:VAL:HG11	2.49	0.42
9:E:87:VAL:C	9:E:89:GLU:N	2.67	0.42
11:G:60:SER:C	11:G:62:ASP:N	2.71	0.42
13:I:8:PHE:HE1	22:I:1032:BCR:C9	2.32	0.42
16:L:127:PRO:O	16:L:128:ASP:C	2.58	0.42
19:4:1205:CLA:HED2	19:4:1205:CLA:H2A	2.02	0.42
2:2:205:PHE:O	2:2:206:ALA:HB2	2.19	0.42
22:3:1225:BCR:H341	22:3:1225:BCR:H11C	1.57	0.42
6:B:477:PRO:O	6:B:478:LEU:HD22	2.18	0.42
12:H:45:ALA:HA	12:H:48:THR:OG1	2.19	0.42
6:B:216:LEU:HD22	6:B:218:TYR:H	1.84	0.42
11:G:80:ILE:O	11:G:81:VAL:C	2.58	0.42
8:D:152:GLN:O	8:D:154:TYR:N	2.53	0.42
5:A:34:TRP:O	5:A:35:ALA:HB3	2.20	0.42
8:D:24:THR:OG1	8:D:24:THR:O	2.30	0.42
4:4:139:ASN:HA	4:4:140:PRO:HD3	1.84	0.42
19:A:1774:CLA:H2	19:A:1774:CLA:HMB2	2.02	0.42
19:A:1776:CLA:H112	19:A:1776:CLA:H91	1.82	0.42
19:A:1777:CLA:O2D	19:A:1777:CLA:OBD	2.37	0.42
5:A:351:THR:CA	19:A:1780:CLA:H191	2.49	0.42
19:A:1789:CLA:HBC2	19:B:1741:CLA:HBC1	2.01	0.42
5:A:193:LEU:HA	5:A:196:PHE:HE2	1.80	0.42
5:A:281:LEU:HB2	5:A:301:HIS:CD2	2.52	0.42
5:A:584:PRO:HB2	7:C:67:VAL:HB	2.01	0.42
5:A:648:THR:C	5:A:650:ASN:H	2.23	0.42
5:A:672:LEU:CD2	5:A:672:LEU:H	2.32	0.42
19:B:1742:CLA:HBD	19:B:1742:CLA:CGA	2.50	0.42
19:B:1754:CLA:H161	19:B:1754:CLA:H141	1.65	0.42
19:B:1765:CLA:ND	19:B:1766:CLA:CBB	2.82	0.42
19:B:1771:CLA:C19	13:I:21:MET:CE	2.98	0.42
21:B:8054:SUC:HO2	21:B:8054:SUC:H1'1	1.80	0.42
11:G:5:SER:O	11:G:7:VAL:CG1	2.68	0.42
12:H:45:ALA:N	12:H:46:PRO:HD2	2.34	0.42
17:N:4:GLU:OE2	17:N:5:GLU:CB	2.61	0.42
20:A:1809:LMU:H12	20:A:1809:LMU:H41	1.70	0.42
17:N:14:LYS:HB2	17:N:17:ASN:OD1	2.20	0.42
6:B:541:ALA:HB2	6:B:572:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:179:THR:HB	1:1:180:HIS:H	1.54	0.42
2:2:37:ASP:OD2	3:3:41:ASP:HB2	2.18	0.42
4:4:142:ASN:O	4:4:143:PHE:HB2	2.19	0.42
5:A:334:HIS:HB3	19:A:1777:CLA:CHB	2.49	0.42
19:A:1777:CLA:C1C	19:A:1777:CLA:H52	2.49	0.42
19:A:1777:CLA:H3A	19:A:1777:CLA:HBA2	1.62	0.42
5:A:177:LEU:HA	5:A:177:LEU:HD22	1.89	0.42
19:A:1781:CLA:CBB	19:A:1794:CLA:HMA1	2.49	0.42
5:A:207:LEU:HD11	5:A:313:ALA:CB	2.49	0.42
5:A:210:LEU:HD23	5:A:211:LEU:N	2.35	0.42
5:A:467:MET:HB3	5:A:467:MET:HE3	1.73	0.42
19:B:1735:CLA:HBC3	19:B:1735:CLA:HHD	2.01	0.42
6:B:167:TRP:CD1	19:B:1743:CLA:HED1	2.55	0.42
6:B:326:ILE:CG2	19:B:1755:CLA:HBC3	2.48	0.42
24:B:1784:LMG:O8	24:B:1784:LMG:C11	2.68	0.42
6:B:260:GLY:O	6:B:262:HIS:NE2	2.52	0.42
6:B:350:GLN:HG3	6:B:372:TYR:HE1	1.84	0.42
6:B:439:HIS:HB2	19:B:1764:CLA:C1C	2.49	0.42
6:B:707:LEU:HG	6:B:708:VAL:N	2.34	0.42
10:F:128:SER:C	10:F:130:LEU:HD23	2.40	0.42
10:F:131:PHE:O	10:F:132:ARG:C	2.56	0.42
10:F:96:TRP:CZ3	10:F:134:PHE:N	2.87	0.42
16:L:63:LEU:CG	16:L:64:LEU:H	2.27	0.42
3:3:96:GLY:C	3:3:97:PHE:CG	2.92	0.42
17:N:45:ASN:HA	17:N:57:LYS:HZ2	1.83	0.42
17:N:57:LYS:O	17:N:58:VAL:C	2.57	0.42
17:N:72:LYS:CB	17:N:74:LYS:H	2.21	0.42
1:1:109:GLU:HB3	19:1:1195:CLA:HMA3	2.01	0.42
15:K:44:GLU:O	15:K:45:SER:HB2	2.19	0.42
6:B:503:GLU:CA	6:B:507:SER:HB2	2.50	0.42
5:A:570:PRO:C	5:A:572:LYS:N	2.73	0.42
3:3:206:VAL:HB	3:3:207:GLY:H	1.69	0.42
12:H:77:LEU:CD2	12:H:78:PRO:HD2	2.50	0.42
5:A:164:LEU:CA	5:A:167:THR:HG23	2.47	0.42
19:A:1761:CLA:C4B	19:A:1785:CLA:HMB2	2.50	0.42
5:A:183:TRP:C	5:A:185:HIS:H	2.23	0.42
5:A:345:GLY:C	5:A:347:TYR:N	2.66	0.42
5:A:430:ASP:O	5:A:434:ARG:N	2.45	0.42
20:A:7006:LMU:C6B	20:A:7006:LMU:H3'	2.50	0.42
5:A:79:PHE:CE2	5:A:185:HIS:CG	2.94	0.42
6:B:262:HIS:ND1	6:B:265:THR:O	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:292:ARG:NE	6:B:292:ARG:CA	2.64	0.42
6:B:10:GLN:HB2	6:B:35:ASP:OD2	2.19	0.42
6:B:366:THR:C	6:B:368:GLN:N	2.73	0.42
6:B:429:LEU:HA	6:B:429:LEU:HD23	1.64	0.42
6:B:269:TRP:CG	6:B:497:TRP:HH2	2.38	0.42
6:B:661:PHE:O	6:B:662:MET:O	2.37	0.42
6:B:724:PHE:CZ	19:B:1786:CLA:HMD1	2.55	0.42
9:E:37:LYS:HD2	9:E:47:LYS:HE3	2.02	0.42
11:G:28:ARG:HG2	11:G:29:GLU:CB	2.50	0.42
11:G:62:ASP:HB2	11:G:63:PRO:CD	2.45	0.42
16:L:33:ILE:HG13	16:L:37:LEU:HD21	2.02	0.42
16:L:56:VAL:CB	19:L:1167:CLA:HED2	2.50	0.42
18:R:38:UNK:C	18:R:42:UNK:CA	2.97	0.42
20:A:7032:LMU:H31	20:A:7032:LMU:H4B	2.02	0.42
15:K:8:ASN:CB	15:K:9:LEU:HD23	2.50	0.42
8:D:49:THR:C	8:D:50:TRP:HD1	2.23	0.42
5:A:630:ASP:C	5:A:632:GLY:H	2.21	0.42
2:2:208:PHE:CE1	2:2:209:THR:O	2.73	0.42
11:G:79:HIS:CG	11:G:79:HIS:O	2.72	0.42
5:A:667:SER:O	5:A:667:SER:OG	2.37	0.42
4:4:88:SER:C	4:4:90:LEU:HD13	2.39	0.42
5:A:132:LEU:HD21	5:A:674:ALA:HB2	2.02	0.42
5:A:737:HIS:CE1	19:A:1796:CLA:NA	2.88	0.42
19:A:1797:CLA:H102	19:A:1797:CLA:H51	2.02	0.42
19:A:1799:CLA:CGA	19:A:1799:CLA:CHA	2.98	0.42
5:A:210:LEU:N	5:A:213:LEU:N	2.68	0.42
6:B:190:TRP:CE2	19:B:1749:CLA:CMD	3.03	0.42
22:B:1775:BCR:H343	11:G:21:PHE:CE1	2.55	0.42
6:B:534:LEU:CD2	6:B:579:ALA:HB2	2.50	0.42
6:B:583:MET:O	6:B:587:ILE:HB	2.20	0.42
6:B:594:TRP:HD1	6:B:595:HIS:CB	2.33	0.42
5:A:680:LEU:HG	6:B:617:MET:HB2	2.02	0.42
11:G:32:ALA:O	11:G:34:GLN:C	2.58	0.42
11:G:44:PHE:CA	11:G:46:ALA:HB2	2.49	0.42
16:L:149:SER:C	16:L:151:VAL:N	2.73	0.42
16:L:160:VAL:C	16:L:161:LEU:O	2.58	0.42
3:3:92:TRP:HZ2	5:A:250:LEU:CD1	2.28	0.42
3:3:106:TYR:CB	3:3:107:TRP:HD1	2.32	0.42
6:B:470:THR:H	6:B:501:ILE:HG23	1.84	0.42
5:A:586:ARG:HG3	7:C:49:VAL:CG2	2.43	0.42
2:2:81:THR:O	2:2:82:ALA:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:37:LEU:O	14:J:38:THR:OG1	2.35	0.42
12:H:36:GLN:CG	12:H:36:GLN:O	2.68	0.42
6:B:213:LEU:HD12	6:B:214:ASP:H	1.83	0.42
16:L:135:GLY:HA2	16:L:138:LYS:HE2	2.02	0.42
2:2:103:GLY:HA2	19:2:1222:CLA:CAB	2.49	0.42
4:4:121:PHE:CD1	4:4:143:PHE:CZ	3.08	0.42
4:4:147:LEU:HD13	4:4:148:GLU:CA	2.43	0.42
5:A:150:PHE:O	5:A:151:GLN:HG3	2.20	0.42
5:A:224:HIS:CE1	19:A:1771:CLA:C1D	3.02	0.42
5:A:466:THR:HG21	19:B:1740:CLA:HBB1	2.01	0.42
5:A:604:TRP:O	5:A:605:MET:C	2.59	0.42
5:A:621:GLN:HG2	5:A:637:ILE:CD1	2.40	0.42
5:A:680:LEU:HD21	6:B:617:MET:SD	2.60	0.42
6:B:230:TRP:CH2	11:G:11:SER:CB	2.94	0.42
6:B:25:ILE:H	6:B:25:ILE:HG13	1.57	0.42
6:B:310:PRO:CG	6:B:311:PRO:CD	2.88	0.42
6:B:381:PHE:HA	6:B:583:MET:SD	2.60	0.42
6:B:707:LEU:O	6:B:710:LEU:CB	2.68	0.42
7:C:63:LEU:CD1	7:C:64:SER:H	2.32	0.42
8:D:139:LYS:NZ	9:E:41:ARG:HH11	2.18	0.42
11:G:24:PHE:HB3	11:G:28:ARG:HH11	1.85	0.42
11:G:43:HIS:C	11:G:45:GLU:CA	2.88	0.42
11:G:50:ARG:CB	11:G:51:ALA:CA	2.97	0.42
16:L:46:ALA:N	16:L:52:ARG:HH12	2.18	0.42
19:4:1205:CLA:CHD	19:4:1205:CLA:HBC2	2.50	0.42
20:A:7041:LMU:H4B	20:A:7041:LMU:H1B	1.53	0.42
17:N:44:GLU:C	17:N:46:PHE:N	2.68	0.42
10:F:23:LYS:C	10:F:26:GLN:H	2.23	0.42
5:A:338:PHE:C	5:A:338:PHE:CD2	2.93	0.42
5:A:274:TRP:CZ2	5:A:278:ALA:HA	2.55	0.42
16:L:12:GLN:HA	16:L:13:PRO:HD3	1.82	0.42
5:A:349:ILE:CD1	5:A:422:TYR:HB3	2.50	0.42
20:A:7025:LMU:H52	20:A:7025:LMU:H21	1.82	0.42
19:L:1166:CLA:H11	19:L:1166:CLA:C4D	2.50	0.42
10:F:65:SER:C	10:F:67:GLY:H	2.23	0.42
19:2:1213:CLA:C4	19:2:1213:CLA:CHD	2.97	0.41
2:2:59:ALA:HB3	2:2:172:LEU:HD22	1.99	0.41
2:2:66:GLU:HB3	2:2:67:PHE:H	1.54	0.41
4:4:36:ASN:OD1	4:4:37:LEU:N	2.52	0.41
4:4:86:SER:O	4:4:87:SER:C	2.56	0.41
19:A:1764:CLA:H3A	19:A:1764:CLA:HBA2	1.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1771:CLA:CGD	19:A:1771:CLA:C2A	2.95	0.41
5:A:207:LEU:CD1	19:A:1776:CLA:HBB2	2.50	0.41
19:A:1794:CLA:CMC	19:A:1794:CLA:CBC	2.96	0.41
5:A:183:TRP:C	5:A:185:HIS:N	2.73	0.41
5:A:216:LEU:CD1	22:A:1802:BCR:H11C	2.50	0.41
5:A:694:PHE:HZ	6:B:661:PHE:CE1	2.38	0.41
5:A:87:SER:O	5:A:88:ILE:HB	2.19	0.41
5:A:92:TRP:C	5:A:94:SER:H	2.22	0.41
6:B:16:PRO:HG3	7:C:74:THR:HG22	2.02	0.41
6:B:304:ILE:CD1	19:B:1750:CLA:HED3	2.50	0.41
19:B:1738:CLA:H192	19:B:1758:CLA:H141	2.02	0.41
6:B:266:GLN:NE2	6:B:363:GLN:HG2	2.34	0.41
6:B:373:THR:C	6:B:376:GLN:H	2.24	0.41
6:B:393:PHE:CZ	6:B:398:TYR:HD2	2.37	0.41
6:B:587:ILE:CG2	6:B:587:ILE:O	2.67	0.41
6:B:588:GLY:O	6:B:592:PHE:CB	2.52	0.41
5:A:680:LEU:CG	6:B:617:MET:HB2	2.50	0.41
9:E:34:SER:O	9:E:35:LYS:CB	2.64	0.41
10:F:75:GLY:O	19:F:1156:CLA:HAC2	2.19	0.41
11:G:20:ARG:NH2	11:G:61:ASN:C	2.74	0.41
20:A:7036:LMU:H101	20:A:7036:LMU:H72	1.66	0.41
19:1:1192:CLA:H121	19:1:1192:CLA:HBC3	2.02	0.41
3:3:94:ARG:CA	3:3:97:PHE:HE1	2.33	0.41
17:N:57:LYS:O	17:N:60:PHE:HD1	1.99	0.41
17:N:64:ASP:HB3	17:N:65:LEU:H	1.43	0.41
3:3:52:LYS:O	3:3:56:TYR:CB	2.68	0.41
20:A:7037:LMU:H121	20:A:7051:LMU:H41	2.00	0.41
2:2:181:HIS:HE1	19:2:1214:CLA:CHA	2.32	0.41
5:A:536:THR:O	5:A:537:ALA:HB3	2.20	0.41
3:3:207:GLY:O	3:3:208:PRO:C	2.58	0.41
1:1:38:ARG:CZ	1:1:139:LYS:HB3	2.50	0.41
5:A:527:VAL:HG12	5:A:528:ALA:O	2.20	0.41
2:2:51:HIS:HA	2:2:54:TRP:CD1	2.55	0.41
4:4:103:ILE:HD13	4:4:103:ILE:H	1.84	0.41
4:4:148:GLU:HB3	4:4:149:ALA:H	1.78	0.41
5:A:163:GLN:CG	5:A:164:LEU:N	2.83	0.41
5:A:127:VAL:CG2	19:A:1765:CLA:HBB2	2.50	0.41
5:A:224:HIS:CE1	19:A:1771:CLA:NC	2.88	0.41
19:A:1781:CLA:C5	19:A:1782:CLA:CED	2.86	0.41
19:A:1783:CLA:H202	22:A:1807:BCR:H15C	1.99	0.41
22:A:1803:BCR:HC8	22:A:1803:BCR:C31	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:657:LEU:HD23	19:A:1810:CLA:C2D	2.50	0.41
5:A:79:PHE:HZ	5:A:185:HIS:NE2	2.08	0.41
5:A:244:LEU:H	5:A:244:LEU:HD12	1.85	0.41
5:A:357:GLN:NE2	5:A:360:ILE:HG23	2.35	0.41
5:A:408:VAL:O	5:A:411:ALA:HB3	2.20	0.41
5:A:650:ASN:HD22	6:B:635:ILE:CD1	2.33	0.41
20:A:7003:LMU:H22	20:A:7003:LMU:O2'	2.20	0.41
20:A:7006:LMU:H2'	20:A:7006:LMU:C2	2.49	0.41
5:A:98:PHE:CD1	5:A:98:PHE:C	2.94	0.41
6:B:116:ALA:CB	6:B:121:TYR:CD2	3.04	0.41
6:B:348:VAL:HG22	19:B:1759:CLA:HMD3	2.02	0.41
6:B:431:PHE:CD2	19:B:1763:CLA:CMA	3.03	0.41
6:B:486:LEU:HD12	19:B:1766:CLA:CMD	2.49	0.41
22:B:1782:BCR:H24C	22:B:1782:BCR:H371	1.01	0.41
6:B:387:PHE:CB	6:B:534:LEU:HD13	2.49	0.41
6:B:534:LEU:HD21	6:B:579:ALA:HB2	2.01	0.41
6:B:560:ASP:CG	7:C:66:ARG:CZ	2.89	0.41
9:E:60:LYS:CG	9:E:61:THR:H	2.19	0.41
10:F:126:ALA:HB1	10:F:129:LEU:HD12	2.02	0.41
10:F:144:LEU:CD1	10:F:149:LEU:HD13	2.50	0.41
11:G:18:LEU:HD23	11:G:18:LEU:N	2.35	0.41
10:F:125:LEU:HD11	14:J:18:TRP:CZ3	2.55	0.41
16:L:149:SER:C	16:L:151:VAL:H	2.23	0.41
16:L:68:PHE:CD1	16:L:68:PHE:N	2.88	0.41
20:A:7042:LMU:H52	20:A:7042:LMU:H81	1.59	0.41
18:R:41:UNK:N	18:R:42:UNK:CB	2.83	0.41
19:1:1308:CLA:C2	19:J:1044:CLA:HED1	2.50	0.41
5:A:21:LEU:CD1	5:A:21:LEU:C	2.59	0.41
10:F:24:LYS:HA	10:F:26:GLN:H	1.79	0.41
20:A:7039:LMU:H61	20:A:7039:LMU:H92	1.69	0.41
6:B:325:THR:HG21	6:B:403:ASN:HD21	1.86	0.41
1:1:63:LEU:CG	1:1:63:LEU:O	2.67	0.41
20:A:7004:LMU:C1B	20:A:7004:LMU:O3'	2.68	0.41
8:D:93:LYS:CB	8:D:93:LYS:HZ2	2.30	0.41
1:1:38:ARG:HH12	1:1:138:LYS:HD2	1.85	0.41
4:4:144:ALA:HB2	4:4:148:GLU:O	2.18	0.41
19:A:1772:CLA:H43	19:A:1772:CLA:H12	1.90	0.41
19:A:1778:CLA:CBA	19:A:1778:CLA:HED2	2.50	0.41
5:A:334:HIS:CD2	19:A:1777:CLA:C1B	3.03	0.41
5:A:378:SER:HG	5:A:512:SER:HG	1.68	0.41
5:A:663:GLN:OE1	5:A:753:ARG:CZ	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:175:LEU:HD11	19:B:1750:CLA:HMA1	2.03	0.41
19:B:1769:CLA:H161	19:B:1769:CLA:H203	1.91	0.41
6:B:188:LEU:HD21	22:B:1776:BCR:H281	2.03	0.41
22:B:1781:BCR:H353	19:B:1788:CLA:H122	2.02	0.41
19:B:1788:CLA:H141	19:B:1788:CLA:H161	1.73	0.41
6:B:262:HIS:HA	6:B:263:PRO:HD2	1.93	0.41
6:B:347:LEU:O	6:B:351:HIS:HB2	2.20	0.41
6:B:557:PHE:HE2	7:C:66:ARG:NE	2.16	0.41
9:E:43:SER:O	9:E:46:PHE:HB2	2.20	0.41
10:F:147:GLY:O	10:F:149:LEU:O	2.38	0.41
10:F:80:TRP:HZ3	19:F:1156:CLA:HMC3	1.82	0.41
19:G:1099:CLA:O1D	19:G:1099:CLA:C1A	2.64	0.41
11:G:28:ARG:HG3	11:G:29:GLU:CB	2.50	0.41
13:I:10:PRO:O	13:I:11:LEU:C	2.58	0.41
16:L:33:ILE:O	16:L:35:TRP:N	2.53	0.41
4:4:75:TRP:CG	19:4:1205:CLA:CMD	2.93	0.41
20:A:7016:LMU:H1'	20:A:7016:LMU:H6D	1.44	0.41
19:3:1224:CLA:H52	19:3:1224:CLA:H12	1.77	0.41
20:A:7032:LMU:H91	20:A:7032:LMU:H121	1.84	0.41
3:3:111:TYR:HB2	3:3:112:THR:CG2	2.51	0.41
19:2:1217:CLA:H42	19:2:1217:CLA:H11	1.87	0.41
16:L:10:VAL:HG13	16:L:12:GLN:HE22	1.85	0.41
6:B:70:TRP:N	6:B:70:TRP:CD1	2.88	0.41
2:2:188:PRO:C	2:2:190:ASP:N	2.72	0.41
6:B:332:PHE:CE1	6:B:408:LEU:HD21	2.55	0.41
6:B:152:ALA:O	6:B:153:GLY:O	2.37	0.41
15:K:46:GLY:O	15:K:47:ILE:HB	2.20	0.41
5:A:66:SER:O	5:A:67:HIS:CB	2.67	0.41
11:G:83:TYR:O	11:G:83:TYR:CD1	2.72	0.41
12:H:77:LEU:HD23	12:H:78:PRO:HD2	2.02	0.41
3:3:153:SER:C	3:3:161:GLY:HA2	2.41	0.41
2:2:54:TRP:NE1	2:2:109:ARG:HD2	2.32	0.41
2:2:57:LEU:C	2:2:57:LEU:HD23	2.40	0.41
4:4:142:ASN:O	4:4:143:PHE:CB	2.67	0.41
4:4:35:GLU:HB3	4:4:36:ASN:CB	2.24	0.41
19:A:1762:CLA:H12	19:A:1762:CLA:HBA2	1.78	0.41
5:A:182:GLY:C	19:A:1767:CLA:HAC1	2.40	0.41
5:A:224:HIS:CE1	19:A:1771:CLA:CHD	2.99	0.41
5:A:376:MET:HE3	19:A:1784:CLA:OBD	2.20	0.41
5:A:87:SER:HA	5:A:90:PHE:HB2	2.02	0.41
5:A:88:ILE:O	5:A:92:TRP:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:97:TYR:HA	5:A:153:TRP:HZ2	1.85	0.41
19:B:1736:CLA:HMC3	19:B:1738:CLA:OBD	2.20	0.41
23:B:1774:PQN:H141	23:B:1774:PQN:H161	1.41	0.41
19:B:1759:CLA:C19	22:B:1777:BCR:H14C	2.51	0.41
5:A:693:LEU:HD13	6:B:665:ILE:HD13	2.02	0.41
6:B:674:LEU:HA	6:B:677:THR:HG23	2.03	0.41
6:B:75:GLU:HB2	6:B:132:ASN:CB	2.42	0.41
7:C:6:LYS:O	7:C:63:LEU:CD2	2.68	0.41
7:C:74:THR:HB	7:C:80:ALA:HB2	1.97	0.41
11:G:17:PHE:N	11:G:17:PHE:CD2	2.87	0.41
13:I:11:LEU:O	13:I:11:LEU:HD13	2.21	0.41
16:L:64:LEU:CA	16:L:67:PRO:HG2	2.46	0.41
17:N:72:LYS:HB3	17:N:74:LYS:HB2	1.99	0.41
19:3:1224:CLA:CBD	19:3:1224:CLA:HAA2	2.49	0.41
8:D:100:PHE:O	8:D:113:HIS:HB2	2.21	0.41
4:4:56:ALA:O	4:4:57:GLY:C	2.59	0.41
6:B:68:VAL:O	6:B:69:ALA:CB	2.68	0.41
20:A:1809:LMU:H21	20:A:1809:LMU:H1'	1.59	0.41
2:2:152:SER:C	2:2:154:GLN:H	2.24	0.41
2:2:57:LEU:O	2:2:60:ALA:N	2.48	0.41
2:2:91:THR:N	2:2:94:LEU:HB2	2.35	0.41
4:4:115:VAL:O	4:4:116:ASN:C	2.57	0.41
4:4:160:MET:HA	4:4:163:PHE:CB	2.44	0.41
4:4:36:ASN:O	4:4:39:TRP:CA	2.68	0.41
5:A:126:ILE:HG13	5:A:126:ILE:H	1.58	0.41
5:A:81:ALA:CA	19:A:1760:CLA:HMA1	2.44	0.41
19:3:1212:CLA:HBC3	19:A:1770:CLA:C1D	2.50	0.41
19:A:1781:CLA:H11	19:A:1794:CLA:CAD	2.51	0.41
19:A:1781:CLA:HAA1	19:A:1781:CLA:CED	2.50	0.41
19:A:1799:CLA:H152	22:L:1170:BCR:C35	2.47	0.41
19:A:1810:CLA:HHD	19:A:1810:CLA:CBC	2.43	0.41
5:A:75:SER:HB3	5:A:354:TRP:HZ2	1.83	0.41
5:A:599:PHE:CD1	5:A:600:LEU:HD23	2.36	0.41
5:A:684:PHE:HB2	19:A:1811:CLA:HAA1	2.02	0.41
5:A:690:LEU:O	5:A:694:PHE:N	2.42	0.41
6:B:293:THR:HG21	19:B:1743:CLA:HMA3	2.02	0.41
6:B:196:HIS:CE1	19:B:1746:CLA:C1D	3.04	0.41
19:B:1761:CLA:HBA2	19:B:1761:CLA:H3A	1.47	0.41
6:B:180:SER:OG	6:B:285:LEU:HA	2.20	0.41
6:B:190:TRP:C	6:B:192:GLY:N	2.73	0.41
6:B:362:ALA:HA	6:B:365:PHE:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:393:PHE:CE2	6:B:398:TYR:HD2	2.38	0.41
6:B:486:LEU:CD1	19:B:1766:CLA:CMD	2.99	0.41
11:G:60:SER:C	11:G:63:PRO:HD2	2.41	0.41
6:B:690:LEU:HD21	16:L:129:GLN:HA	2.01	0.41
16:L:33:ILE:HD12	16:L:36:TYR:HD1	1.85	0.41
17:N:53:ALA:C	17:N:54:LYS:HD2	2.41	0.41
20:A:7033:LMU:C2'	20:A:7033:LMU:O6B	2.68	0.41
6:B:120:VAL:O	6:B:123:TRP:HD1	2.02	0.41
19:3:3011:CLA:C17	19:3:3011:CLA:H122	2.31	0.41
3:3:158:TYR:C	3:3:160:GLY:N	2.70	0.41
10:F:151:ASP:OD2	10:F:154:PHE:CG	2.73	0.41
10:F:113:LYS:HA	10:F:114:PRO:HD3	1.63	0.41
5:A:490:GLN:C	5:A:490:GLN:HE21	2.24	0.41
19:2:1223:CLA:CBC	19:2:1223:CLA:CMC	2.93	0.41
4:4:30:LEU:O	4:4:30:LEU:CG	2.66	0.41
5:A:158:ILE:HA	5:A:243:PRO:O	2.20	0.41
19:A:1761:CLA:H41	22:A:1803:BCR:C31	2.51	0.41
19:A:1797:CLA:H122	19:A:1797:CLA:H72	1.88	0.41
5:A:509:ALA:O	5:A:510:SER:CB	2.68	0.41
19:B:1748:CLA:H2	19:B:1757:CLA:HBB1	2.02	0.41
6:B:174:ARG:HH12	19:B:1755:CLA:HMD2	1.85	0.41
19:B:1756:CLA:HBA2	19:B:1756:CLA:H3A	1.39	0.41
6:B:586:THR:O	6:B:590:VAL:HG12	2.21	0.41
11:G:20:ARG:NH2	11:G:61:ASN:HA	2.36	0.41
16:L:123:ARG:C	16:L:124:LYS:HD3	2.41	0.41
16:L:68:PHE:HD1	16:L:68:PHE:H	1.68	0.41
4:4:76:TYR:HD1	4:4:76:TYR:O	1.97	0.41
20:N:1086:LMU:C6'	20:N:1086:LMU:C4	2.92	0.41
2:2:202:ALA:O	2:2:203:THR:OG1	2.29	0.41
19:1:1014:CLA:H111	19:1:1014:CLA:H143	1.56	0.41
3:3:197:TYR:CE1	19:3:1214:CLA:CAB	3.03	0.41
3:3:197:TYR:OH	19:3:1214:CLA:C1C	2.68	0.41
20:K:1086:LMU:H122	20:K:1086:LMU:H91	1.27	0.41
10:F:23:LYS:O	10:F:26:GLN:CB	2.48	0.41
3:3:87:GLU:CA	22:3:1225:BCR:H382	2.50	0.41
15:K:51:ASP:N	15:K:52:PRO:HD2	2.36	0.41
19:2:1217:CLA:HED3	19:2:1217:CLA:CAD	2.27	0.41
12:H:37:SER:C	12:H:39:PHE:H	2.23	0.41
19:L:1166:CLA:HED2	19:L:1166:CLA:CAA	2.47	0.41
5:A:35:ALA:O	5:A:36:LYS:HB2	2.21	0.41
8:D:77:LEU:HD23	8:D:77:LEU:HA	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:160:MET:CA	4:4:163:PHE:HB2	2.47	0.41
4:4:80:LYS:O	4:4:81:GLU:HG2	2.21	0.41
19:A:1761:CLA:H141	19:A:1761:CLA:H161	1.63	0.41
19:A:1791:CLA:HBC1	22:A:1805:BCR:C3	2.39	0.41
22:A:1804:BCR:C8	22:A:1804:BCR:C32	2.98	0.41
5:A:205:HIS:CG	19:A:1769:CLA:HMC2	2.55	0.41
5:A:445:HIS:CD2	19:A:1786:CLA:HMB1	2.56	0.41
5:A:571:ASP:HB3	7:C:53:ARG:HH12	1.84	0.41
5:A:76:ARG:NE	5:A:192:LYS:HA	2.35	0.41
19:B:1753:CLA:HBA2	19:B:1753:CLA:H3A	1.43	0.41
6:B:192:GLY:HA2	19:B:1746:CLA:HMC3	2.03	0.41
6:B:448:THR:OG1	6:B:451:LYS:HB2	2.20	0.41
6:B:522:ALA:O	6:B:589:TRP:HE3	2.03	0.41
6:B:594:TRP:CD1	6:B:595:HIS:HB2	2.53	0.41
6:B:710:LEU:HA	6:B:710:LEU:HD22	1.94	0.41
6:B:603:ARG:HB2	6:B:732:LYS:HD3	2.03	0.41
7:C:7:ILE:HG12	7:C:8:TYR:N	2.35	0.41
9:E:36:VAL:HG11	9:E:87:VAL:HG11	2.03	0.41
16:L:95:LEU:HD13	22:L:1169:BCR:H313	1.98	0.41
17:N:45:ASN:CG	17:N:57:LYS:HZ1	2.17	0.41
20:A:7048:LMU:H5B	20:A:7048:LMU:O2B	2.21	0.41
10:F:22:LEU:HA	10:F:25:LEU:HD13	2.03	0.41
19:4:4007:CLA:H52	19:4:4007:CLA:H11	1.86	0.41
16:L:15:ASN:N	16:L:24:GLU:OE1	2.53	0.41
20:A:7038:LMU:H62	20:A:7038:LMU:H91	1.94	0.41
8:D:53:PRO:HB2	8:D:54:LYS:H	1.63	0.41
4:4:108:ASP:O	4:4:111:ASN:O	2.39	0.41
4:4:127:PRO:HB2	4:4:128:ALA:H	1.52	0.41
4:4:44:GLU:HB3	4:4:45:LEU:H	1.73	0.41
19:A:1767:CLA:H111	19:A:1767:CLA:H72	1.49	0.41
5:A:344:LYS:HE2	5:A:344:LYS:HB3	1.89	0.41
5:A:57:LEU:O	5:A:61:ALA:HB2	2.21	0.41
19:B:1752:CLA:HBC3	22:B:1775:BCR:HC7	2.01	0.41
19:B:1757:CLA:H8	22:B:1778:BCR:C12	2.45	0.41
19:B:1739:CLA:H193	19:B:1758:CLA:H192	2.02	0.41
5:A:554:LEU:CD2	19:B:1788:CLA:O2D	2.69	0.41
6:B:309:ILE:CD1	6:B:312:GLY:HA3	2.51	0.41
6:B:525:LEU:CD2	6:B:525:LEU:O	2.55	0.41
6:B:657:TRP:HB3	6:B:658:ALA:H	1.58	0.41
6:B:658:ALA:O	6:B:661:PHE:CD2	2.69	0.41
20:A:7003:LMU:H3B	21:B:8054:SUC:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:5:VAL:HG23	7:C:65:VAL:HG21	1.23	0.41
7:C:69:LEU:O	7:C:71:HIS:N	2.53	0.41
7:C:62:PHE:CZ	9:E:42:GLU:CB	3.04	0.41
16:L:90:GLY:O	16:L:94:ILE:N	2.49	0.41
17:N:65:LEU:O	17:N:67:LEU:CA	2.69	0.41
17:N:69:CYS:O	17:N:72:LYS:HE3	2.20	0.41
17:N:72:LYS:CD	17:N:74:LYS:HG3	2.44	0.41
3:3:189:LEU:C	3:3:191:MET:N	2.74	0.41
3:3:49:ILE:CA	3:3:51:PRO:HD2	2.51	0.41
19:3:1222:CLA:H111	19:3:1222:CLA:H143	1.60	0.41
19:4:4007:CLA:H41	19:4:4007:CLA:H61	1.64	0.41
8:D:111:TYR:CD2	8:D:114:PRO:CG	3.04	0.41
17:N:35:VAL:HG12	17:N:35:VAL:O	2.20	0.41
2:2:191:ASN:ND2	2:2:196:HIS:ND1	2.69	0.41
21:B:8061:SUC:O1'	21:B:8061:SUC:O3'	2.29	0.41
5:A:124:TRP:HE3	5:A:124:TRP:HA	1.84	0.41
19:A:1759:CLA:HBB2	19:A:1760:CLA:C1C	2.51	0.41
5:A:177:LEU:C	5:A:179:LEU:N	2.74	0.41
19:A:1785:CLA:HBD	19:A:1785:CLA:HAA1	2.02	0.41
22:A:1803:BCR:H11C	22:A:1803:BCR:H341	1.69	0.41
22:A:1806:BCR:C23	22:A:1806:BCR:C39	2.74	0.41
5:A:432:LEU:O	5:A:434:ARG:N	2.53	0.41
5:A:436:LEU:O	5:A:438:HIS:O	2.37	0.41
5:A:44:ILE:HG13	5:A:44:ILE:H	1.57	0.41
5:A:76:ARG:HE	5:A:192:LYS:HA	1.86	0.41
6:B:122:GLN:HG3	6:B:361:ILE:CG1	2.44	0.41
19:B:1744:CLA:CMC	19:B:1744:CLA:CBC	2.91	0.41
19:B:1753:CLA:H51	19:B:1753:CLA:CBB	2.50	0.41
19:B:1752:CLA:CBA	19:B:1753:CLA:O1A	2.68	0.41
6:B:431:PHE:HD2	19:B:1763:CLA:HMA3	1.85	0.41
19:B:1765:CLA:HMD2	19:B:1766:CLA:CMC	2.51	0.41
19:B:1771:CLA:H191	13:I:21:MET:HE1	2.03	0.41
19:B:1763:CLA:C7	22:B:1780:BCR:H402	2.50	0.41
23:B:1774:PQN:C17	22:B:1781:BCR:C33	2.93	0.41
19:B:1738:CLA:C7	24:B:1784:LMG:H381	2.49	0.41
6:B:303:TYR:H	6:B:306:GLU:HB2	1.84	0.41
6:B:307:ALA:O	6:B:308:HIS:O	2.38	0.41
6:B:606:VAL:O	6:B:608:GLN:N	2.53	0.41
6:B:696:LYS:NZ	8:D:39:LYS:HE3	2.35	0.41
11:G:44:PHE:HA	11:G:46:ALA:HB2	2.03	0.41
14:J:19:PHE:C	14:J:19:PHE:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1782:CLA:H2	19:A:1782:CLA:H62	1.90	0.41
5:A:227:LEU:HG	5:A:296:LEU:HB2	2.03	0.41
5:A:430:ASP:O	5:A:432:LEU:N	2.54	0.41
5:A:449:VAL:HG21	19:A:1794:CLA:CHC	2.50	0.41
5:A:703:LEU:HA	5:A:703:LEU:HD22	1.66	0.41
19:B:1763:CLA:HBD	19:B:1763:CLA:HBA1	2.01	0.41
19:B:1765:CLA:ND	19:B:1766:CLA:HBB2	2.36	0.41
6:B:416:GLU:O	6:B:420:SER:OG	2.39	0.41
6:B:577:TYR:CD2	6:B:577:TYR:C	2.93	0.41
11:G:23:PHE:CE2	11:G:24:PHE:HB2	2.56	0.41
6:B:694:ARG:HD2	13:I:28:VAL:CG1	2.51	0.41
19:1:1188:CLA:H8	19:1:1188:CLA:H41	0.50	0.41
17:N:57:LYS:CG	17:N:58:VAL:N	2.27	0.41
19:1:1014:CLA:O2D	19:1:1014:CLA:CAA	2.65	0.41
3:3:47:GLY:O	3:3:48:PHE:CD2	2.74	0.41
19:J:1043:CLA:CHA	19:J:1043:CLA:HED2	2.45	0.41
10:F:17:ARG:O	10:F:21:ALA:HB3	2.21	0.41
10:F:17:ARG:CA	10:F:17:ARG:NE	2.83	0.41
10:F:26:GLN:C	10:F:28:SER:H	2.24	0.41
1:1:142:GLU:OE1	19:1:1187:CLA:HMD3	2.20	0.41
20:A:7020:LMU:H62	20:A:7020:LMU:H92	1.26	0.41
20:R:1056:LMU:O2'	20:R:1056:LMU:C2	2.68	0.41
20:R:1056:LMU:H6D	20:R:1056:LMU:C5B	2.50	0.41
20:A:7014:LMU:H1'	20:A:7014:LMU:H4'	1.86	0.41
3:3:158:TYR:CB	3:3:159:PRO:CD	2.82	0.41
8:D:86:LEU:HA	8:D:90:LEU:HB2	2.02	0.41
5:A:277:TYR:HD2	5:A:279:ASP:H	1.68	0.41
16:L:6:PRO:HB2	16:L:9:GLN:O	2.20	0.41
16:L:14:LEU:HD21	16:L:21:GLY:O	2.20	0.41
1:1:36:LEU:O	1:1:40:LYS:N	2.54	0.41
5:A:523:VAL:HG13	5:A:524:GLY:N	2.36	0.41
8:D:70:GLU:OE1	8:D:71:GLY:O	2.39	0.41
19:B:1767:CLA:HBA2	19:B:1767:CLA:H3A	1.67	0.41
3:3:120:LEU:O	3:3:123:PHE:HB3	2.21	0.41
6:B:605:ASN:HD22	6:B:605:ASN:C	2.24	0.41
2:2:52:SER:C	2:2:54:TRP:N	2.75	0.41
3:3:84:ILE:N	3:3:85:PRO:HD3	2.36	0.41
19:A:1774:CLA:H152	19:A:1774:CLA:H8	2.02	0.41
19:A:1789:CLA:HBA1	19:A:1789:CLA:H3A	1.84	0.41
5:A:614:PHE:HE1	19:A:1810:CLA:H62	1.86	0.41
5:A:370:ILE:CD1	19:A:1781:CLA:CGD	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:376:MET:CE	19:A:1784:CLA:OBD	2.69	0.41
19:B:1763:CLA:HAA1	22:B:1779:BCR:H16C	2.03	0.41
19:B:1756:CLA:H42	19:B:1769:CLA:CBA	2.51	0.41
22:B:1777:BCR:C33	22:B:1777:BCR:C8	2.86	0.41
22:B:1777:BCR:H15C	22:B:1777:BCR:H351	1.78	0.41
5:A:554:LEU:HD21	19:B:1788:CLA:O2D	2.20	0.41
6:B:301:ILE:O	6:B:301:ILE:HG23	2.21	0.41
6:B:334:LEU:HD22	19:B:1737:CLA:CHD	2.51	0.41
6:B:696:LYS:HE2	6:B:696:LYS:HB2	1.83	0.41
11:G:58:LEU:HB2	11:G:59:LYS:H	1.35	0.41
19:1:1192:CLA:H62	19:1:1192:CLA:H41	1.76	0.41
3:3:92:TRP:O	3:3:95:THR:CG2	2.68	0.41
17:N:45:ASN:ND2	17:N:54:LYS:CD	2.73	0.41
20:B:1783:LMU:H91	20:B:1783:LMU:H62	1.67	0.41
5:A:316:MET:HA	5:A:317:TYR:HA	1.69	0.41
20:A:7026:LMU:C4	20:A:7026:LMU:H81	2.40	0.41
5:A:141:ARG:CD	10:F:40:LEU:H	2.34	0.41
19:4:1211:CLA:CBC	19:4:1211:CLA:CHD	2.83	0.41
20:A:7013:LMU:O3'	20:A:7013:LMU:C1B	2.65	0.41
16:L:112:PRO:O	16:L:113:SER:CB	2.68	0.41
19:L:1166:CLA:HBC2	19:L:1166:CLA:CHD	2.51	0.41
8:D:96:ILE:O	8:D:97:LYS:CB	2.69	0.41
1:1:121:LYS:HB3	1:1:124:PRO:HG3	2.03	0.41
17:N:9:LYS:HB3	17:N:9:LYS:HE2	1.86	0.41
2:2:109:ARG:O	2:2:113:ILE:HG23	2.21	0.40
2:2:42:ARG:CG	2:2:45:VAL:HB	2.47	0.40
4:4:127:PRO:O	4:4:129:GLY:N	2.37	0.40
5:A:112:ASP:N	5:A:113:PRO:HD3	2.36	0.40
5:A:156:SER:HB2	5:A:159:THR:H	1.86	0.40
19:A:1761:CLA:H3A	19:A:1761:CLA:HBA1	1.66	0.40
19:A:1762:CLA:H71	19:A:1762:CLA:C2	2.51	0.40
5:A:369:THR:HG22	19:A:1784:CLA:HMC1	2.02	0.40
19:A:1787:CLA:H72	19:A:1800:CLA:HBA1	2.04	0.40
22:A:1807:BCR:H311	22:A:1807:BCR:C8	2.51	0.40
5:A:226:SER:O	5:A:230:ASN:OD1	2.39	0.40
5:A:392:GLN:O	5:A:392:GLN:CD	2.60	0.40
5:A:541:VAL:HA	5:A:544:ILE:HG22	2.03	0.40
5:A:588:GLY:N	6:B:668:ARG:CZ	2.84	0.40
5:A:691:MET:HE3	23:A:1801:PQN:H2M1	2.01	0.40
5:A:744:ALA:HB2	22:A:1806:BCR:C30	2.36	0.40
19:B:1750:CLA:HMD3	19:B:1752:CLA:C3B	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:693:TRP:HE1	19:B:1771:CLA:CHD	2.33	0.40
6:B:197:VAL:HG22	6:B:207:VAL:HG11	2.03	0.40
6:B:308:HIS:ND1	6:B:309:ILE:N	2.68	0.40
6:B:51:PHE:CD1	19:B:1744:CLA:HED1	2.56	0.40
6:B:53:GLN:O	6:B:54:LEU:HB2	2.21	0.40
6:B:593:TYR:CD1	19:B:1768:CLA:HMC2	2.56	0.40
7:C:73:THR:HB	7:C:74:THR:H	1.17	0.40
13:I:20:ALA:O	13:I:24:LEU:N	2.54	0.40
16:L:104:ILE:HD12	16:L:104:ILE:C	2.42	0.40
20:1:1199:LMU:H1'	20:1:1199:LMU:H6D	1.87	0.40
2:2:182:ILE:HG22	2:2:205:PHE:HB2	2.03	0.40
10:F:23:LYS:HD2	10:F:23:LYS:HA	1.60	0.40
10:F:46:MET:C	10:F:50:LYS:HB2	2.41	0.40
10:F:68:LEU:HA	10:F:69:PRO:HD3	1.88	0.40
13:I:1:MET:O	13:I:2:ILE:CG2	2.59	0.40
12:H:55:LYS:O	12:H:56:PHE:HB2	2.21	0.40
5:A:483:GLN:HA	5:A:483:GLN:OE1	2.21	0.40
2:2:70:LYS:HE3	2:2:70:LYS:HB3	1.70	0.40
4:4:99:HIS:C	4:4:103:ILE:HD11	2.41	0.40
4:4:32:GLU:CD	4:4:32:GLU:H	2.23	0.40
5:A:281:LEU:CD2	19:A:1772:CLA:CMA	3.00	0.40
5:A:382:TYR:CD2	19:A:1784:CLA:HED3	2.56	0.40
5:A:445:HIS:CE1	19:A:1786:CLA:CMB	3.04	0.40
19:A:1789:CLA:C4	16:L:64:LEU:CD2	2.94	0.40
19:A:1796:CLA:HBA2	19:A:1796:CLA:H3A	1.66	0.40
5:A:225:VAL:C	5:A:228:PRO:HD2	2.42	0.40
5:A:364:MET:HG3	19:A:1780:CLA:HMB2	2.01	0.40
5:A:414:ALA:O	5:A:417:PHE:HB3	2.21	0.40
20:A:7003:LMU:H111	20:A:7006:LMU:H6'1	2.02	0.40
5:A:753:ARG:HH11	5:A:753:ARG:HD3	1.73	0.40
19:B:1735:CLA:HBA2	19:B:1735:CLA:C4A	2.50	0.40
6:B:256:THR:HG23	6:B:272:ASP:OD1	2.22	0.40
6:B:260:GLY:H	6:B:269:TRP:HE1	1.69	0.40
6:B:285:LEU:HD12	22:B:1775:BCR:C17	2.51	0.40
6:B:288:GLY:O	6:B:289:LEU:HD12	2.21	0.40
6:B:691:ILE:O	6:B:691:ILE:HG22	2.21	0.40
6:B:560:ASP:CG	7:C:52:LYS:HZ3	2.24	0.40
8:D:109:VAL:O	8:D:110:GLN:HG3	2.21	0.40
10:F:77:GLN:O	10:F:78:ARG:HG2	2.21	0.40
16:L:125:LYS:C	16:L:127:PRO:CD	2.88	0.40
17:N:58:VAL:O	17:N:59:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:50:GLU:HG3	3:3:51:PRO:N	2.36	0.40
1:1:109:GLU:OE2	19:1:1195:CLA:C1B	2.69	0.40
12:H:19:GLY:O	12:H:20:GLN:CB	2.69	0.40
8:D:48:ILE:CA	8:D:100:PHE:HB3	2.51	0.40
5:A:583:GLY:O	5:A:589:THR:HB	2.21	0.40
5:A:639:ALA:O	5:A:640:GLY:C	2.59	0.40
10:F:142:ARG:NH1	10:F:142:ARG:HA	2.35	0.40
2:2:124:ILE:O	2:2:125:PHE:CG	2.74	0.40
19:A:1762:CLA:HAA2	19:A:1762:CLA:CB	2.52	0.40
19:A:1764:CLA:H112	19:A:1783:CLA:H91	2.02	0.40
5:A:451:ILE:HD13	19:A:1788:CLA:CED	2.42	0.40
19:A:1811:CLA:CED	19:A:1811:CLA:C3D	2.98	0.40
5:A:46:LYS:HG2	5:A:46:LYS:H	1.80	0.40
5:A:567:ARG:CB	5:A:567:ARG:HH21	2.34	0.40
19:A:1795:CLA:NC	19:B:1735:CLA:HBC2	2.36	0.40
6:B:299:HIS:NE2	19:B:1752:CLA:CED	2.85	0.40
19:B:1772:CLA:H3A	19:B:1772:CLA:HBA2	1.76	0.40
6:B:22:TRP:CZ2	19:B:1771:CLA:HMB1	2.57	0.40
6:B:353:TYR:HB2	6:B:594:TRP:CH2	2.56	0.40
7:C:51:CYS:HB2	7:C:53:ARG:H	1.85	0.40
7:C:3:HIS:ND1	7:C:69:LEU:HD12	2.37	0.40
12:H:62:GLY:O	13:I:15:LEU:HD22	2.20	0.40
19:1:1188:CLA:CBB	19:1:1192:CLA:HHC	2.51	0.40
4:4:192:THR:CG2	4:4:193:ILE:N	2.84	0.40
3:3:192:LEU:C	3:3:194:ILE:H	2.23	0.40
20:A:7033:LMU:H5'	20:A:7033:LMU:H1B	1.31	0.40
10:F:29:LEU:HB3	10:F:30:LYS:H	1.72	0.40
10:F:51:LYS:C	10:F:53:PHE:N	2.74	0.40
15:K:5:SER:C	15:K:7:THR:N	2.75	0.40
21:B:8053:SUC:C2	21:B:8053:SUC:C5'	2.97	0.40
10:F:6:THR:HB	10:F:7:PRO:HD2	2.02	0.40
16:L:77:THR:HG21	16:L:82:ALA:CB	2.47	0.40
16:L:9:GLN:HG3	16:L:10:VAL:N	2.36	0.40
11:G:71:VAL:O	11:G:76:SER:OG	2.39	0.40
10:F:116:GLN:HE21	10:F:116:GLN:HB2	1.61	0.40
4:4:187:ASP:HA	4:4:188:PRO:HD3	1.81	0.40
2:2:95:PHE:O	2:2:99:LEU:N	2.44	0.40
4:4:147:LEU:HD22	4:4:148:GLU:HG2	2.02	0.40
4:4:166:PHE:O	4:4:169:GLN:CB	2.55	0.40
5:A:150:PHE:N	5:A:153:TRP:HE3	2.19	0.40
5:A:173:VAL:HG23	5:A:174:PHE:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1806:BCR:H371	22:A:1806:BCR:H24C	1.79	0.40
5:A:242:ILE:CG1	5:A:243:PRO:HD3	2.44	0.40
5:A:413:HIS:HA	5:A:416:ILE:HD12	2.03	0.40
5:A:416:ILE:O	5:A:420:ARG:O	2.38	0.40
5:A:606:TYR:HH	19:A:1810:CLA:HED3	1.87	0.40
5:A:751:LEU:H	5:A:751:LEU:HG	1.69	0.40
19:B:1740:CLA:H93	19:B:1740:CLA:H61	1.85	0.40
22:B:1782:BCR:H321	22:B:1782:BCR:HC7	1.92	0.40
6:B:285:LEU:O	6:B:288:GLY:O	2.39	0.40
6:B:122:GLN:HB2	6:B:358:TYR:HB3	2.02	0.40
6:B:387:PHE:O	6:B:391:PRO:CD	2.67	0.40
10:F:96:TRP:HE3	10:F:134:PHE:N	2.17	0.40
11:G:28:ARG:CD	11:G:33:LYS:HE2	2.48	0.40
11:G:58:LEU:HA	11:G:61:ASN:OD1	2.21	0.40
13:I:12:VAL:HG23	13:I:13:GLY:H	1.87	0.40
16:L:33:ILE:HG13	16:L:37:LEU:CD2	2.52	0.40
3:3:56:TYR:CD1	3:3:185:LYS:NZ	2.84	0.40
21:B:8055:SUC:O1'	21:B:8055:SUC:O3'	2.29	0.40
7:C:11:CYS:C	7:C:13:GLY:N	2.74	0.40
16:L:21:GLY:C	16:L:23:LEU:H	2.24	0.40
6:B:137:THR:HA	6:B:140:ILE:CD1	2.52	0.40
6:B:500:ALA:HB3	6:B:507:SER:O	2.21	0.40
6:B:52:GLY:O	6:B:56:ILE:HG12	2.21	0.40
4:4:184:HIS:ND1	4:4:184:HIS:C	2.74	0.40
19:4:1198:CLA:HMB1	19:4:1198:CLA:CBB	2.50	0.40
5:A:126:ILE:O	5:A:126:ILE:HD12	2.22	0.40
5:A:652:TRP:CE2	19:A:1810:CLA:H142	2.56	0.40
5:A:213:LEU:O	22:A:1803:BCR:C17	2.70	0.40
5:A:396:PHE:CE2	5:A:616:PHE:CD1	3.09	0.40
5:A:40:PHE:CG	5:A:40:PHE:O	2.74	0.40
5:A:701:GLN:NE2	5:A:724:ALA:H	2.20	0.40
6:B:174:ARG:O	6:B:175:LEU:CB	2.67	0.40
22:B:1775:BCR:H341	22:B:1775:BCR:H11C	1.73	0.40
23:A:1801:PQN:H152	22:B:1779:BCR:H322	2.02	0.40
6:B:188:LEU:O	6:B:190:TRP:N	2.55	0.40
6:B:193:HIS:O	6:B:194:LEU:C	2.58	0.40
6:B:203:ARG:HB3	6:B:270:LEU:CD1	2.51	0.40
6:B:300:SER:O	6:B:302:LYS:O	2.40	0.40
6:B:435:GLY:HA3	19:B:1764:CLA:HBB1	2.02	0.40
6:B:471:THR:O	6:B:472:TYR:C	2.60	0.40
19:B:1736:CLA:C4C	22:I:1032:BCR:H401	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:1167:CLA:HAC1	22:L:1169:BCR:H322	2.03	0.40
19:1:1192:CLA:CAA	20:1:1199:LMU:O3'	2.62	0.40
15:K:11:MET:SD	15:K:15:THR:OG1	2.79	0.40
6:B:222:LEU:O	6:B:223:GLY:C	2.60	0.40
12:H:53:LEU:O	12:H:54:LEU:HB3	2.22	0.40
20:A:7031:LMU:H4'	20:A:7031:LMU:C3B	2.47	0.40
6:B:227:THR:O	6:B:229:GLN:N	2.54	0.40

All (62) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:1225:BCR:C28	20:B:1783:LMU:C5[2_556]	0.48	1.72
22:3:1225:BCR:C40	20:B:1783:LMU:C8[2_556]	0.57	1.63
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	0.69	1.51
3:3:181:LEU:CG	6:B:490:ARG:NH2[1_556]	0.72	1.48
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.72	1.48
22:3:1225:BCR:C38	20:B:1783:LMU:C12[2_556]	0.82	1.38
4:4:130:GLU:C	16:L:159:TYR:OH[1_655]	0.88	1.32
3:3:182:LYS:NZ	6:B:491:ASN:ND2[1_556]	0.89	1.31
11:G:31:MET:CE	17:N:85:TRP:CD1[2_546]	1.03	1.17
3:3:181:LEU:CD1	6:B:490:ARG:NH2[1_556]	1.08	1.12
22:3:1225:BCR:C29	20:B:1783:LMU:C7[2_556]	1.12	1.08
22:3:1225:BCR:C26	20:B:1783:LMU:C11[2_556]	1.15	1.05
22:3:1225:BCR:C29	20:B:1783:LMU:C6[2_556]	1.21	0.99
22:3:1225:BCR:C28	20:B:1783:LMU:C6[2_556]	1.26	0.94
11:G:31:MET:SD	17:N:85:TRP:CD2[2_546]	1.27	0.93
22:3:1225:BCR:C25	20:B:1783:LMU:C10[2_556]	1.30	0.90
22:3:1225:BCR:C38	20:B:1783:LMU:C11[2_556]	1.37	0.83
22:3:1225:BCR:C30	20:B:1783:LMU:C6[2_556]	1.40	0.80
22:3:1225:BCR:C30	20:B:1783:LMU:C7[2_556]	1.42	0.78
11:G:31:MET:CE	17:N:85:TRP:CE2[2_546]	1.43	0.77
22:3:1225:BCR:C25	20:B:1783:LMU:C9[2_556]	1.50	0.70
22:3:1225:BCR:C25	20:B:1783:LMU:C6[2_556]	1.52	0.68
22:3:1225:BCR:C40	20:B:1783:LMU:C9[2_556]	1.53	0.67
22:3:1225:BCR:C24	20:B:1783:LMU:C10[2_556]	1.53	0.67
22:3:1225:BCR:C30	20:B:1783:LMU:C8[2_556]	1.59	0.61
22:3:1225:BCR:C29	20:B:1783:LMU:C5[2_556]	1.62	0.58
22:3:1225:BCR:C30	20:B:1783:LMU:C9[2_556]	1.65	0.55
11:G:31:MET:SD	17:N:85:TRP:CG[2_546]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:1225:BCR:C27	20:B:1783:LMU:C6[2_556]	1.68	0.52
22:3:1225:BCR:C26	20:B:1783:LMU:C10[2_556]	1.69	0.51
22:3:1225:BCR:C26	20:B:1783:LMU:C6[2_556]	1.69	0.51
11:G:31:MET:CE	17:N:85:TRP:CG[2_546]	1.71	0.49
11:G:34:GLN:NE2	20:A:7047:LMU:C7[2_646]	1.71	0.49
22:3:1225:BCR:C24	20:B:1783:LMU:C9[2_556]	1.72	0.48
19:1:1193:CLA:O1A	19:1:1142:CLA:O2A[1_654]	1.74	0.46
22:3:1225:BCR:C40	20:B:1783:LMU:C7[2_556]	1.78	0.42
22:3:1225:BCR:C25	20:B:1783:LMU:C11[2_556]	1.81	0.39
6:B:295:PHE:CE1	17:N:85:TRP:CH2[2_546]	1.85	0.35
22:3:1225:BCR:C28	20:B:1783:LMU:C4[2_556]	1.85	0.35
22:3:1225:BCR:C38	20:B:1783:LMU:C10[2_556]	1.86	0.34
11:G:30:ASN:OD1	20:A:7047:LMU:C9[2_646]	1.88	0.32
11:G:31:MET:CE	17:N:85:TRP:CD2[2_546]	1.89	0.31
22:3:1225:BCR:C26	20:B:1783:LMU:C12[2_556]	1.89	0.31
11:G:31:MET:SD	17:N:85:TRP:CE2[2_546]	1.89	0.31
3:3:182:LYS:NZ	6:B:491:ASN:CG[1_556]	1.91	0.29
6:B:3:LEU:CD2	10:F:34:ASP:OD2[2_546]	1.93	0.27
4:4:130:GLU:CA	16:L:159:TYR:OH[1_655]	1.94	0.26
4:4:126:LEU:CD2	16:L:74:LEU:O[1_655]	1.95	0.25
22:3:1225:BCR:C27	20:B:1783:LMU:C5[2_556]	1.96	0.24
20:A:7009:LMU:C6B	20:R:1056:LMU:C12[1_654]	1.97	0.23
20:A:7009:LMU:C6B	20:R:1056:LMU:C10[1_654]	2.02	0.18
11:G:31:MET:SD	17:N:85:TRP:CE3[2_546]	2.05	0.15
4:4:131:VAL:N	16:L:159:TYR:OH[1_655]	2.05	0.15
4:4:133:TYR:OH	16:L:156:PHE:O[1_655]	2.07	0.13
20:A:7009:LMU:O3B	20:R:1056:LMU:C10[1_654]	2.08	0.12
20:A:7009:LMU:O6B	20:R:1056:LMU:C12[1_654]	2.08	0.12
6:B:295:PHE:CE1	17:N:85:TRP:CZ3[2_546]	2.10	0.10
3:3:87:GLU:O	20:B:1783:LMU:C12[2_556]	2.13	0.07
4:4:126:LEU:O	16:L:78:GLU:N[1_655]	2.14	0.06
3:3:181:LEU:CB	6:B:490:ARG:NH2[1_556]	2.14	0.06
20:2:1224:LMU:O2B	19:A:1791:CLA:CMB[1_655]	2.16	0.04
3:3:87:GLU:C	20:B:1783:LMU:C12[2_556]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	160/241 (66%)	83 (52%)	47 (29%)	30 (19%)	0	2
2	2	174/269 (65%)	62 (36%)	48 (28%)	64 (37%)	0	0
3	3	154/276 (56%)	77 (50%)	42 (27%)	35 (23%)	0	1
4	4	164/251 (65%)	56 (34%)	47 (29%)	61 (37%)	0	0
5	A	726/758 (96%)	333 (46%)	198 (27%)	195 (27%)	0	0
6	B	731/734 (100%)	362 (50%)	186 (25%)	183 (25%)	0	1
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	49 (36%)	41 (30%)	46 (34%)	0	0
9	E	63/143 (44%)	28 (44%)	15 (24%)	20 (32%)	0	0
10	F	152/231 (66%)	69 (45%)	41 (27%)	42 (28%)	0	0
11	G	93/167 (56%)	37 (40%)	25 (27%)	31 (33%)	0	0
12	H	67/144 (46%)	28 (42%)	15 (22%)	24 (36%)	0	0
13	I	28/40 (70%)	10 (36%)	11 (39%)	7 (25%)	0	1
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	1
15	K	82/131 (63%)	54 (66%)	12 (15%)	16 (20%)	0	2
16	L	159/216 (74%)	65 (41%)	46 (29%)	48 (30%)	0	0
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0
All	All	3091/4108 (75%)	1377 (44%)	833 (27%)	881 (28%)	0	0

All (881) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	90	PRO
1	1	130	PRO
1	1	137	PRO
1	1	161	PHE
1	1	178	ALA
1	1	183	ASP
2	2	37	ASP
2	2	40	SER

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Mol	Chain	Res	Type
2	2	41	LEU
2	2	42	ARG
2	2	45	VAL
2	2	66	GLU
2	2	70	LYS
2	2	74	LEU
2	2	75	ASN
2	2	81	THR
2	2	104	TRP
2	2	120	ASN
2	2	125	PHE
2	2	128	ASN
2	2	129	LYS
2	2	130	LEU
2	2	149	GLY
2	2	154	GLN
2	2	159	LEU
2	2	160	ARG
2	2	188	PRO
2	2	189	ILE
2	2	190	ASP
2	2	197	LEU
2	2	200	PRO
2	2	204	ILE
2	2	207	ALA
2	2	209	THR
2	2	210	PRO
3	3	48	PHE
3	3	49	ILE
3	3	85	PRO
3	3	97	PHE
3	3	107	TRP
3	3	108	ALA
3	3	110	SER
3	3	111	TYR
3	3	113	LEU
3	3	134	LYS
3	3	135	PRO
3	3	142	TYR
3	3	158	TYR
3	3	159	PRO
3	3	164	PHE

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Mol	Chain	Res	Type
3	3	166	PRO
3	3	167	LEU
3	3	172	ASP
3	3	206	VAL
3	3	210	GLN
4	4	32	GLU
4	4	34	PRO
4	4	35	GLU
4	4	38	ARG
4	4	45	LEU
4	4	60	LEU
4	4	66	SER
4	4	69	ILE
4	4	73	PRO
4	4	74	LYS
4	4	82	GLU
4	4	84	PHE
4	4	87	SER
4	4	88	SER
4	4	107	GLN
4	4	115	VAL
4	4	121	PHE
4	4	122	LYS
4	4	125	SER
4	4	126	LEU
4	4	128	ALA
4	4	141	LEU
4	4	143	PHE
4	4	148	GLU
4	4	150	LYS
4	4	171	ASN
4	4	172	VAL
4	4	173	THR
4	4	175	LYS
4	4	178	PHE
4	4	192	THR
4	4	193	ILE
5	A	22	VAL
5	A	23	ASP
5	A	25	ASP
5	A	26	PRO
5	A	27	ILE

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Mol	Chain	Res	Type
5	A	28	LYS
5	A	35	ALA
5	A	36	LYS
5	A	40	PHE
5	A	60	ASP
5	A	67	HIS
5	A	69	SER
5	A	71	LEU
5	A	82	HIS
5	A	83	PHE
5	A	88	ILE
5	A	99	HIS
5	A	104	SER
5	A	155	ALA
5	A	156	SER
5	A	157	GLY
5	A	158	ILE
5	A	159	THR
5	A	160	SER
5	A	175	ALA
5	A	193	LEU
5	A	205	HIS
5	A	221	HIS
5	A	237	VAL
5	A	244	LEU
5	A	247	GLU
5	A	250	LEU
5	A	252	ARG
5	A	258	LEU
5	A	268	PRO
5	A	279	ASP
5	A	280	PHE
5	A	281	LEU
5	A	282	THR
5	A	283	PHE
5	A	286	GLY
5	A	299	ILE
5	A	307	ALA
5	A	310	PHE
5	A	328	LYS
5	A	329	ASP
5	A	333	ALA

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Mol	Chain	Res	Type
5	A	339	THR
5	A	346	LEU
5	A	349	ILE
5	A	361	ASN
5	A	386	ALA
5	A	389	TYR
5	A	423	ASP
5	A	427	ARG
5	A	428	TYR
5	A	429	ASN
5	A	433	ASP
5	A	473	PRO
5	A	474	GLN
5	A	477	PHE
5	A	486	PRO
5	A	489	ALA
5	A	498	LEU
5	A	507	ALA
5	A	508	THR
5	A	509	ALA
5	A	510	SER
5	A	521	VAL
5	A	523	VAL
5	A	553	VAL
5	A	578	ARG
5	A	579	PHE
5	A	594	ALA
5	A	643	ALA
5	A	657	LEU
5	A	673	SER
5	A	679	PHE
5	A	727	ILE
5	A	735	VAL
5	A	750	PHE
5	A	751	LEU
5	A	752	ALA
5	A	757	VAL
6	B	5	ILE
6	B	6	PRO
6	B	26	ALA
6	B	35	ASP
6	B	68	VAL

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Mol	Chain	Res	Type
6	B	69	ALA
6	B	77	TRP
6	B	80	ASP
6	B	83	HIS
6	B	86	PRO
6	B	99	PRO
6	B	104	PHE
6	B	120	VAL
6	B	129	LEU
6	B	136	TYR
6	B	140	ILE
6	B	142	LEU
6	B	159	PRO
6	B	160	LYS
6	B	167	TRP
6	B	182	LEU
6	B	187	SER
6	B	198	ALA
6	B	208	ARG
6	B	231	ASN
6	B	248	GLN
6	B	265	THR
6	B	292	ARG
6	B	293	THR
6	B	294	ASN
6	B	308	HIS
6	B	310	PRO
6	B	320	LYS
6	B	321	GLY
6	B	362	ALA
6	B	375	HIS
6	B	378	ILE
6	B	382	ILE
6	B	383	MET
6	B	405	ASP
6	B	420	SER
6	B	450	GLU
6	B	479	SER
6	B	480	SER
6	B	490	ARG
6	B	494	LEU
6	B	495	PRO

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Mol	Chain	Res	Type
6	B	505	SER
6	B	506	ASN
6	B	512	ILE
6	B	528	HIS
6	B	539	LEU
6	B	545	LYS
6	B	555	TYR
6	B	569	ASP
6	B	587	ILE
6	B	599	ILE
6	B	603	ARG
6	B	605	ASN
6	B	610	ASN
6	B	629	SER
6	B	636	THR
6	B	639	VAL
6	B	657	TRP
6	B	661	PHE
6	B	662	MET
6	B	668	ARG
6	B	681	ALA
6	B	682	HIS
6	B	691	ILE
6	B	707	LEU
6	B	710	LEU
6	B	731	GLY
7	C	8	TYR
7	C	21	CYS
7	C	32	GLY
7	C	49	VAL
7	C	56	SER
7	C	59	PRO
7	C	62	PHE
7	C	65	VAL
7	C	66	ARG
7	C	75	ARG
8	D	32	SER
8	D	36	LEU
8	D	38	ARG
8	D	65	ALA
8	D	70	GLU
8	D	78	ALA

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Mol	Chain	Res	Type
8	D	94	TYR
8	D	95	LYS
8	D	97	LYS
8	D	109	VAL
8	D	114	PRO
8	D	115	LYS
8	D	119	TYR
8	D	120	PRO
8	D	121	GLU
8	D	124	ASN
8	D	132	LEU
8	D	139	LYS
8	D	146	VAL
8	D	151	LYS
8	D	153	PRO
9	E	35	LYS
9	E	46	PHE
9	E	53	VAL
9	E	54	ALA
9	E	60	LYS
9	E	64	PRO
9	E	65	VAL
9	E	72	VAL
9	E	73	ASN
9	E	86	GLU
9	E	87	VAL
9	E	90	VAL
10	F	2	ILE
10	F	7	PRO
10	F	12	LYS
10	F	21	ALA
10	F	25	LEU
10	F	26	GLN
10	F	31	LEU
10	F	35	ASP
10	F	38	PRO
10	F	42	ILE
10	F	47	GLU
10	F	52	ARG
10	F	54	ASP
10	F	58	LYS
10	F	59	TYR

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Mol	Chain	Res	Type
10	F	77	GLN
10	F	109	ARG
10	F	116	GLN
10	F	127	SER
10	F	130	LEU
10	F	152	ASN
10	F	153	ASN
11	G	31	MET
11	G	33	LYS
11	G	34	GLN
11	G	38	GLN
11	G	42	SER
11	G	50	ARG
11	G	59	LYS
11	G	61	ASN
11	G	70	ASP
11	G	74	TRP
11	G	81	VAL
11	G	86	LEU
11	G	87	ALA
11	G	94	ASP
12	H	15	ALA
12	H	17	THR
12	H	20	GLN
12	H	24	TYR
12	H	31	PRO
12	H	41	GLU
12	H	46	PRO
12	H	50	ARG
12	H	52	LEU
12	H	56	PHE
12	H	71	ASN
12	H	77	LEU
13	I	22	ALA
13	I	23	SER
14	J	5	LYS
14	J	6	THR
14	J	10	VAL
14	J	22	LEU
14	J	39	PHE
15	K	41	GLU
15	K	44	GLU

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Mol	Chain	Res	Type
15	K	47	ILE
15	K	52	PRO
15	K	75	VAL
16	L	6	PRO
16	L	8	TYR
16	L	10	VAL
16	L	37	LEU
16	L	43	TYR
16	L	44	ARG
16	L	46	ALA
16	L	63	LEU
16	L	75	ARG
16	L	76	ASN
16	L	88	ALA
16	L	97	MET
16	L	121	THR
16	L	123	ARG
16	L	125	LYS
16	L	127	PRO
16	L	128	ASP
16	L	129	GLN
16	L	149	SER
16	L	154	ALA
16	L	158	MET
16	L	163	LEU
16	L	164	PRO
17	N	2	VAL
17	N	7	LEU
17	N	11	LYS
17	N	24	THR
17	N	27	ALA
17	N	28	ASN
17	N	40	CYS
17	N	43	PRO
17	N	45	ASN
17	N	47	THR
17	N	51	ASP
17	N	58	VAL
17	N	61	LEU
17	N	63	ASP
17	N	66	ASP
17	N	68	GLU

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Mol	Chain	Res	Type
17	N	75	TYR
17	N	76	LYS
17	N	77	CYS
17	N	80	ASN
17	N	82	PHE
17	N	83	TRP
1	1	21	ASP
1	1	27	LEU
1	1	28	GLY
1	1	29	LEU
1	1	61	GLU
2	2	69	THR
2	2	71	LEU
2	2	73	ILE
2	2	82	ALA
2	2	91	THR
2	2	103	GLY
2	2	113	ILE
2	2	136	GLY
2	2	163	GLU
2	2	168	ARG
2	2	192	LEU
2	2	194	ALA
2	2	205	PHE
2	2	206	ALA
2	2	208	PHE
3	3	52	LYS
3	3	77	ILE
3	3	95	THR
3	3	106	TYR
3	3	137	SER
3	3	162	PRO
3	3	208	PRO
4	4	36	ASN
4	4	59	LEU
4	4	70	ILE
4	4	71	ASN
4	4	85	ALA
4	4	91	PHE
4	4	106	TRP
4	4	127	PRO
4	4	129	GLY

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Mol	Chain	Res	Type
4	4	154	ILE
4	4	162	ALA
4	4	167	ILE
4	4	186	SER
4	4	188	PRO
5	A	39	HIS
5	A	45	ALA
5	A	57	LEU
5	A	74	ILE
5	A	96	MET
5	A	105	ASN
5	A	130	GLU
5	A	144	GLN
5	A	149	PHE
5	A	184	PHE
5	A	189	ALA
5	A	210	LEU
5	A	213	LEU
5	A	215	SER
5	A	234	ASN
5	A	242	ILE
5	A	243	PRO
5	A	263	ALA
5	A	266	ALA
5	A	278	ALA
5	A	290	LEU
5	A	292	GLY
5	A	308	ILE
5	A	313	ALA
5	A	337	PRO
5	A	347	TYR
5	A	373	ALA
5	A	400	MET
5	A	421	ASP
5	A	424	PRO
5	A	431	LEU
5	A	439	ARG
5	A	446	LEU
5	A	476	MET
5	A	479	ASP
5	A	505	PRO
5	A	511	THR

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Mol	Chain	Res	Type
5	A	514	THR
5	A	516	GLY
5	A	518	GLY
5	A	538	ASP
5	A	574	ASN
5	A	592	VAL
5	A	624	VAL
5	A	637	ILE
5	A	640	GLY
5	A	649	ILE
5	A	661	ALA
5	A	671	SER
5	A	701	GLN
5	A	742	GLY
6	B	20	ARG
6	B	42	LEU
6	B	103	ALA
6	B	105	THR
6	B	115	ASN
6	B	128	GLY
6	B	153	GLY
6	B	188	LEU
6	B	207	VAL
6	B	222	LEU
6	B	224	PRO
6	B	228	GLY
6	B	230	TRP
6	B	232	LEU
6	B	234	ALA
6	B	237	PRO
6	B	247	THR
6	B	267	SER
6	B	318	GLY
6	B	330	ILE
6	B	371	LEU
6	B	437	TYR
6	B	464	GLN
6	B	469	LYS
6	B	481	THR
6	B	503	GLU
6	B	514	PRO
6	B	554	GLY

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Mol	Chain	Res	Type
6	B	592	PHE
6	B	664	LEU
6	B	690	LEU
6	B	716	GLY
6	B	733	PHE
7	C	10	THR
7	C	22	PRO
7	C	43	PRO
7	C	61	ASP
7	C	64	SER
7	C	68	TYR
7	C	70	TRP
8	D	26	SER
8	D	31	GLY
8	D	35	GLY
8	D	53	PRO
8	D	63	GLY
8	D	110	GLN
8	D	129	GLY
8	D	130	VAL
8	D	138	GLY
8	D	150	GLY
9	E	30	PRO
9	E	42	GLU
9	E	89	GLU
9	E	91	ALA
10	F	46	MET
10	F	126	ALA
10	F	138	VAL
10	F	141	TYR
11	G	22	VAL
11	G	28	ARG
11	G	46	ALA
11	G	63	PRO
11	G	80	ILE
11	G	85	ILE
11	G	93	TYR
12	H	23	VAL
12	H	34	SER
12	H	37	SER
12	H	44	ALA
12	H	75	ASP

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Mol	Chain	Res	Type
13	I	25	PHE
14	J	26	LEU
14	J	37	LEU
15	K	27	ALA
15	K	32	ARG
15	K	35	THR
15	K	40	LEU
15	K	45	SER
15	K	73	GLY
15	K	79	LYS
16	L	11	ILE
16	L	24	GLU
16	L	27	VAL
16	L	36	TYR
16	L	64	LEU
16	L	89	ALA
16	L	108	LYS
16	L	120	LEU
16	L	161	LEU
17	N	35	VAL
17	N	42	PHE
17	N	48	GLY
17	N	54	LYS
17	N	69	CYS
17	N	71	GLY
17	N	74	LYS
17	N	78	GLY
1	1	55	PRO
1	1	78	PRO
1	1	79	GLY
1	1	118	PRO
1	1	122	LYS
1	1	133	TYR
1	1	184	PRO
2	2	53	ARG
2	2	94	LEU
2	2	96	ILE
2	2	114	LEU
3	3	88	THR
3	3	91	PRO
3	3	153	SER
3	3	157	ALA

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Mol	Chain	Res	Type
4	4	93	ILE
4	4	119	PRO
4	4	145	PRO
5	A	41	SER
5	A	63	ASP
5	A	73	GLU
5	A	114	THR
5	A	116	ILE
5	A	124	TRP
5	A	127	VAL
5	A	151	GLN
5	A	200	GLU
5	A	225	VAL
5	A	305	ALA
5	A	317	TYR
5	A	354	TRP
5	A	355	HIS
5	A	404	GLY
5	A	426	THR
5	A	485	GLN
5	A	537	ALA
5	A	659	ALA
5	A	717	ALA
6	B	8	PHE
6	B	41	ARG
6	B	43	TYR
6	B	71	GLN
6	B	161	TRP
6	B	173	SER
6	B	178	HIS
6	B	179	LEU
6	B	189	ALA
6	B	223	GLY
6	B	225	LEU
6	B	239	SER
6	B	240	SER
6	B	272	ASP
6	B	273	VAL
6	B	278	LEU
6	B	281	ALA
6	B	309	ILE
6	B	361	ILE

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Mol	Chain	Res	Type
6	B	400	PRO
6	B	468	GLY
6	B	474	PHE
6	B	477	PRO
6	B	482	ASN
6	B	493	TRP
6	B	501	ILE
6	B	558	PRO
6	B	732	LYS
7	C	37	LYS
8	D	55	GLU
8	D	93	LYS
8	D	128	GLN
10	F	11	SER
10	F	34	ASP
10	F	44	ALA
10	F	53	PHE
10	F	63	CYS
10	F	114	PRO
11	G	84	TYR
11	G	89	ALA
12	H	27	ASP
12	H	45	ALA
13	I	2	ILE
14	J	9	SER
14	J	23	ALA
14	J	38	THR
15	K	48	GLN
16	L	113	SER
16	L	147	GLY
17	N	9	LYS
17	N	21	ARG
17	N	56	LYS
17	N	81	VAL
1	1	124	PRO
1	1	140	LEU
1	1	177	LEU
2	2	57	LEU
2	2	109	ARG
2	2	150	SER
2	2	180	GLN
2	2	186	THR

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Mol	Chain	Res	Type
2	2	198	ALA
3	3	75	PRO
3	3	141	GLN
3	3	156	PRO
3	3	169	PHE
4	4	57	GLY
4	4	72	VAL
4	4	112	PRO
4	4	139	ASN
4	4	177	PRO
4	4	187	ASP
5	A	31	PHE
5	A	37	PRO
5	A	135	ASP
5	A	230	ASN
5	A	276	LYS
5	A	410	ALA
5	A	422	TYR
5	A	571	ASP
5	A	702	GLU
5	A	738	TYR
6	B	54	LEU
6	B	164	SER
6	B	170	ASN
6	B	217	PRO
6	B	227	THR
6	B	229	GLN
6	B	270	LEU
6	B	335	GLY
6	B	354	SER
6	B	379	ALA
6	B	451	LYS
6	B	475	ASP
6	B	476	ILE
6	B	478	LEU
6	B	540	ASP
6	B	595	HIS
6	B	596	TRP
6	B	623	TYR
6	B	627	ASN
6	B	687	LEU
6	B	730	SER

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Mol	Chain	Res	Type
7	C	9	ASP
7	C	12	ILE
7	C	28	MET
8	D	46	TYR
8	D	60	MET
8	D	106	SER
8	D	143	PRO
9	E	61	THR
9	E	84	LEU
10	F	39	ALA
10	F	83	PHE
10	F	117	LYS
10	F	128	SER
10	F	132	ARG
10	F	151	ASP
11	G	36	PRO
11	G	56	SER
11	G	96	SER
12	H	18	THR
13	I	9	VAL
15	K	29	SER
16	L	48	ASN
16	L	50	LEU
16	L	85	SER
16	L	86	LEU
16	L	112	PRO
17	N	17	ASN
17	N	25	THR
17	N	49	CYS
17	N	70	GLU
1	1	84	TYR
2	2	68	LEU
2	2	115	ASN
2	2	140	GLY
2	2	146	LEU
2	2	179	PHE
2	2	187	GLY
4	4	92	VAL
4	4	137	ILE
5	A	95	GLY
5	A	186	TYR
5	A	235	ALA

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Mol	Chain	Res	Type
5	A	269	PHE
5	A	306	ILE
5	A	353	SER
5	A	375	HIS
5	A	472	ARG
5	A	503	THR
5	A	580	PRO
5	A	709	TRP
5	A	720	THR
6	B	139	ALA
6	B	206	TYR
6	B	212	PHE
6	B	421	HIS
6	B	460	ALA
6	B	472	TYR
6	B	550	LYS
6	B	559	CYS
6	B	586	THR
6	B	593	TYR
6	B	598	HIS
6	B	704	GLN
6	B	708	VAL
7	C	30	PRO
7	C	35	LYS
7	C	52	LYS
7	C	58	CYS
7	C	73	THR
8	D	22	PRO
8	D	40	ALA
8	D	104	PHE
8	D	125	PRO
8	D	148	PHE
9	E	52	VAL
10	F	73	VAL
11	G	91	ASN
12	H	16	ASN
12	H	74	GLN
13	I	5	PRO
16	L	61	GLY
16	L	135	GLY
16	L	159	TYR
17	N	34	THR

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Mol	Chain	Res	Type
17	N	50	GLN
17	N	62	SER
1	1	32	VAL
1	1	125	GLY
1	1	145	VAL
2	2	116	PRO
4	4	118	ASP
5	A	29	THR
5	A	48	PRO
5	A	86	LEU
5	A	179	LEU
5	A	239	PRO
5	A	259	TYR
5	A	500	PRO
5	A	570	PRO
5	A	721	GLN
6	B	94	PRO
6	B	162	LYS
6	B	219	PRO
6	B	360	PHE
6	B	367	THR
6	B	391	PRO
6	B	498	LEU
6	B	564	ARG
6	B	630	GLN
7	C	55	GLU
8	D	34	GLY
10	F	37	ALA
10	F	61	LEU
10	F	102	ARG
11	G	67	ASN
12	H	72	ALA
15	K	34	ALA
15	K	51	ASP
16	L	69	VAL
16	L	157	LEU
4	4	168	ILE
5	A	223	VAL
5	A	229	ILE
5	A	531	PRO
5	A	584	PRO
5	A	696	GLY

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Mol	Chain	Res	Type
5	A	754	ILE
6	B	557	PHE
6	B	711	VAL
4	4	165	GLY
5	A	190	ALA
5	A	716	VAL
6	B	606	VAL
8	D	67	ILE
9	E	55	VAL
11	G	64	VAL
11	G	71	VAL
16	L	53	GLY
16	L	72	GLY
16	L	150	GLY
17	N	59	PRO
2	2	182	ILE
6	B	87	ILE
6	B	463	ILE
8	D	28	ILE
11	G	35	VAL
1	1	89	VAL
1	1	173	PRO
2	2	135	VAL
2	2	167	GLY
5	A	718	PRO
6	B	113	VAL
12	H	60	GLY
13	I	12	VAL
4	4	63	VAL
16	L	16	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	126/190 (66%)	99 (79%)	27 (21%)	<b>1</b> <b>7</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	141/216 (65%)	78 (55%)	63 (45%)	0	0
3	3	118/215 (55%)	78 (66%)	40 (34%)	0	2
4	4	139/201 (69%)	73 (52%)	66 (48%)	0	0
5	A	592/618 (96%)	395 (67%)	197 (33%)	0	2
6	B	598/600 (100%)	369 (62%)	229 (38%)	0	1
7	C	70/70 (100%)	40 (57%)	30 (43%)	0	1
8	D	118/173 (68%)	75 (64%)	43 (36%)	0	1
9	E	56/114 (49%)	36 (64%)	20 (36%)	0	1
10	F	127/190 (67%)	74 (58%)	53 (42%)	0	1
11	G	79/144 (55%)	47 (60%)	32 (40%)	0	1
12	H	57/115 (50%)	26 (46%)	31 (54%)	0	0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0	3
14	J	36/39 (92%)	24 (67%)	12 (33%)	0	2
15	K	61/102 (60%)	39 (64%)	22 (36%)	0	1
16	L	124/169 (73%)	81 (65%)	43 (35%)	0	2
17	N	74/139 (53%)	33 (45%)	41 (55%)	0	0
All	All	2542/3331 (76%)	1585 (62%)	957 (38%)	0	1

All (957) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	17	SER
1	1	27	LEU
1	1	37	GLU
1	1	43	GLU
1	1	47	CYS
1	1	52	LEU
1	1	57	ILE
1	1	63	LEU
1	1	65	TYR
1	1	85	LEU
1	1	105	ILE
1	1	110	HIS
1	1	111	GLN
1	1	117	ASP
1	1	120	LYS

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Mol	Chain	Res	Type
1	1	121	LYS
1	1	129	ASP
1	1	133	TYR
1	1	134	SER
1	1	136	ASP
1	1	139	LYS
1	1	140	LEU
1	1	142	GLU
1	1	179	THR
1	1	181	LEU
1	1	183	ASP
1	1	185	TRP
2	2	37	ASP
2	2	41	LEU
2	2	42	ARG
2	2	53	ARG
2	2	57	LEU
2	2	63	PHE
2	2	64	ILE
2	2	66	GLU
2	2	67	PHE
2	2	69	THR
2	2	70	LYS
2	2	73	ILE
2	2	75	ASN
2	2	76	THR
2	2	78	SER
2	2	79	TRP
2	2	80	TYR
2	2	85	GLN
2	2	86	GLU
2	2	87	TYR
2	2	89	THR
2	2	92	THR
2	2	95	PHE
2	2	97	VAL
2	2	98	GLU
2	2	99	LEU
2	2	100	VAL
2	2	101	PHE
2	2	109	ARG
2	2	110	TRP

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Mol	Chain	Res	Type
2	2	112	ASP
2	2	115	ASN
2	2	118	CYS
2	2	120	ASN
2	2	122	ASP
2	2	127	ASN
2	2	131	THR
2	2	133	THR
2	2	137	TYR
2	2	143	PHE
2	2	144	ASP
2	2	146	LEU
2	2	150	SER
2	2	157	LYS
2	2	159	LEU
2	2	160	ARG
2	2	161	THR
2	2	162	LYS
2	2	164	ILE
2	2	171	MET
2	2	179	PHE
2	2	180	GLN
2	2	183	TYR
2	2	189	ILE
2	2	190	ASP
2	2	191	ASN
2	2	193	PHE
2	2	196	HIS
2	2	199	ASP
2	2	201	HIS
2	2	204	ILE
2	2	205	PHE
2	2	211	LYS
3	3	50	GLU
3	3	60	ILE
3	3	67	LEU
3	3	73	ILE
3	3	76	GLU
3	3	78	LEU
3	3	83	LEU
3	3	84	ILE
3	3	86	GLN

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Mol	Chain	Res	Type
3	3	90	LEU
3	3	93	PHE
3	3	94	ARG
3	3	95	THR
3	3	97	PHE
3	3	106	TYR
3	3	107	TRP
3	3	109	ASP
3	3	111	TYR
3	3	112	THR
3	3	128	ARG
3	3	131	ASP
3	3	141	GLN
3	3	146	LEU
3	3	150	LEU
3	3	163	PHE
3	3	164	PHE
3	3	165	ASN
3	3	171	LYS
3	3	181	LEU
3	3	182	LYS
3	3	185	LYS
3	3	188	ARG
3	3	191	MET
3	3	192	LEU
3	3	195	LEU
3	3	198	PHE
3	3	200	GLN
3	3	204	THR
3	3	209	TYR
3	3	210	GLN
4	4	32	GLU
4	4	35	GLU
4	4	38	ARG
4	4	45	LEU
4	4	49	ARG
4	4	50	TRP
4	4	52	MET
4	4	59	LEU
4	4	60	LEU
4	4	64	PHE
4	4	66	SER

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Mol	Chain	Res	Type
4	4	67	ILE
4	4	75	TRP
4	4	76	TYR
4	4	82	GLU
4	4	83	TYR
4	4	84	PHE
4	4	87	SER
4	4	90	LEU
4	4	91	PHE
4	4	92	VAL
4	4	93	ILE
4	4	94	GLU
4	4	95	PHE
4	4	97	LEU
4	4	99	HIS
4	4	101	VAL
4	4	103	ILE
4	4	104	ARG
4	4	105	ARG
4	4	107	GLN
4	4	109	ILE
4	4	118	ASP
4	4	120	ILE
4	4	121	PHE
4	4	122	LYS
4	4	125	SER
4	4	126	LEU
4	4	131	VAL
4	4	139	ASN
4	4	146	THR
4	4	147	LEU
4	4	150	LYS
4	4	151	GLU
4	4	152	LYS
4	4	154	ILE
4	4	156	ASN
4	4	158	ARG
4	4	159	LEU
4	4	160	MET
4	4	161	LEU
4	4	163	PHE
4	4	164	LEU

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Mol	Chain	Res	Type
4	4	167	ILE
4	4	168	ILE
4	4	169	GLN
4	4	172	VAL
4	4	175	LYS
4	4	178	PHE
4	4	180	ASN
4	4	184	HIS
4	4	186	SER
4	4	187	ASP
4	4	189	TRP
4	4	190	HIS
4	4	192	THR
5	A	21	LEU
5	A	24	ARG
5	A	27	ILE
5	A	31	PHE
5	A	34	TRP
5	A	40	PHE
5	A	44	ILE
5	A	46	LYS
5	A	50	THR
5	A	52	THR
5	A	60	ASP
5	A	62	HIS
5	A	63	ASP
5	A	68	THR
5	A	69	SER
5	A	71	LEU
5	A	72	GLU
5	A	78	VAL
5	A	82	HIS
5	A	83	PHE
5	A	86	LEU
5	A	88	ILE
5	A	94	SER
5	A	102	ARG
5	A	103	PHE
5	A	107	GLU
5	A	109	TRP
5	A	111	ASN
5	A	114	THR

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Mol	Chain	Res	Type
5	A	124	TRP
5	A	130	GLU
5	A	131	ILE
5	A	133	ASN
5	A	135	ASP
5	A	141	ARG
5	A	144	GLN
5	A	164	LEU
5	A	167	THR
5	A	172	LEU
5	A	177	LEU
5	A	180	PHE
5	A	188	LYS
5	A	193	LEU
5	A	197	GLN
5	A	203	LEU
5	A	207	LEU
5	A	213	LEU
5	A	223	VAL
5	A	224	HIS
5	A	227	LEU
5	A	230	ASN
5	A	231	GLN
5	A	232	PHE
5	A	238	ASP
5	A	242	ILE
5	A	248	PHE
5	A	249	ILE
5	A	251	ASN
5	A	253	ASP
5	A	254	LEU
5	A	255	LEU
5	A	261	SER
5	A	262	PHE
5	A	277	TYR
5	A	281	LEU
5	A	284	ARG
5	A	287	LEU
5	A	290	LEU
5	A	296	LEU
5	A	297	THR
5	A	298	ASP

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Mol	Chain	Res	Type
5	A	299	ILE
5	A	304	LEU
5	A	308	ILE
5	A	309	LEU
5	A	316	MET
5	A	331	LEU
5	A	332	GLU
5	A	334	HIS
5	A	339	THR
5	A	341	GLN
5	A	352	THR
5	A	353	SER
5	A	357	GLN
5	A	361	ASN
5	A	368	LEU
5	A	369	THR
5	A	375	HIS
5	A	376	MET
5	A	377	TYR
5	A	379	MET
5	A	384	TYR
5	A	387	THR
5	A	391	THR
5	A	392	GLN
5	A	393	LEU
5	A	397	THR
5	A	400	MET
5	A	402	ILE
5	A	405	PHE
5	A	420	ARG
5	A	422	TYR
5	A	426	THR
5	A	427	ARG
5	A	433	ASP
5	A	434	ARG
5	A	435	VAL
5	A	438	HIS
5	A	439	ARG
5	A	440	ASP
5	A	444	SER
5	A	446	LEU
5	A	458	PHE

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Mol	Chain	Res	Type
5	A	462	ILE
5	A	464	ASN
5	A	466	THR
5	A	477	PHE
5	A	479	ASP
5	A	480	THR
5	A	488	PHE
5	A	490	GLN
5	A	495	THR
5	A	498	LEU
5	A	503	THR
5	A	514	THR
5	A	520	LEU
5	A	521	VAL
5	A	529	LEU
5	A	530	LEU
5	A	532	ILE
5	A	536	THR
5	A	539	PHE
5	A	540	LEU
5	A	547	PHE
5	A	548	THR
5	A	553	VAL
5	A	554	LEU
5	A	555	ILE
5	A	557	LEU
5	A	558	LYS
5	A	561	LEU
5	A	564	ARG
5	A	567	ARG
5	A	568	LEU
5	A	569	ILE
5	A	572	LYS
5	A	575	LEU
5	A	577	PHE
5	A	578	ARG
5	A	590	CYS
5	A	591	GLN
5	A	600	LEU
5	A	605	MET
5	A	607	ASN
5	A	613	ILE

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Mol	Chain	Res	Type
5	A	614	PHE
5	A	623	ASP
5	A	629	ASN
5	A	630	ASP
5	A	631	GLN
5	A	633	VAL
5	A	637	ILE
5	A	638	THR
5	A	641	ASN
5	A	642	PHE
5	A	644	GLN
5	A	645	SER
5	A	646	SER
5	A	653	LEU
5	A	654	ARG
5	A	657	LEU
5	A	660	GLN
5	A	662	SER
5	A	663	GLN
5	A	664	VAL
5	A	673	SER
5	A	677	LEU
5	A	684	PHE
5	A	685	VAL
5	A	689	SER
5	A	691	MET
5	A	692	PHE
5	A	697	ARG
5	A	703	LEU
5	A	707	ILE
5	A	715	LYS
5	A	723	ARG
5	A	726	SER
5	A	727	ILE
5	A	728	VAL
5	A	733	VAL
5	A	735	VAL
5	A	736	THR
5	A	740	LEU
5	A	745	THR
5	A	751	LEU
5	A	754	ILE

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Mol	Chain	Res	Type
6	B	3	LEU
6	B	4	ARG
6	B	5	ILE
6	B	6	PRO
6	B	9	SER
6	B	14	GLN
6	B	15	ASP
6	B	17	THR
6	B	19	ARG
6	B	20	ARG
6	B	25	ILE
6	B	35	ASP
6	B	41	ARG
6	B	45	ASN
6	B	46	ILE
6	B	50	HIS
6	B	51	PHE
6	B	53	GLN
6	B	57	ILE
6	B	67	HIS
6	B	70	TRP
6	B	71	GLN
6	B	75	GLU
6	B	83	HIS
6	B	84	VAL
6	B	91	ILE
6	B	104	PHE
6	B	110	LEU
6	B	113	VAL
6	B	114	ASN
6	B	121	TYR
6	B	122	GLN
6	B	123	TRP
6	B	124	TRP
6	B	127	ILE
6	B	129	LEU
6	B	130	ARG
6	B	132	ASN
6	B	134	ASP
6	B	136	TYR
6	B	137	THR
6	B	140	ILE

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Mol	Chain	Res	Type
6	B	142	LEU
6	B	143	LEU
6	B	144	PHE
6	B	145	LEU
6	B	151	LEU
6	B	154	TRP
6	B	157	LEU
6	B	160	LYS
6	B	161	TRP
6	B	164	SER
6	B	175	LEU
6	B	177	HIS
6	B	178	HIS
6	B	180	SER
6	B	188	LEU
6	B	195	VAL
6	B	199	ILE
6	B	203	ARG
6	B	206	TYR
6	B	208	ARG
6	B	210	ASN
6	B	214	ASP
6	B	216	LEU
6	B	226	LEU
6	B	229	GLN
6	B	231	ASN
6	B	232	LEU
6	B	243	LEU
6	B	246	THR
6	B	248	GLN
6	B	257	ILE
6	B	258	LEU
6	B	262	HIS
6	B	265	THR
6	B	266	GLN
6	B	269	TRP
6	B	270	LEU
6	B	271	THR
6	B	272	ASP
6	B	278	LEU
6	B	285	LEU
6	B	292	ARG

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Mol	Chain	Res	Type
6	B	294	ASN
6	B	295	PHE
6	B	297	ILE
6	B	299	HIS
6	B	300	SER
6	B	301	ILE
6	B	309	ILE
6	B	315	LEU
6	B	317	ARG
6	B	325	THR
6	B	326	ILE
6	B	330	ILE
6	B	332	PHE
6	B	348	VAL
6	B	350	GLN
6	B	352	MET
6	B	353	TYR
6	B	355	LEU
6	B	361	ILE
6	B	363	GLN
6	B	364	ASP
6	B	365	PHE
6	B	372	TYR
6	B	374	HIS
6	B	382	ILE
6	B	383	MET
6	B	384	THR
6	B	387	PHE
6	B	393	PHE
6	B	396	ARG
6	B	403	ASN
6	B	406	ASN
6	B	407	VAL
6	B	410	ARG
6	B	412	LEU
6	B	418	ILE
6	B	419	ILE
6	B	420	SER
6	B	422	LEU
6	B	423	SER
6	B	427	LEU
6	B	428	PHE

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Mol	Chain	Res	Type
6	B	431	PHE
6	B	436	LEU
6	B	437	TYR
6	B	438	VAL
6	B	440	ASN
6	B	443	MET
6	B	446	PHE
6	B	448	THR
6	B	452	GLN
6	B	454	LEU
6	B	458	ILE
6	B	461	GLN
6	B	464	GLN
6	B	471	THR
6	B	472	TYR
6	B	478	LEU
6	B	481	THR
6	B	486	LEU
6	B	492	ILE
6	B	494	LEU
6	B	501	ILE
6	B	502	ASN
6	B	504	ASN
6	B	508	LEU
6	B	509	PHE
6	B	510	LEU
6	B	512	ILE
6	B	514	PRO
6	B	516	ASP
6	B	517	PHE
6	B	521	HIS
6	B	525	LEU
6	B	527	LEU
6	B	528	HIS
6	B	532	LEU
6	B	533	ILE
6	B	539	LEU
6	B	540	ASP
6	B	544	SER
6	B	545	LYS
6	B	551	LYS
6	B	555	TYR

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Mol	Chain	Res	Type
6	B	560	ASP
6	B	564	ARG
6	B	569	ASP
6	B	577	TYR
6	B	578	LEU
6	B	580	VAL
6	B	583	MET
6	B	584	LEU
6	B	587	ILE
6	B	592	PHE
6	B	594	TRP
6	B	596	TRP
6	B	601	LEU
6	B	603	ARG
6	B	605	ASN
6	B	606	VAL
6	B	607	SER
6	B	608	GLN
6	B	611	GLU
6	B	615	TYR
6	B	616	LEU
6	B	617	MET
6	B	620	LEU
6	B	621	ARG
6	B	622	ASP
6	B	629	SER
6	B	631	LEU
6	B	633	ASN
6	B	638	LEU
6	B	640	CYS
6	B	643	LEU
6	B	645	VAL
6	B	649	MET
6	B	651	LEU
6	B	659	THR
6	B	662	MET
6	B	664	LEU
6	B	665	ILE
6	B	670	TYR
6	B	672	GLN
6	B	674	LEU
6	B	676	GLU

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Mol	Chain	Res	Type
6	B	677	THR
6	B	682	HIS
6	B	685	THR
6	B	689	ASN
6	B	690	LEU
6	B	691	ILE
6	B	692	ARG
6	B	700	LEU
6	B	702	ILE
6	B	703	VAL
6	B	710	LEU
6	B	712	HIS
6	B	715	VAL
6	B	718	ILE
6	B	719	PHE
6	B	721	TYR
6	B	725	LEU
6	B	732	LYS
6	B	733	PHE
7	C	2	SER
7	C	4	SER
7	C	7	ILE
7	C	10	THR
7	C	12	ILE
7	C	15	THR
7	C	16	GLN
7	C	18	VAL
7	C	23	THR
7	C	24	ASP
7	C	28	MET
7	C	37	LYS
7	C	38	GLN
7	C	45	THR
7	C	48	CYS
7	C	52	LYS
7	C	58	CYS
7	C	59	PRO
7	C	62	PHE
7	C	63	LEU
7	C	66	ARG
7	C	67	VAL
7	C	68	TYR

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Mol	Chain	Res	Type
7	C	69	LEU
7	C	70	TRP
7	C	73	THR
7	C	74	THR
7	C	77	MET
7	C	79	LEU
7	C	81	TYR
8	D	26	SER
8	D	28	ILE
8	D	41	GLN
8	D	44	GLU
8	D	46	TYR
8	D	47	VAL
8	D	48	ILE
8	D	49	THR
8	D	50	TRP
8	D	56	GLN
8	D	57	ILE
8	D	58	PHE
8	D	69	ARG
8	D	70	GLU
8	D	73	ASN
8	D	75	LEU
8	D	79	ARG
8	D	81	GLU
8	D	82	GLN
8	D	83	CYS
8	D	86	LEU
8	D	89	ARG
8	D	92	SER
8	D	93	LYS
8	D	95	LYS
8	D	96	ILE
8	D	98	TYR
8	D	104	PHE
8	D	105	PRO
8	D	111	TYR
8	D	116	ASP
8	D	121	GLU
8	D	122	LYS
8	D	123	VAL
8	D	127	ARG

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Mol	Chain	Res	Type
8	D	128	GLN
8	D	134	MET
8	D	135	ARG
8	D	137	ILE
8	D	139	LYS
8	D	144	ILE
8	D	147	LYS
8	D	151	LYS
9	E	28	ILE
9	E	31	LYS
9	E	32	ARG
9	E	35	LYS
9	E	36	VAL
9	E	39	LEU
9	E	40	ARG
9	E	42	GLU
9	E	45	TRP
9	E	47	LYS
9	E	48	ASN
9	E	55	VAL
9	E	56	ASP
9	E	58	ASP
9	E	61	THR
9	E	68	ARG
9	E	73	ASN
9	E	76	ASN
9	E	79	THR
9	E	84	LEU
10	F	8	CYS
10	F	9	LYS
10	F	12	LYS
10	F	13	GLN
10	F	14	PHE
10	F	17	ARG
10	F	18	GLU
10	F	20	GLN
10	F	23	LYS
10	F	24	LYS
10	F	25	LEU
10	F	26	GLN
10	F	28	SER
10	F	29	LEU

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Mol	Chain	Res	Type
10	F	31	LEU
10	F	43	LYS
10	F	48	LYS
10	F	51	LYS
10	F	52	ARG
10	F	53	PHE
10	F	61	LEU
10	F	71	LEU
10	F	77	GLN
10	F	78	ARG
10	F	79	HIS
10	F	83	PHE
10	F	88	ILE
10	F	91	LEU
10	F	92	TYR
10	F	93	ILE
10	F	96	TRP
10	F	100	VAL
10	F	104	TYR
10	F	106	ILE
10	F	108	ILE
10	F	110	ASP
10	F	111	GLU
10	F	113	LYS
10	F	115	THR
10	F	116	GLN
10	F	119	ILE
10	F	121	ILE
10	F	123	VAL
10	F	135	SER
10	F	136	TRP
10	F	137	PRO
10	F	138	VAL
10	F	141	TYR
10	F	142	ARG
10	F	143	GLU
10	F	146	ASN
10	F	153	ASN
10	F	154	PHE
11	G	7	VAL
11	G	10	LEU
11	G	12	THR

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Mol	Chain	Res	Type
11	G	15	SER
11	G	17	PHE
11	G	18	LEU
11	G	22	VAL
11	G	24	PHE
11	G	28	ARG
11	G	30	ASN
11	G	31	MET
11	G	33	LYS
11	G	39	ASN
11	G	41	MET
11	G	42	SER
11	G	43	HIS
11	G	44	PHE
11	G	45	GLU
11	G	48	ASP
11	G	49	THR
11	G	50	ARG
11	G	55	VAL
11	G	57	LEU
11	G	58	LEU
11	G	62	ASP
11	G	71	VAL
11	G	76	SER
11	G	83	TYR
11	G	88	THR
11	G	91	ASN
11	G	93	TYR
11	G	97	PHE
12	H	11	LEU
12	H	14	ILE
12	H	17	THR
12	H	20	GLN
12	H	21	TRP
12	H	24	TYR
12	H	30	SER
12	H	32	TYR
12	H	33	ASN
12	H	35	LEU
12	H	36	GLN
12	H	37	SER
12	H	41	GLU

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Mol	Chain	Res	Type
12	H	42	THR
12	H	43	PHE
12	H	47	PHE
12	H	48	THR
12	H	49	LYS
12	H	52	LEU
12	H	53	LEU
12	H	54	LEU
12	H	55	LYS
12	H	56	PHE
12	H	57	LEU
12	H	59	LEU
12	H	64	LEU
12	H	66	THR
12	H	67	TYR
12	H	69	SER
12	H	75	ASP
12	H	77	LEU
13	I	3	ASN
13	I	7	LEU
13	I	9	VAL
13	I	11	LEU
13	I	12	VAL
13	I	16	PHE
13	I	26	LEU
13	I	30	LYS
14	J	2	ARG
14	J	3	ASP
14	J	4	PHE
14	J	5	LYS
14	J	9	SER
14	J	13	VAL
14	J	14	LEU
14	J	16	THR
14	J	19	PHE
14	J	35	ASP
14	J	37	LEU
14	J	41	PHE
15	K	3	ILE
15	K	9	LEU
15	K	10	ILE
15	K	11	MET

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Mol	Chain	Res	Type
15	K	13	THR
15	K	15	THR
15	K	17	LEU
15	K	19	LEU
15	K	20	PHE
15	K	23	ARG
15	K	32	ARG
15	K	40	LEU
15	K	41	GLU
15	K	43	ARG
15	K	44	GLU
15	K	45	SER
15	K	48	GLN
15	K	56	THR
15	K	59	ASP
15	K	63	CYS
15	K	69	ILE
15	K	72	VAL
16	L	5	LYS
16	L	8	TYR
16	L	9	GLN
16	L	10	VAL
16	L	14	LEU
16	L	15	ASN
16	L	20	ILE
16	L	30	SER
16	L	32	LEU
16	L	38	SER
16	L	39	ASN
16	L	40	LEU
16	L	44	ARG
16	L	52	ARG
16	L	54	VAL
16	L	58	LEU
16	L	63	LEU
16	L	68	PHE
16	L	70	LYS
16	L	74	LEU
16	L	76	ASN
16	L	77	THR
16	L	79	TYR
16	L	94	ILE

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Mol	Chain	Res	Type
16	L	97	MET
16	L	107	PHE
16	L	108	LYS
16	L	111	GLU
16	L	118	LEU
16	L	120	LEU
16	L	123	ARG
16	L	124	LYS
16	L	134	ASP
16	L	136	TRP
16	L	140	THR
16	L	145	PHE
16	L	149	SER
16	L	152	THR
16	L	158	MET
16	L	159	TYR
16	L	161	LEU
16	L	163	LEU
16	L	165	TYR
17	N	4	GLU
17	N	5	GLU
17	N	6	TYR
17	N	10	SER
17	N	11	LYS
17	N	16	LEU
17	N	25	THR
17	N	28	ASN
17	N	29	PHE
17	N	33	TYR
17	N	37	PHE
17	N	39	SER
17	N	40	CYS
17	N	41	LYS
17	N	46	PHE
17	N	49	CYS
17	N	50	GLN
17	N	51	ASP
17	N	52	LEU
17	N	54	LYS
17	N	55	GLN
17	N	57	LYS
17	N	58	VAL

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Mol	Chain	Res	Type
17	N	60	PHE
17	N	61	LEU
17	N	62	SER
17	N	64	ASP
17	N	65	LEU
17	N	66	ASP
17	N	67	LEU
17	N	68	GLU
17	N	69	CYS
17	N	70	GLU
17	N	72	LYS
17	N	73	ASP
17	N	75	TYR
17	N	79	SER
17	N	81	VAL
17	N	82	PHE
17	N	83	TRP
17	N	84	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	111	GLN
2	2	115	ASN
2	2	128	ASN
2	2	181	HIS
2	2	191	ASN
3	3	105	ASN
3	3	126	HIS
3	3	165	ASN
4	4	71	ASN
4	4	169	GLN
4	4	170	HIS
4	4	180	ASN
5	A	58	HIS
5	A	99	HIS
5	A	121	GLN
5	A	129	GLN
5	A	144	GLN
5	A	197	GLN
5	A	224	HIS
5	A	230	ASN

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Mol	Chain	Res	Type
5	A	231	GLN
5	A	246	HIS
5	A	302	HIS
5	A	303	HIS
5	A	343	HIS
5	A	361	ASN
5	A	375	HIS
5	A	398	HIS
5	A	447	ASN
5	A	464	ASN
5	A	474	GLN
5	A	490	GLN
5	A	542	HIS
5	A	545	HIS
5	A	591	GLN
5	A	607	ASN
5	A	629	ASN
5	A	636	HIS
5	A	641	ASN
5	A	660	GLN
5	A	683	HIS
5	A	701	GLN
5	A	711	HIS
6	B	14	GLN
6	B	29	HIS
6	B	34	HIS
6	B	50	HIS
6	B	67	HIS
6	B	71	GLN
6	B	95	HIS
6	B	122	GLN
6	B	158	GLN
6	B	178	HIS
6	B	193	HIS
6	B	220	GLN
6	B	266	GLN
6	B	277	HIS
6	B	328	ASN
6	B	333	GLN
6	B	375	HIS
6	B	399	ASN
6	B	403	ASN

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Mol	Chain	Res	Type
6	B	406	ASN
6	B	432	HIS
6	B	461	GLN
6	B	502	ASN
6	B	504	ASN
6	B	506	ASN
6	B	521	HIS
6	B	528	HIS
6	B	595	HIS
6	B	605	ASN
6	B	608	GLN
6	B	610	ASN
6	B	630	GLN
6	B	633	ASN
6	B	641	ASN
6	B	672	GLN
6	B	712	HIS
7	C	71	HIS
8	D	41	GLN
8	D	56	GLN
8	D	73	ASN
8	D	82	GLN
8	D	128	GLN
8	D	133	ASN
8	D	152	GLN
9	E	48	ASN
9	E	73	ASN
10	F	77	GLN
10	F	116	GLN
10	F	146	ASN
10	F	152	ASN
10	F	153	ASN
11	G	61	ASN
11	G	67	ASN
12	H	16	ASN
12	H	33	ASN
12	H	36	GLN
12	H	71	ASN
14	J	30	ASN
15	K	80	ASN
16	L	12	GLN
16	L	15	ASN

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Mol	Chain	Res	Type
16	L	39	ASN
16	L	48	ASN
16	L	131	GLN
17	N	45	ASN
17	N	55	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 262 ligands modelled in this entry, 1 is unknown - leaving 261 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	CLA	1	1010	-	16,32,73	1.80	3 (18%)	21,54,113	3.20	12 (57%)
19	CLA	1	1014	-	51,69,73	2.06	13 (25%)	56,108,113	4.77	27 (48%)
19	CLA	1	1142	-	32,53,73	2.51	11 (34%)	37,89,113	5.57	15 (40%)
19	CLA	1	1145	-	45,63,73	2.38	15 (33%)	49,101,113	5.77	23 (46%)
19	CLA	1	1146	-	40,58,73	2.50	15 (37%)	44,95,113	5.40	21 (47%)
19	CLA	1	1148	-	45,63,73	2.31	13 (28%)	49,101,113	4.74	19 (38%)
19	CLA	1	1149	-	36,54,73	2.67	13 (36%)	42,90,113	4.93	25 (59%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	1	1187	1	36,54,73	2.50	14 (38%)	41,90,113	5.55	26 (63%)
19	CLA	1	1188	19	47,65,73	2.12	14 (29%)	50,103,113	5.06	24 (48%)
19	CLA	1	1189	-	37,55,73	2.42	10 (27%)	42,91,113	5.12	18 (42%)
19	CLA	1	1190	-	36,54,73	2.53	11 (30%)	41,90,113	4.45	17 (41%)
19	CLA	1	1191	-	16,32,73	1.72	5 (31%)	21,54,113	4.20	14 (66%)
19	CLA	1	1192	19	51,69,73	2.12	10 (19%)	56,108,113	3.69	17 (30%)
19	CLA	1	1193	-	41,59,73	2.43	14 (34%)	44,96,113	4.89	21 (47%)
19	CLA	1	1194	-	16,32,73	2.05	7 (43%)	21,54,113	4.15	12 (57%)
19	CLA	1	1195	1	24,44,73	2.82	8 (33%)	28,78,113	4.34	11 (39%)
19	CLA	1	1196	-	41,59,73	2.95	18 (43%)	44,96,113	5.39	22 (50%)
19	CLA	1	1197	-	16,32,73	1.81	4 (25%)	21,54,113	3.36	12 (57%)
19	CLA	1	1198	-	16,32,73	1.78	4 (25%)	21,54,113	3.77	12 (57%)
20	LMU	1	1199	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
20	LMU	1	1200	-	36,36,36	0.80	0	47,47,47	2.18	16 (34%)
19	CLA	1	1241	-	45,63,73	2.25	10 (22%)	49,101,113	4.83	19 (38%)
19	CLA	1	1303	-	16,32,73	1.77	6 (37%)	21,54,113	2.91	10 (47%)
19	CLA	1	1307	-	16,32,73	1.94	7 (43%)	21,54,113	3.81	14 (66%)
19	CLA	1	1308	-	38,56,73	2.38	12 (31%)	42,92,113	5.25	16 (38%)
19	CLA	1	1309	-	16,32,73	1.80	5 (31%)	21,54,113	3.93	10 (47%)
19	CLA	1	1505	-	45,63,73	2.20	12 (26%)	49,101,113	4.68	20 (40%)
19	CLA	2	1212	-	41,59,73	2.29	11 (26%)	44,96,113	5.18	17 (38%)
19	CLA	2	1213	-	55,73,73	2.01	11 (20%)	61,113,113	3.68	20 (32%)
19	CLA	2	1214	-	16,32,73	1.92	7 (43%)	21,54,113	3.71	12 (57%)
19	CLA	2	1215	-	40,58,73	2.27	11 (27%)	44,95,113	4.49	17 (38%)
19	CLA	2	1216	-	16,32,73	1.93	7 (43%)	21,54,113	3.57	12 (57%)
19	CLA	2	1217	2	55,73,73	2.14	11 (20%)	61,113,113	4.44	19 (31%)
19	CLA	2	1218	-	55,73,73	2.01	9 (16%)	61,113,113	4.08	21 (34%)
19	CLA	2	1219	-	16,32,73	1.70	3 (18%)	21,54,113	3.15	12 (57%)
19	CLA	2	1220	-	24,44,73	2.66	8 (33%)	28,78,113	5.04	16 (57%)
19	CLA	2	1221	-	16,32,73	1.73	3 (18%)	21,54,113	3.16	12 (57%)
19	CLA	2	1222	2	40,58,73	2.32	10 (25%)	44,95,113	4.34	18 (40%)
19	CLA	2	1223	-	40,58,73	2.38	10 (25%)	44,95,113	5.00	16 (36%)
20	LMU	2	1224	-	36,36,36	0.80	1 (2%)	47,47,47	0.94	2 (4%)
21	SUC	2	1225	-	23,23,24	1.10	2 (8%)	35,35,36	2.24	12 (34%)
19	CLA	2	2010	-	16,32,73	1.79	4 (25%)	21,54,113	2.85	8 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	3	1212	3	40,58,73	2.41	13 (32%)	44,95,113	4.97	22 (50%)
19	CLA	3	1213	-	16,32,73	2.02	7 (43%)	21,54,113	3.33	12 (57%)
19	CLA	3	1214	-	24,44,73	2.73	8 (33%)	28,78,113	4.06	13 (46%)
19	CLA	3	1215	-	16,32,73	1.97	5 (31%)	21,54,113	3.29	12 (57%)
19	CLA	3	1216	-	16,32,73	1.83	5 (31%)	21,54,113	3.26	11 (52%)
19	CLA	3	1217	-	16,32,73	1.83	5 (31%)	21,54,113	3.27	12 (57%)
19	CLA	3	1218	-	32,50,73	2.43	9 (28%)	36,85,113	5.45	19 (52%)
19	CLA	3	1219	-	55,73,73	2.01	9 (16%)	61,113,113	4.19	19 (31%)
19	CLA	3	1220	-	16,32,73	1.63	3 (18%)	21,54,113	3.01	11 (52%)
19	CLA	3	1221	-	16,32,73	2.01	6 (37%)	21,54,113	3.60	12 (57%)
19	CLA	3	1222	3	55,73,73	2.22	16 (29%)	61,113,113	5.29	21 (34%)
19	CLA	3	1223	-	16,32,73	2.07	6 (37%)	21,54,113	4.68	14 (66%)
19	CLA	3	1224	-	55,73,73	2.23	13 (23%)	61,113,113	5.00	20 (32%)
22	BCR	3	1225	-	41,41,41	2.05	5 (12%)	56,56,56	5.88	21 (37%)
21	SUC	3	1226	-	24,24,24	0.90	0	36,36,36	2.21	8 (22%)
19	CLA	3	3001	-	16,32,73	1.94	4 (25%)	21,54,113	3.30	11 (52%)
19	CLA	3	3008	-	40,58,73	2.33	8 (20%)	44,95,113	4.42	18 (40%)
19	CLA	3	3011	-	55,73,73	1.87	10 (18%)	61,113,113	3.98	17 (27%)
19	CLA	3	3015	-	16,32,73	1.99	6 (37%)	21,54,113	3.77	11 (52%)
19	CLA	4	1196	4	45,63,73	2.23	12 (26%)	49,101,113	4.91	17 (34%)
19	CLA	4	1197	-	24,44,73	2.84	8 (33%)	28,78,113	4.76	16 (57%)
19	CLA	4	1198	-	55,73,73	2.30	16 (29%)	61,113,113	4.57	24 (39%)
19	CLA	4	1199	-	45,63,73	2.12	10 (22%)	49,101,113	4.29	17 (34%)
19	CLA	4	1200	-	40,58,73	2.46	12 (30%)	44,95,113	6.11	23 (52%)
19	CLA	4	1201	4	42,60,73	2.74	20 (47%)	45,97,113	5.78	32 (71%)
19	CLA	4	1202	-	24,44,73	2.72	9 (37%)	28,78,113	4.49	13 (46%)
19	CLA	4	1203	-	16,32,73	2.46	7 (43%)	21,54,113	4.02	12 (57%)
19	CLA	4	1204	-	16,32,73	1.90	6 (37%)	21,54,113	3.13	10 (47%)
19	CLA	4	1205	-	45,63,73	2.26	9 (20%)	49,101,113	4.46	17 (34%)
19	CLA	4	1206	-	55,73,73	2.01	11 (20%)	61,113,113	4.46	20 (32%)
19	CLA	4	1207	-	16,32,73	1.74	4 (25%)	21,54,113	3.28	11 (52%)
19	CLA	4	1208	-	16,32,73	1.59	2 (12%)	21,54,113	3.30	13 (61%)
19	CLA	4	1209	4	24,44,73	2.67	8 (33%)	28,78,113	5.08	15 (53%)
19	CLA	4	1210	4	16,32,73	1.72	4 (25%)	21,54,113	2.62	11 (52%)
19	CLA	4	1211	-	36,54,73	2.68	15 (41%)	41,90,113	5.09	15 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMU	4	1212	-	36,36,36	0.73	0	47,47,47	1.20	4 (8%)
19	CLA	4	4007	-	42,60,73	2.71	16 (38%)	45,97,113	5.28	21 (46%)
19	CLA	4	4014	20	37,55,73	2.34	11 (29%)	42,91,113	5.25	16 (38%)
19	CLA	A	1759	-	40,58,73	2.38	13 (32%)	44,95,113	5.05	19 (43%)
19	CLA	A	1760	19	45,63,73	2.33	12 (26%)	49,101,113	3.53	17 (34%)
19	CLA	A	1761	-	55,73,73	2.00	11 (20%)	61,113,113	3.97	19 (31%)
19	CLA	A	1762	-	45,63,73	2.19	10 (22%)	49,101,113	4.90	19 (38%)
19	CLA	A	1763	5,22	36,54,73	2.77	16 (44%)	41,90,113	6.33	20 (48%)
19	CLA	A	1764	5	55,73,73	2.11	13 (23%)	61,113,113	4.10	21 (34%)
19	CLA	A	1765	-	42,60,73	2.19	10 (23%)	45,97,113	4.47	19 (42%)
19	CLA	A	1766	-	32,53,73	2.52	9 (28%)	37,89,113	5.25	19 (51%)
19	CLA	A	1767	19,5	55,73,73	2.07	11 (20%)	61,113,113	3.99	22 (36%)
19	CLA	A	1768	5	44,62,73	2.17	11 (25%)	47,99,113	4.12	15 (31%)
19	CLA	A	1769	-	44,62,73	2.08	11 (25%)	47,99,113	4.06	20 (42%)
19	CLA	A	1770	-	32,53,73	2.63	9 (28%)	37,89,113	4.66	15 (40%)
19	CLA	A	1771	5	40,58,73	2.74	16 (40%)	44,95,113	5.73	29 (65%)
19	CLA	A	1772	5	44,62,73	2.38	13 (29%)	47,99,113	5.01	20 (42%)
19	CLA	A	1773	-	42,60,73	2.34	11 (26%)	45,97,113	5.00	16 (35%)
19	CLA	A	1774	-	55,73,73	1.99	11 (20%)	61,113,113	3.64	20 (32%)
19	CLA	A	1775	-	16,32,73	1.81	3 (18%)	21,54,113	2.78	8 (38%)
19	CLA	A	1776	-	55,73,73	1.94	9 (16%)	61,113,113	4.02	20 (32%)
19	CLA	A	1777	-	41,59,73	2.32	11 (26%)	44,96,113	4.90	17 (38%)
19	CLA	A	1778	5	32,50,73	2.48	10 (31%)	36,85,113	5.20	16 (44%)
19	CLA	A	1779	-	45,63,73	2.22	11 (24%)	49,101,113	4.58	18 (36%)
19	CLA	A	1780	-	55,73,73	1.83	10 (18%)	61,113,113	3.61	19 (31%)
19	CLA	A	1781	-	55,73,73	1.93	11 (20%)	61,113,113	4.42	17 (27%)
19	CLA	A	1782	19	55,73,73	1.94	11 (20%)	61,113,113	4.42	17 (27%)
19	CLA	A	1783	-	55,73,73	2.00	10 (18%)	61,113,113	4.28	20 (32%)
19	CLA	A	1784	5	45,63,73	2.24	11 (24%)	49,101,113	4.54	16 (32%)
19	CLA	A	1785	-	55,73,73	1.97	12 (21%)	61,113,113	4.05	22 (36%)
19	CLA	A	1786	-	40,58,73	2.26	10 (25%)	44,95,113	5.05	21 (47%)
19	CLA	A	1787	5	55,73,73	2.02	10 (18%)	61,113,113	4.09	20 (32%)
19	CLA	A	1788	-	55,73,73	1.97	11 (20%)	61,113,113	4.30	18 (29%)
19	CLA	A	1789	-	45,63,73	2.14	11 (24%)	49,101,113	4.80	22 (44%)
19	CLA	A	1790	19,5	40,58,73	2.27	10 (25%)	44,95,113	4.51	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	A	1791	19,5	32,53,73	2.41	10 (31%)	37,89,113	5.69	19 (51%)
19	CLA	A	1792	-	39,57,73	2.40	10 (25%)	43,93,113	4.88	17 (39%)
19	CLA	A	1793	-	55,73,73	2.06	12 (21%)	61,113,113	4.17	19 (31%)
19	CLA	A	1794	-	37,55,73	2.33	11 (29%)	42,91,113	4.27	14 (33%)
19	CLA	A	1795	-	37,55,73	2.51	12 (32%)	42,91,113	4.91	19 (45%)
19	CLA	A	1796	-	55,73,73	2.07	10 (18%)	61,113,113	4.36	20 (32%)
19	CLA	A	1797	19	55,73,73	2.26	14 (25%)	61,113,113	4.78	25 (40%)
19	CLA	A	1798	-	40,58,73	2.29	9 (22%)	44,95,113	5.02	17 (38%)
19	CLA	A	1799	-	55,73,73	1.98	12 (21%)	61,113,113	4.45	20 (32%)
19	CLA	A	1800	-	45,63,73	2.29	9 (20%)	49,101,113	4.20	18 (36%)
23	PQN	A	1801	-	34,34,34	1.54	3 (8%)	44,45,45	1.44	7 (15%)
22	BCR	A	1802	5	41,41,41	1.92	4 (9%)	56,56,56	5.89	19 (33%)
22	BCR	A	1803	-	41,41,41	2.02	3 (7%)	56,56,56	5.93	19 (33%)
22	BCR	A	1804	-	41,41,41	1.99	5 (12%)	56,56,56	5.92	22 (39%)
22	BCR	A	1805	-	41,41,41	2.07	4 (9%)	56,56,56	5.91	23 (41%)
22	BCR	A	1806	-	41,41,41	2.05	5 (12%)	56,56,56	5.93	23 (41%)
22	BCR	A	1807	19	41,41,41	1.92	4 (9%)	56,56,56	5.91	19 (33%)
20	LMU	A	1808	-	36,36,36	0.84	0	47,47,47	1.45	7 (14%)
20	LMU	A	1809	-	36,36,36	0.84	1 (2%)	47,47,47	1.76	11 (23%)
19	CLA	A	1810	-	55,73,73	2.09	13 (23%)	61,113,113	4.48	20 (32%)
19	CLA	A	1811	-	55,73,73	2.02	12 (21%)	61,113,113	4.19	19 (31%)
19	CLA	A	1812	-	55,73,73	2.14	11 (20%)	61,113,113	4.39	19 (31%)
20	LMU	A	7003	-	36,36,36	0.39	0	47,47,47	0.73	1 (2%)
20	LMU	A	7004	-	36,36,36	0.37	0	47,47,47	0.71	1 (2%)
20	LMU	A	7005	-	36,36,36	0.70	0	47,47,47	1.94	12 (25%)
20	LMU	A	7006	-	36,36,36	0.38	0	47,47,47	0.73	1 (2%)
20	LMU	A	7009	20	35,35,36	0.29	0	46,46,47	0.73	1 (2%)
20	LMU	A	7010	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
20	LMU	A	7013	-	36,36,36	0.43	0	47,47,47	1.64	11 (23%)
20	LMU	A	7014	-	36,36,36	1.01	2 (5%)	47,47,47	2.53	15 (31%)
20	LMU	A	7015	-	36,36,36	0.82	1 (2%)	47,47,47	1.48	7 (14%)
20	LMU	A	7016	-	36,36,36	0.67	1 (2%)	47,47,47	1.98	12 (25%)
20	LMU	A	7017	-	36,36,36	0.68	2 (5%)	47,47,47	2.35	15 (31%)
20	LMU	A	7019	-	36,36,36	0.92	1 (2%)	47,47,47	1.43	7 (14%)
20	LMU	A	7020	-	36,36,36	0.42	0	47,47,47	1.81	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMU	A	7021	-	36,36,36	0.77	0	47,47,47	2.09	14 (29%)
20	LMU	A	7022	-	36,36,36	0.75	0	47,47,47	2.23	17 (36%)
20	LMU	A	7023	-	36,36,36	0.77	1 (2%)	47,47,47	2.00	18 (38%)
20	LMU	A	7024	-	36,36,36	0.83	1 (2%)	47,47,47	1.72	11 (23%)
20	LMU	A	7025	-	36,36,36	0.86	1 (2%)	47,47,47	1.59	11 (23%)
20	LMU	A	7026	21	36,36,36	1.11	3 (8%)	47,47,47	3.17	22 (46%)
20	LMU	A	7027	-	36,36,36	1.03	1 (2%)	47,47,47	2.02	15 (31%)
20	LMU	A	7028	-	36,36,36	0.79	2 (5%)	47,47,47	1.92	17 (36%)
20	LMU	A	7030	-	36,36,36	0.97	1 (2%)	47,47,47	2.38	15 (31%)
20	LMU	A	7031	-	36,36,36	0.98	1 (2%)	47,47,47	1.38	5 (10%)
20	LMU	A	7032	-	36,36,36	1.03	4 (11%)	47,47,47	2.82	18 (38%)
20	LMU	A	7033	-	36,36,36	1.00	2 (5%)	47,47,47	2.27	14 (29%)
20	LMU	A	7034	19	36,36,36	0.72	1 (2%)	47,47,47	1.38	4 (8%)
20	LMU	A	7035	-	36,36,36	0.76	1 (2%)	47,47,47	1.65	9 (19%)
20	LMU	A	7036	-	35,35,36	1.28	4 (11%)	46,46,47	2.37	16 (34%)
20	LMU	A	7037	20	36,36,36	0.91	2 (5%)	47,47,47	3.13	25 (53%)
20	LMU	A	7038	-	36,36,36	0.66	0	47,47,47	2.47	17 (36%)
20	LMU	A	7039	-	36,36,36	0.99	2 (5%)	47,47,47	2.65	14 (29%)
20	LMU	A	7040	-	36,36,36	1.00	3 (8%)	47,47,47	2.54	13 (27%)
20	LMU	A	7041	-	36,36,36	0.66	1 (2%)	47,47,47	1.90	13 (27%)
20	LMU	A	7042	-	36,36,36	0.52	0	47,47,47	2.12	14 (29%)
20	LMU	A	7043	-	36,36,36	0.75	0	47,47,47	2.26	14 (29%)
20	LMU	A	7047	-	36,36,36	1.02	1 (2%)	47,47,47	1.49	4 (8%)
20	LMU	A	7048	-	36,36,36	0.46	0	47,47,47	2.19	17 (36%)
20	LMU	A	7049	-	36,36,36	0.58	1 (2%)	47,47,47	1.42	8 (17%)
20	LMU	A	7050	-	36,36,36	1.01	3 (8%)	47,47,47	2.77	19 (40%)
20	LMU	A	7051	20	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
19	CLA	B	1735	-	55,73,73	2.14	12 (21%)	61,113,113	3.73	24 (39%)
19	CLA	B	1736	-	32,53,73	2.36	10 (31%)	37,89,113	4.51	15 (40%)
19	CLA	B	1737	-	50,68,73	2.08	10 (20%)	55,107,113	4.66	21 (38%)
19	CLA	B	1738	-	55,73,73	2.02	13 (23%)	61,113,113	4.34	28 (45%)
19	CLA	B	1739	-	55,73,73	2.15	11 (20%)	61,113,113	4.41	20 (32%)
19	CLA	B	1740	6	55,73,73	1.88	11 (20%)	61,113,113	4.47	17 (27%)
19	CLA	B	1741	-	50,68,73	2.06	11 (22%)	55,107,113	4.51	19 (34%)
19	CLA	B	1742	6	44,62,73	2.47	10 (22%)	49,100,113	3.24	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	B	1743	6	45,63,73	2.07	12 (26%)	49,101,113	4.30	21 (42%)
19	CLA	B	1744	-	48,66,73	2.54	17 (35%)	52,104,113	4.99	22 (42%)
19	CLA	B	1745	-	55,73,73	2.07	11 (20%)	61,113,113	3.55	19 (31%)
19	CLA	B	1746	6	50,68,73	2.05	9 (18%)	55,107,113	4.17	18 (32%)
19	CLA	B	1747	-	36,54,73	2.46	10 (27%)	41,90,113	4.75	16 (39%)
19	CLA	B	1748	-	49,67,73	2.05	10 (20%)	53,105,113	3.75	18 (33%)
19	CLA	B	1749	-	50,68,73	1.98	11 (22%)	55,107,113	4.55	18 (32%)
19	CLA	B	1750	-	51,69,73	1.97	11 (21%)	56,108,113	4.50	19 (33%)
19	CLA	B	1751	-	40,58,73	2.25	12 (30%)	44,95,113	4.46	16 (36%)
19	CLA	B	1752	-	36,54,73	2.37	10 (27%)	41,90,113	4.97	15 (36%)
19	CLA	B	1753	6	45,63,73	2.26	9 (20%)	49,101,113	4.83	18 (36%)
19	CLA	B	1754	-	55,73,73	2.56	18 (32%)	61,113,113	4.63	19 (31%)
19	CLA	B	1755	-	44,62,73	2.30	12 (27%)	47,99,113	4.39	21 (44%)
19	CLA	B	1756	-	48,66,73	2.13	12 (25%)	52,104,113	4.76	16 (30%)
19	CLA	B	1757	6	55,73,73	1.94	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	B	1758	-	55,73,73	2.11	11 (20%)	61,113,113	4.39	20 (32%)
19	CLA	B	1759	-	55,73,73	2.04	12 (21%)	61,113,113	4.02	20 (32%)
19	CLA	B	1760	-	55,73,73	1.96	13 (23%)	61,113,113	4.21	18 (29%)
19	CLA	B	1761	-	40,58,73	2.40	8 (20%)	44,95,113	4.17	20 (45%)
19	CLA	B	1762	6	40,58,73	2.21	10 (25%)	44,95,113	4.93	18 (40%)
19	CLA	B	1763	6	55,73,73	2.07	13 (23%)	61,113,113	4.39	19 (31%)
19	CLA	B	1764	6	40,58,73	2.38	12 (30%)	44,95,113	4.75	21 (47%)
19	CLA	B	1765	19	32,53,73	2.69	11 (34%)	37,89,113	5.08	14 (37%)
19	CLA	B	1766	19	32,53,73	2.51	10 (31%)	37,89,113	5.46	15 (40%)
19	CLA	B	1767	-	41,59,73	2.40	11 (26%)	44,96,113	4.81	17 (38%)
19	CLA	B	1768	-	50,68,73	2.01	11 (22%)	55,107,113	4.48	15 (27%)
19	CLA	B	1769	6	55,73,73	1.91	11 (20%)	61,113,113	3.92	17 (27%)
19	CLA	B	1770	-	37,55,73	2.29	10 (27%)	42,91,113	4.46	17 (40%)
19	CLA	B	1771	-	55,73,73	1.95	10 (18%)	61,113,113	4.10	22 (36%)
19	CLA	B	1772	-	55,73,73	1.93	12 (21%)	61,113,113	3.95	22 (36%)
19	CLA	B	1773	-	24,44,73	2.79	8 (33%)	28,78,113	4.92	16 (57%)
23	PQN	B	1774	-	34,34,34	1.47	2 (5%)	44,45,45	1.51	5 (11%)
22	BCR	B	1775	-	41,41,41	1.96	4 (9%)	56,56,56	5.89	20 (35%)
22	BCR	B	1776	-	41,41,41	2.10	5 (12%)	56,56,56	5.92	22 (39%)
22	BCR	B	1777	-	41,41,41	1.90	4 (9%)	56,56,56	5.03	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	BCR	B	1778	-	41,41,41	2.15	5 (12%)	56,56,56	5.93	25 (44%)
22	BCR	B	1779	-	41,41,41	1.98	4 (9%)	56,56,56	5.88	18 (32%)
22	BCR	B	1780	-	41,41,41	2.99	14 (34%)	56,56,56	6.07	31 (55%)
22	BCR	B	1781	-	41,41,41	2.09	4 (9%)	56,56,56	5.92	20 (35%)
22	BCR	B	1782	-	41,41,41	2.81	17 (41%)	56,56,56	5.39	30 (53%)
20	LMU	B	1783	-	36,36,36	0.98	1 (2%)	47,47,47	2.43	16 (34%)
24	LMG	B	1784	-	49,49,55	0.93	2 (4%)	57,57,63	1.04	3 (5%)
25	SF4	B	1785	5,6	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	B	1786	-	55,73,73	1.97	11 (20%)	61,113,113	4.25	23 (37%)
19	CLA	B	1787	-	55,73,73	1.98	13 (23%)	61,113,113	4.12	23 (37%)
19	CLA	B	1788	-	55,73,73	2.01	11 (20%)	61,113,113	3.93	19 (31%)
21	SUC	B	8051	-	24,24,24	0.64	0	36,36,36	1.40	2 (5%)
21	SUC	B	8052	-	24,24,24	0.93	0	36,36,36	1.70	9 (25%)
21	SUC	B	8053	-	24,24,24	0.74	0	36,36,36	1.68	10 (27%)
21	SUC	B	8054	-	24,24,24	1.25	3 (12%)	36,36,36	1.76	9 (25%)
21	SUC	B	8055	-	24,24,24	0.96	0	36,36,36	1.27	3 (8%)
21	SUC	B	8056	-	24,24,24	1.11	1 (4%)	36,36,36	1.88	14 (38%)
21	SUC	B	8059	-	24,24,24	1.09	2 (8%)	36,36,36	2.11	12 (33%)
21	SUC	B	8060	-	24,24,24	1.10	0	36,36,36	1.86	7 (19%)
21	SUC	B	8061	-	24,24,24	0.94	1 (4%)	36,36,36	2.31	15 (41%)
21	SUC	B	8062	20	24,24,24	1.07	3 (12%)	36,36,36	2.80	16 (44%)
25	SF4	C	1082	7	0,12,12	0.00	-	0,24,24	0.00	-
25	SF4	C	1083	7	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	F	1155	-	24,44,73	2.73	8 (33%)	28,78,113	3.66	14 (50%)
19	CLA	F	1156	19	30,49,73	2.48	10 (33%)	34,84,113	5.81	17 (50%)
19	CLA	F	1157	19	43,61,73	2.60	15 (34%)	46,98,113	4.73	18 (39%)
21	SUC	F	1158	10	24,24,24	0.95	1 (4%)	36,36,36	1.59	9 (25%)
19	CLA	G	1099	-	41,59,73	2.46	14 (34%)	44,96,113	5.41	18 (40%)
19	CLA	I	1031	-	50,68,73	2.05	11 (22%)	55,107,113	4.89	16 (29%)
22	BCR	I	1032	-	41,41,41	2.80	9 (21%)	56,56,56	6.52	29 (51%)
19	CLA	J	1043	-	51,69,73	2.05	12 (23%)	56,108,113	4.61	17 (30%)
19	CLA	J	1044	-	51,69,73	2.05	12 (23%)	56,108,113	4.68	26 (46%)
19	CLA	K	1085	20	40,58,73	2.26	11 (27%)	44,95,113	5.18	18 (40%)
20	LMU	K	1086	19	36,36,36	0.77	1 (2%)	47,47,47	2.40	12 (25%)
19	CLA	L	1166	16	40,58,73	2.35	10 (25%)	44,95,113	5.08	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	L	1167	22,16	37,55,73	2.36	10 (27%)	42,91,113	5.16	21 (50%)
19	CLA	L	1168	-	40,58,73	2.45	14 (35%)	44,95,113	5.64	17 (38%)
22	BCR	L	1169	-	41,41,41	2.53	10 (24%)	56,56,56	5.72	20 (35%)
22	BCR	L	1170	19	41,41,41	3.43	20 (48%)	56,56,56	6.42	27 (48%)
20	LMU	L	1171	-	36,36,36	0.85	1 (2%)	47,47,47	1.54	11 (23%)
20	LMU	N	1086	17	36,36,36	0.54	0	47,47,47	2.15	13 (27%)
19	CLA	R	1054	-	47,65,73	2.14	12 (25%)	50,103,113	4.89	18 (36%)
19	CLA	R	1055	-	48,66,73	2.49	15 (31%)	52,104,113	4.47	23 (44%)
20	LMU	R	1056	20	36,36,36	0.36	0	47,47,47	0.72	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1014	-	4/4/19/25	1/33/131/135	0/0/9/9
19	CLA	1	1142	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	1	1145	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	1	1146	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	1	1148	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1149	-	5/5/16/25	0/16/112/135	0/0/9/9
19	CLA	1	1187	1	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1188	19	4/4/18/25	1/28/126/135	0/0/9/9
19	CLA	1	1189	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	1190	-	3/3/16/25	1/15/113/135	0/0/9/9
19	CLA	1	1191	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1192	19	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1193	-	4/4/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1194	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1195	1	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1196	-	4/4/17/25	1/21/119/135	0/0/9/9
19	CLA	1	1197	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1198	-	3/3/7/25	0/0/66/135	0/0/8/9
20	LMU	1	1199	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMU	1	1200	-	-	0/21/61/61	0/2/2/2
19	CLA	1	1241	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1303	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1307	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1308	-	3/3/16/25	0/17/115/135	0/0/9/9
19	CLA	1	1309	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1505	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	2	1212	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	2	1213	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	1214	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1215	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1216	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1217	2	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	2	1218	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	1219	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1220	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	2	1221	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1222	2	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1223	-	3/3/17/25	0/19/117/135	0/0/9/9
20	LMU	2	1224	-	-	0/21/61/61	0/2/2/2
21	SUC	2	1225	-	1/1/9/9	0/10/49/51	0/2/2/2
19	CLA	2	2010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1212	3	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	3	1213	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1214	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	1215	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1216	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1217	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1218	-	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	3	1219	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1220	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1221	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1222	3	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1223	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1224	-	4/4/20/25	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	3	1225	-	-	1/29/63/63	0/2/2/2
21	SUC	3	1226	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	3	3001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3008	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	3	3011	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3015	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1196	4	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1197	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1198	-	5/5/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1199	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1200	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	4	1201	4	4/4/17/25	0/22/120/135	0/0/9/9
19	CLA	4	1202	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1203	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1204	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1205	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1206	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1207	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1208	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1209	4	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1210	4	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
20	LMU	4	1212	-	-	0/21/61/61	0/2/2/2
19	CLA	4	4007	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4014	20	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1759	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1760	19	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1761	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1762	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1763	5,22	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	1764	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1765	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	1766	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1767	19,5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1768	5	3/3/17/25	0/24/122/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1769	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1770	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1771	5	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1772	5	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1773	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	1774	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1775	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	A	1776	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1777	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1778	5	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	A	1779	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1780	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1781	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1782	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1783	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1784	5	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1785	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1786	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1787	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1788	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1789	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1790	19,5	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1791	19,5	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1792	-	3/3/16/25	0/18/116/135	0/0/9/9
19	CLA	A	1793	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1794	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1795	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1796	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1797	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1798	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1799	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1800	-	4/4/18/25	0/25/123/135	0/0/9/9
23	PQN	A	1801	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	A	1802	5	-	1/29/63/63	0/2/2/2
22	BCR	A	1803	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	1804	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1805	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1806	-	-	1/29/63/63	0/2/2/2
22	BCR	A	1807	19	-	0/29/63/63	0/2/2/2
20	LMU	A	1808	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1809	-	-	1/21/61/61	0/2/2/2
19	CLA	A	1810	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1811	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1812	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	A	7003	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7004	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7005	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7006	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7009	20	-	0/20/60/61	0/2/2/2
20	LMU	A	7010	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7013	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7014	-	1/1/10/10	0/21/61/61	0/2/2/2
20	LMU	A	7015	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7016	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7017	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7019	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7020	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7021	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7022	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7023	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7024	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7025	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7026	21	-	0/21/61/61	0/2/2/2
20	LMU	A	7027	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7028	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7030	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7031	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7032	-	-	1/21/61/61	0/2/2/2
20	LMU	A	7033	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7034	19	-	0/21/61/61	0/2/2/2
20	LMU	A	7035	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7036	-	-	0/20/60/61	0/2/2/2
20	LMU	A	7037	20	-	0/21/61/61	0/2/2/2
20	LMU	A	7038	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7039	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7040	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7041	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMU	A	7042	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7043	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7047	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7048	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7049	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7050	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7051	20	-	1/21/61/61	0/2/2/2
19	CLA	B	1735	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1736	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1737	-	4/4/19/25	1/31/129/135	0/0/9/9
19	CLA	B	1738	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1739	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1740	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1741	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1742	6	4/4/18/25	0/25/121/135	0/0/9/9
19	CLA	B	1743	6	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1744	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	B	1745	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1746	6	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1747	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1748	-	4/4/18/25	0/30/128/135	0/0/9/9
19	CLA	B	1749	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1750	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	B	1751	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1752	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1753	6	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1754	-	3/3/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1755	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	B	1756	-	4/4/18/25	1/29/127/135	0/0/9/9
19	CLA	B	1757	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1758	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1759	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1760	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1761	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	B	1762	6	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1763	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1764	6	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1765	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1766	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1767	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	B	1768	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1769	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1770	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	B	1771	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1772	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1773	-	3/3/14/25	0/0/96/135	0/0/9/9
23	PQN	B	1774	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	B	1775	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1776	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1777	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1778	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1779	-	-	1/29/63/63	0/2/2/2
22	BCR	B	1780	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1781	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1782	-	-	0/29/63/63	0/2/2/2
20	LMU	B	1783	-	-	0/21/61/61	0/2/2/2
24	LMG	B	1784	-	-	0/44/64/70	0/1/1/1
25	SF4	B	1785	5,6	-	0/0/48/48	0/6/5/5
19	CLA	B	1786	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1787	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1788	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	B	8051	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8052	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8053	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8054	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8055	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8056	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8059	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8060	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8061	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8062	20	1/1/9/9	0/12/51/51	0/2/2/2
25	SF4	C	1082	7	-	0/0/48/48	0/6/5/5
25	SF4	C	1083	7	-	0/0/48/48	1/6/5/5
19	CLA	F	1155	-	3/3/14/25	0/0/96/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	F	1156	19	3/3/15/25	0/8/106/135	0/0/9/9
19	CLA	F	1157	19	6/6/17/25	1/23/121/135	0/0/9/9
21	SUC	F	1158	10	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	G	1099	-	3/3/17/25	1/21/119/135	0/0/9/9
19	CLA	I	1031	-	4/4/19/25	0/31/129/135	0/0/9/9
22	BCR	I	1032	-	-	1/29/63/63	0/2/2/2
19	CLA	J	1043	-	4/4/19/25	1/33/131/135	0/0/9/9
19	CLA	J	1044	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	K	1085	20	3/3/17/25	0/19/117/135	0/0/9/9
20	LMU	K	1086	19	-	0/21/61/61	0/2/2/2
19	CLA	L	1166	16	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	L	1167	22,16	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	L	1168	-	4/4/17/25	0/19/117/135	0/0/9/9
22	BCR	L	1169	-	-	2/29/63/63	0/2/2/2
22	BCR	L	1170	19	-	0/29/63/63	0/2/2/2
20	LMU	L	1171	-	-	0/21/61/61	0/2/2/2
20	LMU	N	1086	17	-	0/21/61/61	0/2/2/2
19	CLA	R	1054	-	4/4/18/25	1/28/126/135	0/0/9/9
19	CLA	R	1055	-	4/4/18/25	0/29/127/135	0/0/9/9
20	LMU	R	1056	20	-	0/21/61/61	0/2/2/2

All (1984) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1170	BCR	C21-C22	-11.56	1.20	1.35
22	B	1782	BCR	C21-C22	-10.75	1.21	1.35
22	B	1780	BCR	C21-C22	-10.23	1.22	1.35
22	L	1170	BCR	C20-C21	-10.19	1.12	1.43
22	I	1032	BCR	C21-C22	-9.52	1.23	1.35
19	F	1157	CLA	C3B-CAB	-9.19	1.28	1.47
19	R	1055	CLA	C3B-CAB	-9.13	1.28	1.47
22	L	1169	BCR	C20-C21	-8.95	1.15	1.43
19	4	4007	CLA	C3B-CAB	-8.87	1.29	1.47
19	1	1196	CLA	C3B-CAB	-8.83	1.29	1.47
22	L	1169	BCR	C21-C22	-8.80	1.24	1.35
22	B	1780	BCR	C20-C21	-8.75	1.16	1.43
19	4	1202	CLA	CAB-C3B	-8.68	1.33	1.51
19	4	1197	CLA	CAB-C3B	-8.65	1.34	1.51
19	B	1754	CLA	C3B-CAB	-8.60	1.29	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1782	BCR	C20-C21	-8.53	1.17	1.43
19	A	1771	CLA	C3B-CAB	-8.50	1.29	1.47
19	B	1742	CLA	CAB-C3B	-8.49	1.34	1.51
22	B	1778	BCR	C20-C21	-8.48	1.17	1.43
22	B	1781	BCR	C20-C21	-8.46	1.17	1.43
22	B	1776	BCR	C20-C21	-8.45	1.17	1.43
22	A	1805	BCR	C20-C21	-8.37	1.17	1.43
22	B	1778	BCR	C21-C22	-8.32	1.24	1.35
22	A	1803	BCR	C20-C21	-8.29	1.18	1.43
22	3	1225	BCR	C20-C21	-8.25	1.18	1.43
22	A	1806	BCR	C20-C21	-8.23	1.18	1.43
19	1	1195	CLA	CAB-C3B	-8.19	1.34	1.51
19	B	1773	CLA	CAB-C3B	-8.19	1.34	1.51
22	L	1170	BCR	C17-C18	-8.18	1.24	1.35
22	B	1779	BCR	C20-C21	-8.17	1.18	1.43
22	A	1807	BCR	C20-C21	-8.16	1.18	1.43
22	B	1775	BCR	C20-C21	-8.16	1.18	1.43
22	A	1802	BCR	C20-C21	-8.15	1.18	1.43
19	B	1754	CLA	C4C-C3C	-8.15	1.30	1.45
22	A	1804	BCR	C20-C21	-8.15	1.18	1.43
19	B	1739	CLA	C3B-CAB	-8.13	1.30	1.47
19	2	1217	CLA	C3B-CAB	-8.11	1.30	1.47
22	B	1776	BCR	C21-C22	-8.09	1.25	1.35
19	4	1209	CLA	CAB-C3B	-8.09	1.35	1.51
19	A	1763	CLA	C3B-CAB	-8.06	1.30	1.47
19	2	1220	CLA	CAB-C3B	-7.97	1.35	1.51
22	I	1032	BCR	C20-C21	-7.96	1.19	1.43
19	4	1198	CLA	C3B-CAB	-7.96	1.30	1.47
22	B	1781	BCR	C21-C22	-7.94	1.25	1.35
22	B	1777	BCR	C20-C21	-7.93	1.19	1.43
19	3	1214	CLA	CAB-C3B	-7.92	1.35	1.51
22	A	1805	BCR	C21-C22	-7.85	1.25	1.35
22	A	1803	BCR	C21-C22	-7.85	1.25	1.35
19	1	1145	CLA	C3B-CAB	-7.84	1.31	1.47
19	1	1149	CLA	CAB-C3B	-7.83	1.35	1.51
19	4	1200	CLA	C3B-CAB	-7.79	1.31	1.47
22	A	1806	BCR	C21-C22	-7.76	1.25	1.35
19	4	1211	CLA	C3B-CAB	-7.74	1.31	1.47
19	2	1222	CLA	C3B-CAB	-7.74	1.31	1.47
22	3	1225	BCR	C21-C22	-7.73	1.25	1.35
19	A	1797	CLA	C3B-CAB	-7.69	1.31	1.47
19	B	1738	CLA	C3B-CAB	-7.68	1.31	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1779	BCR	C21-C22	-7.64	1.25	1.35
19	3	1212	CLA	C3B-CAB	-7.62	1.31	1.47
19	B	1744	CLA	C3B-CAB	-7.59	1.31	1.47
22	A	1804	BCR	C21-C22	-7.59	1.25	1.35
19	B	1735	CLA	C3B-CAB	-7.58	1.31	1.47
19	A	1812	CLA	C3B-CAB	-7.54	1.31	1.47
19	A	1764	CLA	C3B-CAB	-7.49	1.31	1.47
19	3	1222	CLA	C3B-CAB	-7.46	1.32	1.47
22	A	1807	BCR	C21-C22	-7.45	1.25	1.35
19	F	1155	CLA	CAB-C3B	-7.42	1.36	1.51
22	A	1802	BCR	C21-C22	-7.40	1.26	1.35
19	A	1783	CLA	C3B-CAB	-7.38	1.32	1.47
19	B	1755	CLA	C3B-CAB	-7.38	1.32	1.47
22	B	1775	BCR	C21-C22	-7.35	1.26	1.35
19	B	1765	CLA	C3B-CAB	-7.34	1.32	1.47
19	4	1201	CLA	C4C-C3C	-7.30	1.31	1.45
19	A	1793	CLA	C3B-CAB	-7.29	1.32	1.47
19	B	1788	CLA	C3B-CAB	-7.24	1.32	1.47
19	A	1784	CLA	C3B-CAB	-7.14	1.32	1.47
19	A	1792	CLA	C3B-CAB	-7.02	1.32	1.47
19	2	1212	CLA	C3B-CAB	-7.01	1.32	1.47
19	B	1772	CLA	C3B-CAB	-6.99	1.33	1.47
19	1	1014	CLA	C3B-CAB	-6.96	1.33	1.47
22	I	1032	BCR	C30-C25	-6.95	1.43	1.53
19	B	1759	CLA	C3B-CAB	-6.94	1.33	1.47
19	G	1099	CLA	C3B-CAB	-6.93	1.33	1.47
19	1	1148	CLA	C3B-CAB	-6.92	1.33	1.47
19	3	1224	CLA	C4C-C3C	-6.92	1.32	1.45
19	3	1224	CLA	C3B-CAB	-6.91	1.33	1.47
19	1	1146	CLA	C3B-CAB	-6.90	1.33	1.47
19	B	1758	CLA	C3B-CAB	-6.90	1.33	1.47
19	B	1753	CLA	C3B-CAB	-6.88	1.33	1.47
19	A	1811	CLA	C3B-CAB	-6.82	1.33	1.47
19	B	1769	CLA	C3B-CAB	-6.81	1.33	1.47
19	A	1772	CLA	C3B-CAB	-6.81	1.33	1.47
19	B	1763	CLA	C3B-CAB	-6.77	1.33	1.47
22	B	1777	BCR	C21-C22	-6.74	1.26	1.35
19	A	1765	CLA	C3B-CAB	-6.74	1.33	1.47
19	J	1044	CLA	C3B-CAB	-6.71	1.33	1.47
19	B	1756	CLA	C3B-CAB	-6.71	1.33	1.47
19	L	1167	CLA	C3B-CAB	-6.70	1.33	1.47
19	A	1759	CLA	C3B-CAB	-6.70	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1789	CLA	C3B-CAB	-6.68	1.33	1.47
19	1	1188	CLA	C3B-CAB	-6.66	1.33	1.47
19	B	1766	CLA	C3B-CAB	-6.64	1.33	1.47
19	A	1767	CLA	C3B-CAB	-6.63	1.33	1.47
19	B	1786	CLA	C3B-CAB	-6.63	1.33	1.47
19	B	1768	CLA	C3B-CAB	-6.63	1.33	1.47
19	A	1795	CLA	C3B-CAB	-6.62	1.33	1.47
19	B	1761	CLA	C3B-CAB	-6.59	1.33	1.47
19	4	4014	CLA	C3B-CAB	-6.58	1.33	1.47
19	1	1308	CLA	C3B-CAB	-6.57	1.33	1.47
19	A	1781	CLA	C3B-CAB	-6.57	1.33	1.47
19	1	1142	CLA	C3B-CAB	-6.56	1.33	1.47
19	I	1031	CLA	C3B-CAB	-6.55	1.33	1.47
19	A	1761	CLA	C3B-CAB	-6.53	1.34	1.47
19	B	1767	CLA	C3B-CAB	-6.52	1.34	1.47
19	B	1787	CLA	C3B-CAB	-6.51	1.34	1.47
19	B	1757	CLA	C3B-CAB	-6.51	1.34	1.47
19	A	1788	CLA	C3B-CAB	-6.50	1.34	1.47
19	F	1156	CLA	C3B-CAB	-6.50	1.34	1.47
19	K	1085	CLA	C3B-CAB	-6.47	1.34	1.47
19	3	1222	CLA	C4C-C3C	-6.46	1.33	1.45
19	B	1745	CLA	C3B-CAB	-6.45	1.34	1.47
19	A	1799	CLA	C3B-CAB	-6.45	1.34	1.47
19	A	1796	CLA	C3B-CAB	-6.44	1.34	1.47
19	A	1782	CLA	C3B-CAB	-6.44	1.34	1.47
19	1	1196	CLA	C4C-C3C	-6.43	1.33	1.45
19	A	1794	CLA	C3B-CAB	-6.43	1.34	1.47
19	A	1778	CLA	C3B-CAB	-6.42	1.34	1.47
19	B	1744	CLA	C4C-C3C	-6.41	1.33	1.45
19	J	1043	CLA	C3B-CAB	-6.40	1.34	1.47
19	4	1196	CLA	C3B-CAB	-6.40	1.34	1.47
19	A	1810	CLA	C3B-CAB	-6.39	1.34	1.47
19	B	1740	CLA	C3B-CAB	-6.38	1.34	1.47
19	1	1189	CLA	C3B-CAB	-6.35	1.34	1.47
19	A	1790	CLA	C3B-CAB	-6.35	1.34	1.47
19	A	1779	CLA	C3B-CAB	-6.30	1.34	1.47
19	A	1787	CLA	C3B-CAB	-6.29	1.34	1.47
19	B	1764	CLA	C3B-CAB	-6.29	1.34	1.47
19	A	1800	CLA	C3B-CAB	-6.25	1.34	1.47
19	1	1193	CLA	C3B-CAB	-6.24	1.34	1.47
19	4	1199	CLA	C3B-CAB	-6.19	1.34	1.47
19	B	1762	CLA	C3B-CAB	-6.17	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1168	CLA	C3B-CAB	-6.15	1.34	1.47
19	A	1786	CLA	C3B-CAB	-6.15	1.34	1.47
19	B	1754	CLA	C3B-C2B	-6.13	1.32	1.40
19	A	1773	CLA	C3B-CAB	-6.11	1.34	1.47
19	1	1196	CLA	C3B-C2B	-6.07	1.32	1.40
19	1	1192	CLA	C3B-CAB	-6.06	1.34	1.47
19	1	1187	CLA	C3B-CAB	-6.06	1.34	1.47
19	2	1218	CLA	C3B-CAB	-6.05	1.35	1.47
19	1	1241	CLA	C3B-CAB	-6.04	1.35	1.47
19	B	1760	CLA	C3B-CAB	-6.03	1.35	1.47
19	2	1223	CLA	C3B-CAB	-6.02	1.35	1.47
19	3	1219	CLA	C3B-CAB	-6.01	1.35	1.47
19	L	1166	CLA	C3B-CAB	-6.00	1.35	1.47
22	B	1780	BCR	C30-C25	-6.00	1.45	1.53
19	B	1747	CLA	C3B-CAB	-5.98	1.35	1.47
19	3	3011	CLA	C3B-CAB	-5.97	1.35	1.47
19	1	1190	CLA	C3B-CAB	-5.95	1.35	1.47
19	A	1798	CLA	C3B-CAB	-5.94	1.35	1.47
19	B	1751	CLA	C3B-CAB	-5.91	1.35	1.47
19	A	1774	CLA	C3B-CAB	-5.91	1.35	1.47
19	B	1737	CLA	C3B-CAB	-5.91	1.35	1.47
19	4	1201	CLA	C1C-C2C	-5.90	1.32	1.44
19	3	1218	CLA	C3B-CAB	-5.88	1.35	1.47
19	A	1780	CLA	C3B-CAB	-5.87	1.35	1.47
19	A	1760	CLA	C3B-CAB	-5.86	1.35	1.47
19	A	1770	CLA	C3B-CAB	-5.80	1.35	1.47
19	A	1766	CLA	C3B-CAB	-5.80	1.35	1.47
19	B	1743	CLA	C3B-CAB	-5.80	1.35	1.47
19	B	1746	CLA	C3B-CAB	-5.80	1.35	1.47
19	A	1785	CLA	C3B-CAB	-5.76	1.35	1.47
19	B	1771	CLA	C3B-CAB	-5.75	1.35	1.47
19	3	3008	CLA	C3B-CAB	-5.74	1.35	1.47
19	4	1205	CLA	C3B-CAB	-5.72	1.35	1.47
19	G	1099	CLA	C4C-C3C	-5.71	1.34	1.45
19	B	1750	CLA	C3B-CAB	-5.70	1.35	1.47
19	4	1206	CLA	C3B-CAB	-5.70	1.35	1.47
19	2	1215	CLA	C3B-CAB	-5.68	1.35	1.47
22	L	1170	BCR	C20-C19	-5.66	1.19	1.34
19	A	1791	CLA	C3B-CAB	-5.66	1.35	1.47
19	R	1055	CLA	C3B-C2B	-5.65	1.32	1.40
19	4	4007	CLA	C1C-C2C	-5.64	1.33	1.44
19	B	1749	CLA	C3B-CAB	-5.63	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1762	CLA	C3B-CAB	-5.62	1.35	1.47
19	F	1157	CLA	C3B-C2B	-5.59	1.33	1.40
19	B	1748	CLA	C3B-CAB	-5.57	1.36	1.47
19	B	1736	CLA	C3B-CAB	-5.51	1.36	1.47
19	1	1505	CLA	C3B-CAB	-5.50	1.36	1.47
19	4	1198	CLA	C3B-C2B	-5.50	1.33	1.40
19	A	1777	CLA	C3B-CAB	-5.47	1.36	1.47
19	B	1741	CLA	C3B-CAB	-5.47	1.36	1.47
19	R	1054	CLA	C3B-CAB	-5.40	1.36	1.47
19	3	1212	CLA	C3B-C2B	-5.39	1.33	1.40
19	A	1772	CLA	C3B-C2B	-5.35	1.33	1.40
22	I	1032	BCR	C26-C25	-5.33	1.25	1.34
19	2	1217	CLA	C4C-C3C	-5.27	1.35	1.45
19	A	1769	CLA	C3B-CAB	-5.26	1.36	1.47
19	1	1146	CLA	C1C-C2C	-5.24	1.34	1.44
19	B	1770	CLA	C3B-CAB	-5.23	1.36	1.47
19	4	1203	CLA	C1C-NC	-5.17	1.28	1.37
19	4	1200	CLA	C4C-C3C	-5.16	1.35	1.45
19	A	1776	CLA	C3B-CAB	-5.15	1.36	1.47
19	1	1146	CLA	C4C-C3C	-5.15	1.35	1.45
19	A	1771	CLA	C4C-C3C	-5.14	1.35	1.45
19	A	1768	CLA	C3B-CAB	-5.06	1.37	1.47
19	1	1196	CLA	C3D-CAD	-5.05	1.31	1.45
19	B	1752	CLA	C3B-CAB	-4.92	1.37	1.47
19	4	1198	CLA	C1C-C2C	-4.90	1.34	1.44
19	4	1211	CLA	C4C-C3C	-4.87	1.36	1.45
19	2	1213	CLA	C3B-CAB	-4.85	1.37	1.47
19	B	1744	CLA	C1C-C2C	-4.84	1.34	1.44
19	B	1744	CLA	C3B-C2B	-4.80	1.34	1.40
22	L	1170	BCR	C10-C9	-4.73	1.29	1.35
19	A	1772	CLA	C4C-C3C	-4.73	1.36	1.45
22	B	1780	BCR	C1-C6	-4.72	1.47	1.53
19	4	1201	CLA	C3B-CAB	-4.71	1.37	1.47
19	R	1055	CLA	C4C-C3C	-4.69	1.36	1.45
19	A	1797	CLA	C4C-C3C	-4.68	1.36	1.45
19	2	1217	CLA	C1C-C2C	-4.67	1.35	1.44
19	4	1211	CLA	C3B-C2B	-4.66	1.34	1.40
19	3	1224	CLA	C1C-C2C	-4.59	1.35	1.44
19	4	4007	CLA	C4C-C3C	-4.57	1.36	1.45
19	3	1222	CLA	C1C-C2C	-4.54	1.35	1.44
19	1	1188	CLA	C1C-C2C	-4.53	1.35	1.44
19	A	1797	CLA	C1C-C2C	-4.51	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1145	CLA	C1C-C2C	-4.50	1.35	1.44
19	2	1217	CLA	C3B-C2B	-4.50	1.34	1.40
19	A	1770	CLA	C3B-C2B	-4.49	1.34	1.40
19	A	1810	CLA	C4C-C3C	-4.49	1.36	1.45
19	4	1198	CLA	C4C-C3C	-4.48	1.36	1.45
22	L	1169	BCR	C20-C19	-4.42	1.22	1.34
22	B	1780	BCR	C14-C13	-4.41	1.29	1.35
19	A	1763	CLA	C4C-C3C	-4.40	1.37	1.45
19	1	1196	CLA	C1C-C2C	-4.40	1.35	1.44
22	I	1032	BCR	C1-C6	-4.36	1.47	1.53
19	1	1148	CLA	C3B-C2B	-4.35	1.34	1.40
19	A	1797	CLA	C3B-C2B	-4.33	1.34	1.40
19	3	1223	CLA	C4C-NC	-4.28	1.30	1.37
19	A	1796	CLA	C4C-C3C	-4.26	1.37	1.45
19	4	1201	CLA	C2A-C1A	-4.25	1.43	1.52
19	R	1055	CLA	C1C-C2C	-4.25	1.36	1.44
19	A	1763	CLA	C1C-C2C	-4.24	1.36	1.44
19	F	1157	CLA	C4C-C3C	-4.23	1.37	1.45
19	1	1145	CLA	C4C-C3C	-4.21	1.37	1.45
19	A	1763	CLA	C3B-C2B	-4.18	1.34	1.40
19	A	1765	CLA	C1C-C2C	-4.17	1.36	1.44
22	B	1780	BCR	C20-C19	-4.13	1.23	1.34
19	B	1754	CLA	C1C-C2C	-4.10	1.36	1.44
22	B	1780	BCR	C17-C18	-4.10	1.30	1.35
19	A	1771	CLA	C3B-C2B	-4.09	1.34	1.40
19	1	1308	CLA	C4C-C3C	-4.07	1.37	1.45
22	L	1169	BCR	C17-C18	-4.07	1.30	1.35
19	4	1203	CLA	C3C-C4C	-4.06	1.33	1.43
19	1	1148	CLA	C4C-C3C	-4.05	1.37	1.45
19	1	1014	CLA	C4C-C3C	-4.05	1.37	1.45
19	B	1744	CLA	C3D-CAD	-4.04	1.34	1.45
19	3	3015	CLA	C4C-NC	-4.02	1.30	1.37
19	A	1771	CLA	C1C-NC	-4.01	1.31	1.37
22	B	1782	BCR	C20-C19	-4.00	1.24	1.34
19	3	1224	CLA	C3B-C2B	-3.99	1.35	1.40
19	J	1043	CLA	C4C-C3C	-3.98	1.37	1.45
19	4	4007	CLA	C3B-C2B	-3.97	1.35	1.40
19	A	1795	CLA	C1C-C2C	-3.97	1.36	1.44
19	4	1203	CLA	C4C-NC	-3.97	1.31	1.37
19	1	1142	CLA	C4C-C3C	-3.97	1.37	1.45
19	1	1014	CLA	C1C-C2C	-3.96	1.36	1.44
19	4	1196	CLA	C4C-C3C	-3.96	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1187	CLA	C4C-C3C	-3.95	1.37	1.45
19	4	1205	CLA	C4C-C3C	-3.95	1.37	1.45
19	A	1795	CLA	C4C-C3C	-3.93	1.37	1.45
19	B	1754	CLA	C1C-NC	-3.91	1.31	1.37
19	A	1774	CLA	C4C-C3C	-3.91	1.38	1.45
19	B	1765	CLA	C4C-C3C	-3.90	1.38	1.45
19	A	1771	CLA	C1C-C2C	-3.90	1.36	1.44
22	B	1782	BCR	C5-C6	-3.89	1.28	1.34
19	A	1800	CLA	C4C-C3C	-3.89	1.38	1.45
19	B	1738	CLA	C1C-C2C	-3.88	1.36	1.44
19	1	1187	CLA	C1C-C2C	-3.84	1.36	1.44
19	B	1764	CLA	C1C-C2C	-3.81	1.36	1.44
19	B	1756	CLA	C4C-C3C	-3.77	1.38	1.45
19	3	1212	CLA	C4C-C3C	-3.76	1.38	1.45
19	4	1203	CLA	C2C-C1C	-3.75	1.34	1.43
19	3	1222	CLA	C4C-NC	-3.73	1.31	1.37
19	1	1196	CLA	C3D-C2D	-3.73	1.31	1.40
19	B	1760	CLA	C4C-C3C	-3.71	1.38	1.45
19	4	1211	CLA	C1C-C2C	-3.71	1.37	1.44
19	B	1754	CLA	C4C-NC	-3.69	1.31	1.37
22	B	1778	BCR	C20-C19	-3.68	1.24	1.34
19	B	1788	CLA	C4C-C3C	-3.68	1.38	1.45
19	B	1738	CLA	C3B-C2B	-3.67	1.35	1.40
19	A	1772	CLA	C3D-CAD	-3.64	1.35	1.45
22	B	1776	BCR	C20-C19	-3.63	1.25	1.34
22	B	1781	BCR	C20-C19	-3.62	1.25	1.34
19	G	1099	CLA	C3B-C2B	-3.62	1.35	1.40
19	3	1212	CLA	C1C-NC	-3.59	1.31	1.37
19	B	1757	CLA	C4C-C3C	-3.59	1.38	1.45
20	A	7036	LMU	O1B-C4'	-3.58	1.34	1.43
22	A	1803	BCR	C20-C19	-3.58	1.25	1.34
19	G	1099	CLA	C1C-C2C	-3.58	1.37	1.44
19	A	1759	CLA	C4C-C3C	-3.57	1.38	1.45
19	1	1193	CLA	C2A-C1A	-3.57	1.44	1.52
19	B	1754	CLA	C3D-CAD	-3.54	1.35	1.45
19	B	1739	CLA	C1C-C2C	-3.54	1.37	1.44
19	B	1735	CLA	C3B-C2B	-3.54	1.35	1.40
19	R	1055	CLA	C3D-CAD	-3.54	1.35	1.45
19	3	1224	CLA	C1C-NC	-3.52	1.31	1.37
19	4	4014	CLA	C4C-C3C	-3.52	1.38	1.45
19	4	1196	CLA	C1C-C2C	-3.51	1.37	1.44
19	4	1201	CLA	C4C-NC	-3.51	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	I	1031	CLA	C4C-C3C	-3.50	1.38	1.45
19	1	1014	CLA	C3B-C2B	-3.50	1.35	1.40
19	B	1770	CLA	C4C-C3C	-3.50	1.38	1.45
19	1	1145	CLA	C3D-CAD	-3.49	1.35	1.45
19	B	1737	CLA	C1C-C2C	-3.49	1.37	1.44
19	A	1782	CLA	C4C-C3C	-3.49	1.38	1.45
19	A	1764	CLA	C4C-C3C	-3.49	1.38	1.45
19	A	1781	CLA	C4C-C3C	-3.47	1.38	1.45
19	4	4007	CLA	C3D-CAD	-3.46	1.36	1.45
19	B	1769	CLA	C4C-C3C	-3.44	1.38	1.45
19	3	1215	CLA	C1C-NC	-3.43	1.31	1.37
19	4	1211	CLA	C3D-CAD	-3.43	1.36	1.45
22	A	1805	BCR	C20-C19	-3.43	1.25	1.34
22	A	1806	BCR	C20-C19	-3.43	1.25	1.34
19	3	1224	CLA	C3D-CAD	-3.42	1.36	1.45
19	A	1767	CLA	C1C-C2C	-3.42	1.37	1.44
19	F	1156	CLA	C4C-C3C	-3.41	1.38	1.45
19	B	1750	CLA	C4C-C3C	-3.41	1.38	1.45
19	2	1212	CLA	C4C-C3C	-3.41	1.38	1.45
22	3	1225	BCR	C20-C19	-3.41	1.25	1.34
19	1	1142	CLA	C1C-C2C	-3.40	1.37	1.44
19	A	1763	CLA	C3D-CAD	-3.40	1.36	1.45
19	A	1791	CLA	C4C-C3C	-3.39	1.38	1.45
19	L	1166	CLA	C4C-C3C	-3.38	1.38	1.45
19	1	1148	CLA	C3D-CAD	-3.38	1.36	1.45
22	B	1782	BCR	C26-C25	-3.38	1.28	1.34
22	I	1032	BCR	C38-C26	-3.38	1.45	1.51
19	A	1788	CLA	C1C-C2C	-3.37	1.37	1.44
19	A	1774	CLA	C3B-C2B	-3.37	1.35	1.40
19	1	1188	CLA	C4C-C3C	-3.36	1.39	1.45
22	A	1807	BCR	C20-C19	-3.36	1.25	1.34
19	B	1759	CLA	C4C-C3C	-3.36	1.39	1.45
19	A	1788	CLA	C4C-C3C	-3.36	1.39	1.45
19	K	1085	CLA	C4C-C3C	-3.35	1.39	1.45
19	A	1791	CLA	C1C-C2C	-3.35	1.37	1.44
19	1	1187	CLA	C3D-CAD	-3.35	1.36	1.45
22	B	1779	BCR	C20-C19	-3.35	1.25	1.34
22	B	1775	BCR	C20-C19	-3.35	1.25	1.34
19	1	1188	CLA	C3B-C2B	-3.34	1.35	1.40
19	3	3015	CLA	C1C-NC	-3.34	1.32	1.37
19	B	1749	CLA	C4C-C3C	-3.33	1.39	1.45
19	R	1055	CLA	C1C-NC	-3.32	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	1044	CLA	C4C-C3C	-3.32	1.39	1.45
19	3	1213	CLA	C3C-C4C	-3.32	1.35	1.43
22	A	1804	BCR	C20-C19	-3.32	1.25	1.34
19	3	1213	CLA	C1C-NC	-3.32	1.32	1.37
22	I	1032	BCR	C20-C19	-3.31	1.25	1.34
19	A	1782	CLA	C1C-C2C	-3.30	1.38	1.44
19	1	1308	CLA	C1C-C2C	-3.29	1.38	1.44
19	A	1771	CLA	C3A-C2A	-3.29	1.44	1.54
19	B	1735	CLA	C4C-C3C	-3.29	1.39	1.45
19	A	1777	CLA	C4C-C3C	-3.29	1.39	1.45
19	4	1201	CLA	C3A-C2A	-3.29	1.44	1.54
19	1	1148	CLA	C1C-NC	-3.28	1.32	1.37
19	B	1738	CLA	C4C-C3C	-3.28	1.39	1.45
19	A	1789	CLA	C1C-C2C	-3.26	1.38	1.44
19	2	1215	CLA	C4C-C3C	-3.26	1.39	1.45
22	A	1802	BCR	C20-C19	-3.25	1.25	1.34
19	B	1754	CLA	C2A-C1A	-3.25	1.45	1.52
19	4	1204	CLA	C2B-C1B	-3.25	1.34	1.40
19	3	1222	CLA	C1C-NC	-3.24	1.32	1.37
19	B	1766	CLA	C4C-C3C	-3.24	1.39	1.45
19	3	1222	CLA	C3D-CAD	-3.24	1.36	1.45
19	A	1810	CLA	C3B-C2B	-3.24	1.36	1.40
22	B	1780	BCR	C29-C30	-3.24	1.46	1.54
19	K	1085	CLA	C1C-C2C	-3.23	1.38	1.44
19	B	1764	CLA	C4C-C3C	-3.23	1.39	1.45
19	2	1214	CLA	C4C-NC	-3.23	1.32	1.37
19	3	1213	CLA	C4C-NC	-3.23	1.32	1.37
19	A	1772	CLA	C1C-C2C	-3.22	1.38	1.44
19	A	1771	CLA	C2A-C1A	-3.22	1.45	1.52
19	1	1196	CLA	C1C-NC	-3.22	1.32	1.37
19	3	1212	CLA	C1C-C2C	-3.22	1.38	1.44
19	B	1771	CLA	C1C-C2C	-3.21	1.38	1.44
19	B	1744	CLA	CBD-CGD	-3.21	1.41	1.52
19	1	1188	CLA	C3D-CAD	-3.21	1.36	1.45
19	4	1200	CLA	C3B-C2B	-3.20	1.36	1.40
19	A	1773	CLA	C4C-C3C	-3.20	1.39	1.45
19	A	1764	CLA	C3B-C2B	-3.20	1.36	1.40
19	A	1769	CLA	C1C-C2C	-3.20	1.38	1.44
19	B	1756	CLA	C1C-C2C	-3.20	1.38	1.44
19	1	1309	CLA	C3C-C4C	-3.19	1.35	1.43
19	G	1099	CLA	C1C-NC	-3.19	1.32	1.37
19	A	1812	CLA	C4C-C3C	-3.19	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1784	CLA	C3B-C2B	-3.19	1.36	1.40
19	1	1307	CLA	C1C-NC	-3.18	1.32	1.37
19	B	1740	CLA	C4C-C3C	-3.16	1.39	1.45
22	L	1170	BCR	C14-C13	-3.16	1.31	1.35
19	4	1206	CLA	C4C-C3C	-3.15	1.39	1.45
19	A	1760	CLA	C4C-C3C	-3.14	1.39	1.45
19	3	1221	CLA	C2C-C1C	-3.14	1.35	1.43
19	1	1307	CLA	C2B-C1B	-3.14	1.34	1.40
19	J	1044	CLA	C1C-C2C	-3.13	1.38	1.44
19	4	1201	CLA	CAA-C2A	-3.13	1.47	1.54
19	3	1223	CLA	C2C-C1C	-3.13	1.35	1.43
22	L	1170	BCR	C30-C25	-3.12	1.49	1.53
20	A	7050	LMU	O5B-C5B	-3.11	1.36	1.44
19	B	1769	CLA	C1C-C2C	-3.11	1.38	1.44
19	B	1737	CLA	C4C-C3C	-3.10	1.39	1.45
19	J	1043	CLA	C1C-C2C	-3.10	1.38	1.44
19	B	1788	CLA	C1C-C2C	-3.08	1.38	1.44
19	A	1799	CLA	C4C-C3C	-3.08	1.39	1.45
22	L	1170	BCR	C29-C30	-3.08	1.46	1.54
19	B	1747	CLA	C4C-C3C	-3.07	1.39	1.45
22	L	1169	BCR	C30-C25	-3.07	1.49	1.53
19	A	1770	CLA	C1C-C2C	-3.07	1.38	1.44
19	4	1206	CLA	C1C-C2C	-3.06	1.38	1.44
20	A	7039	LMU	O5B-C5B	-3.06	1.36	1.44
19	4	1201	CLA	C3D-CAD	-3.05	1.37	1.45
20	A	7036	LMU	C3'-C4'	-3.05	1.43	1.52
19	1	1194	CLA	C1C-NC	-3.04	1.32	1.37
19	1	1190	CLA	C1C-C2C	-3.04	1.38	1.44
19	L	1168	CLA	C4C-C3C	-3.04	1.39	1.45
19	1	1192	CLA	C4C-C3C	-3.04	1.39	1.45
19	A	1769	CLA	C4C-C3C	-3.04	1.39	1.45
19	B	1767	CLA	C4C-C3C	-3.03	1.39	1.45
19	3	1213	CLA	C2C-C1C	-3.03	1.35	1.43
20	A	7036	LMU	C4'-C5'	-3.02	1.44	1.52
19	A	1781	CLA	C1C-C2C	-3.02	1.38	1.44
19	2	1216	CLA	C4C-NC	-3.02	1.32	1.37
19	B	1747	CLA	C1C-C2C	-3.02	1.38	1.44
19	B	1760	CLA	C3D-CAD	-3.02	1.37	1.45
19	B	1763	CLA	C4C-C3C	-3.01	1.39	1.45
19	A	1811	CLA	C4C-C3C	-3.01	1.39	1.45
19	A	1812	CLA	C1C-C2C	-3.00	1.38	1.44
19	1	1190	CLA	C4C-C3C	-3.00	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1201	CLA	C1C-NC	-3.00	1.32	1.37
19	B	1786	CLA	C4C-C3C	-3.00	1.39	1.45
19	B	1758	CLA	C4C-C3C	-3.00	1.39	1.45
19	2	1216	CLA	C2C-C1C	-2.99	1.36	1.43
19	B	1739	CLA	C4C-C3C	-2.98	1.39	1.45
19	B	1752	CLA	C4C-C3C	-2.98	1.39	1.45
19	A	1768	CLA	C1C-C2C	-2.96	1.38	1.44
19	1	1194	CLA	C2C-C1C	-2.96	1.36	1.43
19	B	1787	CLA	C4C-C3C	-2.94	1.39	1.45
22	I	1032	BCR	C10-C9	-2.94	1.31	1.35
19	B	1741	CLA	C4C-C3C	-2.94	1.39	1.45
19	A	1792	CLA	C1C-C2C	-2.94	1.38	1.44
22	L	1170	BCR	C40-C30	-2.93	1.47	1.53
19	B	1772	CLA	C3B-C2B	-2.93	1.36	1.40
19	A	1793	CLA	C1C-C2C	-2.93	1.38	1.44
19	A	1762	CLA	C1C-C2C	-2.92	1.38	1.44
19	1	1149	CLA	C1C-C2C	-2.92	1.38	1.44
19	A	1771	CLA	C3A-C4A	-2.92	1.42	1.51
19	1	1303	CLA	C1C-NC	-2.92	1.32	1.37
19	1	1193	CLA	C4C-C3C	-2.92	1.39	1.45
19	2	1216	CLA	C3C-C4C	-2.91	1.36	1.43
19	1	1148	CLA	C1C-C2C	-2.91	1.38	1.44
19	A	1783	CLA	C1C-C2C	-2.91	1.38	1.44
19	A	1759	CLA	C1C-C2C	-2.91	1.38	1.44
19	A	1794	CLA	C4C-C3C	-2.91	1.39	1.45
19	2	1217	CLA	C3D-CAD	-2.91	1.37	1.45
19	1	1194	CLA	C2B-C1B	-2.90	1.35	1.40
19	A	1763	CLA	C2A-C1A	-2.89	1.46	1.52
19	4	1198	CLA	C1C-NC	-2.89	1.32	1.37
19	A	1766	CLA	C4C-C3C	-2.89	1.39	1.45
19	B	1757	CLA	C1C-C2C	-2.89	1.38	1.44
19	2	1214	CLA	C1C-NC	-2.88	1.32	1.37
19	B	1771	CLA	C4C-C3C	-2.88	1.39	1.45
19	A	1761	CLA	C1C-C2C	-2.87	1.38	1.44
19	B	1758	CLA	C1C-C2C	-2.87	1.38	1.44
22	L	1170	BCR	C39-C30	-2.87	1.47	1.53
19	4	1199	CLA	C1C-C2C	-2.86	1.38	1.44
19	B	1762	CLA	C4C-C3C	-2.86	1.39	1.45
19	1	1145	CLA	C3A-C2A	-2.86	1.46	1.54
19	A	1764	CLA	C2A-C1A	-2.86	1.46	1.52
22	B	1778	BCR	C30-C25	-2.85	1.49	1.53
19	1	1145	CLA	CBD-CGD	-2.85	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	1155	CLA	C1C-C2C	-2.85	1.38	1.44
19	4	1198	CLA	C3D-CAD	-2.85	1.37	1.45
19	4	1202	CLA	C1C-C2C	-2.84	1.38	1.44
19	B	1740	CLA	C1C-C2C	-2.84	1.38	1.44
19	A	1793	CLA	C4C-C3C	-2.84	1.39	1.45
19	4	1198	CLA	C3D-C2D	-2.84	1.33	1.40
19	A	1768	CLA	C4C-C3C	-2.84	1.39	1.45
19	B	1760	CLA	C1C-C2C	-2.83	1.38	1.44
19	F	1156	CLA	C1C-C2C	-2.82	1.38	1.44
19	A	1760	CLA	C1C-C2C	-2.82	1.38	1.44
22	B	1782	BCR	C1-C6	-2.82	1.49	1.53
19	A	1776	CLA	C1C-C2C	-2.82	1.38	1.44
19	A	1785	CLA	C3B-C2B	-2.82	1.36	1.40
19	3	1215	CLA	C2C-C1C	-2.82	1.36	1.43
19	3	1219	CLA	C4C-C3C	-2.81	1.39	1.45
19	3	1215	CLA	C3C-C4C	-2.81	1.36	1.43
19	1	1303	CLA	C4C-NC	-2.80	1.33	1.37
19	4	4014	CLA	C1C-C2C	-2.80	1.39	1.44
19	A	1797	CLA	C3D-CAD	-2.80	1.37	1.45
19	3	3015	CLA	C3C-C4C	-2.80	1.36	1.43
19	4	1204	CLA	C1C-NC	-2.79	1.32	1.37
19	1	1309	CLA	C1C-NC	-2.79	1.32	1.37
19	1	1190	CLA	C3D-CAD	-2.79	1.37	1.45
19	1	1188	CLA	C1C-NC	-2.78	1.33	1.37
19	B	1753	CLA	C1C-C2C	-2.78	1.39	1.44
19	B	1748	CLA	C1C-C2C	-2.78	1.39	1.44
19	4	1211	CLA	CBD-CGD	-2.77	1.42	1.52
19	2	1212	CLA	C1C-C2C	-2.77	1.39	1.44
22	L	1170	BCR	C31-C1	-2.77	1.47	1.53
19	A	1760	CLA	C3B-C2B	-2.77	1.36	1.40
19	B	1763	CLA	C1C-C2C	-2.77	1.39	1.44
19	G	1099	CLA	C3D-CAD	-2.77	1.37	1.45
19	A	1778	CLA	C1C-C2C	-2.77	1.39	1.44
19	1	1145	CLA	C3B-C2B	-2.76	1.36	1.40
19	1	1187	CLA	C3D-C2D	-2.76	1.33	1.40
19	A	1759	CLA	C3B-C2B	-2.76	1.36	1.40
19	4	1202	CLA	C4C-C3C	-2.76	1.39	1.44
20	A	7040	LMU	O5B-C5B	-2.75	1.37	1.44
22	3	1225	BCR	C1-C6	-2.75	1.49	1.53
19	1	1146	CLA	C3D-CAD	-2.75	1.38	1.45
19	B	1746	CLA	C4C-C3C	-2.75	1.40	1.45
19	1	1146	CLA	C1C-NC	-2.74	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1740	CLA	C3D-CAD	-2.74	1.38	1.45
20	A	7040	LMU	C4B-C5B	-2.73	1.47	1.53
22	B	1776	BCR	C1-C6	-2.73	1.49	1.53
21	B	8056	SUC	O5-C5	-2.72	1.37	1.44
19	A	1766	CLA	C1C-C2C	-2.71	1.39	1.44
22	B	1782	BCR	C4-C5	-2.71	1.45	1.51
19	3	3015	CLA	C2C-C1C	-2.71	1.36	1.43
22	B	1781	BCR	C1-C6	-2.70	1.50	1.53
22	A	1806	BCR	C1-C6	-2.70	1.50	1.53
19	B	1763	CLA	C3D-CAD	-2.70	1.38	1.45
19	B	1787	CLA	C3B-C2B	-2.70	1.36	1.40
19	B	1761	CLA	C1C-C2C	-2.69	1.39	1.44
21	B	8054	SUC	O3'-C3'	-2.69	1.37	1.42
19	2	1214	CLA	C2C-C1C	-2.68	1.36	1.43
19	A	1774	CLA	C1C-C2C	-2.68	1.39	1.44
19	B	1744	CLA	C3D-C2D	-2.68	1.33	1.40
19	B	1736	CLA	C3B-C2B	-2.68	1.36	1.40
22	B	1780	BCR	C39-C30	-2.67	1.48	1.53
19	1	1149	CLA	C2A-C1A	-2.67	1.46	1.52
20	A	7032	LMU	O5'-C5'	-2.67	1.37	1.44
19	1	1146	CLA	C3B-C2B	-2.67	1.36	1.40
19	1	1195	CLA	C4C-C3C	-2.67	1.39	1.44
19	A	1794	CLA	C3B-C2B	-2.67	1.36	1.40
19	F	1157	CLA	CAA-C2A	-2.67	1.48	1.54
19	F	1157	CLA	C1C-C2C	-2.67	1.39	1.44
19	1	1145	CLA	C1C-NC	-2.66	1.33	1.37
20	A	7028	LMU	C4B-C5B	-2.66	1.47	1.53
22	L	1170	BCR	C2-C1	-2.65	1.47	1.54
22	B	1782	BCR	C29-C30	-2.65	1.47	1.54
19	4	1201	CLA	CAC-C3C	-2.65	1.43	1.51
19	A	1783	CLA	C4C-C3C	-2.64	1.40	1.45
19	B	1744	CLA	C4C-NC	-2.64	1.33	1.37
19	A	1771	CLA	CAA-C2A	-2.64	1.48	1.54
19	2	1213	CLA	C1C-C2C	-2.63	1.39	1.44
19	2	1223	CLA	C3D-CAD	-2.63	1.38	1.45
19	3	1218	CLA	C1C-C2C	-2.63	1.39	1.44
22	B	1780	BCR	C40-C30	-2.63	1.48	1.53
22	B	1777	BCR	C20-C19	-2.63	1.27	1.34
19	A	1791	CLA	C3D-CAD	-2.63	1.38	1.45
19	1	1148	CLA	C3D-C2D	-2.61	1.33	1.40
19	B	1735	CLA	C2A-C1A	-2.61	1.47	1.52
19	B	1739	CLA	C3B-C2B	-2.61	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1170	BCR	C34-C9	-2.61	1.45	1.50
19	B	1763	CLA	C3B-C2B	-2.61	1.36	1.40
19	A	1795	CLA	C3B-C2B	-2.61	1.36	1.40
19	A	1767	CLA	C4C-C3C	-2.61	1.40	1.45
22	A	1805	BCR	C30-C25	-2.61	1.50	1.53
19	2	1223	CLA	C4C-C3C	-2.60	1.40	1.45
19	B	1770	CLA	C1C-C2C	-2.60	1.39	1.44
21	2	1225	SUC	O5-C5	-2.60	1.38	1.44
19	3	1223	CLA	C3C-C4C	-2.60	1.36	1.43
19	B	1743	CLA	C4C-C3C	-2.59	1.40	1.45
19	2	1222	CLA	C1C-C2C	-2.59	1.39	1.44
19	B	1768	CLA	C3D-CAD	-2.58	1.38	1.45
19	A	1792	CLA	C4C-C3C	-2.58	1.40	1.45
19	B	1773	CLA	C1C-C2C	-2.58	1.39	1.44
19	A	1773	CLA	C1C-C2C	-2.58	1.39	1.44
19	J	1044	CLA	C3B-C2B	-2.58	1.36	1.40
19	1	1142	CLA	C3B-C2B	-2.58	1.36	1.40
19	4	4007	CLA	C3A-C2A	-2.57	1.46	1.54
19	2	1218	CLA	C1C-C2C	-2.57	1.39	1.44
19	4	4007	CLA	C1C-NC	-2.57	1.33	1.37
22	L	1169	BCR	C40-C30	-2.57	1.48	1.53
20	A	7050	LMU	C4'-C5'	-2.56	1.45	1.52
19	A	1798	CLA	C1C-C2C	-2.56	1.39	1.44
22	L	1170	BCR	C4-C5	-2.56	1.45	1.51
19	A	1762	CLA	C4C-C3C	-2.55	1.40	1.45
20	A	7030	LMU	C4B-C5B	-2.55	1.47	1.53
19	4	1198	CLA	CBD-CHA	-2.55	1.39	1.52
19	1	1505	CLA	C4C-C3C	-2.55	1.40	1.45
19	4	1201	CLA	C3B-C2B	-2.55	1.37	1.40
19	1	1189	CLA	C3D-CAD	-2.54	1.38	1.45
19	I	1031	CLA	C3D-CAD	-2.54	1.38	1.45
22	B	1782	BCR	C32-C1	-2.54	1.48	1.53
19	B	1751	CLA	C4C-C3C	-2.53	1.40	1.45
19	A	1779	CLA	C4C-C3C	-2.53	1.40	1.45
19	B	1758	CLA	C3D-CAD	-2.53	1.38	1.45
19	1	1149	CLA	C3D-CAD	-2.52	1.38	1.45
19	B	1742	CLA	C1C-C2C	-2.51	1.39	1.44
19	A	1763	CLA	C3A-C2A	-2.51	1.47	1.54
19	4	1206	CLA	C3D-CAD	-2.50	1.38	1.45
22	L	1170	BCR	C37-C22	-2.50	1.45	1.50
19	A	1772	CLA	C1C-NC	-2.50	1.33	1.37
19	B	1742	CLA	C4C-C3C	-2.50	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1736	CLA	C4C-C3C	-2.49	1.40	1.45
19	I	1031	CLA	C1C-C2C	-2.49	1.39	1.44
19	4	1196	CLA	C3B-C2B	-2.48	1.37	1.40
20	A	7037	LMU	C4B-C3B	-2.48	1.45	1.52
19	3	1214	CLA	C4C-C3C	-2.48	1.39	1.44
19	1	1194	CLA	C3C-C4C	-2.48	1.37	1.43
19	A	1761	CLA	C3B-C2B	-2.48	1.37	1.40
19	1	1187	CLA	CMD-C2D	-2.47	1.46	1.51
19	1	1014	CLA	C3D-CAD	-2.47	1.38	1.45
20	A	7037	LMU	C4'-C5'	-2.47	1.46	1.52
22	B	1775	BCR	C30-C25	-2.46	1.50	1.53
19	B	1764	CLA	C1C-NC	-2.46	1.33	1.37
19	B	1752	CLA	C3D-CAD	-2.46	1.38	1.45
19	2	1214	CLA	C3C-C4C	-2.46	1.37	1.43
20	A	7023	LMU	C4B-C5B	-2.45	1.47	1.53
22	B	1780	BCR	C10-C9	-2.45	1.32	1.35
19	1	1505	CLA	C1C-C2C	-2.44	1.39	1.44
19	1	1198	CLA	C2B-C1B	-2.44	1.35	1.40
19	B	1764	CLA	C3D-CAD	-2.44	1.38	1.45
19	B	1741	CLA	C3D-CAD	-2.44	1.38	1.45
22	3	1225	BCR	C30-C25	-2.44	1.50	1.53
19	B	1755	CLA	C3B-C2B	-2.43	1.37	1.40
19	B	1754	CLA	CAC-C3C	-2.43	1.44	1.51
22	A	1804	BCR	C1-C6	-2.43	1.50	1.53
19	B	1754	CLA	C3C-C2C	-2.43	1.31	1.36
19	A	1767	CLA	C3B-C2B	-2.42	1.37	1.40
19	A	1786	CLA	C1C-C2C	-2.42	1.39	1.44
19	1	1187	CLA	C1C-NC	-2.42	1.33	1.37
19	B	1754	CLA	O2D-CED	-2.42	1.39	1.45
19	A	1799	CLA	C3D-CAD	-2.42	1.38	1.45
19	B	1749	CLA	C1C-C2C	-2.42	1.39	1.44
19	A	1764	CLA	C3D-CAD	-2.41	1.38	1.45
19	1	1308	CLA	C3B-C2B	-2.41	1.37	1.40
19	B	1744	CLA	C3A-C2A	-2.41	1.47	1.54
19	A	1771	CLA	C4C-NC	-2.41	1.33	1.37
19	1	1303	CLA	C2C-C1C	-2.41	1.37	1.43
19	3	1221	CLA	C4C-NC	-2.41	1.33	1.37
19	4	1200	CLA	C1C-C2C	-2.41	1.39	1.44
19	B	1786	CLA	C1C-C2C	-2.40	1.39	1.44
19	A	1789	CLA	C3A-C2A	-2.40	1.47	1.54
19	1	1191	CLA	C3C-C4C	-2.40	1.37	1.43
22	L	1169	BCR	C31-C1	-2.40	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1191	CLA	C2C-C1C	-2.40	1.37	1.43
19	J	1043	CLA	C3D-CAD	-2.40	1.39	1.45
22	B	1778	BCR	C1-C6	-2.40	1.50	1.53
19	F	1155	CLA	C4C-C3C	-2.40	1.39	1.44
22	A	1806	BCR	C30-C25	-2.39	1.50	1.53
22	L	1170	BCR	C36-C18	-2.39	1.45	1.50
22	B	1782	BCR	C30-C25	-2.39	1.50	1.53
19	4	1197	CLA	C4C-C3C	-2.38	1.39	1.44
22	L	1170	BCR	C5-C6	-2.38	1.30	1.34
19	F	1157	CLA	C1C-NC	-2.38	1.33	1.37
19	R	1054	CLA	C4C-C3C	-2.38	1.40	1.45
19	4	1200	CLA	C3D-CAD	-2.38	1.39	1.45
19	1	1188	CLA	C3A-C2A	-2.37	1.47	1.54
19	1	1309	CLA	C2C-C1C	-2.37	1.37	1.43
19	3	1215	CLA	C4C-NC	-2.37	1.33	1.37
22	B	1780	BCR	C32-C1	-2.37	1.48	1.53
19	3	1216	CLA	C2C-C1C	-2.37	1.37	1.43
19	B	1741	CLA	C1C-C2C	-2.37	1.39	1.44
19	B	1751	CLA	C3D-CAD	-2.37	1.39	1.45
19	A	1784	CLA	C1C-C2C	-2.37	1.39	1.44
19	A	1786	CLA	C3D-CAD	-2.37	1.39	1.45
19	1	1308	CLA	C3D-CAD	-2.36	1.39	1.45
19	B	1738	CLA	C1C-NC	-2.36	1.33	1.37
19	A	1780	CLA	C3D-CAD	-2.36	1.39	1.45
19	R	1054	CLA	C3D-CAD	-2.36	1.39	1.45
19	A	1799	CLA	C1C-C2C	-2.36	1.39	1.44
20	A	7032	LMU	C1B-C2B	-2.36	1.45	1.52
19	B	1788	CLA	C1C-NC	-2.36	1.33	1.37
19	A	1811	CLA	C1C-C2C	-2.36	1.39	1.44
19	A	1787	CLA	C4C-C3C	-2.35	1.40	1.45
22	B	1779	BCR	C30-C25	-2.35	1.50	1.53
19	B	1745	CLA	C3B-C2B	-2.35	1.37	1.40
21	F	1158	SUC	O3'-C3'	-2.35	1.37	1.42
19	2	1213	CLA	C4C-C3C	-2.35	1.40	1.45
19	B	1772	CLA	C1C-C2C	-2.35	1.39	1.44
19	A	1796	CLA	C3B-C2B	-2.35	1.37	1.40
19	4	1209	CLA	C1C-C2C	-2.35	1.39	1.44
19	B	1786	CLA	C3B-C2B	-2.34	1.37	1.40
19	A	1777	CLA	C1C-C2C	-2.34	1.39	1.44
22	L	1169	BCR	C1-C6	-2.34	1.50	1.53
19	A	1785	CLA	C4C-C3C	-2.34	1.40	1.45
19	1	1142	CLA	C3D-CAD	-2.34	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1201	CLA	C3A-C4A	-2.34	1.44	1.51
19	B	1755	CLA	C1C-C2C	-2.33	1.39	1.44
19	A	1773	CLA	C3D-CAD	-2.33	1.39	1.45
19	1	1196	CLA	C4C-NC	-2.33	1.34	1.37
19	4	1197	CLA	C1C-C2C	-2.33	1.39	1.44
20	A	7036	LMU	C4B-C3B	-2.33	1.46	1.52
22	B	1782	BCR	C10-C9	-2.32	1.32	1.35
19	2	1215	CLA	C1C-C2C	-2.32	1.39	1.44
19	J	1044	CLA	C3A-C2A	-2.32	1.47	1.54
19	B	1766	CLA	C3D-CAD	-2.32	1.39	1.45
19	4	1196	CLA	C3D-CAD	-2.32	1.39	1.45
19	A	1780	CLA	C1C-C2C	-2.32	1.39	1.44
19	1	1241	CLA	C1C-C2C	-2.32	1.39	1.44
19	B	1765	CLA	C1C-C2C	-2.32	1.39	1.44
19	B	1756	CLA	C3B-C2B	-2.32	1.37	1.40
19	A	1764	CLA	C1C-C2C	-2.31	1.39	1.44
19	B	1743	CLA	C1C-C2C	-2.31	1.39	1.44
19	4	1211	CLA	C1C-NC	-2.31	1.33	1.37
20	A	7016	LMU	O5'-C5'	-2.31	1.38	1.44
19	4	1204	CLA	C2C-C1C	-2.30	1.37	1.43
19	B	1745	CLA	C4C-C3C	-2.30	1.40	1.45
20	A	7017	LMU	C4B-C5B	-2.30	1.48	1.53
19	3	1212	CLA	C4C-NC	-2.30	1.34	1.37
20	A	7033	LMU	O1B-C4'	-2.30	1.38	1.43
19	2	1216	CLA	C1C-NC	-2.29	1.33	1.37
19	1	1303	CLA	C3C-C4C	-2.29	1.37	1.43
19	A	1811	CLA	C3B-C2B	-2.29	1.37	1.40
22	B	1782	BCR	C34-C9	-2.29	1.46	1.50
19	B	1744	CLA	CAA-C2A	-2.29	1.49	1.54
20	K	1086	LMU	C4B-C5B	-2.29	1.48	1.53
19	1	1189	CLA	C4C-C3C	-2.28	1.40	1.45
19	B	1759	CLA	C3B-C2B	-2.28	1.37	1.40
19	3	1214	CLA	C1C-C2C	-2.28	1.40	1.44
19	A	1784	CLA	C4C-C3C	-2.28	1.40	1.45
19	3	1217	CLA	C2C-C1C	-2.28	1.37	1.43
19	A	1793	CLA	C3B-C2B	-2.27	1.37	1.40
19	1	1149	CLA	C3A-C2A	-2.27	1.47	1.54
19	A	1797	CLA	C1C-NC	-2.27	1.33	1.37
19	A	1799	CLA	C3B-C2B	-2.27	1.37	1.40
22	L	1170	BCR	C16-C15	-2.27	1.29	1.35
19	B	1756	CLA	C3D-CAD	-2.26	1.39	1.45
19	3	1224	CLA	C4C-NC	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1779	CLA	C3D-CAD	-2.26	1.39	1.45
19	B	1744	CLA	C1C-NC	-2.26	1.34	1.37
19	A	1778	CLA	C4C-C3C	-2.25	1.41	1.45
21	B	8062	SUC	O5-C1	-2.25	1.36	1.41
22	L	1170	BCR	C32-C1	-2.25	1.48	1.53
19	B	1757	CLA	C3D-CAD	-2.25	1.39	1.45
19	R	1055	CLA	C3D-C2D	-2.23	1.34	1.40
20	A	7032	LMU	C3B-C2B	-2.23	1.46	1.52
19	L	1166	CLA	C1C-C2C	-2.23	1.40	1.44
19	B	1768	CLA	C4C-C3C	-2.23	1.41	1.45
19	A	1810	CLA	C3D-CAD	-2.23	1.39	1.45
19	B	1754	CLA	CBD-CHA	-2.23	1.41	1.52
20	A	7041	LMU	C4B-C5B	-2.23	1.48	1.53
19	L	1168	CLA	C3B-C2B	-2.23	1.37	1.40
19	1	1145	CLA	C3D-C2D	-2.22	1.34	1.40
19	1	1187	CLA	C3C-C2C	-2.22	1.31	1.36
19	A	1812	CLA	C1C-NC	-2.22	1.34	1.37
19	A	1771	CLA	C3D-CAD	-2.22	1.39	1.45
19	4	4007	CLA	C4C-NC	-2.22	1.34	1.37
22	B	1780	BCR	C37-C22	-2.22	1.46	1.50
19	A	1785	CLA	C1C-C2C	-2.21	1.40	1.44
19	J	1043	CLA	C3B-C2B	-2.21	1.37	1.40
19	L	1168	CLA	C3A-C2A	-2.21	1.48	1.54
22	A	1804	BCR	C30-C25	-2.20	1.50	1.53
19	1	1198	CLA	C1C-NC	-2.20	1.33	1.37
19	3	1217	CLA	C3C-C4C	-2.20	1.37	1.43
19	L	1168	CLA	C3D-CAD	-2.20	1.39	1.45
22	L	1169	BCR	C26-C25	-2.20	1.30	1.34
19	B	1750	CLA	C3D-CAD	-2.20	1.39	1.45
19	A	1797	CLA	C3D-C2D	-2.20	1.34	1.40
19	3	1216	CLA	C3C-C4C	-2.19	1.37	1.43
22	B	1782	BCR	C40-C30	-2.19	1.49	1.53
19	B	1765	CLA	C3D-CAD	-2.19	1.39	1.45
19	1	1192	CLA	C1C-C2C	-2.19	1.40	1.44
19	4	1201	CLA	C3D-C2D	-2.19	1.34	1.40
21	B	8059	SUC	O5-C5	-2.19	1.38	1.44
21	2	1225	SUC	O2'-C5'	-2.19	1.38	1.43
19	B	1759	CLA	C3D-CAD	-2.18	1.39	1.45
19	B	1745	CLA	C1C-C2C	-2.18	1.40	1.44
19	J	1044	CLA	C3A-C4A	-2.18	1.44	1.51
19	4	1204	CLA	C3B-C4B	-2.18	1.36	1.40
19	1	1194	CLA	C4C-NC	-2.17	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1146	CLA	CMC-C2C	-2.17	1.46	1.50
22	B	1782	BCR	C23-C22	-2.17	1.41	1.45
19	1	1241	CLA	C4C-C3C	-2.17	1.41	1.45
19	1	1188	CLA	C3D-C2D	-2.16	1.34	1.40
19	3	3011	CLA	C4C-C3C	-2.16	1.41	1.45
19	4	1198	CLA	C3A-C2A	-2.16	1.48	1.54
19	B	1765	CLA	C1C-NC	-2.16	1.34	1.37
19	3	3011	CLA	C1C-C2C	-2.15	1.40	1.44
19	A	1779	CLA	C1C-C2C	-2.15	1.40	1.44
19	A	1778	CLA	C3B-C2B	-2.15	1.37	1.40
19	1	1505	CLA	C3B-C2B	-2.15	1.37	1.40
19	2	1220	CLA	C4C-C3C	-2.14	1.40	1.44
19	A	1777	CLA	C3D-CAD	-2.14	1.39	1.45
19	L	1168	CLA	CBD-CGD	-2.14	1.44	1.52
19	4	4007	CLA	C3D-C2D	-2.14	1.34	1.40
19	B	1787	CLA	C1C-C2C	-2.14	1.40	1.44
19	B	1750	CLA	C1C-C2C	-2.14	1.40	1.44
19	2	1220	CLA	C3D-CAD	-2.14	1.39	1.45
19	2	1213	CLA	C3D-CAD	-2.14	1.39	1.45
19	1	1193	CLA	CAA-C2A	-2.14	1.49	1.54
19	1	1307	CLA	C4C-NC	-2.14	1.34	1.37
19	B	1736	CLA	C1C-C2C	-2.14	1.40	1.44
19	B	1754	CLA	CMB-C2B	-2.13	1.47	1.51
22	B	1782	BCR	C33-C5	-2.13	1.47	1.51
19	1	1191	CLA	C1C-NC	-2.13	1.34	1.37
19	A	1765	CLA	C3D-CAD	-2.13	1.39	1.45
19	A	1795	CLA	C4C-NC	-2.12	1.34	1.37
19	A	1810	CLA	C1C-C2C	-2.12	1.40	1.44
19	L	1167	CLA	C1C-C2C	-2.12	1.40	1.44
21	B	8059	SUC	O2'-C5'	-2.12	1.38	1.43
19	B	1773	CLA	C4C-C3C	-2.12	1.40	1.44
19	A	1763	CLA	C1C-NC	-2.12	1.34	1.37
19	3	1222	CLA	C3B-C2B	-2.12	1.37	1.40
19	A	1788	CLA	C3D-CAD	-2.11	1.39	1.45
19	A	1794	CLA	C1C-C2C	-2.11	1.40	1.44
19	B	1760	CLA	C3A-C2A	-2.11	1.48	1.54
19	B	1767	CLA	C3D-CAD	-2.11	1.39	1.45
19	F	1157	CLA	C3D-CAD	-2.11	1.39	1.45
19	1	1193	CLA	C3A-C2A	-2.11	1.48	1.54
19	B	1751	CLA	C1C-C2C	-2.11	1.40	1.44
19	L	1167	CLA	C3D-CAD	-2.11	1.39	1.45
19	A	1772	CLA	C3D-C2D	-2.11	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1790	CLA	C1C-C2C	-2.10	1.40	1.44
19	1	1193	CLA	C3D-CAD	-2.10	1.39	1.45
19	1	1196	CLA	CBD-CGD	-2.10	1.45	1.52
19	4	1204	CLA	C3C-C4C	-2.10	1.38	1.43
22	A	1802	BCR	C1-C6	-2.10	1.50	1.53
19	B	1772	CLA	C3D-CAD	-2.10	1.39	1.45
19	B	1766	CLA	C1C-C2C	-2.10	1.40	1.44
22	B	1782	BCR	C37-C22	-2.10	1.46	1.50
19	1	1505	CLA	C3D-CAD	-2.10	1.39	1.45
19	A	1789	CLA	C3D-CAD	-2.09	1.39	1.45
19	1	1195	CLA	C1C-C2C	-2.09	1.40	1.44
19	2	1222	CLA	C3D-CAD	-2.09	1.39	1.45
19	4	1198	CLA	CBD-CGD	-2.09	1.45	1.52
19	4	1201	CLA	C3C-C2C	-2.09	1.32	1.36
20	A	7040	LMU	C3B-C2B	-2.09	1.46	1.52
20	A	7050	LMU	O1B-C4'	-2.08	1.38	1.43
19	B	1759	CLA	C1C-C2C	-2.08	1.40	1.44
19	B	1762	CLA	C3D-CAD	-2.08	1.39	1.45
19	B	1767	CLA	C3B-C2B	-2.08	1.37	1.40
19	B	1749	CLA	C3D-CAD	-2.08	1.39	1.45
19	2	1212	CLA	C3D-CAD	-2.08	1.39	1.45
22	B	1782	BCR	C2-C1	-2.08	1.49	1.54
19	A	1759	CLA	C3D-CAD	-2.07	1.39	1.45
19	3	1222	CLA	C2A-C1A	-2.07	1.48	1.52
19	A	1781	CLA	C3D-CAD	-2.07	1.39	1.45
19	4	4014	CLA	C3D-CAD	-2.07	1.39	1.45
19	R	1054	CLA	C1C-C2C	-2.07	1.40	1.44
19	A	1763	CLA	C4C-NC	-2.07	1.34	1.37
19	A	1769	CLA	C3D-CAD	-2.07	1.39	1.45
20	A	7032	LMU	C4B-C5B	-2.07	1.48	1.53
19	4	1207	CLA	C3C-C4C	-2.07	1.38	1.43
19	4	1203	CLA	C2B-C1B	-2.07	1.36	1.40
19	3	1222	CLA	C3D-C2D	-2.07	1.35	1.40
19	4	1202	CLA	C3D-CAD	-2.06	1.39	1.45
21	B	8054	SUC	O5-C5	-2.06	1.39	1.44
22	B	1780	BCR	C26-C25	-2.06	1.30	1.34
21	B	8062	SUC	O3-C3	-2.06	1.38	1.43
19	F	1157	CLA	C4C-NC	-2.06	1.34	1.37
22	L	1169	BCR	C2-C1	-2.06	1.49	1.54
21	B	8062	SUC	O5-C5	-2.06	1.39	1.44
19	B	1748	CLA	C4C-C3C	-2.06	1.41	1.45
19	B	1738	CLA	C3D-CAD	-2.05	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	1224	CLA	C3C-C2C	-2.05	1.32	1.36
19	1	1307	CLA	C3C-C4C	-2.04	1.38	1.43
19	4	1199	CLA	C4C-C3C	-2.04	1.41	1.45
19	A	1785	CLA	C3D-CAD	-2.04	1.40	1.45
22	A	1807	BCR	C1-C6	-2.04	1.50	1.53
19	4	1211	CLA	CMC-C2C	-2.04	1.46	1.50
21	B	8054	SUC	O2'-C2'	-2.04	1.37	1.42
19	G	1099	CLA	CBD-CGD	-2.04	1.45	1.52
22	I	1032	BCR	C37-C22	-2.04	1.46	1.50
19	3	1221	CLA	C1C-NC	-2.04	1.34	1.37
19	3	1213	CLA	C2B-C1B	-2.03	1.36	1.40
19	A	1782	CLA	C3B-C2B	-2.03	1.37	1.40
22	B	1776	BCR	C30-C25	-2.03	1.50	1.53
19	B	1735	CLA	C1C-C2C	-2.03	1.40	1.44
19	R	1055	CLA	C4C-NC	-2.03	1.34	1.37
19	1	1014	CLA	C1C-NC	-2.03	1.34	1.37
19	K	1085	CLA	C3D-CAD	-2.03	1.40	1.45
19	4	1209	CLA	C3D-CAD	-2.03	1.40	1.45
19	B	1787	CLA	C3D-CAD	-2.03	1.40	1.45
22	L	1170	BCR	C35-C13	-2.03	1.46	1.50
19	B	1743	CLA	C3D-CAD	-2.03	1.40	1.45
20	A	7028	LMU	O5'-C5'	-2.03	1.39	1.44
19	3	1221	CLA	C3C-C4C	-2.03	1.38	1.43
19	1	1196	CLA	CMB-C2B	-2.03	1.47	1.51
19	A	1790	CLA	C3D-CAD	-2.02	1.40	1.45
19	1	1146	CLA	C3A-C4A	-2.02	1.45	1.51
19	A	1759	CLA	C1C-NC	-2.02	1.34	1.37
19	B	1769	CLA	C3D-CAD	-2.02	1.40	1.45
19	A	1811	CLA	C3D-CAD	-2.02	1.40	1.45
19	F	1156	CLA	C3D-CAD	-2.01	1.40	1.45
21	B	8061	SUC	C4-C3	-2.01	1.47	1.52
19	B	1772	CLA	C4C-C3C	-2.01	1.41	1.45
19	3	1223	CLA	C1C-NC	-2.01	1.34	1.37
19	B	1751	CLA	C3A-C2A	-2.01	1.48	1.54
19	1	1146	CLA	O2A-C1	-2.00	1.40	1.46
19	A	1787	CLA	C1C-C2C	-2.00	1.40	1.44
19	3	1212	CLA	C3D-CAD	-2.00	1.40	1.45
19	3	1218	CLA	C4C-C3C	-2.00	1.41	1.45
19	3	3011	CLA	C1B-CHB	2.00	1.45	1.39
20	A	7014	LMU	O1'-C1'	2.01	1.43	1.40
19	B	1760	CLA	C2-C3	2.01	1.36	1.33
19	B	1743	CLA	C2-C3	2.01	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1768	CLA	C2-C3	2.02	1.36	1.33
20	A	7025	LMU	O1'-C1'	2.02	1.43	1.40
19	1	1188	CLA	OBD-CAD	2.02	1.25	1.22
19	B	1763	CLA	C1A-CHA	2.03	1.51	1.43
19	B	1736	CLA	C1B-CHB	2.04	1.45	1.39
19	A	1761	CLA	C1A-CHA	2.04	1.51	1.43
19	1	1303	CLA	C4B-CHC	2.05	1.47	1.43
19	2	1215	CLA	C1A-CHA	2.05	1.51	1.43
22	B	1777	BCR	C23-C22	2.05	1.50	1.45
19	2	1216	CLA	CHA-C1A	2.06	1.47	1.41
19	B	1787	CLA	C1A-CHA	2.06	1.51	1.43
19	A	1798	CLA	C1B-CHB	2.07	1.45	1.39
19	B	1740	CLA	C1B-CHB	2.07	1.45	1.39
23	A	1801	PQN	O1-C1	2.07	1.27	1.23
19	G	1099	CLA	C1B-CHB	2.07	1.45	1.39
19	1	1187	CLA	C1B-CHB	2.07	1.45	1.39
20	A	7033	LMU	O1'-C1'	2.08	1.43	1.40
19	4	1203	CLA	CHA-C1A	2.08	1.47	1.41
19	A	1810	CLA	C1B-CHB	2.08	1.45	1.39
19	B	1768	CLA	C2-C3	2.09	1.37	1.33
19	B	1755	CLA	C1A-CHA	2.09	1.51	1.43
19	1	1197	CLA	C1B-CHB	2.09	1.48	1.43
19	B	1787	CLA	C1B-CHB	2.09	1.45	1.39
19	4	1211	CLA	OBD-CAD	2.10	1.25	1.22
19	4	4007	CLA	C1B-CHB	2.11	1.45	1.39
19	B	1771	CLA	C1B-CHB	2.11	1.45	1.39
19	2	1214	CLA	CHA-C1A	2.12	1.47	1.41
19	A	1810	CLA	C2-C3	2.15	1.37	1.33
19	A	1769	CLA	C1B-CHB	2.17	1.45	1.39
20	B	1783	LMU	O1'-C1'	2.17	1.44	1.40
19	1	1307	CLA	CHA-C1A	2.17	1.47	1.41
20	A	7035	LMU	O1'-C1'	2.18	1.44	1.40
20	A	7049	LMU	O1'-C1'	2.19	1.44	1.40
19	R	1054	CLA	C2-C3	2.19	1.37	1.33
19	1	1196	CLA	CBA-CGA	2.19	1.57	1.50
19	R	1055	CLA	C4B-CHC	2.20	1.45	1.39
19	3	1212	CLA	C4B-CHC	2.20	1.45	1.39
19	3	1213	CLA	C4B-CHC	2.20	1.48	1.43
20	A	7017	LMU	O1'-C1'	2.20	1.44	1.40
19	4	1209	CLA	C1B-CHB	2.21	1.45	1.39
19	A	1793	CLA	C1B-CHB	2.23	1.46	1.39
20	L	1171	LMU	O5B-C1B	2.23	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1795	CLA	C1B-CHB	2.23	1.46	1.39
19	A	1790	CLA	C1B-CHB	2.23	1.46	1.39
19	B	1744	CLA	OBD-CAD	2.23	1.25	1.22
19	1	1145	CLA	C1B-CHB	2.23	1.46	1.39
19	B	1738	CLA	C1B-CHB	2.23	1.46	1.39
19	2	1223	CLA	C1B-CHB	2.24	1.46	1.39
19	3	3001	CLA	C1B-CHB	2.25	1.48	1.43
19	2	1213	CLA	C1B-CHB	2.25	1.46	1.39
19	1	1241	CLA	C1B-CHB	2.26	1.46	1.39
19	B	1755	CLA	C1B-CHB	2.26	1.46	1.39
19	J	1043	CLA	C1B-CHB	2.26	1.46	1.39
19	B	1739	CLA	C1B-CHB	2.26	1.46	1.39
19	A	1772	CLA	OBD-CAD	2.26	1.25	1.22
19	B	1737	CLA	C1B-CHB	2.26	1.46	1.39
19	A	1770	CLA	C1B-CHB	2.26	1.46	1.39
19	A	1764	CLA	C2-C3	2.27	1.37	1.33
19	A	1812	CLA	C1B-CHB	2.27	1.46	1.39
19	F	1155	CLA	C1B-CHB	2.27	1.46	1.39
19	A	1793	CLA	C2-C3	2.27	1.37	1.33
19	1	1188	CLA	C4B-CHC	2.28	1.46	1.39
19	1	1142	CLA	C1B-CHB	2.29	1.46	1.39
19	4	1196	CLA	C1B-CHB	2.29	1.46	1.39
19	4	1201	CLA	C4B-CHC	2.30	1.46	1.39
19	A	1780	CLA	C1B-CHB	2.31	1.46	1.39
19	4	1198	CLA	C4B-CHC	2.32	1.46	1.39
19	1	1308	CLA	C1B-CHB	2.32	1.46	1.39
19	1	1193	CLA	C2-C3	2.33	1.37	1.33
19	3	3015	CLA	CHD-C4C	2.33	1.46	1.41
19	A	1811	CLA	C1B-CHB	2.34	1.46	1.39
19	I	1031	CLA	C1B-CHB	2.34	1.46	1.39
19	4	1201	CLA	OBD-CAD	2.34	1.25	1.22
19	L	1167	CLA	C1B-CHB	2.34	1.46	1.39
19	4	1207	CLA	CHA-C1A	2.35	1.48	1.41
19	B	1752	CLA	C1B-CHB	2.35	1.46	1.39
19	A	1767	CLA	C1B-CHB	2.35	1.46	1.39
19	4	1200	CLA	C1B-CHB	2.36	1.46	1.39
19	A	1797	CLA	C1B-CHB	2.36	1.46	1.39
20	A	7034	LMU	O1'-C1'	2.37	1.44	1.40
19	A	1760	CLA	C1B-CHB	2.37	1.46	1.39
19	2	2010	CLA	C1B-CHB	2.39	1.48	1.43
19	A	1760	CLA	C2-C3	2.39	1.37	1.33
19	A	1796	CLA	C1B-CHB	2.40	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	7039	LMU	C4B-C3B	2.41	1.58	1.52
20	A	7026	LMU	O5'-C1'	2.41	1.48	1.41
19	1	1190	CLA	C1B-CHB	2.42	1.46	1.39
19	B	1756	CLA	C1B-CHB	2.42	1.46	1.39
19	A	1777	CLA	C1B-CHB	2.44	1.46	1.39
19	2	2010	CLA	CHA-C1A	2.45	1.48	1.41
19	A	1779	CLA	C1B-CHB	2.45	1.46	1.39
19	A	1763	CLA	C1B-CHB	2.46	1.46	1.39
19	4	1210	CLA	C1B-CHB	2.46	1.48	1.43
19	1	1196	CLA	OBD-CAD	2.47	1.26	1.22
19	3	1222	CLA	C4B-CHC	2.48	1.46	1.39
19	2	1214	CLA	C4B-CHC	2.49	1.48	1.43
19	B	1788	CLA	C1B-CHB	2.49	1.46	1.39
19	B	1758	CLA	C1B-CHB	2.49	1.46	1.39
19	A	1766	CLA	C1B-CHB	2.49	1.46	1.39
19	B	1755	CLA	C2-C3	2.50	1.37	1.33
19	B	1772	CLA	C1B-CHB	2.52	1.46	1.39
19	A	1788	CLA	C1B-CHB	2.52	1.46	1.39
19	1	1194	CLA	C4B-CHC	2.52	1.48	1.43
19	2	1221	CLA	CHA-C1A	2.53	1.48	1.41
19	3	1220	CLA	CHA-C1A	2.54	1.48	1.41
19	2	1217	CLA	O2A-CGA	2.54	1.41	1.33
19	A	1762	CLA	C1B-CHB	2.54	1.46	1.39
19	4	1211	CLA	C1B-CHB	2.55	1.46	1.39
19	3	1224	CLA	C4B-CHC	2.55	1.46	1.39
19	B	1738	CLA	OBD-CAD	2.56	1.26	1.22
19	B	1746	CLA	C1B-CHB	2.56	1.46	1.39
20	A	7024	LMU	O1'-C1'	2.56	1.44	1.40
19	B	1765	CLA	C1B-CHB	2.56	1.46	1.39
19	2	1216	CLA	C4B-CHC	2.57	1.49	1.43
19	A	1763	CLA	OBD-CAD	2.57	1.26	1.22
19	1	1014	CLA	C1B-CHB	2.57	1.46	1.39
20	A	7015	LMU	O1'-C1'	2.58	1.44	1.40
19	A	1768	CLA	C1B-CHB	2.58	1.47	1.39
19	2	1215	CLA	C1B-CHB	2.60	1.47	1.39
19	4	1197	CLA	C1B-CHB	2.60	1.47	1.39
19	B	1786	CLA	C1B-CHB	2.60	1.47	1.39
19	1	1191	CLA	C4B-CHC	2.60	1.49	1.43
19	B	1753	CLA	C1B-CHB	2.61	1.47	1.39
19	A	1775	CLA	CHA-C1A	2.62	1.49	1.41
19	B	1754	CLA	O2D-CGD	2.63	1.39	1.33
19	4	1198	CLA	O2A-CGA	2.64	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1773	CLA	C1B-CHB	2.64	1.47	1.39
19	B	1766	CLA	C1B-CHB	2.65	1.47	1.39
19	A	1759	CLA	C1B-CHB	2.65	1.47	1.39
19	L	1168	CLA	C1B-CHB	2.65	1.47	1.39
19	B	1762	CLA	C1B-CHB	2.66	1.47	1.39
19	A	1794	CLA	C1B-CHB	2.67	1.47	1.39
19	B	1745	CLA	C1B-CHB	2.67	1.47	1.39
19	4	4014	CLA	C1B-CHB	2.67	1.47	1.39
19	B	1741	CLA	C1B-CHB	2.68	1.47	1.39
19	A	1774	CLA	C1B-CHB	2.68	1.47	1.39
19	B	1749	CLA	OBD-CAD	2.69	1.26	1.22
19	B	1757	CLA	C1B-CHB	2.69	1.47	1.39
20	2	1224	LMU	O1'-C1'	2.69	1.45	1.40
19	1	1197	CLA	CHA-C1A	2.70	1.49	1.41
19	1	1149	CLA	CMA-C3A	2.70	1.59	1.53
19	3	1220	CLA	C4B-CHC	2.71	1.49	1.43
19	3	1222	CLA	OBD-CAD	2.71	1.26	1.22
19	I	1031	CLA	OBD-CAD	2.71	1.26	1.22
19	A	1776	CLA	C1B-CHB	2.71	1.47	1.39
19	1	1196	CLA	C4B-CHC	2.72	1.47	1.39
19	B	1767	CLA	C1B-CHB	2.72	1.47	1.39
19	4	4007	CLA	OBD-CAD	2.72	1.26	1.22
19	A	1782	CLA	C1B-CHB	2.72	1.47	1.39
19	K	1085	CLA	C1B-CHB	2.72	1.47	1.39
19	3	1216	CLA	C4B-CHC	2.73	1.49	1.43
19	4	1200	CLA	CHD-C4C	2.73	1.47	1.41
20	A	7027	LMU	O1'-C1'	2.73	1.45	1.40
20	A	7026	LMU	O1'-C1'	2.73	1.45	1.40
19	4	1202	CLA	C1B-CHB	2.74	1.47	1.39
19	B	1735	CLA	C1B-CHB	2.74	1.47	1.39
19	4	1199	CLA	C1B-CHB	2.74	1.47	1.39
19	1	1505	CLA	C1B-CHB	2.74	1.47	1.39
19	1	1010	CLA	CHA-C1A	2.75	1.49	1.41
19	2	1212	CLA	C1B-CHB	2.75	1.47	1.39
19	B	1748	CLA	C1B-CHB	2.75	1.47	1.39
19	F	1156	CLA	C1B-CHB	2.76	1.47	1.39
19	4	1210	CLA	CHA-C1A	2.76	1.49	1.41
19	A	1784	CLA	C1B-CHB	2.76	1.47	1.39
19	3	1213	CLA	CHD-C4C	2.77	1.47	1.41
19	B	1763	CLA	C1B-CHB	2.77	1.47	1.39
19	A	1781	CLA	C1B-CHB	2.77	1.47	1.39
19	3	1224	CLA	CHD-C4C	2.77	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1198	CLA	C4B-CHC	2.79	1.49	1.43
19	1	1307	CLA	C4B-CHC	2.79	1.49	1.43
19	A	1783	CLA	C1B-CHB	2.80	1.47	1.39
20	A	1809	LMU	O1'-C1'	2.80	1.45	1.40
19	3	1217	CLA	CHA-C1A	2.81	1.49	1.41
19	2	1217	CLA	C4B-CHC	2.82	1.47	1.39
19	B	1764	CLA	C1B-CHB	2.82	1.47	1.39
19	A	1787	CLA	C1B-CHB	2.82	1.47	1.39
19	B	1743	CLA	C1B-CHB	2.82	1.47	1.39
19	1	1195	CLA	C1B-CHB	2.83	1.47	1.39
19	4	4007	CLA	O2A-CGA	2.83	1.41	1.33
19	A	1772	CLA	O2A-CGA	2.83	1.41	1.33
19	3	1216	CLA	CHA-C1A	2.84	1.49	1.41
19	B	1742	CLA	C1B-CHB	2.84	1.47	1.39
19	B	1740	CLA	O2A-CGA	2.84	1.41	1.33
19	B	1744	CLA	CHD-C4C	2.85	1.47	1.41
19	B	1760	CLA	C1B-CHB	2.85	1.47	1.39
19	3	3015	CLA	C4B-CHC	2.86	1.49	1.43
19	3	1217	CLA	C4B-CHC	2.87	1.49	1.43
19	B	1744	CLA	O2D-CGD	2.87	1.40	1.33
19	A	1763	CLA	O2A-CGA	2.87	1.42	1.32
19	3	1221	CLA	CHA-C1A	2.88	1.49	1.41
19	F	1157	CLA	C1B-CHB	2.88	1.47	1.39
19	A	1789	CLA	C1B-CHB	2.88	1.47	1.39
19	B	1747	CLA	C1B-CHB	2.89	1.47	1.39
19	A	1765	CLA	C4B-CHC	2.89	1.47	1.39
19	2	1217	CLA	C1B-CHB	2.90	1.47	1.39
19	A	1786	CLA	C1B-CHB	2.90	1.47	1.39
19	2	1219	CLA	C4B-CHC	2.90	1.49	1.43
19	4	1206	CLA	C1B-CHB	2.90	1.47	1.39
19	A	1785	CLA	C1B-CHB	2.91	1.47	1.39
19	3	3008	CLA	C1B-CHB	2.92	1.47	1.39
19	2	1218	CLA	C1B-CHB	2.92	1.47	1.39
19	1	1197	CLA	C4B-CHC	2.92	1.49	1.43
19	1	1014	CLA	O2A-CGA	2.93	1.42	1.33
19	B	1773	CLA	C1B-CHB	2.93	1.47	1.39
19	A	1791	CLA	C1B-CHB	2.93	1.47	1.39
20	A	7026	LMU	O3B-C3B	2.93	1.50	1.43
19	A	1761	CLA	OBD-CAD	2.94	1.26	1.22
19	A	1795	CLA	C4B-CHC	2.94	1.47	1.39
19	A	1765	CLA	C1B-CHB	2.94	1.47	1.39
20	A	7014	LMU	O2B-C2B	2.95	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1149	CLA	C1B-CHB	2.95	1.48	1.39
19	A	1771	CLA	C4B-CHC	2.95	1.48	1.39
19	1	1193	CLA	C1B-CHB	2.95	1.48	1.39
19	1	1146	CLA	OBD-CAD	2.96	1.26	1.22
19	A	1763	CLA	C4B-CHC	2.96	1.48	1.39
19	4	1203	CLA	CHD-C4C	2.97	1.48	1.41
19	B	1750	CLA	C1B-CHB	2.97	1.48	1.39
19	R	1055	CLA	C1B-CHB	2.98	1.48	1.39
19	3	3001	CLA	CHA-C1A	2.98	1.50	1.41
19	1	1309	CLA	C4B-CHC	2.98	1.49	1.43
19	B	1769	CLA	C1B-CHB	2.99	1.48	1.39
19	3	1214	CLA	C1B-CHB	2.99	1.48	1.39
19	2	1222	CLA	C1B-CHB	3.00	1.48	1.39
19	4	1211	CLA	O2D-CGD	3.00	1.40	1.33
19	3	1223	CLA	C4B-CHC	3.02	1.50	1.43
19	1	1189	CLA	C1B-CHB	3.02	1.48	1.39
19	1	1188	CLA	O2A-CGA	3.03	1.42	1.33
19	1	1309	CLA	CHD-C4C	3.03	1.48	1.41
19	B	1744	CLA	O2A-CGA	3.04	1.42	1.33
19	4	1211	CLA	CHD-C4C	3.04	1.48	1.41
19	A	1799	CLA	C1B-CHB	3.04	1.48	1.39
19	1	1014	CLA	C4B-CHC	3.04	1.48	1.39
19	4	4007	CLA	C4B-CHC	3.05	1.48	1.39
19	B	1770	CLA	C1B-CHB	3.06	1.48	1.39
19	4	1201	CLA	O2A-CGA	3.07	1.42	1.33
19	2	1219	CLA	CHA-C1A	3.07	1.50	1.41
19	4	1200	CLA	O2A-CGA	3.07	1.42	1.33
19	B	1749	CLA	C1B-CHB	3.08	1.48	1.39
19	1	1148	CLA	OBD-CAD	3.09	1.27	1.22
19	B	1751	CLA	C1B-CHB	3.09	1.48	1.39
19	B	1769	CLA	C4B-CHC	3.09	1.48	1.39
19	B	1754	CLA	O2A-CGA	3.10	1.42	1.33
19	A	1761	CLA	C1B-CHB	3.10	1.48	1.39
19	B	1754	CLA	CHD-C4C	3.10	1.48	1.41
19	A	1775	CLA	C4B-CHC	3.10	1.50	1.43
19	R	1054	CLA	C1B-CHB	3.11	1.48	1.39
19	3	1222	CLA	CHD-C4C	3.13	1.48	1.41
20	A	7019	LMU	O1'-C1'	3.14	1.45	1.40
19	4	1207	CLA	C4B-CHC	3.14	1.50	1.43
19	2	1220	CLA	C1B-CHB	3.15	1.48	1.39
19	3	1218	CLA	C1B-CHB	3.15	1.48	1.39
19	A	1792	CLA	C1B-CHB	3.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	1212	CLA	CHD-C4C	3.16	1.48	1.41
19	A	1797	CLA	C4B-CHC	3.16	1.48	1.39
19	A	1797	CLA	CHD-C4C	3.17	1.48	1.41
19	B	1738	CLA	C4B-CHC	3.17	1.48	1.39
19	L	1166	CLA	C1B-CHB	3.17	1.48	1.39
19	B	1772	CLA	C4B-CHC	3.20	1.48	1.39
19	3	1219	CLA	C1B-CHB	3.20	1.48	1.39
19	3	1223	CLA	CHD-C4C	3.21	1.48	1.41
19	1	1145	CLA	C4B-CHC	3.22	1.48	1.39
19	4	1210	CLA	C4B-CHC	3.22	1.50	1.43
19	A	1791	CLA	C4B-CHC	3.24	1.48	1.39
19	B	1768	CLA	C4B-CHC	3.24	1.48	1.39
19	1	1187	CLA	CHC-C1C	3.25	1.45	1.35
19	3	1212	CLA	O2A-CGA	3.27	1.43	1.33
19	1	1303	CLA	CHD-C4C	3.27	1.48	1.41
19	A	1778	CLA	C1B-CHB	3.28	1.48	1.39
19	1	1146	CLA	O2A-CGA	3.28	1.43	1.33
19	2	1214	CLA	CHD-C4C	3.28	1.48	1.41
19	4	1199	CLA	C4B-CHC	3.29	1.48	1.39
19	A	1759	CLA	C4B-CHC	3.29	1.48	1.39
19	1	1196	CLA	C1B-CHB	3.30	1.48	1.39
19	B	1737	CLA	C4B-CHC	3.30	1.48	1.39
19	B	1768	CLA	OBD-CAD	3.31	1.27	1.22
19	3	1222	CLA	C1B-CHB	3.31	1.49	1.39
19	B	1760	CLA	C4B-CHC	3.31	1.49	1.39
19	1	1191	CLA	CHD-C4C	3.31	1.49	1.41
19	2	2010	CLA	C4B-CHC	3.33	1.50	1.43
19	R	1055	CLA	CHD-C4C	3.33	1.49	1.41
19	1	1192	CLA	C1B-CHB	3.33	1.49	1.39
19	A	1761	CLA	C4B-CHC	3.34	1.49	1.39
19	A	1800	CLA	C1B-CHB	3.34	1.49	1.39
19	J	1044	CLA	O2A-CGA	3.35	1.43	1.33
19	R	1054	CLA	OBD-CAD	3.35	1.27	1.22
19	A	1774	CLA	C4B-CHC	3.36	1.49	1.39
19	3	1218	CLA	C4B-CHC	3.36	1.49	1.39
19	1	1014	CLA	OBD-CAD	3.36	1.27	1.22
20	A	7031	LMU	O1'-C1'	3.37	1.46	1.40
19	F	1157	CLA	O2A-CGA	3.37	1.43	1.33
19	B	1759	CLA	C1B-CHB	3.37	1.49	1.39
19	1	1196	CLA	CHD-C4C	3.38	1.49	1.41
19	B	1768	CLA	C1B-CHB	3.38	1.49	1.39
19	A	1772	CLA	CHD-C4C	3.38	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1205	CLA	C1B-CHB	3.38	1.49	1.39
19	R	1055	CLA	OBD-CAD	3.39	1.27	1.22
19	A	1789	CLA	C4B-CHC	3.39	1.49	1.39
19	A	1764	CLA	C4B-CHC	3.39	1.49	1.39
19	4	1200	CLA	C4B-CHC	3.40	1.49	1.39
19	B	1770	CLA	OBD-CAD	3.40	1.27	1.22
19	1	1187	CLA	CHD-C4C	3.40	1.49	1.41
19	3	1222	CLA	CHC-C1C	3.41	1.46	1.35
19	3	1222	CLA	O2A-CGA	3.41	1.43	1.33
19	B	1754	CLA	C4B-CHC	3.41	1.49	1.39
19	G	1099	CLA	C4B-CHC	3.41	1.49	1.39
19	1	1010	CLA	C4B-CHC	3.42	1.50	1.43
19	4	1211	CLA	C4B-CHC	3.42	1.49	1.39
19	4	1196	CLA	C4B-CHC	3.43	1.49	1.39
19	4	1208	CLA	C4B-CHC	3.44	1.50	1.43
19	4	1206	CLA	C4B-CHC	3.44	1.49	1.39
19	B	1739	CLA	C4B-CHC	3.45	1.49	1.39
19	A	1769	CLA	C4B-CHC	3.46	1.49	1.39
19	1	1142	CLA	C4B-CHC	3.46	1.49	1.39
20	A	7047	LMU	O1'-C1'	3.46	1.46	1.40
19	1	1149	CLA	C4B-CHC	3.47	1.49	1.39
19	1	1145	CLA	O2D-CGD	3.47	1.42	1.33
19	1	1308	CLA	C4B-CHC	3.48	1.49	1.39
19	A	1788	CLA	C4B-CHC	3.48	1.49	1.39
19	B	1751	CLA	OBD-CAD	3.48	1.27	1.22
19	A	1793	CLA	C4B-CHC	3.49	1.49	1.39
19	J	1044	CLA	C4B-CHC	3.50	1.49	1.39
19	A	1799	CLA	C4B-CHC	3.50	1.49	1.39
19	1	1307	CLA	CHD-C4C	3.51	1.49	1.41
19	J	1044	CLA	CHD-C4C	3.51	1.49	1.41
19	1	1187	CLA	O2A-CGA	3.51	1.44	1.32
19	A	1783	CLA	O2A-CGA	3.52	1.43	1.33
19	B	1788	CLA	OBD-CAD	3.53	1.27	1.22
19	B	1769	CLA	OBD-CAD	3.53	1.27	1.22
19	B	1760	CLA	CHD-C4C	3.54	1.49	1.41
19	2	1216	CLA	CHD-C4C	3.54	1.49	1.41
19	B	1750	CLA	C4B-CHC	3.55	1.49	1.39
19	A	1778	CLA	C4B-CHC	3.56	1.49	1.39
19	B	1741	CLA	C4B-CHC	3.56	1.49	1.39
19	B	1747	CLA	O2A-CGA	3.56	1.45	1.32
19	A	1782	CLA	C4B-CHC	3.57	1.49	1.39
19	J	1043	CLA	C4B-CHC	3.57	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1204	CLA	CHD-C4C	3.57	1.49	1.41
19	A	1771	CLA	O2A-CGA	3.57	1.44	1.33
19	B	1745	CLA	C4B-CHC	3.58	1.49	1.39
19	4	1198	CLA	OBD-CAD	3.59	1.27	1.22
19	B	1736	CLA	C4B-CHC	3.59	1.49	1.39
19	4	1208	CLA	CHD-C4C	3.60	1.49	1.41
19	B	1744	CLA	C4B-CHC	3.60	1.49	1.39
19	B	1756	CLA	C4B-CHC	3.60	1.49	1.39
19	B	1750	CLA	OBD-CAD	3.61	1.27	1.22
19	A	1771	CLA	CHD-C4C	3.61	1.49	1.41
19	3	1212	CLA	OBD-CAD	3.62	1.27	1.22
19	4	4014	CLA	OBD-CAD	3.62	1.27	1.22
19	A	1790	CLA	C4B-CHC	3.62	1.49	1.39
19	A	1786	CLA	OBD-CAD	3.63	1.27	1.22
19	A	1811	CLA	OBD-CAD	3.63	1.27	1.22
19	F	1157	CLA	CHD-C4C	3.63	1.49	1.41
19	A	1784	CLA	C4B-CHC	3.63	1.49	1.39
19	1	1145	CLA	O2A-CGA	3.64	1.44	1.33
19	A	1772	CLA	C4B-CHC	3.64	1.49	1.39
19	1	1190	CLA	C4B-CHC	3.64	1.49	1.39
19	2	1217	CLA	O2D-CGD	3.65	1.42	1.33
19	1	1146	CLA	C4B-CHC	3.66	1.49	1.39
19	A	1780	CLA	C4B-CHC	3.67	1.50	1.39
19	B	1743	CLA	OBD-CAD	3.67	1.28	1.22
19	A	1785	CLA	C4B-CHC	3.68	1.50	1.39
19	K	1085	CLA	C4B-CHC	3.68	1.50	1.39
19	1	1188	CLA	CHD-C4C	3.68	1.49	1.41
19	B	1755	CLA	C4B-CHC	3.68	1.50	1.39
19	A	1790	CLA	OBD-CAD	3.69	1.28	1.22
19	A	1760	CLA	C4B-CHC	3.69	1.50	1.39
19	A	1789	CLA	OBD-CAD	3.70	1.28	1.22
19	A	1780	CLA	OBD-CAD	3.70	1.28	1.22
19	1	1505	CLA	C4B-CHC	3.71	1.50	1.39
19	2	1218	CLA	C4B-CHC	3.72	1.50	1.39
19	B	1735	CLA	O2A-CGA	3.72	1.44	1.33
19	A	1794	CLA	C4B-CHC	3.72	1.50	1.39
19	B	1749	CLA	C4B-CHC	3.73	1.50	1.39
19	A	1794	CLA	OBD-CAD	3.74	1.28	1.22
19	A	1781	CLA	C4B-CHC	3.74	1.50	1.39
19	B	1788	CLA	C4B-CHC	3.74	1.50	1.39
19	A	1769	CLA	OBD-CAD	3.74	1.28	1.22
19	A	1762	CLA	C4B-CHC	3.75	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1749	CLA	O2A-CGA	3.76	1.44	1.33
19	A	1797	CLA	OBD-CAD	3.76	1.28	1.22
19	4	1209	CLA	CHD-C4C	3.76	1.50	1.41
19	B	1763	CLA	OBD-CAD	3.76	1.28	1.22
19	B	1762	CLA	C4B-CHC	3.76	1.50	1.39
19	4	1211	CLA	O2A-CGA	3.77	1.45	1.32
19	4	1198	CLA	O2D-CGD	3.77	1.42	1.33
19	4	1202	CLA	OBD-CAD	3.78	1.28	1.22
19	1	1146	CLA	CHD-C4C	3.78	1.50	1.41
19	F	1155	CLA	C4B-CHC	3.78	1.50	1.39
19	A	1810	CLA	OBD-CAD	3.78	1.28	1.22
19	B	1743	CLA	C4B-CHC	3.79	1.50	1.39
19	B	1759	CLA	O2A-CGA	3.79	1.44	1.33
19	1	1148	CLA	CHD-C4C	3.80	1.50	1.41
19	2	1222	CLA	OBD-CAD	3.80	1.28	1.22
19	2	1220	CLA	OBD-CAD	3.80	1.28	1.22
19	1	1188	CLA	CHC-C1C	3.80	1.47	1.35
19	A	1774	CLA	OBD-CAD	3.81	1.28	1.22
19	4	1197	CLA	C4B-CHC	3.81	1.50	1.39
19	B	1753	CLA	C4B-CHC	3.82	1.50	1.39
19	A	1812	CLA	O2A-CGA	3.82	1.44	1.33
19	2	1215	CLA	C4B-CHC	3.82	1.50	1.39
19	1	1188	CLA	O2D-CGD	3.82	1.43	1.33
19	A	1763	CLA	O2D-CGD	3.82	1.43	1.33
19	2	1217	CLA	CHD-C4C	3.82	1.50	1.41
19	B	1771	CLA	C4B-CHC	3.83	1.50	1.39
19	B	1739	CLA	O2A-CGA	3.83	1.44	1.33
19	4	1201	CLA	CHD-C4C	3.83	1.50	1.41
19	A	1787	CLA	C4B-CHC	3.83	1.50	1.39
19	3	1215	CLA	CHD-C4C	3.84	1.50	1.41
19	2	1222	CLA	C4B-CHC	3.84	1.50	1.39
19	R	1054	CLA	C4B-CHC	3.84	1.50	1.39
19	A	1798	CLA	C4B-CHC	3.84	1.50	1.39
19	1	1014	CLA	CHC-C1C	3.84	1.47	1.35
19	B	1764	CLA	C4B-CHC	3.85	1.50	1.39
19	A	1794	CLA	O2A-CGA	3.85	1.44	1.33
19	2	1221	CLA	CHD-C4C	3.85	1.50	1.41
19	A	1776	CLA	OBD-CAD	3.85	1.28	1.22
19	K	1085	CLA	O2A-CGA	3.85	1.44	1.33
19	B	1773	CLA	C4B-CHC	3.85	1.50	1.39
19	2	1221	CLA	C4B-CHC	3.86	1.51	1.43
19	A	1786	CLA	C4B-CHC	3.86	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1759	CLA	CHD-C4C	3.86	1.50	1.41
19	A	1765	CLA	O2D-CGD	3.87	1.43	1.33
19	4	1202	CLA	C4B-CHC	3.87	1.50	1.39
19	F	1157	CLA	C4B-CHC	3.87	1.50	1.39
19	A	1770	CLA	C4B-CHC	3.87	1.50	1.39
19	B	1735	CLA	C4B-CHC	3.87	1.50	1.39
19	4	4014	CLA	C4B-CHC	3.87	1.50	1.39
19	3	3001	CLA	C4B-CHC	3.87	1.51	1.43
19	B	1786	CLA	O2A-CGA	3.87	1.45	1.33
24	B	1784	LMG	O7-C10	3.88	1.45	1.34
19	3	3011	CLA	C4B-CHC	3.88	1.50	1.39
19	F	1156	CLA	C4B-CHC	3.90	1.50	1.39
19	A	1811	CLA	C4B-CHC	3.90	1.50	1.39
19	1	1149	CLA	OBD-CAD	3.90	1.28	1.22
19	A	1781	CLA	OBD-CAD	3.91	1.28	1.22
19	A	1782	CLA	O2A-CGA	3.92	1.45	1.33
19	B	1758	CLA	O2A-CGA	3.92	1.45	1.33
19	A	1765	CLA	CHC-C1C	3.92	1.47	1.35
19	2	1212	CLA	C4B-CHC	3.92	1.50	1.39
19	A	1792	CLA	C4B-CHC	3.93	1.50	1.39
19	B	1762	CLA	OBD-CAD	3.93	1.28	1.22
19	A	1799	CLA	O2A-CGA	3.93	1.45	1.33
19	B	1757	CLA	C4B-CHC	3.94	1.50	1.39
19	A	1800	CLA	C4B-CHC	3.95	1.50	1.39
19	A	1768	CLA	OBD-CAD	3.95	1.28	1.22
19	L	1166	CLA	C4B-CHC	3.95	1.50	1.39
19	1	1190	CLA	O2A-CGA	3.96	1.46	1.32
19	A	1783	CLA	O2D-CGD	3.96	1.43	1.33
19	L	1167	CLA	C4B-CHC	3.97	1.50	1.39
19	B	1752	CLA	C4B-CHC	3.97	1.50	1.39
19	1	1194	CLA	CHD-C4C	3.98	1.50	1.41
19	R	1055	CLA	CHC-C1C	3.98	1.47	1.35
19	B	1760	CLA	OBD-CAD	3.99	1.28	1.22
19	A	1767	CLA	C4B-CHC	3.99	1.50	1.39
19	3	3008	CLA	O2A-CGA	3.99	1.45	1.33
19	B	1743	CLA	CHD-C4C	3.99	1.50	1.41
19	B	1748	CLA	C4B-CHC	3.99	1.50	1.39
19	B	1757	CLA	CHD-C4C	4.00	1.50	1.41
19	1	1148	CLA	O2A-CGA	4.00	1.45	1.33
19	1	1014	CLA	CHD-C4C	4.01	1.50	1.41
19	3	1214	CLA	C4B-CHC	4.01	1.50	1.39
19	1	1241	CLA	C4B-CHC	4.02	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1771	CLA	O2D-CGD	4.02	1.43	1.33
19	A	1796	CLA	C4B-CHC	4.02	1.50	1.39
19	G	1099	CLA	CHD-C4C	4.02	1.50	1.41
19	2	1223	CLA	C4B-CHC	4.03	1.50	1.39
19	G	1099	CLA	O2A-CGA	4.03	1.45	1.33
19	1	1196	CLA	O2A-CGA	4.04	1.45	1.33
19	2	1220	CLA	C4B-CHC	4.04	1.51	1.39
19	I	1031	CLA	C4B-CHC	4.04	1.51	1.39
19	B	1786	CLA	C4B-CHC	4.04	1.51	1.39
19	4	1205	CLA	C4B-CHC	4.05	1.51	1.39
19	A	1773	CLA	C4B-CHC	4.05	1.51	1.39
19	2	1217	CLA	CHC-C1C	4.05	1.48	1.35
19	1	1148	CLA	C4B-CHC	4.06	1.51	1.39
19	A	1810	CLA	O2A-CGA	4.06	1.45	1.33
19	B	1761	CLA	OBD-CAD	4.06	1.28	1.22
19	F	1157	CLA	O2D-CGD	4.06	1.43	1.33
19	A	1812	CLA	C4B-CHC	4.06	1.51	1.39
19	B	1740	CLA	C4B-CHC	4.07	1.51	1.39
19	3	1224	CLA	CHC-C1C	4.07	1.48	1.35
19	B	1762	CLA	CHD-C4C	4.08	1.50	1.41
19	1	1193	CLA	C4B-CHC	4.08	1.51	1.39
19	G	1099	CLA	OBD-CAD	4.08	1.28	1.22
19	A	1783	CLA	C4B-CHC	4.08	1.51	1.39
19	4	1209	CLA	C4B-CHC	4.08	1.51	1.39
19	B	1767	CLA	C4B-CHC	4.08	1.51	1.39
19	1	1192	CLA	C4B-CHC	4.08	1.51	1.39
19	B	1770	CLA	CHD-C4C	4.08	1.50	1.41
19	1	1308	CLA	OBD-CAD	4.09	1.28	1.22
19	B	1760	CLA	O2A-CGA	4.09	1.45	1.33
19	4	1197	CLA	CHD-C4C	4.09	1.50	1.41
19	1	1192	CLA	CHD-C4C	4.09	1.50	1.41
19	B	1787	CLA	C4B-CHC	4.09	1.51	1.39
19	A	1764	CLA	O2D-CGD	4.09	1.43	1.33
19	B	1765	CLA	CHD-C4C	4.10	1.50	1.41
24	B	1784	LMG	O8-C28	4.11	1.45	1.33
19	B	1759	CLA	C4B-CHC	4.11	1.51	1.39
19	B	1765	CLA	C4B-CHC	4.11	1.51	1.39
19	2	1219	CLA	CHD-C4C	4.11	1.50	1.41
19	B	1740	CLA	OBD-CAD	4.11	1.28	1.22
19	B	1761	CLA	C4B-CHC	4.11	1.51	1.39
19	A	1763	CLA	CHC-C1C	4.11	1.48	1.35
19	4	4007	CLA	CHC-C1C	4.11	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1746	CLA	CHD-C4C	4.12	1.50	1.41
19	4	1210	CLA	CHD-C4C	4.12	1.50	1.41
19	B	1756	CLA	OBD-CAD	4.12	1.28	1.22
19	A	1766	CLA	C4B-CHC	4.13	1.51	1.39
19	4	1196	CLA	O2A-CGA	4.13	1.45	1.33
19	B	1772	CLA	OBD-CAD	4.13	1.28	1.22
19	B	1768	CLA	O2D-CGD	4.13	1.43	1.33
19	1	1308	CLA	O2A-CGA	4.13	1.45	1.33
19	3	1212	CLA	CHC-C1C	4.13	1.48	1.35
19	B	1738	CLA	O2A-CGA	4.14	1.45	1.33
19	A	1779	CLA	C4B-CHC	4.14	1.51	1.39
19	A	1781	CLA	O2A-CGA	4.14	1.45	1.33
19	B	1737	CLA	OBD-CAD	4.14	1.28	1.22
19	4	1202	CLA	CHD-C4C	4.16	1.51	1.41
19	2	1212	CLA	O2A-CGA	4.16	1.45	1.33
19	B	1766	CLA	C4B-CHC	4.16	1.51	1.39
19	R	1055	CLA	O2D-CGD	4.16	1.43	1.33
19	B	1756	CLA	O2A-CGA	4.17	1.45	1.33
19	B	1754	CLA	CHC-C1C	4.17	1.48	1.35
19	A	1768	CLA	C4B-CHC	4.17	1.51	1.39
19	L	1168	CLA	CMA-C3A	4.17	1.62	1.53
19	B	1771	CLA	OBD-CAD	4.18	1.28	1.22
19	B	1757	CLA	O2A-CGA	4.18	1.45	1.33
19	B	1769	CLA	O2D-CGD	4.19	1.43	1.33
19	A	1791	CLA	OBD-CAD	4.19	1.28	1.22
19	J	1043	CLA	O2A-CGA	4.20	1.46	1.33
19	A	1810	CLA	CHD-C4C	4.20	1.51	1.41
19	A	1800	CLA	CHD-C4C	4.20	1.51	1.41
19	L	1167	CLA	OBD-CAD	4.20	1.28	1.22
19	A	1784	CLA	OBD-CAD	4.20	1.28	1.22
19	B	1758	CLA	OBD-CAD	4.21	1.28	1.22
19	A	1780	CLA	O2A-CGA	4.21	1.46	1.33
19	B	1757	CLA	OBD-CAD	4.21	1.28	1.22
19	B	1762	CLA	CHC-C1C	4.22	1.48	1.35
19	A	1793	CLA	OBD-CAD	4.22	1.28	1.22
19	3	1220	CLA	CHD-C4C	4.23	1.51	1.41
19	B	1751	CLA	C4B-CHC	4.23	1.51	1.39
19	B	1788	CLA	CHD-C4C	4.23	1.51	1.41
19	K	1085	CLA	CHD-C4C	4.23	1.51	1.41
19	J	1044	CLA	OBD-CAD	4.23	1.28	1.22
19	4	4014	CLA	O2A-CGA	4.23	1.46	1.33
19	L	1167	CLA	O2A-CGA	4.24	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1145	CLA	CHD-C4C	4.24	1.51	1.41
19	A	1762	CLA	O2A-CGA	4.24	1.46	1.33
19	1	1146	CLA	CHC-C1C	4.24	1.48	1.35
19	A	1764	CLA	OBD-CAD	4.24	1.28	1.22
19	A	1782	CLA	OBD-CAD	4.24	1.28	1.22
19	B	1758	CLA	C4B-CHC	4.24	1.51	1.39
19	4	1205	CLA	O2A-CGA	4.24	1.46	1.33
19	A	1777	CLA	C4B-CHC	4.24	1.51	1.39
19	B	1770	CLA	C4B-CHC	4.24	1.51	1.39
19	L	1168	CLA	C4B-CHC	4.25	1.51	1.39
19	B	1772	CLA	CHD-C4C	4.25	1.51	1.41
19	B	1751	CLA	CHD-C4C	4.25	1.51	1.41
19	A	1785	CLA	O2A-CGA	4.25	1.46	1.33
19	B	1747	CLA	C4B-CHC	4.26	1.51	1.39
19	R	1055	CLA	O2A-CGA	4.26	1.46	1.33
19	A	1759	CLA	O2A-CGA	4.26	1.46	1.33
19	A	1795	CLA	CHD-C4C	4.27	1.51	1.41
19	B	1755	CLA	O2A-CGA	4.27	1.46	1.33
19	G	1099	CLA	CHC-C1C	4.27	1.48	1.35
19	A	1780	CLA	O2D-CGD	4.28	1.44	1.33
19	B	1770	CLA	O2A-CGA	4.28	1.46	1.33
19	1	1142	CLA	OBD-CAD	4.28	1.28	1.22
19	B	1764	CLA	CHC-C1C	4.28	1.48	1.35
19	A	1789	CLA	CHC-C1C	4.28	1.48	1.35
19	A	1776	CLA	C4B-CHC	4.28	1.51	1.39
19	A	1767	CLA	OBD-CAD	4.28	1.28	1.22
19	J	1043	CLA	OBD-CAD	4.28	1.28	1.22
19	K	1085	CLA	OBD-CAD	4.29	1.28	1.22
19	2	1215	CLA	OBD-CAD	4.29	1.28	1.22
19	B	1764	CLA	O2A-CGA	4.29	1.46	1.33
19	B	1749	CLA	CHD-C4C	4.29	1.51	1.41
19	3	1214	CLA	OBD-CAD	4.29	1.28	1.22
19	A	1764	CLA	O2A-CGA	4.30	1.46	1.33
19	B	1763	CLA	C4B-CHC	4.31	1.51	1.39
19	F	1156	CLA	CHD-C4C	4.31	1.51	1.41
19	J	1043	CLA	CHD-C4C	4.31	1.51	1.41
19	B	1786	CLA	CHD-C4C	4.33	1.51	1.41
19	2	1212	CLA	CHD-C4C	4.33	1.51	1.41
19	B	1750	CLA	CHD-C4C	4.33	1.51	1.41
19	2	1212	CLA	OBD-CAD	4.33	1.29	1.22
19	B	1764	CLA	OBD-CAD	4.33	1.29	1.22
19	B	1753	CLA	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1742	CLA	C4B-CHC	4.34	1.51	1.39
19	3	3011	CLA	O2A-CGA	4.35	1.46	1.33
19	A	1771	CLA	CHC-C1C	4.35	1.49	1.35
19	B	1766	CLA	CHD-C4C	4.35	1.51	1.41
19	2	1223	CLA	CHD-C4C	4.35	1.51	1.41
19	G	1099	CLA	O2D-CGD	4.35	1.44	1.33
19	3	1224	CLA	O2A-CGA	4.36	1.46	1.33
19	1	1148	CLA	O2D-CGD	4.36	1.44	1.33
19	A	1786	CLA	CHD-C4C	4.36	1.51	1.41
19	1	1196	CLA	CHC-C1C	4.37	1.49	1.35
19	A	1782	CLA	CHD-C4C	4.37	1.51	1.41
19	A	1798	CLA	O2A-CGA	4.37	1.46	1.33
19	2	1215	CLA	O2A-CGA	4.37	1.46	1.33
19	4	4007	CLA	CHD-C4C	4.38	1.51	1.41
19	1	1196	CLA	O2D-CGD	4.38	1.44	1.33
19	B	1773	CLA	CHD-C4C	4.38	1.51	1.41
19	B	1787	CLA	OBD-CAD	4.38	1.29	1.22
19	A	1777	CLA	O2A-CGA	4.39	1.46	1.33
19	B	1772	CLA	O2D-CGD	4.39	1.44	1.33
19	A	1781	CLA	CHD-C4C	4.39	1.51	1.41
19	1	1198	CLA	CHD-C4C	4.40	1.51	1.41
19	B	1740	CLA	CHD-C4C	4.40	1.51	1.41
19	1	1308	CLA	CHD-C4C	4.40	1.51	1.41
19	A	1796	CLA	CHD-C4C	4.40	1.51	1.41
19	1	1145	CLA	CHC-C1C	4.40	1.49	1.35
19	B	1746	CLA	OBD-CAD	4.41	1.29	1.22
19	A	1773	CLA	CHD-C4C	4.42	1.51	1.41
19	A	1792	CLA	CHD-C4C	4.42	1.51	1.41
19	A	1765	CLA	OBD-CAD	4.42	1.29	1.22
19	A	1788	CLA	O2D-CGD	4.42	1.44	1.33
19	B	1762	CLA	O2A-CGA	4.43	1.46	1.33
19	B	1772	CLA	CHC-C1C	4.43	1.49	1.35
19	B	1746	CLA	C4B-CHC	4.43	1.52	1.39
19	F	1156	CLA	OBD-CAD	4.43	1.29	1.22
19	L	1166	CLA	CHD-C4C	4.43	1.51	1.41
19	I	1031	CLA	O2D-CGD	4.44	1.44	1.33
19	A	1760	CLA	O2D-CGD	4.44	1.44	1.33
19	3	1216	CLA	CHD-C4C	4.44	1.51	1.41
19	L	1168	CLA	OBD-CAD	4.45	1.29	1.22
19	4	1207	CLA	CHD-C4C	4.45	1.51	1.41
19	2	2010	CLA	CHD-C4C	4.45	1.51	1.41
19	A	1788	CLA	CHC-C1C	4.46	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	1217	CLA	CHD-C4C	4.46	1.51	1.41
19	1	1010	CLA	CHD-C4C	4.47	1.51	1.41
19	A	1785	CLA	OBD-CAD	4.47	1.29	1.22
19	4	1199	CLA	O2A-CGA	4.47	1.46	1.33
19	B	1763	CLA	CHD-C4C	4.47	1.51	1.41
19	A	1779	CLA	OBD-CAD	4.48	1.29	1.22
19	A	1795	CLA	O2A-CGA	4.48	1.46	1.33
19	4	4014	CLA	CHD-C4C	4.48	1.51	1.41
19	B	1763	CLA	O2D-CGD	4.49	1.44	1.33
19	4	1196	CLA	OBD-CAD	4.49	1.29	1.22
19	A	1773	CLA	OBD-CAD	4.49	1.29	1.22
19	4	1198	CLA	CHC-C1C	4.49	1.49	1.35
19	1	1505	CLA	O2A-CGA	4.50	1.46	1.33
19	1	1190	CLA	CHD-C4C	4.50	1.51	1.41
19	2	1222	CLA	O2A-CGA	4.50	1.46	1.33
19	L	1168	CLA	O2A-CGA	4.50	1.46	1.33
19	A	1765	CLA	O2A-CGA	4.50	1.46	1.33
19	4	1206	CLA	CHD-C4C	4.50	1.51	1.41
19	B	1746	CLA	O2A-CGA	4.51	1.46	1.33
19	A	1787	CLA	O2A-CGA	4.51	1.46	1.33
19	4	4014	CLA	O2D-CGD	4.52	1.44	1.33
19	B	1743	CLA	O2A-CGA	4.53	1.47	1.33
19	B	1736	CLA	O2D-CGD	4.53	1.44	1.33
19	A	1788	CLA	CHD-C4C	4.53	1.51	1.41
19	2	1213	CLA	C4B-CHC	4.53	1.52	1.39
19	A	1794	CLA	CHD-C4C	4.53	1.51	1.41
19	B	1738	CLA	CHC-C1C	4.54	1.49	1.35
19	B	1748	CLA	OBD-CAD	4.54	1.29	1.22
19	1	1193	CLA	CHD-C4C	4.54	1.51	1.41
19	B	1764	CLA	CHD-C4C	4.54	1.51	1.41
19	A	1776	CLA	O2A-CGA	4.54	1.47	1.33
19	A	1797	CLA	CHC-C1C	4.55	1.49	1.35
19	A	1786	CLA	O2D-CGD	4.55	1.44	1.33
19	B	1738	CLA	CHD-C4C	4.55	1.51	1.41
19	1	1193	CLA	OBD-CAD	4.55	1.29	1.22
19	L	1168	CLA	CHD-C4C	4.55	1.51	1.41
19	1	1192	CLA	O2A-CGA	4.55	1.47	1.33
19	A	1769	CLA	CHD-C4C	4.56	1.51	1.41
19	1	1189	CLA	O2A-CGA	4.56	1.47	1.33
19	B	1756	CLA	CHD-C4C	4.56	1.52	1.41
19	B	1787	CLA	O2A-CGA	4.56	1.47	1.33
19	B	1769	CLA	O2A-CGA	4.56	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1810	CLA	C4B-CHC	4.57	1.52	1.39
19	A	1796	CLA	OBD-CAD	4.57	1.29	1.22
19	B	1757	CLA	CHC-C1C	4.57	1.49	1.35
19	A	1812	CLA	CHC-C1C	4.57	1.49	1.35
19	B	1741	CLA	CHC-C1C	4.57	1.49	1.35
19	A	1800	CLA	O2A-CGA	4.57	1.47	1.33
19	1	1142	CLA	CHD-C4C	4.58	1.52	1.41
19	1	1195	CLA	C4B-CHC	4.58	1.52	1.39
19	A	1788	CLA	OBD-CAD	4.58	1.29	1.22
19	2	1220	CLA	CHD-C4C	4.58	1.52	1.41
19	4	1202	CLA	CHC-C1C	4.58	1.49	1.35
19	1	1241	CLA	O2A-CGA	4.59	1.47	1.33
19	B	1772	CLA	O2A-CGA	4.59	1.47	1.33
19	L	1166	CLA	OBD-CAD	4.59	1.29	1.22
19	A	1782	CLA	CHC-C1C	4.60	1.49	1.35
19	F	1157	CLA	CHC-C1C	4.60	1.49	1.35
19	K	1085	CLA	CHC-C1C	4.61	1.49	1.35
19	A	1778	CLA	CHC-C1C	4.61	1.49	1.35
19	A	1761	CLA	CHC-C1C	4.61	1.49	1.35
19	2	1223	CLA	OBD-CAD	4.61	1.29	1.22
19	B	1741	CLA	CHD-C4C	4.61	1.52	1.41
19	I	1031	CLA	CHD-C4C	4.61	1.52	1.41
19	3	1219	CLA	CHD-C4C	4.61	1.52	1.41
19	2	1218	CLA	O2A-CGA	4.61	1.47	1.33
19	A	1789	CLA	O2A-CGA	4.62	1.47	1.33
19	A	1787	CLA	CHC-C1C	4.62	1.49	1.35
19	4	1199	CLA	CHD-C4C	4.62	1.52	1.41
19	3	3008	CLA	C4B-CHC	4.62	1.52	1.39
19	B	1748	CLA	CHD-C4C	4.62	1.52	1.41
19	4	1200	CLA	OBD-CAD	4.62	1.29	1.22
19	A	1769	CLA	O2D-CGD	4.63	1.45	1.33
19	B	1738	CLA	O2D-CGD	4.63	1.45	1.33
19	1	1146	CLA	O2D-CGD	4.63	1.45	1.33
19	B	1760	CLA	CHC-C1C	4.63	1.49	1.35
19	A	1811	CLA	CHD-C4C	4.63	1.52	1.41
19	A	1772	CLA	O2D-CGD	4.63	1.45	1.33
19	A	1783	CLA	OBD-CAD	4.63	1.29	1.22
19	4	1205	CLA	CHD-C4C	4.63	1.52	1.41
19	B	1759	CLA	CHC-C1C	4.64	1.49	1.35
19	A	1793	CLA	O2D-CGD	4.64	1.45	1.33
19	4	1196	CLA	CHD-C4C	4.64	1.52	1.41
19	B	1735	CLA	OBD-CAD	4.64	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1793	CLA	O2A-CGA	4.65	1.47	1.33
19	B	1769	CLA	CHC-C1C	4.65	1.49	1.35
19	B	1755	CLA	CHC-C1C	4.65	1.49	1.35
19	J	1044	CLA	CHC-C1C	4.65	1.49	1.35
19	B	1786	CLA	O2D-CGD	4.65	1.45	1.33
19	F	1155	CLA	OBD-CAD	4.66	1.29	1.22
19	3	3011	CLA	OBD-CAD	4.66	1.29	1.22
19	B	1747	CLA	CHD-C4C	4.67	1.52	1.41
19	A	1779	CLA	CHD-C4C	4.67	1.52	1.41
19	4	1201	CLA	CHC-C1C	4.67	1.50	1.35
19	F	1157	CLA	OBD-CAD	4.67	1.29	1.22
19	2	1215	CLA	CHD-C4C	4.67	1.52	1.41
19	B	1767	CLA	O2A-CGA	4.68	1.47	1.33
19	B	1744	CLA	CHC-C1C	4.68	1.50	1.35
19	B	1786	CLA	OBD-CAD	4.68	1.29	1.22
19	A	1784	CLA	CHD-C4C	4.68	1.52	1.41
19	3	1212	CLA	O2D-CGD	4.69	1.45	1.33
19	1	1505	CLA	OBD-CAD	4.69	1.29	1.22
19	B	1737	CLA	CHC-C1C	4.69	1.50	1.35
19	A	1769	CLA	O2A-CGA	4.69	1.47	1.33
19	B	1756	CLA	O2D-CGD	4.69	1.45	1.33
19	B	1752	CLA	CHD-C4C	4.70	1.52	1.41
19	1	1195	CLA	CHD-C4C	4.70	1.52	1.41
19	4	1200	CLA	O2D-CGD	4.70	1.45	1.33
19	A	1775	CLA	CHD-C4C	4.70	1.52	1.41
19	1	1189	CLA	CHD-C4C	4.71	1.52	1.41
19	A	1799	CLA	CHD-C4C	4.71	1.52	1.41
19	3	1222	CLA	O2D-CGD	4.71	1.45	1.33
19	3	1219	CLA	C4B-CHC	4.71	1.52	1.39
19	3	1218	CLA	CHD-C4C	4.73	1.52	1.41
19	A	1774	CLA	CHD-C4C	4.73	1.52	1.41
19	3	3011	CLA	CHD-C4C	4.73	1.52	1.41
19	A	1796	CLA	O2A-CGA	4.73	1.47	1.33
19	3	1224	CLA	O2D-CGD	4.74	1.45	1.33
19	A	1789	CLA	CHD-C4C	4.74	1.52	1.41
19	A	1787	CLA	CHD-C4C	4.74	1.52	1.41
19	A	1781	CLA	CHC-C1C	4.74	1.50	1.35
19	B	1736	CLA	CHD-C4C	4.75	1.52	1.41
19	A	1776	CLA	CHD-C4C	4.75	1.52	1.41
19	A	1759	CLA	CHD-C4C	4.75	1.52	1.41
19	B	1788	CLA	O2A-CGA	4.75	1.47	1.33
19	2	1222	CLA	O2D-CGD	4.75	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1785	CLA	CHD-C4C	4.75	1.52	1.41
19	1	1197	CLA	CHD-C4C	4.76	1.52	1.41
19	B	1767	CLA	CHD-C4C	4.76	1.52	1.41
19	B	1743	CLA	CHC-C1C	4.76	1.50	1.35
19	B	1768	CLA	CHC-C1C	4.76	1.50	1.35
19	A	1791	CLA	CHD-C4C	4.76	1.52	1.41
19	B	1740	CLA	CHC-C1C	4.76	1.50	1.35
19	B	1771	CLA	O2A-CGA	4.76	1.47	1.33
19	A	1788	CLA	O2A-CGA	4.77	1.47	1.33
19	F	1156	CLA	CHC-C1C	4.77	1.50	1.35
19	B	1740	CLA	O2D-CGD	4.78	1.45	1.33
19	L	1166	CLA	O2A-CGA	4.78	1.47	1.33
19	B	1752	CLA	O2A-CGA	4.78	1.49	1.32
19	A	1792	CLA	O2A-CGA	4.78	1.47	1.33
19	A	1774	CLA	O2A-CGA	4.79	1.47	1.33
19	1	1190	CLA	CHC-C1C	4.79	1.50	1.35
19	A	1798	CLA	CHC-C1C	4.79	1.50	1.35
19	B	1747	CLA	CHC-C1C	4.80	1.50	1.35
19	1	1193	CLA	O2A-CGA	4.80	1.47	1.33
19	3	1221	CLA	CHD-C4C	4.80	1.52	1.41
19	A	1792	CLA	O2D-CGD	4.80	1.45	1.33
19	A	1778	CLA	CHD-C4C	4.81	1.52	1.41
19	B	1748	CLA	CHC-C1C	4.81	1.50	1.35
19	2	1212	CLA	CHC-C1C	4.81	1.50	1.35
19	A	1790	CLA	O2A-CGA	4.81	1.47	1.33
19	2	1222	CLA	CHD-C4C	4.82	1.52	1.41
19	B	1787	CLA	CHD-C4C	4.82	1.52	1.41
19	B	1773	CLA	CHC-C1C	4.82	1.50	1.35
19	4	1206	CLA	OBD-CAD	4.82	1.29	1.22
19	1	1308	CLA	O2D-CGD	4.82	1.45	1.33
19	A	1768	CLA	CHC-C1C	4.82	1.50	1.35
19	B	1786	CLA	CHC-C1C	4.82	1.50	1.35
19	1	1189	CLA	C4B-CHC	4.83	1.53	1.39
19	2	1222	CLA	CHC-C1C	4.83	1.50	1.35
19	A	1759	CLA	CHC-C1C	4.83	1.50	1.35
19	1	1149	CLA	CHD-C4C	4.83	1.52	1.41
19	2	1212	CLA	O2D-CGD	4.84	1.45	1.33
19	4	1199	CLA	CHC-C1C	4.84	1.50	1.35
19	B	1735	CLA	CHD-C4C	4.84	1.52	1.41
19	3	3011	CLA	CHC-C1C	4.84	1.50	1.35
19	B	1736	CLA	CHC-C1C	4.84	1.50	1.35
19	J	1043	CLA	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1213	CLA	CHD-C4C	4.85	1.52	1.41
19	3	3008	CLA	OBD-CAD	4.85	1.29	1.22
19	A	1799	CLA	OBD-CAD	4.86	1.29	1.22
19	B	1743	CLA	O2D-CGD	4.86	1.45	1.33
19	A	1759	CLA	OBD-CAD	4.86	1.29	1.22
19	R	1054	CLA	CHD-C4C	4.86	1.52	1.41
19	B	1750	CLA	O2D-CGD	4.87	1.45	1.33
19	1	1142	CLA	O2D-CGD	4.87	1.45	1.33
19	A	1783	CLA	CHC-C1C	4.87	1.50	1.35
19	B	1753	CLA	OBD-CAD	4.87	1.29	1.22
19	A	1811	CLA	O2D-CGD	4.87	1.45	1.33
19	A	1773	CLA	O2A-CGA	4.87	1.48	1.33
19	B	1741	CLA	OBD-CAD	4.87	1.29	1.22
19	A	1790	CLA	CHD-C4C	4.87	1.52	1.41
19	B	1752	CLA	CHC-C1C	4.87	1.50	1.35
19	1	1189	CLA	OBD-CAD	4.87	1.29	1.22
19	A	1791	CLA	CHC-C1C	4.88	1.50	1.35
19	B	1787	CLA	O2D-CGD	4.88	1.45	1.33
19	A	1780	CLA	CHD-C4C	4.88	1.52	1.41
19	B	1739	CLA	OBD-CAD	4.88	1.29	1.22
19	B	1771	CLA	O2D-CGD	4.88	1.45	1.33
19	B	1755	CLA	CHD-C4C	4.88	1.52	1.41
19	1	1195	CLA	OBD-CAD	4.88	1.29	1.22
19	3	1214	CLA	CHC-C1C	4.88	1.50	1.35
19	B	1751	CLA	CHC-C1C	4.89	1.50	1.35
19	A	1767	CLA	O2D-CGD	4.89	1.45	1.33
19	1	1149	CLA	CHC-C1C	4.89	1.50	1.35
19	4	1199	CLA	O2D-CGD	4.89	1.45	1.33
19	1	1189	CLA	O2D-CGD	4.90	1.45	1.33
19	A	1812	CLA	O2D-CGD	4.90	1.45	1.33
19	B	1768	CLA	CHD-C4C	4.91	1.52	1.41
19	3	1219	CLA	O2A-CGA	4.91	1.48	1.33
19	B	1753	CLA	CHC-C1C	4.91	1.50	1.35
19	L	1168	CLA	CHC-C1C	4.91	1.50	1.35
19	A	1799	CLA	CHC-C1C	4.91	1.50	1.35
19	4	1211	CLA	CHC-C1C	4.91	1.50	1.35
19	B	1750	CLA	O2A-CGA	4.92	1.48	1.33
19	A	1772	CLA	CHC-C1C	4.92	1.50	1.35
19	F	1156	CLA	O2D-CGD	4.92	1.45	1.33
19	A	1799	CLA	O2D-CGD	4.92	1.45	1.33
19	4	1206	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1765	CLA	CHD-C4C	4.93	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1201	CLA	O2D-CGD	4.93	1.45	1.33
19	A	1781	CLA	O2D-CGD	4.93	1.45	1.33
19	2	1220	CLA	CHC-C1C	4.93	1.50	1.35
19	A	1762	CLA	CHC-C1C	4.94	1.50	1.35
19	A	1784	CLA	O2D-CGD	4.94	1.45	1.33
19	B	1745	CLA	CHC-C1C	4.94	1.50	1.35
19	A	1766	CLA	OBD-CAD	4.94	1.29	1.22
19	J	1043	CLA	CHC-C1C	4.94	1.50	1.35
19	B	1788	CLA	O2D-CGD	4.94	1.45	1.33
19	4	1198	CLA	CHD-C4C	4.94	1.52	1.41
19	B	1768	CLA	O2A-CGA	4.94	1.48	1.33
19	1	1308	CLA	CHC-C1C	4.95	1.50	1.35
19	A	1795	CLA	OBD-CAD	4.95	1.29	1.22
19	2	1215	CLA	O2D-CGD	4.95	1.45	1.33
19	A	1767	CLA	CHD-C4C	4.95	1.52	1.41
19	1	1192	CLA	CHC-C1C	4.96	1.50	1.35
19	A	1811	CLA	CHC-C1C	4.96	1.50	1.35
19	4	4014	CLA	CHC-C1C	4.96	1.50	1.35
19	3	1214	CLA	CHD-C4C	4.96	1.52	1.41
19	B	1763	CLA	O2A-CGA	4.96	1.48	1.33
19	A	1780	CLA	CHC-C1C	4.97	1.50	1.35
19	A	1793	CLA	CHC-C1C	4.97	1.50	1.35
19	A	1785	CLA	O2D-CGD	4.97	1.45	1.33
19	R	1054	CLA	CHC-C1C	4.97	1.50	1.35
19	A	1792	CLA	CHC-C1C	4.98	1.50	1.35
23	B	1774	PQN	C10-C5	4.98	1.48	1.40
19	A	1760	CLA	CHD-C4C	4.98	1.52	1.41
19	B	1742	CLA	OBD-CAD	4.98	1.30	1.22
19	A	1792	CLA	OBD-CAD	4.98	1.30	1.22
19	A	1777	CLA	CHD-C4C	4.98	1.53	1.41
19	3	3001	CLA	CHD-C4C	4.98	1.53	1.41
19	B	1769	CLA	CHD-C4C	4.98	1.53	1.41
19	L	1167	CLA	O2D-CGD	4.99	1.45	1.33
19	A	1759	CLA	O2D-CGD	4.99	1.45	1.33
19	4	1209	CLA	CHC-C1C	4.99	1.51	1.35
19	K	1085	CLA	O2D-CGD	4.99	1.45	1.33
19	B	1741	CLA	O2A-CGA	4.99	1.48	1.33
19	A	1773	CLA	CHC-C1C	4.99	1.51	1.35
19	A	1790	CLA	CHC-C1C	5.00	1.51	1.35
19	B	1759	CLA	O2D-CGD	5.01	1.46	1.33
19	A	1764	CLA	CHD-C4C	5.01	1.53	1.41
19	B	1751	CLA	O2A-CGA	5.01	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1745	CLA	CHD-C4C	5.02	1.53	1.41
19	3	3011	CLA	O2D-CGD	5.02	1.46	1.33
19	1	1187	CLA	OBD-CAD	5.02	1.30	1.22
19	B	1757	CLA	O2D-CGD	5.02	1.46	1.33
19	A	1768	CLA	CHD-C4C	5.03	1.53	1.41
19	B	1742	CLA	O2D-CGD	5.03	1.46	1.33
19	4	1196	CLA	O2D-CGD	5.03	1.46	1.33
19	B	1787	CLA	CHC-C1C	5.03	1.51	1.35
19	A	1782	CLA	O2D-CGD	5.03	1.46	1.33
23	A	1801	PQN	C10-C5	5.04	1.48	1.40
19	3	1219	CLA	OBD-CAD	5.04	1.30	1.22
19	B	1756	CLA	CHC-C1C	5.04	1.51	1.35
19	1	1241	CLA	CHD-C4C	5.04	1.53	1.41
19	2	1213	CLA	CHC-C1C	5.04	1.51	1.35
19	A	1795	CLA	CHC-C1C	5.04	1.51	1.35
19	3	1218	CLA	CHC-C1C	5.04	1.51	1.35
19	B	1760	CLA	O2D-CGD	5.04	1.46	1.33
19	B	1766	CLA	OBD-CAD	5.04	1.30	1.22
19	1	1142	CLA	CHC-C1C	5.04	1.51	1.35
19	A	1785	CLA	CHC-C1C	5.04	1.51	1.35
19	1	1505	CLA	CHC-C1C	5.05	1.51	1.35
19	3	3008	CLA	CHD-C4C	5.05	1.53	1.41
19	I	1031	CLA	O2A-CGA	5.05	1.48	1.33
19	B	1737	CLA	O2A-CGA	5.06	1.48	1.33
19	1	1505	CLA	CHD-C4C	5.06	1.53	1.41
19	A	1774	CLA	O2D-CGD	5.06	1.46	1.33
19	4	1209	CLA	OBD-CAD	5.06	1.30	1.22
19	A	1798	CLA	OBD-CAD	5.06	1.30	1.22
19	4	1196	CLA	CHC-C1C	5.07	1.51	1.35
19	4	1206	CLA	O2A-CGA	5.07	1.48	1.33
19	B	1751	CLA	O2D-CGD	5.07	1.46	1.33
19	A	1794	CLA	O2D-CGD	5.07	1.46	1.33
19	A	1774	CLA	CHC-C1C	5.07	1.51	1.35
19	A	1793	CLA	CHD-C4C	5.07	1.53	1.41
19	A	1784	CLA	CHC-C1C	5.07	1.51	1.35
19	B	1788	CLA	CHC-C1C	5.08	1.51	1.35
19	3	1218	CLA	OBD-CAD	5.08	1.30	1.22
19	B	1758	CLA	O2D-CGD	5.08	1.46	1.33
19	B	1750	CLA	CHC-C1C	5.08	1.51	1.35
19	B	1742	CLA	CHC-C1C	5.08	1.51	1.35
19	2	1218	CLA	CHC-C1C	5.08	1.51	1.35
19	A	1810	CLA	CHC-C1C	5.08	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1752	CLA	OBD-CAD	5.08	1.30	1.22
19	B	1770	CLA	O2D-CGD	5.09	1.46	1.33
19	B	1755	CLA	OBD-CAD	5.09	1.30	1.22
19	4	1197	CLA	CHC-C1C	5.09	1.51	1.35
19	A	1767	CLA	CHC-C1C	5.09	1.51	1.35
19	1	1193	CLA	O2D-CGD	5.10	1.46	1.33
19	B	1739	CLA	CHC-C1C	5.10	1.51	1.35
19	A	1779	CLA	CHC-C1C	5.10	1.51	1.35
19	A	1763	CLA	CHD-C4C	5.10	1.53	1.41
19	L	1167	CLA	CHC-C1C	5.11	1.51	1.35
19	A	1786	CLA	CHC-C1C	5.11	1.51	1.35
19	A	1779	CLA	O2A-CGA	5.12	1.48	1.33
19	A	1767	CLA	O2A-CGA	5.12	1.48	1.33
19	B	1771	CLA	CHC-C1C	5.12	1.51	1.35
19	F	1155	CLA	CHC-C1C	5.12	1.51	1.35
19	A	1762	CLA	CHD-C4C	5.12	1.53	1.41
19	A	1761	CLA	CHD-C4C	5.13	1.53	1.41
19	B	1748	CLA	O2A-CGA	5.14	1.48	1.33
19	A	1811	CLA	O2A-CGA	5.14	1.48	1.33
19	1	1149	CLA	O2A-CGA	5.14	1.48	1.33
19	B	1742	CLA	CHD-C4C	5.15	1.53	1.41
19	A	1797	CLA	O2A-CGA	5.15	1.48	1.33
19	A	1769	CLA	CHC-C1C	5.15	1.51	1.35
19	2	1213	CLA	OBD-CAD	5.15	1.30	1.22
19	1	1241	CLA	OBD-CAD	5.15	1.30	1.22
19	A	1760	CLA	CHC-C1C	5.15	1.51	1.35
19	B	1739	CLA	CHD-C4C	5.15	1.53	1.41
19	B	1761	CLA	O2A-CGA	5.15	1.48	1.33
19	1	1148	CLA	CHC-C1C	5.15	1.51	1.35
19	L	1167	CLA	CHD-C4C	5.16	1.53	1.41
19	1	1241	CLA	CHC-C1C	5.18	1.51	1.35
19	1	1014	CLA	O2D-CGD	5.18	1.46	1.33
19	A	1777	CLA	OBD-CAD	5.18	1.30	1.22
19	4	1199	CLA	OBD-CAD	5.19	1.30	1.22
19	3	1219	CLA	O2D-CGD	5.19	1.46	1.33
19	B	1763	CLA	CHC-C1C	5.20	1.51	1.35
19	B	1766	CLA	CHC-C1C	5.20	1.51	1.35
19	B	1771	CLA	CHD-C4C	5.20	1.53	1.41
19	A	1798	CLA	O2D-CGD	5.21	1.46	1.33
19	A	1770	CLA	CHC-C1C	5.21	1.51	1.35
19	4	1200	CLA	CHC-C1C	5.22	1.51	1.35
19	A	1787	CLA	OBD-CAD	5.22	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1770	CLA	CHD-C4C	5.22	1.53	1.41
19	B	1753	CLA	CHD-C4C	5.23	1.53	1.41
19	4	1205	CLA	OBD-CAD	5.23	1.30	1.22
19	A	1778	CLA	OBD-CAD	5.23	1.30	1.22
19	A	1784	CLA	O2A-CGA	5.23	1.49	1.33
19	B	1737	CLA	CHD-C4C	5.24	1.53	1.41
19	3	1219	CLA	CHC-C1C	5.24	1.51	1.35
19	B	1745	CLA	OBD-CAD	5.24	1.30	1.22
19	A	1786	CLA	O2A-CGA	5.25	1.49	1.33
19	B	1765	CLA	CHC-C1C	5.25	1.51	1.35
19	B	1761	CLA	CHD-C4C	5.26	1.53	1.41
19	A	1796	CLA	O2D-CGD	5.27	1.46	1.33
19	F	1155	CLA	CHD-C4C	5.27	1.53	1.41
19	2	1223	CLA	CHC-C1C	5.28	1.51	1.35
19	A	1768	CLA	O2D-CGD	5.28	1.46	1.33
19	A	1791	CLA	O2D-CGD	5.28	1.46	1.33
19	A	1777	CLA	CHC-C1C	5.29	1.51	1.35
19	B	1737	CLA	O2D-CGD	5.30	1.46	1.33
19	A	1768	CLA	O2A-CGA	5.30	1.49	1.33
19	A	1800	CLA	CHC-C1C	5.31	1.52	1.35
19	1	1190	CLA	O2D-CGD	5.32	1.46	1.33
19	2	1213	CLA	O2A-CGA	5.32	1.49	1.33
19	B	1749	CLA	O2D-CGD	5.32	1.46	1.33
19	R	1054	CLA	O2D-CGD	5.32	1.46	1.33
19	A	1796	CLA	CHC-C1C	5.33	1.52	1.35
19	2	1218	CLA	CHD-C4C	5.33	1.53	1.41
19	A	1789	CLA	O2D-CGD	5.33	1.46	1.33
19	4	1205	CLA	CHC-C1C	5.34	1.52	1.35
19	B	1749	CLA	CHC-C1C	5.34	1.52	1.35
19	A	1783	CLA	CHD-C4C	5.34	1.53	1.41
19	1	1195	CLA	CHC-C1C	5.34	1.52	1.35
19	L	1166	CLA	CHC-C1C	5.34	1.52	1.35
19	B	1746	CLA	O2D-CGD	5.36	1.46	1.33
19	1	1189	CLA	CHC-C1C	5.36	1.52	1.35
19	B	1761	CLA	CHC-C1C	5.36	1.52	1.35
19	L	1168	CLA	O2D-CGD	5.37	1.46	1.33
19	A	1794	CLA	CHC-C1C	5.37	1.52	1.35
19	B	1759	CLA	OBD-CAD	5.37	1.30	1.22
19	A	1764	CLA	CHC-C1C	5.38	1.52	1.35
19	A	1766	CLA	O2D-CGD	5.38	1.46	1.33
19	A	1777	CLA	O2D-CGD	5.38	1.46	1.33
19	B	1748	CLA	O2D-CGD	5.38	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	1044	CLA	O2D-CGD	5.39	1.47	1.33
19	3	3008	CLA	CHC-C1C	5.39	1.52	1.35
19	B	1758	CLA	CHC-C1C	5.39	1.52	1.35
19	B	1736	CLA	OBD-CAD	5.40	1.30	1.22
19	B	1755	CLA	O2D-CGD	5.40	1.47	1.33
19	A	1760	CLA	OBD-CAD	5.40	1.30	1.22
19	A	1776	CLA	CHC-C1C	5.40	1.52	1.35
19	A	1762	CLA	OBD-CAD	5.41	1.30	1.22
19	2	1218	CLA	OBD-CAD	5.41	1.30	1.22
19	1	1193	CLA	CHC-C1C	5.43	1.52	1.35
19	I	1031	CLA	CHC-C1C	5.43	1.52	1.35
19	B	1735	CLA	CHC-C1C	5.44	1.52	1.35
19	B	1746	CLA	CHC-C1C	5.44	1.52	1.35
19	2	1213	CLA	O2D-CGD	5.44	1.47	1.33
19	A	1798	CLA	CHD-C4C	5.45	1.54	1.41
19	R	1054	CLA	O2A-CGA	5.45	1.49	1.33
19	B	1767	CLA	O2D-CGD	5.46	1.47	1.33
19	B	1741	CLA	O2D-CGD	5.46	1.47	1.33
19	B	1747	CLA	O2D-CGD	5.47	1.47	1.33
19	B	1745	CLA	O2A-CGA	5.47	1.49	1.33
19	4	1206	CLA	O2D-CGD	5.48	1.47	1.33
19	A	1766	CLA	CHD-C4C	5.49	1.54	1.41
19	B	1766	CLA	O2D-CGD	5.49	1.47	1.33
19	A	1795	CLA	O2D-CGD	5.49	1.47	1.33
19	B	1767	CLA	OBD-CAD	5.49	1.30	1.22
19	A	1761	CLA	O2D-CGD	5.50	1.47	1.33
19	A	1760	CLA	O2A-CGA	5.51	1.49	1.33
19	B	1762	CLA	O2D-CGD	5.51	1.47	1.33
19	B	1735	CLA	O2D-CGD	5.51	1.47	1.33
19	B	1742	CLA	O2A-CGA	5.52	1.49	1.33
19	A	1761	CLA	O2A-CGA	5.52	1.50	1.33
19	1	1187	CLA	O2D-CGD	5.53	1.47	1.33
19	4	4007	CLA	O2D-CGD	5.53	1.47	1.33
19	B	1770	CLA	CHC-C1C	5.53	1.52	1.35
19	A	1812	CLA	OBD-CAD	5.54	1.30	1.22
19	B	1758	CLA	CHD-C4C	5.56	1.54	1.41
19	2	1218	CLA	O2D-CGD	5.56	1.47	1.33
19	B	1767	CLA	CHC-C1C	5.57	1.52	1.35
19	A	1787	CLA	O2D-CGD	5.57	1.47	1.33
19	B	1739	CLA	O2D-CGD	5.57	1.47	1.33
19	A	1766	CLA	CHC-C1C	5.58	1.52	1.35
19	B	1773	CLA	OBD-CAD	5.58	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1192	CLA	O2D-CGD	5.58	1.47	1.33
19	B	1745	CLA	O2D-CGD	5.59	1.47	1.33
19	B	1765	CLA	O2D-CGD	5.62	1.47	1.33
19	A	1779	CLA	O2D-CGD	5.63	1.47	1.33
19	L	1166	CLA	O2D-CGD	5.64	1.47	1.33
19	B	1764	CLA	O2D-CGD	5.64	1.47	1.33
19	A	1800	CLA	O2D-CGD	5.64	1.47	1.33
19	2	1223	CLA	O2A-CGA	5.64	1.50	1.33
19	B	1752	CLA	O2D-CGD	5.65	1.47	1.33
19	A	1762	CLA	O2D-CGD	5.65	1.47	1.33
19	A	1797	CLA	O2D-CGD	5.66	1.47	1.33
19	A	1776	CLA	O2D-CGD	5.68	1.47	1.33
19	B	1747	CLA	OBD-CAD	5.69	1.31	1.22
19	2	1215	CLA	CHC-C1C	5.71	1.53	1.35
19	A	1790	CLA	O2D-CGD	5.73	1.47	1.33
19	A	1812	CLA	CHD-C4C	5.73	1.54	1.41
19	4	1197	CLA	OBD-CAD	5.73	1.31	1.22
19	B	1753	CLA	O2D-CGD	5.76	1.47	1.33
19	A	1778	CLA	O2D-CGD	5.76	1.47	1.33
19	A	1773	CLA	O2D-CGD	5.77	1.47	1.33
19	A	1770	CLA	O2D-CGD	5.81	1.48	1.33
19	2	1223	CLA	O2D-CGD	5.84	1.48	1.33
19	1	1149	CLA	O2D-CGD	5.85	1.48	1.33
19	A	1810	CLA	O2D-CGD	5.86	1.48	1.33
19	4	1205	CLA	O2D-CGD	5.86	1.48	1.33
19	1	1505	CLA	O2D-CGD	5.87	1.48	1.33
23	B	1774	PQN	C3-C2	5.88	1.49	1.35
19	A	1770	CLA	OBD-CAD	5.89	1.31	1.22
19	1	1241	CLA	O2D-CGD	5.90	1.48	1.33
19	3	1218	CLA	O2D-CGD	5.92	1.48	1.33
19	B	1761	CLA	O2D-CGD	5.96	1.48	1.33
23	A	1801	PQN	C3-C2	5.96	1.49	1.35
19	1	1192	CLA	OBD-CAD	5.96	1.31	1.22
19	A	1800	CLA	OBD-CAD	6.01	1.31	1.22
19	B	1765	CLA	OBD-CAD	6.12	1.31	1.22
19	3	3008	CLA	O2D-CGD	6.31	1.49	1.33
19	1	1190	CLA	OBD-CAD	6.80	1.32	1.22

All (4178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1763	CLA	OBD-CAD-CBD	-22.01	92.73	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1145	CLA	OBD-CAD-CBD	-21.73	93.14	125.94
19	3	1222	CLA	OBD-CAD-CBD	-21.06	94.17	125.94
19	4	1200	CLA	OBD-CAD-CBD	-20.75	94.63	125.94
19	3	1224	CLA	OBD-CAD-CBD	-17.75	99.15	125.94
19	A	1771	CLA	OBD-CAD-CBD	-17.63	99.33	125.94
19	B	1749	CLA	OBD-CAD-CBD	-16.92	100.40	125.94
19	4	1206	CLA	OBD-CAD-CBD	-16.70	100.73	125.94
19	4	1201	CLA	OBD-CAD-CBD	-16.48	101.08	125.94
19	3	1222	CLA	OBD-CAD-C3D	-16.15	95.40	128.35
19	A	1798	CLA	OBD-CAD-CBD	-16.05	101.72	125.94
19	2	1223	CLA	OBD-CAD-CBD	-15.77	102.14	125.94
19	A	1810	CLA	OBD-CAD-CBD	-15.72	102.21	125.94
19	1	1196	CLA	OBD-CAD-C3D	-15.67	96.38	128.35
19	B	1758	CLA	OBD-CAD-CBD	-15.64	102.34	125.94
19	A	1799	CLA	OBD-CAD-CBD	-15.44	102.63	125.94
19	1	1241	CLA	OBD-CAD-CBD	-15.39	102.72	125.94
19	A	1783	CLA	OBD-CAD-CBD	-15.32	102.82	125.94
19	4	1206	CLA	OBD-CAD-C3D	-15.26	97.22	128.35
19	B	1737	CLA	OBD-CAD-CBD	-15.23	102.96	125.94
19	2	1215	CLA	OBD-CAD-CBD	-15.14	103.09	125.94
19	A	1791	CLA	OBD-CAD-C3D	-15.10	97.54	128.35
19	I	1031	CLA	OBD-CAD-CBD	-14.89	103.47	125.94
19	A	1792	CLA	OBD-CAD-CBD	-14.82	103.58	125.94
19	B	1754	CLA	OBD-CAD-CBD	-14.71	103.75	125.94
19	R	1054	CLA	OBD-CAD-CBD	-14.40	104.22	125.94
19	2	1217	CLA	OBD-CAD-CBD	-14.31	104.35	125.94
19	3	1224	CLA	OBD-CAD-C3D	-14.25	99.27	128.35
19	A	1796	CLA	OBD-CAD-CBD	-14.04	104.76	125.94
22	B	1782	BCR	C24-C23-C22	-14.01	104.86	126.22
19	A	1785	CLA	OBD-CAD-CBD	-13.91	104.95	125.94
19	3	1218	CLA	OBD-CAD-CBD	-13.86	105.03	125.94
19	A	1766	CLA	OBD-CAD-CBD	-13.78	105.14	125.94
19	B	1768	CLA	OBD-CAD-C3D	-13.64	100.51	128.35
19	1	1149	CLA	OBD-CAD-C3D	-13.63	100.53	128.35
19	4	1197	CLA	CAB-C3B-C4B	-13.55	105.95	128.36
19	B	1767	CLA	OBD-CAD-CBD	-13.53	105.52	125.94
19	A	1763	CLA	OBD-CAD-C3D	-13.49	100.81	128.35
19	4	1200	CLA	OBD-CAD-C3D	-13.35	101.11	128.35
19	4	4007	CLA	OBD-CAD-C3D	-13.34	101.13	128.35
19	B	1740	CLA	OBD-CAD-C3D	-13.24	101.33	128.35
19	L	1168	CLA	OBD-CAD-CBD	-13.22	105.99	125.94
19	G	1099	CLA	OBD-CAD-CBD	-13.13	106.13	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1750	CLA	OBD-CAD-CBD	-13.11	106.15	125.94
19	L	1166	CLA	OBD-CAD-CBD	-13.10	106.18	125.94
22	L	1170	BCR	C7-C8-C9	-12.99	106.42	126.22
19	1	1146	CLA	OBD-CAD-CBD	-12.97	106.37	125.94
19	B	1741	CLA	OBD-CAD-C3D	-12.91	102.01	128.35
19	A	1768	CLA	OBD-CAD-CBD	-12.88	106.50	125.94
19	B	1773	CLA	CAB-C3B-C4B	-12.87	107.08	128.36
19	B	1758	CLA	OBD-CAD-C3D	-12.81	102.22	128.35
19	I	1031	CLA	OBD-CAD-C3D	-12.77	102.29	128.35
19	L	1168	CLA	OBD-CAD-C3D	-12.73	102.36	128.35
19	B	1744	CLA	OBD-CAD-C3D	-12.72	102.39	128.35
19	A	1772	CLA	OBD-CAD-C3D	-12.72	102.40	128.35
19	B	1753	CLA	OBD-CAD-CBD	-12.71	106.76	125.94
19	B	1786	CLA	OBD-CAD-CBD	-12.68	106.80	125.94
19	A	1784	CLA	OBD-CAD-CBD	-12.65	106.85	125.94
19	A	1764	CLA	OBD-CAD-C3D	-12.61	102.62	128.35
19	B	1752	CLA	OBD-CAD-C3D	-12.56	102.72	128.35
22	I	1032	BCR	C30-C25-C26	-12.50	104.31	122.66
19	A	1770	CLA	OBD-CAD-CBD	-12.48	107.10	125.94
19	4	1209	CLA	CAB-C3B-C4B	-12.47	107.73	128.36
19	1	1148	CLA	OBD-CAD-C3D	-12.46	102.93	128.35
19	2	1223	CLA	OBD-CAD-C3D	-12.41	103.02	128.35
19	1	1149	CLA	CAB-C3B-C4B	-12.39	107.86	128.36
19	1	1148	CLA	OBD-CAD-CBD	-12.37	107.27	125.94
19	A	1781	CLA	OBD-CAD-CBD	-12.33	107.34	125.94
19	A	1762	CLA	OBD-CAD-CBD	-12.33	107.34	125.94
19	4	1201	CLA	OBD-CAD-C3D	-12.23	103.40	128.35
19	1	1187	CLA	OBD-CAD-C3D	-12.17	103.51	128.35
19	F	1157	CLA	OBD-CAD-CBD	-12.15	107.61	125.94
19	4	1202	CLA	CAB-C3B-C4B	-12.11	108.32	128.36
19	A	1799	CLA	OBD-CAD-C3D	-12.10	103.66	128.35
19	K	1085	CLA	OBD-CAD-CBD	-12.10	107.68	125.94
19	2	1220	CLA	CAB-C3B-C4B	-12.10	108.35	128.36
19	B	1741	CLA	OBD-CAD-CBD	-12.09	107.69	125.94
19	A	1779	CLA	OBD-CAD-C3D	-12.09	103.68	128.35
19	B	1757	CLA	OBD-CAD-CBD	-12.07	107.72	125.94
19	A	1786	CLA	OBD-CAD-CBD	-12.06	107.74	125.94
19	B	1770	CLA	OBD-CAD-CBD	-12.05	107.75	125.94
19	A	1782	CLA	OBD-CAD-CBD	-11.97	107.87	125.94
19	4	1196	CLA	OBD-CAD-CBD	-11.96	107.88	125.94
19	B	1744	CLA	OBD-CAD-CBD	-11.96	107.89	125.94
19	B	1754	CLA	OBD-CAD-C3D	-11.93	104.00	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1773	CLA	OBD-CAD-CBD	-11.93	107.94	125.94
19	4	4014	CLA	OBD-CAD-CBD	-11.92	107.95	125.94
19	A	1786	CLA	OBD-CAD-C3D	-11.91	104.05	128.35
19	A	1776	CLA	OBD-CAD-CBD	-11.90	107.98	125.94
19	A	1788	CLA	OBD-CAD-CBD	-11.87	108.03	125.94
19	B	1767	CLA	OBD-CAD-C3D	-11.84	104.18	128.35
19	1	1145	CLA	OBD-CAD-C3D	-11.83	104.21	128.35
19	A	1774	CLA	OBD-CAD-CBD	-11.81	108.12	125.94
19	B	1743	CLA	OBD-CAD-CBD	-11.79	108.14	125.94
19	2	1212	CLA	OBD-CAD-CBD	-11.79	108.15	125.94
19	A	1772	CLA	OBD-CAD-CBD	-11.76	108.19	125.94
19	A	1783	CLA	OBD-CAD-C3D	-11.75	104.37	128.35
19	A	1778	CLA	OBD-CAD-CBD	-11.74	108.22	125.94
19	J	1043	CLA	OBD-CAD-CBD	-11.72	108.25	125.94
19	F	1156	CLA	OBD-CAD-CBD	-11.71	108.26	125.94
19	B	1756	CLA	OBD-CAD-CBD	-11.69	108.31	125.94
19	1	1189	CLA	OBD-CAD-CBD	-11.66	108.35	125.94
19	B	1787	CLA	OBD-CAD-CBD	-11.64	108.37	125.94
19	1	1308	CLA	OBD-CAD-CBD	-11.63	108.38	125.94
19	1	1142	CLA	OBD-CAD-CBD	-11.62	108.41	125.94
19	4	1198	CLA	OBD-CAD-C3D	-11.58	104.71	128.35
19	A	1812	CLA	OBD-CAD-C3D	-11.58	104.72	128.35
19	B	1740	CLA	OBD-CAD-CBD	-11.57	108.47	125.94
19	B	1761	CLA	OBD-CAD-CBD	-11.57	108.47	125.94
19	B	1786	CLA	OBD-CAD-C3D	-11.52	104.84	128.35
19	B	1765	CLA	OBD-CAD-C3D	-11.48	104.92	128.35
19	A	1776	CLA	OBD-CAD-C3D	-11.47	104.94	128.35
19	A	1769	CLA	OBD-CAD-CBD	-11.39	108.76	125.94
19	1	1195	CLA	CAB-C3B-C4B	-11.38	109.54	128.36
19	2	1217	CLA	OBD-CAD-C3D	-11.31	105.27	128.35
19	B	1764	CLA	OBD-CAD-C3D	-11.30	105.30	128.35
19	B	1766	CLA	OBD-CAD-C3D	-11.27	105.36	128.35
19	A	1785	CLA	OBD-CAD-C3D	-11.26	105.36	128.35
19	A	1773	CLA	OBD-CAD-C3D	-11.22	105.46	128.35
19	1	1505	CLA	OBD-CAD-CBD	-11.15	109.11	125.94
19	A	1762	CLA	OBD-CAD-C3D	-11.15	105.60	128.35
19	A	1788	CLA	OBD-CAD-C3D	-11.12	105.67	128.35
19	A	1811	CLA	OBD-CAD-CBD	-11.10	109.19	125.94
19	1	1241	CLA	OBD-CAD-C3D	-11.09	105.73	128.35
19	1	1149	CLA	OBD-CAD-CBD	-11.08	109.22	125.94
19	1	1188	CLA	OBD-CAD-CBD	-11.06	109.24	125.94
19	1	1189	CLA	OBD-CAD-C3D	-11.06	105.78	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	1170	BCR	C15-C16-C17	-11.06	98.94	123.39
19	B	1743	CLA	OBD-CAD-C3D	-10.88	106.14	128.35
19	A	1766	CLA	OBD-CAD-C3D	-10.87	106.17	128.35
19	B	1764	CLA	OBD-CAD-CBD	-10.80	109.64	125.94
19	A	1812	CLA	OBD-CAD-CBD	-10.78	109.68	125.94
22	B	1782	BCR	C7-C8-C9	-10.76	109.81	126.22
19	A	1790	CLA	OBD-CAD-CBD	-10.74	109.73	125.94
19	A	1761	CLA	OBD-CAD-C3D	-10.74	106.44	128.35
19	G	1099	CLA	OBD-CAD-C3D	-10.74	106.44	128.35
19	2	1222	CLA	OBD-CAD-C3D	-10.74	106.44	128.35
19	3	1212	CLA	OBD-CAD-CBD	-10.65	109.87	125.94
19	B	1750	CLA	OBD-CAD-C3D	-10.59	106.73	128.35
19	4	1197	CLA	C3D-CAD-CBD	-10.54	100.71	107.75
19	R	1054	CLA	OBD-CAD-C3D	-10.54	106.85	128.35
19	L	1167	CLA	OBD-CAD-CBD	-10.52	110.06	125.94
19	A	1759	CLA	OBD-CAD-C3D	-10.49	106.94	128.35
19	L	1167	CLA	OBD-CAD-C3D	-10.49	106.95	128.35
19	B	1747	CLA	OBD-CAD-CBD	-10.46	110.15	125.94
19	A	1777	CLA	OBD-CAD-C3D	-10.46	107.01	128.35
19	3	1224	CLA	C1D-CHD-C4C	-10.44	106.80	122.60
19	A	1795	CLA	OBD-CAD-C3D	-10.43	107.06	128.35
19	B	1773	CLA	C3D-CAD-CBD	-10.39	100.81	107.75
19	4	1209	CLA	OBD-CAD-C3D	-10.34	107.25	128.35
22	I	1032	BCR	C24-C23-C22	-10.32	110.48	126.22
19	A	1793	CLA	OBD-CAD-CBD	-10.30	110.40	125.94
19	1	1146	CLA	OBD-CAD-C3D	-10.28	107.38	128.35
19	A	1777	CLA	OBD-CAD-CBD	-10.24	110.48	125.94
19	J	1043	CLA	OBD-CAD-C3D	-10.20	107.54	128.35
19	A	1789	CLA	OBD-CAD-CBD	-10.20	110.55	125.94
19	B	1756	CLA	OBD-CAD-C3D	-10.17	107.60	128.35
19	4	4014	CLA	OBD-CAD-C3D	-10.15	107.65	128.35
19	A	1791	CLA	OBD-CAD-CBD	-10.13	110.65	125.94
19	B	1757	CLA	OBD-CAD-C3D	-10.11	107.72	128.35
19	A	1797	CLA	OBD-CAD-C3D	-10.07	107.80	128.35
19	B	1737	CLA	OBD-CAD-C3D	-10.05	107.84	128.35
19	4	1202	CLA	OBD-CAD-C3D	-10.05	107.84	128.35
19	1	1308	CLA	OBD-CAD-C3D	-10.04	107.86	128.35
19	3	1219	CLA	OBD-CAD-CBD	-10.02	110.82	125.94
19	1	1142	CLA	OBD-CAD-C3D	-10.01	107.93	128.35
19	B	1787	CLA	OBD-CAD-C3D	-10.01	107.94	128.35
19	K	1085	CLA	OBD-CAD-C3D	-9.96	108.02	128.35
19	4	1209	CLA	C3D-CAD-CBD	-9.95	101.11	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1197	CLA	OBD-CAD-C3D	-9.94	108.06	128.35
19	J	1044	CLA	OBD-CAD-CBD	-9.94	110.94	125.94
19	3	1214	CLA	OBD-CAD-C3D	-9.93	108.08	128.35
19	A	1771	CLA	OBD-CAD-C3D	-9.93	108.10	128.35
19	2	1212	CLA	OBD-CAD-C3D	-9.91	108.12	128.35
19	A	1782	CLA	OBD-CAD-C3D	-9.90	108.14	128.35
19	F	1155	CLA	C3D-CAD-CBD	-9.89	101.14	107.75
19	B	1739	CLA	OBD-CAD-CBD	-9.89	111.02	125.94
19	F	1156	CLA	OBD-CAD-C3D	-9.87	108.22	128.35
19	4	1196	CLA	OBD-CAD-C3D	-9.85	108.25	128.35
19	A	1781	CLA	OBD-CAD-C3D	-9.83	108.29	128.35
19	1	1014	CLA	OBD-CAD-C3D	-9.81	108.33	128.35
19	B	1763	CLA	OBD-CAD-C3D	-9.79	108.38	128.35
19	B	1762	CLA	OBD-CAD-CBD	-9.79	111.17	125.94
19	2	1220	CLA	OBD-CAD-C3D	-9.74	108.47	128.35
19	B	1749	CLA	OBD-CAD-C3D	-9.73	108.50	128.35
19	B	1751	CLA	OBD-CAD-C3D	-9.71	108.54	128.35
19	B	1762	CLA	OBD-CAD-C3D	-9.68	108.59	128.35
19	B	1738	CLA	OBD-CAD-C3D	-9.63	108.71	128.35
19	3	1223	CLA	C3A-C4A-CHB	-9.62	114.35	124.06
19	F	1157	CLA	OBD-CAD-C3D	-9.61	108.73	128.35
19	2	1218	CLA	OBD-CAD-CBD	-9.58	111.48	125.94
19	2	1220	CLA	C3D-CAD-CBD	-9.57	101.36	107.75
19	1	1149	CLA	C3D-CAD-CBD	-9.56	94.08	107.60
19	1	1193	CLA	OBD-CAD-CBD	-9.54	111.55	125.94
19	B	1739	CLA	O1D-CGD-CBD	-9.51	111.00	124.62
19	A	1779	CLA	OBD-CAD-CBD	-9.48	111.63	125.94
19	B	1746	CLA	OBD-CAD-C3D	-9.47	109.02	128.35
22	B	1780	BCR	C15-C14-C13	-9.44	113.57	127.20
19	B	1742	CLA	CAB-C3B-C4B	-9.43	112.76	128.36
19	1	1195	CLA	C3D-CAD-CBD	-9.42	101.46	107.75
19	1	1505	CLA	OBD-CAD-C3D	-9.42	109.14	128.35
19	A	1797	CLA	O1D-CGD-CBD	-9.40	111.15	124.62
19	1	1307	CLA	C3A-C4A-CHB	-9.38	114.59	124.06
19	A	1811	CLA	OBD-CAD-C3D	-9.36	109.25	128.35
19	B	1752	CLA	OBD-CAD-CBD	-9.35	111.82	125.94
19	R	1055	CLA	OBD-CAD-C3D	-9.35	109.28	128.35
19	J	1044	CLA	OBD-CAD-C3D	-9.31	109.35	128.35
19	A	1790	CLA	OBD-CAD-C3D	-9.30	109.37	128.35
19	B	1753	CLA	OBD-CAD-C3D	-9.26	109.45	128.35
19	B	1738	CLA	OBD-CAD-CBD	-9.25	111.97	125.94
19	1	1195	CLA	CAB-C3B-C2B	-9.25	106.22	125.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1746	CLA	OBD-CAD-CBD	-9.16	112.11	125.94
22	I	1032	BCR	C1-C6-C5	-9.14	109.23	122.66
19	2	1222	CLA	OBD-CAD-CBD	-9.14	112.14	125.94
19	3	1218	CLA	OBD-CAD-C3D	-9.09	109.81	128.35
19	4	1198	CLA	C3D-CAD-CBD	-9.05	94.80	107.60
19	B	1766	CLA	OBD-CAD-CBD	-9.05	112.28	125.94
19	B	1751	CLA	OBD-CAD-CBD	-9.05	112.28	125.94
22	B	1782	BCR	C3-C4-C5	-9.02	99.55	113.87
19	2	1218	CLA	OBD-CAD-C3D	-9.02	109.94	128.35
19	3	1214	CLA	CAB-C3B-C4B	-8.98	113.51	128.36
19	1	1148	CLA	C1D-CHD-C4C	-8.95	109.06	122.60
20	A	7030	LMU	C3B-C4B-C5B	-8.92	94.64	110.20
19	1	1149	CLA	CAB-C3B-C2B	-8.90	106.94	125.14
19	B	1763	CLA	OBD-CAD-CBD	-8.89	112.52	125.94
19	B	1759	CLA	OBD-CAD-CBD	-8.89	112.52	125.94
19	A	1795	CLA	OBD-CAD-CBD	-8.89	112.53	125.94
22	3	1225	BCR	C16-C17-C18	-8.86	114.41	127.20
19	B	1760	CLA	OBD-CAD-C3D	-8.79	110.41	128.35
19	B	1763	CLA	CAA-C2A-C3A	-8.76	88.04	113.22
19	1	1188	CLA	OBD-CAD-C3D	-8.73	110.54	128.35
19	B	1788	CLA	OBD-CAD-C3D	-8.70	110.60	128.35
19	G	1099	CLA	C1D-CHD-C4C	-8.69	109.45	122.60
19	A	1778	CLA	OBD-CAD-C3D	-8.68	110.65	128.35
19	A	1784	CLA	OBD-CAD-C3D	-8.64	110.72	128.35
21	B	8062	SUC	C1-O5-C5	-8.63	97.00	113.75
19	2	1217	CLA	C1D-CHD-C4C	-8.62	109.56	122.60
19	A	1789	CLA	OBD-CAD-C3D	-8.62	110.77	128.35
19	A	1768	CLA	OBD-CAD-C3D	-8.58	110.84	128.35
19	4	4007	CLA	CAA-C2A-C3A	-8.57	88.59	113.22
20	A	7032	LMU	C1B-C2B-C3B	-8.55	93.12	109.97
19	B	1747	CLA	OBD-CAD-C3D	-8.55	110.90	128.35
19	B	1759	CLA	OBD-CAD-C3D	-8.54	110.94	128.35
19	A	1798	CLA	OBD-CAD-C3D	-8.52	110.96	128.35
19	B	1761	CLA	OBD-CAD-C3D	-8.50	111.00	128.35
19	A	1761	CLA	OBD-CAD-CBD	-8.46	113.17	125.94
19	2	1215	CLA	OBD-CAD-C3D	-8.45	111.10	128.35
19	4	1198	CLA	OBD-CAD-CBD	-8.44	113.20	125.94
19	A	1765	CLA	OBD-CAD-CBD	-8.43	113.21	125.94
19	4	1202	CLA	CAB-C3B-C2B	-8.40	107.96	125.14
19	L	1166	CLA	OBD-CAD-C3D	-8.40	111.22	128.35
19	B	1770	CLA	OBD-CAD-C3D	-8.37	111.26	128.35
19	2	1220	CLA	CAB-C3B-C2B	-8.37	108.03	125.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1222	CLA	O1D-CGD-CBD	-8.35	112.65	124.62
19	A	1793	CLA	OBD-CAD-C3D	-8.35	111.31	128.35
19	1	1192	CLA	OBD-CAD-CBD	-8.35	113.34	125.94
19	B	1769	CLA	OBD-CAD-CBD	-8.33	113.37	125.94
20	B	1783	LMU	C1B-O5B-C5B	-8.32	97.60	113.75
19	1	1194	CLA	C3A-C4A-CHB	-8.30	115.68	124.06
19	4	1199	CLA	OBD-CAD-C3D	-8.27	111.47	128.35
19	A	1796	CLA	OBD-CAD-C3D	-8.26	111.50	128.35
19	A	1810	CLA	OBD-CAD-C3D	-8.24	111.54	128.35
19	4	1202	CLA	C3D-CAD-CBD	-8.23	102.25	107.75
19	2	1213	CLA	OBD-CAD-C3D	-8.22	111.58	128.35
19	B	1765	CLA	OBD-CAD-CBD	-8.18	113.59	125.94
19	4	1198	CLA	C1D-CHD-C4C	-8.16	110.25	122.60
19	B	1768	CLA	OBD-CAD-CBD	-8.13	113.66	125.94
20	A	7033	LMU	C1B-O1B-C4'	-8.12	96.79	118.01
19	3	3015	CLA	C3A-C4A-CHB	-8.11	115.87	124.06
19	A	1765	CLA	OBD-CAD-C3D	-8.11	111.81	128.35
19	4	1205	CLA	OBD-CAD-C3D	-8.08	111.87	128.35
22	L	1170	BCR	C3-C4-C5	-8.04	101.11	113.87
20	A	7017	LMU	C1B-O1B-C4'	-8.03	97.02	118.01
19	4	4007	CLA	OBD-CAD-CBD	-8.02	113.84	125.94
19	B	1773	CLA	OBD-CAD-C3D	-8.00	112.03	128.35
19	4	1211	CLA	O1D-CGD-CBD	-7.98	113.19	124.62
19	3	1223	CLA	C2D-C3D-C4D	-7.98	99.28	106.30
19	1	1014	CLA	C4B-CHC-C1C	-7.97	112.13	129.26
19	3	3011	CLA	OBD-CAD-C3D	-7.97	112.09	128.35
19	1	1193	CLA	OBD-CAD-C3D	-7.96	112.11	128.35
19	A	1787	CLA	OBD-CAD-C3D	-7.95	112.13	128.35
19	4	1197	CLA	C1D-CHD-C4C	-7.93	110.59	122.60
19	1	1188	CLA	C4B-CHC-C1C	-7.91	112.26	129.26
19	1	1187	CLA	OBD-CAD-CBD	-7.91	114.00	125.94
20	A	7026	LMU	C3B-C4B-C5B	-7.88	96.46	110.20
19	B	1773	CLA	CAB-C3B-C2B	-7.87	109.04	125.14
19	4	4007	CLA	C4B-CHC-C1C	-7.86	112.36	129.26
19	B	1736	CLA	OBD-CAD-C3D	-7.85	112.32	128.35
19	B	1744	CLA	C1D-CHD-C4C	-7.84	110.74	122.60
19	3	1212	CLA	OBD-CAD-C3D	-7.83	112.38	128.35
19	A	1771	CLA	C1D-CHD-C4C	-7.82	110.77	122.60
19	1	1187	CLA	C4B-CHC-C1C	-7.81	112.48	129.26
19	A	1764	CLA	OBD-CAD-CBD	-7.79	114.18	125.94
19	3	1214	CLA	C3D-CAD-CBD	-7.76	102.57	107.75
19	4	1200	CLA	C1D-CHD-C4C	-7.74	110.89	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1771	CLA	OBD-CAD-CBD	-7.70	114.32	125.94
19	4	1201	CLA	C1D-CHD-C4C	-7.69	110.96	122.60
19	1	1192	CLA	OBD-CAD-C3D	-7.69	112.66	128.35
19	A	1759	CLA	OBD-CAD-CBD	-7.67	114.36	125.94
19	3	1222	CLA	C4B-CHC-C1C	-7.66	112.80	129.26
20	A	7037	LMU	C1B-O5B-C5B	-7.65	98.90	113.75
19	B	1788	CLA	OBD-CAD-CBD	-7.64	114.42	125.94
22	B	1780	BCR	C30-C25-C26	-7.63	111.45	122.66
19	B	1735	CLA	OBD-CAD-CBD	-7.60	114.48	125.94
19	A	1800	CLA	OBD-CAD-C3D	-7.58	112.88	128.35
20	A	7026	LMU	C1B-C2B-C3B	-7.58	95.04	109.97
19	A	1769	CLA	OBD-CAD-C3D	-7.58	112.89	128.35
19	A	1774	CLA	OBD-CAD-C3D	-7.57	112.90	128.35
19	1	1196	CLA	C1D-CHD-C4C	-7.56	111.15	122.60
19	B	1771	CLA	C4B-CHC-C1C	-7.53	113.09	129.26
22	L	1170	BCR	C15-C14-C13	-7.52	116.34	127.20
19	A	1780	CLA	OBD-CAD-C3D	-7.47	113.12	128.35
19	1	1145	CLA	C3D-CAD-CBD	-7.46	97.05	107.60
19	B	1772	CLA	OBD-CAD-C3D	-7.45	113.16	128.35
19	1	1197	CLA	C3A-C4A-CHB	-7.43	116.56	124.06
19	B	1771	CLA	OBD-CAD-C3D	-7.42	113.21	128.35
19	A	1778	CLA	O1D-CGD-CBD	-7.42	113.99	124.62
19	B	1769	CLA	OBD-CAD-C3D	-7.38	113.29	128.35
20	A	7037	LMU	O2'-C2'-C1'	-7.38	93.85	110.02
19	A	1797	CLA	C4B-CHC-C1C	-7.36	113.44	129.26
22	L	1170	BCR	C4-C5-C6	-7.36	113.41	122.78
19	A	1770	CLA	OBD-CAD-C3D	-7.33	113.39	128.35
22	I	1032	BCR	C34-C9-C10	-7.31	112.11	122.90
20	A	7036	LMU	C2'-C3'-C4'	-7.30	93.57	109.60
22	I	1032	BCR	C16-C15-C14	-7.29	107.27	123.39
19	L	1167	CLA	CAA-C2A-C3A	-7.27	92.32	113.22
19	A	1761	CLA	C4B-CHC-C1C	-7.27	113.65	129.26
19	3	1219	CLA	OBD-CAD-C3D	-7.24	113.57	128.35
19	1	1194	CLA	C3B-C2B-C1B	-7.22	99.97	106.29
19	1	1307	CLA	C3B-C2B-C1B	-7.22	99.98	106.29
19	A	1760	CLA	OBD-CAD-CBD	-7.22	115.05	125.94
20	A	7039	LMU	C1B-O5B-C5B	-7.20	99.77	113.75
19	L	1168	CLA	C1D-CHD-C4C	-7.18	111.73	122.60
19	A	1810	CLA	C3D-CAD-CBD	-7.18	97.45	107.60
19	4	1211	CLA	C1D-CHD-C4C	-7.17	111.75	122.60
19	2	1217	CLA	C4B-CHC-C1C	-7.17	113.86	129.26
22	I	1032	BCR	C38-C26-C25	-7.16	117.58	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7038	LMU	C3'-C4'-C5'	-7.15	94.66	110.84
19	4	1211	CLA	OBD-CAD-C3D	-7.15	113.76	128.35
19	R	1055	CLA	C4B-CHC-C1C	-7.13	113.94	129.26
20	A	7040	LMU	O5B-C5B-C4B	-7.12	96.32	109.68
19	J	1044	CLA	C1D-CHD-C4C	-7.11	111.83	122.60
19	1	1309	CLA	C3A-C4A-CHB	-7.11	116.88	124.06
19	1	1191	CLA	C3A-C4A-CHB	-7.11	116.88	124.06
20	K	1086	LMU	C3B-C4B-C5B	-7.10	97.81	110.20
19	3	1212	CLA	C1D-CHD-C4C	-7.09	111.87	122.60
19	B	1748	CLA	OBD-CAD-CBD	-7.08	115.26	125.94
19	4	1199	CLA	C4B-CHC-C1C	-7.03	114.16	129.26
19	4	1198	CLA	C4B-CHC-C1C	-7.02	114.17	129.26
22	B	1780	BCR	C3-C4-C5	-7.01	102.74	113.87
19	B	1786	CLA	C4B-CHC-C1C	-7.01	114.20	129.26
19	3	3001	CLA	C3A-C4A-CHB	-7.00	116.99	124.06
19	A	1795	CLA	C4B-CHC-C1C	-6.99	114.24	129.26
19	B	1772	CLA	OBD-CAD-CBD	-6.97	115.42	125.94
20	A	7037	LMU	C4B-C3B-C2B	-6.95	97.82	110.79
19	A	1787	CLA	OBD-CAD-CBD	-6.94	115.47	125.94
19	4	1205	CLA	OBD-CAD-CBD	-6.93	115.47	125.94
19	2	1214	CLA	C3A-C4A-CHB	-6.93	117.07	124.06
19	A	1760	CLA	C4B-CHC-C1C	-6.93	114.38	129.26
20	A	7026	LMU	C3'-C4'-C5'	-6.92	95.18	110.84
19	A	1763	CLA	C4B-CHC-C1C	-6.92	114.39	129.26
19	B	1737	CLA	CAA-C2A-C3A	-6.90	93.38	113.22
19	1	1196	CLA	O2A-CGA-O1A	-6.88	105.72	123.49
19	1	1198	CLA	C3A-C4A-CHB	-6.87	117.12	124.06
19	3	3008	CLA	OBD-CAD-CBD	-6.87	115.57	125.94
19	1	1196	CLA	CHD-C4C-C3C	-6.86	114.33	124.94
19	3	1216	CLA	C3A-C4A-CHB	-6.85	117.14	124.06
19	1	1145	CLA	C1D-CHD-C4C	-6.85	112.24	122.60
19	B	1742	CLA	CAB-C3B-C2B	-6.85	111.14	125.14
19	B	1772	CLA	C4B-CHC-C1C	-6.84	114.58	129.26
19	A	1789	CLA	O1D-CGD-CBD	-6.82	114.84	124.62
20	A	7043	LMU	C3B-C4B-C5B	-6.81	98.33	110.20
19	B	1752	CLA	C1D-CHD-C4C	-6.79	112.32	122.60
20	A	7050	LMU	O5'-C5'-C4'	-6.79	95.40	109.75
19	G	1099	CLA	O1D-CGD-CBD	-6.79	114.89	124.62
19	3	1217	CLA	C3A-C4A-CHB	-6.78	117.22	124.06
19	A	1767	CLA	OBD-CAD-C3D	-6.77	114.53	128.35
19	B	1740	CLA	C1D-CHD-C4C	-6.75	112.39	122.60
19	B	1765	CLA	C1D-CHD-C4C	-6.74	112.40	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1792	CLA	OBD-CAD-C3D	-6.71	114.66	128.35
19	4	1211	CLA	OBD-CAD-CBD	-6.70	115.82	125.94
19	A	1767	CLA	OBD-CAD-CBD	-6.70	115.83	125.94
19	B	1737	CLA	C4B-CHC-C1C	-6.69	114.88	129.26
19	1	1146	CLA	C4B-CHC-C1C	-6.69	114.88	129.26
19	4	1197	CLA	CAB-C3B-C2B	-6.69	111.45	125.14
19	A	1788	CLA	C4B-CHC-C1C	-6.69	114.89	129.26
19	A	1797	CLA	C1D-CHD-C4C	-6.69	112.48	122.60
22	3	1225	BCR	C11-C10-C9	-6.69	117.54	127.20
19	A	1772	CLA	C1D-CHD-C4C	-6.68	112.48	122.60
19	4	1203	CLA	C3B-C2B-C1B	-6.68	100.44	106.29
20	A	7050	LMU	O5B-C1B-C2B	-6.67	96.59	110.28
19	1	1191	CLA	C2D-C3D-C4D	-6.66	100.44	106.30
19	4	1203	CLA	C3A-C4A-CHB	-6.65	117.34	124.06
19	A	1765	CLA	C4B-CHC-C1C	-6.62	115.03	129.26
19	B	1742	CLA	OBD-CAD-C3D	-6.62	114.84	128.35
19	B	1736	CLA	OBD-CAD-CBD	-6.62	115.95	125.94
19	1	1188	CLA	C1D-CHD-C4C	-6.59	112.64	122.60
20	A	7050	LMU	C1B-C2B-C3B	-6.58	97.01	109.97
19	R	1055	CLA	C1D-CHD-C4C	-6.56	112.67	122.60
19	B	1754	CLA	C4B-CHC-C1C	-6.55	115.18	129.26
19	2	1218	CLA	C4B-CHC-C1C	-6.55	115.18	129.26
19	4	1199	CLA	OBD-CAD-CBD	-6.55	116.06	125.94
19	B	1760	CLA	C1D-CHD-C4C	-6.53	112.71	122.60
19	I	1031	CLA	C1D-CHD-C4C	-6.53	112.72	122.60
19	A	1810	CLA	C4B-CHC-C1C	-6.53	115.23	129.26
19	3	1224	CLA	CHD-C4C-C3C	-6.52	114.87	124.94
19	4	1205	CLA	C1D-CHD-C4C	-6.51	112.74	122.60
19	1	1196	CLA	C4B-CHC-C1C	-6.51	115.28	129.26
19	B	1760	CLA	C4B-CHC-C1C	-6.50	115.30	129.26
20	A	7043	LMU	C4B-C3B-C2B	-6.49	98.68	110.79
19	1	1192	CLA	C1D-CHD-C4C	-6.49	112.78	122.60
19	3	3008	CLA	OBD-CAD-C3D	-6.49	115.11	128.35
19	4	1201	CLA	C4B-CHC-C1C	-6.48	115.33	129.26
19	1	1014	CLA	C1D-CHD-C4C	-6.48	112.79	122.60
19	3	1224	CLA	C4B-CHC-C1C	-6.48	115.34	129.26
19	1	1148	CLA	C4-C3-C2	-6.47	110.79	123.50
19	B	1769	CLA	C4B-CHC-C1C	-6.46	115.37	129.26
19	A	1792	CLA	C4B-CHC-C1C	-6.45	115.41	129.26
19	4	1207	CLA	C3A-C4A-CHB	-6.44	117.56	124.06
22	B	1780	BCR	C24-C23-C22	-6.43	116.41	126.22
22	B	1782	BCR	C4-C5-C6	-6.41	114.61	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1099	CLA	CHD-C4C-C3C	-6.41	115.03	124.94
19	B	1748	CLA	OBD-CAD-C3D	-6.41	115.28	128.35
19	B	1742	CLA	OBD-CAD-CBD	-6.38	116.32	125.94
19	B	1758	CLA	O1D-CGD-CBD	-6.37	115.49	124.62
19	1	1193	CLA	CBA-CAA-C2A	-6.37	95.75	113.73
19	A	1774	CLA	C4B-CHC-C1C	-6.36	115.59	129.26
19	A	1767	CLA	C1D-CHD-C4C	-6.36	112.97	122.60
19	B	1745	CLA	C4B-CHC-C1C	-6.34	115.63	129.26
19	A	1767	CLA	C4B-CHC-C1C	-6.34	115.64	129.26
19	1	1303	CLA	C3A-C4A-CHB	-6.34	117.66	124.06
19	A	1793	CLA	C4B-CHC-C1C	-6.34	115.64	129.26
19	A	1784	CLA	C4B-CHC-C1C	-6.34	115.64	129.26
22	L	1169	BCR	C27-C26-C25	-6.34	114.71	122.78
19	J	1044	CLA	CAA-C2A-C3A	-6.33	95.01	113.22
19	B	1738	CLA	C1D-CHD-C4C	-6.33	113.02	122.60
19	A	1789	CLA	C4B-CHC-C1C	-6.33	115.67	129.26
19	B	1741	CLA	C4B-CHC-C1C	-6.32	115.69	129.26
19	A	1766	CLA	C4B-CHC-C1C	-6.31	115.71	129.26
19	B	1754	CLA	CHD-C4C-C3C	-6.30	115.20	124.94
19	A	1811	CLA	C1D-CHD-C4C	-6.29	113.08	122.60
19	1	1505	CLA	C4B-CHC-C1C	-6.29	115.75	129.26
19	A	1810	CLA	CHD-C4C-C3C	-6.28	115.23	124.94
19	A	1782	CLA	C4B-CHC-C1C	-6.28	115.77	129.26
19	B	1754	CLA	C6-C5-C3	-6.28	98.70	112.48
19	B	1764	CLA	C4B-CHC-C1C	-6.28	115.77	129.26
19	A	1791	CLA	C4B-CHC-C1C	-6.28	115.78	129.26
19	B	1745	CLA	OBD-CAD-CBD	-6.27	116.47	125.94
19	3	1222	CLA	C1D-CHD-C4C	-6.27	113.11	122.60
19	2	1214	CLA	C2D-C3D-C4D	-6.27	100.78	106.30
19	2	1216	CLA	C2D-C3D-C4D	-6.26	100.79	106.30
19	4	1201	CLA	CMB-C2B-C1B	-6.25	118.03	128.36
19	2	1213	CLA	OBD-CAD-CBD	-6.24	116.52	125.94
19	2	1223	CLA	C1D-CHD-C4C	-6.24	113.15	122.60
19	K	1085	CLA	C4B-CHC-C1C	-6.23	115.87	129.26
19	B	1764	CLA	O1D-CGD-CBD	-6.23	115.70	124.62
19	4	1198	CLA	CAA-C2A-C3A	-6.23	95.31	113.22
19	B	1770	CLA	C1D-CHD-C4C	-6.23	113.18	122.60
19	1	1187	CLA	C1D-CHD-C4C	-6.22	113.19	122.60
19	F	1157	CLA	C1D-CHD-C4C	-6.21	113.20	122.60
20	A	7014	LMU	C4B-C3B-C2B	-6.21	99.21	110.79
19	B	1752	CLA	C4B-CHC-C1C	-6.21	115.93	129.26
19	J	1043	CLA	C1D-CHD-C4C	-6.20	113.22	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1762	CLA	C4B-CHC-C1C	-6.20	115.95	129.26
19	B	1748	CLA	C4B-CHC-C1C	-6.20	115.95	129.26
19	2	1223	CLA	C4B-CHC-C1C	-6.19	115.95	129.26
19	B	1744	CLA	C4B-CHC-C1C	-6.19	115.95	129.26
19	1	1145	CLA	C4B-CHC-C1C	-6.19	115.96	129.26
19	A	1778	CLA	C4B-CHC-C1C	-6.17	116.00	129.26
19	A	1781	CLA	C4B-CHC-C1C	-6.17	116.01	129.26
19	B	1753	CLA	C4B-CHC-C1C	-6.16	116.02	129.26
19	A	1759	CLA	C4B-CHC-C1C	-6.15	116.04	129.26
19	R	1055	CLA	OBD-CAD-CBD	-6.15	116.66	125.94
19	A	1771	CLA	C1-C2-C3	-6.14	116.64	126.71
19	B	1751	CLA	C4B-CHC-C1C	-6.13	116.08	129.26
19	B	1766	CLA	C4B-CHC-C1C	-6.12	116.11	129.26
19	F	1156	CLA	C4B-CHC-C1C	-6.12	116.11	129.26
19	2	1212	CLA	C1D-CHD-C4C	-6.12	113.34	122.60
19	B	1755	CLA	C1D-CHD-C4C	-6.12	113.34	122.60
19	L	1168	CLA	C3D-CAD-CBD	-6.11	98.96	107.60
19	A	1764	CLA	C4B-CHC-C1C	-6.11	116.13	129.26
19	A	1779	CLA	C4B-CHC-C1C	-6.11	116.14	129.26
19	4	1202	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	B	1743	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	B	1740	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	3	1218	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
20	A	7026	LMU	C1'-C2'-C3'	-6.10	97.96	109.97
19	A	1780	CLA	C4B-CHC-C1C	-6.09	116.17	129.26
19	B	1750	CLA	C4B-CHC-C1C	-6.09	116.18	129.26
19	B	1756	CLA	C1D-CHD-C4C	-6.09	113.39	122.60
19	A	1797	CLA	CMD-C2D-C3D	-6.09	113.18	125.09
19	4	1204	CLA	C3A-C4A-CHB	-6.09	117.92	124.06
19	4	1209	CLA	CAB-C3B-C2B	-6.09	112.69	125.14
19	A	1769	CLA	C1D-CHD-C4C	-6.08	113.40	122.60
19	4	1200	CLA	C4B-CHC-C1C	-6.08	116.19	129.26
19	4	1201	CLA	CBA-CAA-C2A	-6.08	96.58	113.73
19	2	1220	CLA	C4B-CHC-C1C	-6.08	116.20	129.26
19	B	1764	CLA	C1D-CHD-C4C	-6.07	113.41	122.60
19	1	1010	CLA	C3A-C4A-CHB	-6.07	117.93	124.06
19	3	1220	CLA	C3A-C4A-CHB	-6.07	117.93	124.06
19	4	1196	CLA	C4B-CHC-C1C	-6.07	116.23	129.26
19	1	1191	CLA	C1D-CHD-C4C	-6.07	110.72	126.32
19	4	4014	CLA	C1D-CHD-C4C	-6.06	113.43	122.60
19	4	1209	CLA	C1D-CHD-C4C	-6.06	113.44	122.60
19	1	1142	CLA	C1D-CHD-C4C	-6.05	113.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1744	CLA	CHD-C4C-C3C	-6.05	115.59	124.94
19	L	1167	CLA	C4B-CHC-C1C	-6.05	116.27	129.26
19	B	1749	CLA	C4B-CHC-C1C	-6.05	116.27	129.26
19	B	1752	CLA	CHD-C4C-C3C	-6.04	115.60	124.94
19	A	1811	CLA	C4B-CHC-C1C	-6.04	116.28	129.26
19	1	1308	CLA	C1D-CHD-C4C	-6.04	113.47	122.60
19	B	1763	CLA	C4B-CHC-C1C	-6.03	116.30	129.26
19	2	1221	CLA	C3A-C4A-CHB	-6.03	117.97	124.06
19	1	1241	CLA	C1D-CHD-C4C	-6.02	113.49	122.60
19	1	1195	CLA	C1D-CHD-C4C	-6.02	113.49	122.60
19	2	1212	CLA	C4B-CHC-C1C	-6.02	116.33	129.26
19	B	1757	CLA	C1D-CHD-C4C	-6.02	113.50	122.60
20	A	7032	LMU	C3B-C4B-C5B	-6.01	99.71	110.20
19	B	1759	CLA	C1D-CHD-C4C	-6.01	113.50	122.60
19	A	1773	CLA	C1D-CHD-C4C	-6.01	113.51	122.60
19	B	1756	CLA	C4B-CHC-C1C	-6.01	116.35	129.26
19	1	1142	CLA	C4B-CHC-C1C	-6.01	116.36	129.26
19	4	4014	CLA	C4B-CHC-C1C	-6.01	116.36	129.26
19	B	1757	CLA	C4B-CHC-C1C	-6.00	116.37	129.26
19	4	1206	CLA	C4B-CHC-C1C	-5.99	116.39	129.26
19	4	1196	CLA	C1D-CHD-C4C	-5.99	113.54	122.60
19	1	1195	CLA	OBD-CAD-C3D	-5.99	116.14	128.35
19	1	1149	CLA	C4B-CHC-C1C	-5.98	116.40	129.26
19	B	1770	CLA	C4B-CHC-C1C	-5.98	116.41	129.26
19	3	1215	CLA	C3A-C4A-CHB	-5.98	118.02	124.06
19	B	1749	CLA	C1D-CHD-C4C	-5.98	113.56	122.60
19	B	1739	CLA	C4B-CHC-C1C	-5.97	116.43	129.26
19	1	1193	CLA	C4B-CHC-C1C	-5.96	116.45	129.26
19	B	1761	CLA	C4B-CHC-C1C	-5.96	116.46	129.26
19	3	1214	CLA	CAB-C3B-C2B	-5.95	112.97	125.14
19	1	1309	CLA	C1D-CHD-C4C	-5.95	111.02	126.32
19	A	1786	CLA	C4B-CHC-C1C	-5.94	116.49	129.26
19	1	1308	CLA	C4B-CHC-C1C	-5.94	116.51	129.26
19	A	1763	CLA	CGD-CBD-CAD	-5.93	90.52	110.62
19	B	1744	CLA	CMD-C2D-C3D	-5.93	113.50	125.09
19	F	1155	CLA	C4B-CHC-C1C	-5.92	116.55	129.26
19	4	1202	CLA	C1D-CHD-C4C	-5.91	113.65	122.60
19	B	1762	CLA	C4B-CHC-C1C	-5.91	116.56	129.26
22	L	1170	BCR	C34-C9-C10	-5.91	114.18	122.90
20	A	7040	LMU	C3B-C4B-C5B	-5.90	99.90	110.20
19	3	1214	CLA	C1D-CHD-C4C	-5.90	113.67	122.60
19	A	1791	CLA	C1D-CHD-C4C	-5.90	113.67	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1156	CLA	C1D-CHD-C4C	-5.90	113.67	122.60
19	4	4007	CLA	C3D-CAD-CBD	-5.90	99.26	107.60
19	1	1196	CLA	CMD-C2D-C3D	-5.90	113.55	125.09
19	3	1223	CLA	C3B-C2B-C1B	-5.89	101.13	106.29
20	A	7050	LMU	O5B-C5B-C4B	-5.89	98.63	109.68
19	2	1222	CLA	C4B-CHC-C1C	-5.89	116.61	129.26
19	B	1735	CLA	C4B-CHC-C1C	-5.89	116.61	129.26
19	3	3011	CLA	OBD-CAD-CBD	-5.88	117.06	125.94
19	A	1785	CLA	C4B-CHC-C1C	-5.88	116.63	129.26
19	R	1054	CLA	C4B-CHC-C1C	-5.87	116.65	129.26
20	A	7048	LMU	C1-O1'-C1'	-5.86	103.70	113.94
19	B	1768	CLA	C1D-CHD-C4C	-5.86	113.74	122.60
19	A	1787	CLA	C4B-CHC-C1C	-5.85	116.69	129.26
20	A	7039	LMU	O5B-C5B-C6B	-5.85	91.58	106.36
19	F	1155	CLA	OBD-CAD-C3D	-5.84	116.43	128.35
19	3	1222	CLA	CHD-C4C-C3C	-5.84	115.92	124.94
19	A	1799	CLA	C4B-CHC-C1C	-5.84	116.72	129.26
19	4	1205	CLA	CHD-C4C-C3C	-5.83	115.93	124.94
19	L	1166	CLA	C1D-CHD-C4C	-5.82	113.79	122.60
19	1	1309	CLA	C3C-C4C-CHD	-5.81	115.75	125.32
19	F	1155	CLA	C1D-CHD-C4C	-5.81	113.80	122.60
19	1	1188	CLA	C3D-CAD-CBD	-5.80	99.40	107.60
19	A	1770	CLA	C4B-CHC-C1C	-5.80	116.80	129.26
19	A	1796	CLA	C1D-CHD-C4C	-5.80	113.82	122.60
19	A	1761	CLA	C1D-CHD-C4C	-5.79	113.83	122.60
19	A	1800	CLA	C1D-CHD-C4C	-5.79	113.83	122.60
19	1	1309	CLA	C3B-C2B-C1B	-5.79	101.22	106.29
19	B	1758	CLA	C1D-CHD-C4C	-5.79	113.84	122.60
19	J	1043	CLA	C4B-CHC-C1C	-5.78	116.84	129.26
19	1	1198	CLA	C3B-C2B-C1B	-5.76	101.25	106.29
20	A	7016	LMU	C1'-O5'-C5'	-5.75	102.58	113.75
19	2	2010	CLA	C3A-C4A-CHB	-5.75	118.26	124.06
19	B	1751	CLA	C1D-CHD-C4C	-5.75	113.90	122.60
19	B	1788	CLA	C1D-CHD-C4C	-5.75	113.90	122.60
19	B	1753	CLA	C1D-CHD-C4C	-5.74	113.92	122.60
19	1	1192	CLA	C4B-CHC-C1C	-5.73	116.94	129.26
19	A	1768	CLA	C4B-CHC-C1C	-5.72	116.97	129.26
19	1	1190	CLA	C1D-CHD-C4C	-5.72	113.94	122.60
19	K	1085	CLA	C1D-CHD-C4C	-5.72	113.94	122.60
19	J	1044	CLA	C4B-CHC-C1C	-5.71	116.99	129.26
19	3	1214	CLA	C4B-CHC-C1C	-5.71	116.99	129.26
22	I	1032	BCR	C11-C10-C9	-5.71	118.95	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7040	LMU	O3B-C3B-C2B	-5.70	97.50	110.34
19	A	1781	CLA	C1D-CHD-C4C	-5.70	113.97	122.60
20	A	7050	LMU	C1B-O1B-C4'	-5.70	103.12	118.01
19	2	1215	CLA	C4B-CHC-C1C	-5.69	117.03	129.26
19	A	1783	CLA	C1D-CHD-C4C	-5.68	114.01	122.60
19	A	1768	CLA	C1D-CHD-C4C	-5.68	114.01	122.60
19	B	1746	CLA	C1D-CHD-C4C	-5.67	114.02	122.60
19	L	1168	CLA	O1D-CGD-CBD	-5.67	116.49	124.62
22	L	1169	BCR	C33-C5-C6	-5.67	119.04	124.61
22	I	1032	BCR	C29-C30-C25	-5.67	101.39	110.36
19	A	1812	CLA	C4B-CHC-C1C	-5.66	117.09	129.26
19	B	1736	CLA	C4B-CHC-C1C	-5.66	117.09	129.26
19	B	1762	CLA	CHD-C4C-C3C	-5.66	116.19	124.94
19	3	3011	CLA	C4B-CHC-C1C	-5.65	117.11	129.26
19	4	1204	CLA	C1D-CHD-C4C	-5.65	111.78	126.32
19	B	1759	CLA	C4B-CHC-C1C	-5.65	117.12	129.26
19	A	1794	CLA	C4B-CHC-C1C	-5.65	117.12	129.26
19	A	1774	CLA	C1D-CHD-C4C	-5.64	114.06	122.60
19	3	1212	CLA	C4B-CHC-C1C	-5.64	117.15	129.26
19	B	1737	CLA	C1D-CHD-C4C	-5.64	114.07	122.60
19	B	1745	CLA	OBD-CAD-C3D	-5.64	116.85	128.35
22	3	1225	BCR	C33-C5-C6	-5.64	119.07	124.61
22	B	1780	BCR	C10-C11-C12	-5.63	105.96	123.13
19	1	1190	CLA	C4B-CHC-C1C	-5.63	117.16	129.26
19	A	1759	CLA	C1D-CHD-C4C	-5.63	114.08	122.60
19	4	1200	CLA	CHD-C4C-C3C	-5.63	116.24	124.94
19	A	1782	CLA	C1D-CHD-C4C	-5.62	114.09	122.60
19	2	1220	CLA	C1D-CHD-C4C	-5.62	114.10	122.60
19	B	1773	CLA	C4B-CHC-C1C	-5.62	117.20	129.26
19	2	1219	CLA	C3A-C4A-CHB	-5.61	118.39	124.06
20	A	7037	LMU	C3B-C4B-C5B	-5.61	100.42	110.20
19	B	1747	CLA	C4B-CHC-C1C	-5.60	117.23	129.26
19	4	1211	CLA	CHD-C4C-C3C	-5.60	116.29	124.94
20	A	7039	LMU	C1B-C2B-C3B	-5.59	98.95	109.97
19	3	1212	CLA	CBA-CAA-C2A	-5.59	97.97	113.73
20	A	7040	LMU	C1B-O1B-C4'	-5.59	103.41	118.01
22	B	1780	BCR	C35-C13-C14	-5.58	114.65	122.90
19	B	1787	CLA	C1D-CHD-C4C	-5.58	114.16	122.60
19	A	1798	CLA	C4B-CHC-C1C	-5.58	117.27	129.26
19	1	1241	CLA	C4B-CHC-C1C	-5.58	117.27	129.26
19	G	1099	CLA	C4B-CHC-C1C	-5.58	117.27	129.26
20	A	7037	LMU	O1'-C1'-C2'	-5.57	101.00	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1789	CLA	C1D-CHD-C4C	-5.57	114.17	122.60
19	B	1742	CLA	C1D-CHD-C4C	-5.57	114.17	122.60
19	4	1208	CLA	C3A-C4A-CHB	-5.57	118.44	124.06
19	B	1747	CLA	O1D-CGD-CBD	-5.56	116.65	124.62
19	4	1209	CLA	C4B-CHC-C1C	-5.56	117.31	129.26
19	A	1794	CLA	C1D-CHD-C4C	-5.56	114.19	122.60
19	B	1763	CLA	C1D-CHD-C4C	-5.56	114.19	122.60
19	A	1778	CLA	C3D-CAD-CBD	-5.56	99.74	107.60
19	3	1213	CLA	C2A-C1A-CHA	-5.55	112.76	122.58
22	I	1032	BCR	C16-C17-C18	-5.55	119.19	127.20
19	4	1206	CLA	C1D-CHD-C4C	-5.55	114.21	122.60
19	B	1772	CLA	C3D-CAD-CBD	-5.55	99.76	107.60
19	A	1790	CLA	C4B-CHC-C1C	-5.54	117.35	129.26
19	1	1192	CLA	CHD-C4C-C3C	-5.54	116.38	124.94
19	1	1194	CLA	C2D-C3D-C4D	-5.53	101.43	106.30
19	B	1768	CLA	O2D-CGD-O1D	-5.53	112.38	123.79
19	B	1747	CLA	C1D-CHD-C4C	-5.52	114.25	122.60
19	A	1769	CLA	C4B-CHC-C1C	-5.52	117.41	129.26
19	B	1742	CLA	C4B-CHC-C1C	-5.51	117.41	129.26
19	A	1777	CLA	C1D-CHD-C4C	-5.51	114.26	122.60
19	1	1188	CLA	O1D-CGD-CBD	-5.51	116.72	124.62
21	3	1226	SUC	C3-C4-C5	-5.51	100.59	110.20
19	A	1765	CLA	C1D-CHD-C4C	-5.51	114.27	122.60
19	1	1189	CLA	C4B-CHC-C1C	-5.50	117.44	129.26
19	A	1777	CLA	C4B-CHC-C1C	-5.50	117.45	129.26
19	1	1193	CLA	CGD-CBD-CAD	-5.50	92.00	110.62
19	A	1775	CLA	C3A-C4A-CHB	-5.50	118.51	124.06
19	A	1795	CLA	C3D-CAD-CBD	-5.49	99.84	107.60
19	B	1755	CLA	C4B-CHC-C1C	-5.48	117.48	129.26
19	4	1203	CLA	C1D-CHD-C4C	-5.48	112.22	126.32
19	A	1797	CLA	C3D-CAD-CBD	-5.48	99.85	107.60
19	A	1796	CLA	CHD-C4C-C3C	-5.48	116.48	124.94
19	B	1767	CLA	C4B-CHC-C1C	-5.47	117.50	129.26
19	1	1148	CLA	CMD-C2D-C3D	-5.47	114.38	125.09
19	B	1736	CLA	C1D-CHD-C4C	-5.47	114.32	122.60
19	1	1196	CLA	CGD-CBD-CAD	-5.47	92.10	110.62
19	A	1773	CLA	C4B-CHC-C1C	-5.46	117.52	129.26
19	1	1505	CLA	C1D-CHD-C4C	-5.46	114.34	122.60
20	A	7014	LMU	C1'-C2'-C3'	-5.45	99.22	109.97
19	B	1750	CLA	C1D-CHD-C4C	-5.45	114.35	122.60
19	1	1195	CLA	C4B-CHC-C1C	-5.44	117.57	129.26
19	B	1768	CLA	C4B-CHC-C1C	-5.44	117.57	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1779	CLA	C1D-CHD-C4C	-5.44	114.37	122.60
19	B	1758	CLA	C4B-CHC-C1C	-5.43	117.59	129.26
19	A	1771	CLA	CHD-C4C-C3C	-5.43	116.54	124.94
19	B	1739	CLA	C3D-CAD-CBD	-5.43	99.92	107.60
19	3	1219	CLA	C4B-CHC-C1C	-5.42	117.61	129.26
19	3	1219	CLA	C1D-CHD-C4C	-5.42	114.40	122.60
20	A	7021	LMU	O3B-C3B-C4B	-5.41	98.15	110.34
19	4	1203	CLA	C3C-C4C-CHD	-5.41	116.41	125.32
19	A	1771	CLA	C4B-CHC-C1C	-5.41	117.63	129.26
19	A	1785	CLA	C1D-CHD-C4C	-5.41	114.41	122.60
19	L	1168	CLA	CHD-C4C-C3C	-5.41	116.58	124.94
19	3	1221	CLA	C2D-C3D-C4D	-5.40	101.55	106.30
19	A	1780	CLA	C1D-CHD-C4C	-5.39	114.44	122.60
20	A	7041	LMU	C6B-C5B-C4B	-5.39	99.73	113.02
19	1	1191	CLA	C3B-C2B-C1B	-5.38	101.58	106.29
19	1	1149	CLA	CMD-C2D-C3D	-5.38	114.57	125.09
19	A	1793	CLA	C1D-CHD-C4C	-5.38	114.46	122.60
19	B	1766	CLA	C1D-CHD-C4C	-5.38	114.47	122.60
19	2	1213	CLA	C4B-CHC-C1C	-5.37	117.72	129.26
19	3	3008	CLA	C4B-CHC-C1C	-5.37	117.72	129.26
19	B	1754	CLA	CBC-CAC-C3C	-5.37	96.00	112.39
19	L	1166	CLA	C4B-CHC-C1C	-5.37	117.73	129.26
19	B	1738	CLA	C4B-CHC-C1C	-5.36	117.74	129.26
20	A	7039	LMU	O5B-C1B-C2B	-5.36	99.27	110.28
19	A	1776	CLA	C1D-CHD-C4C	-5.36	114.49	122.60
19	A	1790	CLA	C1D-CHD-C4C	-5.35	114.50	122.60
19	B	1751	CLA	C3D-CAD-CBD	-5.35	100.03	107.60
22	L	1170	BCR	C10-C11-C12	-5.35	106.82	123.13
22	B	1782	BCR	C28-C27-C26	-5.35	105.38	113.87
21	3	1226	SUC	C4-C3-C2	-5.34	100.83	110.79
20	1	1200	LMU	C3'-C4'-C5'	-5.34	98.77	110.84
19	3	3008	CLA	C1D-CHD-C4C	-5.34	114.53	122.60
22	A	1806	BCR	C16-C17-C18	-5.33	119.49	127.20
19	4	1205	CLA	C4B-CHC-C1C	-5.33	117.81	129.26
19	4	1211	CLA	C4B-CHC-C1C	-5.32	117.82	129.26
22	B	1781	BCR	C16-C17-C18	-5.32	119.52	127.20
19	A	1759	CLA	O1D-CGD-CBD	-5.32	117.00	124.62
21	B	8062	SUC	O5-C1-C2	-5.31	99.37	110.28
19	2	1213	CLA	C1D-CHD-C4C	-5.31	114.56	122.60
22	A	1803	BCR	C15-C14-C13	-5.31	119.52	127.20
19	1	1014	CLA	O2D-CGD-O1D	-5.31	112.82	123.79
19	2	1216	CLA	C2A-C1A-CHA	-5.31	113.18	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1798	CLA	C1D-CHD-C4C	-5.31	114.57	122.60
19	1	1198	CLA	C2A-C1A-CHA	-5.30	113.19	122.58
19	B	1788	CLA	C4B-CHC-C1C	-5.30	117.88	129.26
21	B	8062	SUC	C3-C4-C5	-5.29	100.97	110.20
19	1	1146	CLA	C1D-CHD-C4C	-5.29	114.60	122.60
19	L	1167	CLA	C1D-CHD-C4C	-5.29	114.60	122.60
22	A	1803	BCR	C16-C17-C18	-5.28	119.57	127.20
19	B	1787	CLA	C4B-CHC-C1C	-5.28	117.92	129.26
19	A	1788	CLA	C1D-CHD-C4C	-5.27	114.63	122.60
22	A	1803	BCR	C11-C10-C9	-5.26	119.59	127.20
22	B	1776	BCR	C11-C10-C9	-5.26	119.59	127.20
22	A	1806	BCR	C15-C14-C13	-5.26	119.60	127.20
19	I	1031	CLA	C4B-CHC-C1C	-5.25	117.98	129.26
21	2	1225	SUC	O5-C5-C4	-5.24	100.44	109.53
22	B	1777	BCR	C27-C26-C25	-5.24	116.11	122.78
19	A	1760	CLA	C1D-CHD-C4C	-5.24	114.67	122.60
19	4	1208	CLA	C3B-C2B-C1B	-5.24	101.71	106.29
22	L	1169	BCR	C30-C25-C26	-5.24	114.97	122.66
19	4	1207	CLA	C1D-CHD-C4C	-5.24	112.86	126.32
19	A	1776	CLA	C4B-CHC-C1C	-5.23	118.03	129.26
22	B	1781	BCR	C11-C10-C9	-5.22	119.65	127.20
19	A	1796	CLA	C4B-CHC-C1C	-5.22	118.04	129.26
22	A	1807	BCR	C15-C14-C13	-5.21	119.67	127.20
21	B	8060	SUC	C6'-C5'-C4'	-5.21	102.76	115.08
22	A	1806	BCR	C33-C5-C6	-5.20	119.50	124.61
22	B	1776	BCR	C15-C14-C13	-5.19	119.69	127.20
19	A	1779	CLA	C3D-CAD-CBD	-5.19	100.26	107.60
19	B	1765	CLA	C4B-CHC-C1C	-5.19	118.11	129.26
22	A	1807	BCR	C11-C10-C9	-5.18	119.71	127.20
19	B	1739	CLA	OBD-CAD-C3D	-5.18	117.78	128.35
19	B	1739	CLA	C1D-CHD-C4C	-5.18	114.76	122.60
19	A	1800	CLA	CHD-C4C-C3C	-5.18	116.94	124.94
22	A	1802	BCR	C11-C10-C9	-5.18	119.72	127.20
22	B	1781	BCR	C15-C14-C13	-5.18	119.72	127.20
22	A	1807	BCR	C16-C17-C18	-5.16	119.75	127.20
22	A	1804	BCR	C38-C26-C25	-5.16	119.54	124.61
19	B	1738	CLA	C6-C5-C3	-5.15	101.17	112.48
19	B	1746	CLA	C4B-CHC-C1C	-5.15	118.19	129.26
20	A	7022	LMU	O3B-C3B-C4B	-5.15	98.74	110.34
19	3	1221	CLA	C3A-C4A-CHB	-5.15	118.86	124.06
20	A	7017	LMU	O4'-C4B-C5B	-5.15	95.60	109.24
19	B	1788	CLA	C3D-CAD-CBD	-5.15	100.32	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1800	CLA	C4B-CHC-C1C	-5.14	118.21	129.26
22	B	1776	BCR	C16-C17-C18	-5.14	119.77	127.20
19	A	1784	CLA	C1D-CHD-C4C	-5.14	114.82	122.60
19	B	1767	CLA	C1D-CHD-C4C	-5.13	114.83	122.60
19	1	1149	CLA	C1D-CHD-C4C	-5.13	114.84	122.60
19	1	1193	CLA	C3D-CAD-CBD	-5.12	100.36	107.60
19	A	1797	CLA	CHD-C4C-C3C	-5.12	117.03	124.94
22	B	1778	BCR	C33-C5-C6	-5.12	119.58	124.61
19	A	1786	CLA	C1D-CHD-C4C	-5.11	114.86	122.60
19	A	1778	CLA	C1D-CHD-C4C	-5.11	114.87	122.60
19	R	1055	CLA	CHD-C4C-C3C	-5.11	117.04	124.94
19	B	1759	CLA	CHD-C4C-C3C	-5.10	117.06	124.94
19	B	1741	CLA	C1D-CHD-C4C	-5.10	114.88	122.60
19	1	1189	CLA	C1D-CHD-C4C	-5.10	114.89	122.60
19	1	1014	CLA	CMD-C2D-C3D	-5.09	115.13	125.09
19	A	1772	CLA	CHD-C4C-C3C	-5.09	117.07	124.94
19	1	1187	CLA	CMD-C2D-C3D	-5.09	115.14	125.09
23	B	1774	PQN	C11-C12-C13	-5.08	118.08	126.70
19	A	1767	CLA	CMD-C2D-C3D	-5.08	115.15	125.09
19	B	1762	CLA	C1D-CHD-C4C	-5.08	114.92	122.60
22	B	1777	BCR	C24-C23-C22	-5.07	118.49	126.22
19	A	1772	CLA	C4B-CHC-C1C	-5.07	118.37	129.26
22	B	1779	BCR	C11-C10-C9	-5.07	119.88	127.20
19	3	1213	CLA	C3A-C4A-CHB	-5.07	118.94	124.06
20	A	7036	LMU	C1B-O1B-C4'	-5.07	104.77	118.01
22	A	1806	BCR	C38-C26-C25	-5.07	119.63	124.61
22	A	1802	BCR	C16-C17-C18	-5.06	119.89	127.20
22	B	1778	BCR	C11-C10-C9	-5.06	119.89	127.20
19	3	1217	CLA	C1D-CHD-C4C	-5.06	113.31	126.32
19	4	4007	CLA	C1D-CHD-C4C	-5.06	114.95	122.60
19	3	3015	CLA	C2A-C1A-CHA	-5.06	113.62	122.58
19	4	1198	CLA	O2A-CGA-O1A	-5.05	110.45	123.49
19	1	1194	CLA	C2A-C1A-CHA	-5.05	113.63	122.58
19	A	1810	CLA	C1D-CHD-C4C	-5.05	114.96	122.60
19	3	1216	CLA	C1D-CHD-C4C	-5.05	113.34	126.32
19	1	1193	CLA	C1D-CHD-C4C	-5.05	114.97	122.60
19	A	1775	CLA	C1D-CHD-C4C	-5.04	113.35	126.32
19	B	1750	CLA	CHD-C4C-C3C	-5.04	117.14	124.94
19	1	1148	CLA	O2D-CGD-O1D	-5.04	113.38	123.79
22	B	1779	BCR	C15-C14-C13	-5.04	119.92	127.20
22	A	1805	BCR	C38-C26-C25	-5.04	119.66	124.61
19	4	1197	CLA	C4B-CHC-C1C	-5.03	118.45	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7030	LMU	O5'-C1'-C2'	-5.03	99.95	110.28
19	1	1191	CLA	C2A-C1A-CHA	-5.03	113.67	122.58
22	B	1778	BCR	C38-C26-C25	-5.03	119.67	124.61
19	G	1099	CLA	C3D-CAD-CBD	-5.02	100.49	107.60
19	3	3015	CLA	C1D-CHD-C4C	-5.02	113.40	126.32
19	A	1795	CLA	C1D-CHD-C4C	-5.02	115.00	122.60
19	R	1054	CLA	C1D-CHD-C4C	-5.02	115.00	122.60
19	1	1148	CLA	CHD-C4C-C3C	-5.02	117.18	124.94
19	A	1797	CLA	OBD-CAD-CBD	-5.02	118.37	125.94
19	B	1736	CLA	O2D-CGD-O1D	-5.01	113.44	123.79
22	A	1804	BCR	C33-C5-C6	-5.01	119.69	124.61
20	A	7026	LMU	O5B-C5B-C4B	-5.01	100.28	109.68
19	4	1201	CLA	C3D-CAD-CBD	-5.00	100.52	107.60
22	A	1802	BCR	C15-C14-C13	-5.00	119.97	127.20
19	B	1765	CLA	C3D-CAD-CBD	-5.00	100.53	107.60
19	4	1198	CLA	CMD-C2D-C3D	-5.00	115.31	125.09
19	B	1770	CLA	O1D-CGD-CBD	-4.99	117.47	124.62
22	A	1804	BCR	C11-C10-C9	-4.99	119.98	127.20
22	B	1779	BCR	C16-C17-C18	-4.99	119.99	127.20
22	B	1778	BCR	C15-C14-C13	-4.98	120.00	127.20
22	B	1775	BCR	C15-C14-C13	-4.98	120.00	127.20
19	4	1210	CLA	C3A-C4A-CHB	-4.98	119.03	124.06
19	B	1766	CLA	CHD-C4C-C3C	-4.97	117.25	124.94
19	3	3011	CLA	C1D-CHD-C4C	-4.97	115.08	122.60
19	A	1764	CLA	C1D-CHD-C4C	-4.97	115.08	122.60
19	B	1764	CLA	C3D-CAD-CBD	-4.97	100.58	107.60
19	1	1187	CLA	CAC-C3C-C2C	-4.96	118.81	127.51
21	B	8061	SUC	C3-C4-C5	-4.96	101.55	110.20
22	A	1804	BCR	C16-C17-C18	-4.96	120.03	127.20
19	B	1769	CLA	C1D-CHD-C4C	-4.96	115.10	122.60
19	1	1188	CLA	CMD-C2D-C3D	-4.95	115.40	125.09
19	A	1787	CLA	C1D-CHD-C4C	-4.95	115.11	122.60
22	B	1778	BCR	C16-C17-C18	-4.95	120.05	127.20
19	2	1215	CLA	C1D-CHD-C4C	-4.95	115.11	122.60
19	4	1205	CLA	C3D-CAD-CBD	-4.94	100.61	107.60
19	A	1793	CLA	CMD-C2D-C3D	-4.94	115.43	125.09
22	B	1775	BCR	C11-C10-C9	-4.93	120.07	127.20
19	A	1772	CLA	O1D-CGD-CBD	-4.93	117.56	124.62
19	F	1157	CLA	C4B-CHC-C1C	-4.93	118.67	129.26
19	F	1157	CLA	CHD-C4C-C3C	-4.93	117.32	124.94
20	A	7030	LMU	C4B-C3B-C2B	-4.92	101.61	110.79
19	3	1215	CLA	C2A-C1A-CHA	-4.92	113.86	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1749	CLA	CHD-C4C-C3C	-4.92	117.34	124.94
19	A	1799	CLA	C1D-CHD-C4C	-4.92	115.16	122.60
22	A	1804	BCR	C15-C14-C13	-4.91	120.10	127.20
19	1	1505	CLA	C3D-CAD-CBD	-4.91	100.66	107.60
19	B	1765	CLA	CHD-C4C-C3C	-4.91	117.35	124.94
19	1	1189	CLA	CMD-C2D-C3D	-4.91	115.49	125.09
19	4	1204	CLA	C3B-C2B-C1B	-4.91	102.00	106.29
19	R	1054	CLA	C3D-CAD-CBD	-4.89	100.68	107.60
20	A	7032	LMU	O1'-C1'-C2'	-4.89	101.86	108.04
19	3	1223	CLA	C2A-C1A-CHA	-4.89	113.92	122.58
19	L	1168	CLA	C4B-CHC-C1C	-4.88	118.77	129.26
19	A	1792	CLA	C1D-CHD-C4C	-4.88	115.21	122.60
19	1	1014	CLA	CHD-C4C-C3C	-4.88	117.40	124.94
19	3	1224	CLA	C3D-CAD-CBD	-4.88	100.70	107.60
22	A	1805	BCR	C33-C5-C6	-4.87	119.82	124.61
22	3	1225	BCR	C38-C26-C25	-4.87	119.82	124.61
19	B	1771	CLA	CMD-C2D-C3D	-4.87	115.56	125.09
19	2	1214	CLA	C1D-CHD-C4C	-4.87	113.80	126.32
19	B	1743	CLA	C1D-CHD-C4C	-4.86	115.24	122.60
19	B	1763	CLA	C3D-CAD-CBD	-4.86	100.73	107.60
22	B	1777	BCR	C16-C17-C18	-4.86	120.18	127.20
20	B	1783	LMU	O2B-C2B-C3B	-4.86	99.40	110.34
22	B	1775	BCR	C33-C5-C6	-4.85	119.84	124.61
19	1	1197	CLA	C3B-C2B-C1B	-4.85	102.04	106.29
19	B	1735	CLA	OBD-CAD-C3D	-4.85	118.45	128.35
22	B	1775	BCR	C16-C17-C18	-4.85	120.19	127.20
19	2	1222	CLA	C1D-CHD-C4C	-4.85	115.26	122.60
19	1	1189	CLA	C3D-CAD-CBD	-4.85	100.74	107.60
19	A	1762	CLA	C1D-CHD-C4C	-4.85	115.27	122.60
22	B	1780	BCR	C16-C17-C18	-4.84	120.20	127.20
19	A	1811	CLA	CHD-C4C-C3C	-4.83	117.48	124.94
19	3	3015	CLA	C3C-C4C-CHD	-4.82	117.39	125.32
19	F	1157	CLA	C4-C3-C2	-4.81	114.06	123.50
19	A	1789	CLA	CMD-C2D-C3D	-4.81	115.68	125.09
19	4	4007	CLA	CMD-C2D-C3D	-4.81	115.68	125.09
19	A	1811	CLA	O1D-CGD-CBD	-4.80	117.74	124.62
19	A	1783	CLA	C4B-CHC-C1C	-4.80	118.95	129.26
19	A	1786	CLA	O2D-CGD-O1D	-4.80	113.88	123.79
19	B	1752	CLA	C3D-CAD-CBD	-4.80	100.82	107.60
19	4	1200	CLA	O2A-CGA-O1A	-4.79	111.12	123.49
19	2	2010	CLA	C1D-CHD-C4C	-4.79	114.00	126.32
20	A	7041	LMU	C4B-C3B-C2B	-4.79	101.85	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	8060	SUC	C2'-O1-C1	-4.79	104.91	117.53
22	A	1803	BCR	C38-C26-C25	-4.78	119.92	124.61
22	B	1782	BCR	C37-C22-C21	-4.78	115.85	122.90
19	4	1198	CLA	CHD-C4C-C3C	-4.77	117.56	124.94
19	B	1773	CLA	C1D-CHD-C4C	-4.77	115.38	122.60
22	A	1805	BCR	C11-C10-C9	-4.77	120.31	127.20
19	3	1212	CLA	O1D-CGD-CBD	-4.76	117.80	124.62
22	A	1805	BCR	C16-C17-C18	-4.76	120.33	127.20
22	B	1776	BCR	C33-C5-C6	-4.76	119.94	124.61
20	A	7040	LMU	O3'-C3'-C2'	-4.76	99.63	110.34
19	A	1771	CLA	CAA-C2A-C3A	-4.75	99.56	113.22
19	1	1197	CLA	C1D-CHD-C4C	-4.75	114.11	126.32
19	3	3001	CLA	C1D-CHD-C4C	-4.74	114.12	126.32
19	B	1772	CLA	C1D-CHD-C4C	-4.74	115.42	122.60
21	B	8052	SUC	C3-C4-C5	-4.74	101.93	110.20
19	3	1223	CLA	C2C-C1C-CHC	-4.74	116.72	125.15
19	2	1219	CLA	C1D-CHD-C4C	-4.74	114.12	126.32
19	1	1196	CLA	C3D-CAD-CBD	-4.74	100.90	107.60
22	A	1805	BCR	C15-C14-C13	-4.73	120.36	127.20
19	B	1745	CLA	CMD-C2D-C3D	-4.73	115.84	125.09
22	L	1169	BCR	C3-C4-C5	-4.73	106.36	113.87
22	B	1781	BCR	C33-C5-C6	-4.73	119.96	124.61
19	1	1198	CLA	C2D-C3D-C4D	-4.72	102.14	106.30
19	A	1771	CLA	C3D-CAD-CBD	-4.72	100.92	107.60
20	A	7005	LMU	O3B-C3B-C2B	-4.72	99.71	110.34
19	B	1745	CLA	C3D-CAD-CBD	-4.72	100.92	107.60
19	A	1788	CLA	C3D-CAD-CBD	-4.72	100.93	107.60
19	B	1764	CLA	CHD-C4C-C3C	-4.71	117.66	124.94
19	3	1221	CLA	C2A-C1A-CHA	-4.71	114.24	122.58
19	A	1759	CLA	CHD-C4C-C3C	-4.71	117.67	124.94
19	3	1221	CLA	C3B-C2B-C1B	-4.71	102.17	106.29
19	B	1735	CLA	CHD-C4C-C3C	-4.71	117.67	124.94
22	A	1803	BCR	C33-C5-C6	-4.70	119.99	124.61
19	B	1754	CLA	C2A-C1A-CHA	-4.70	115.23	123.89
22	L	1170	BCR	C16-C17-C18	-4.70	120.41	127.20
22	3	1225	BCR	C7-C8-C9	-4.70	119.06	126.22
19	3	3015	CLA	C3B-C2B-C1B	-4.69	102.18	106.29
19	2	1217	CLA	CHD-C4C-C3C	-4.69	117.70	124.94
19	B	1744	CLA	CGD-CBD-CAD	-4.68	94.75	110.62
19	B	1766	CLA	O1D-CGD-CBD	-4.68	117.91	124.62
22	B	1775	BCR	C38-C26-C25	-4.68	120.01	124.61
19	A	1773	CLA	CHD-C4C-C3C	-4.68	117.71	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1218	CLA	C3D-CAD-CBD	-4.67	101.00	107.60
22	B	1779	BCR	C33-C5-C6	-4.67	120.02	124.61
19	1	1192	CLA	C3D-CAD-CBD	-4.67	101.00	107.60
19	B	1747	CLA	C3D-CAD-CBD	-4.67	101.00	107.60
22	A	1806	BCR	C11-C10-C9	-4.66	120.46	127.20
19	B	1740	CLA	C3D-CAD-CBD	-4.66	101.00	107.60
19	1	1010	CLA	C1D-CHD-C4C	-4.66	114.33	126.32
19	A	1767	CLA	C3D-CAD-CBD	-4.65	101.02	107.60
19	B	1769	CLA	O2D-CGD-O1D	-4.65	114.19	123.79
19	B	1755	CLA	OBD-CAD-CBD	-4.64	118.93	125.94
22	L	1169	BCR	C7-C8-C9	-4.64	119.14	126.22
19	1	1505	CLA	CMD-C2D-C3D	-4.63	116.03	125.09
19	A	1798	CLA	C3D-CAD-CBD	-4.63	101.05	107.60
22	A	1807	BCR	C38-C26-C25	-4.62	120.06	124.61
19	3	1213	CLA	C3C-C4C-CHD	-4.62	117.72	125.32
19	3	1221	CLA	C2C-C1C-CHC	-4.62	116.94	125.15
19	L	1166	CLA	CHD-C4C-C3C	-4.62	117.80	124.94
19	A	1773	CLA	C3D-CAD-CBD	-4.62	101.07	107.60
20	A	1809	LMU	C3B-C4B-C5B	-4.61	102.16	110.20
19	4	1201	CLA	CHD-C4C-C3C	-4.61	117.82	124.94
21	B	8054	SUC	O1'-C1'-C2'	-4.61	97.18	111.91
20	K	1086	LMU	O5B-C5B-C4B	-4.61	101.04	109.68
19	3	1218	CLA	C1D-CHD-C4C	-4.60	115.64	122.60
19	A	1812	CLA	C1D-CHD-C4C	-4.60	115.64	122.60
19	B	1766	CLA	C3D-CAD-CBD	-4.60	101.10	107.60
19	B	1754	CLA	O2D-CGD-O1D	-4.60	114.30	123.79
19	4	1201	CLA	O2A-CGA-O1A	-4.60	111.63	123.49
19	A	1797	CLA	CMC-C2C-C1C	-4.59	117.91	125.02
19	4	1208	CLA	C2A-C1A-CHA	-4.59	114.45	122.58
19	1	1198	CLA	C1D-CHD-C4C	-4.59	114.52	126.32
19	A	1799	CLA	CHD-C4C-C3C	-4.59	117.85	124.94
19	1	1014	CLA	C6-C5-C3	-4.58	102.43	112.48
19	R	1055	CLA	C3D-CAD-CBD	-4.58	101.12	107.60
19	A	1770	CLA	C1D-CHD-C4C	-4.58	115.67	122.60
19	4	1201	CLA	CBC-CAC-C3C	-4.57	98.43	112.39
19	B	1751	CLA	CHD-C4C-C3C	-4.57	117.87	124.94
19	A	1759	CLA	C3D-CAD-CBD	-4.57	101.13	107.60
19	A	1798	CLA	CMD-C2D-C3D	-4.57	116.15	125.09
19	3	3015	CLA	C2D-C3D-C4D	-4.57	102.28	106.30
19	2	1221	CLA	C3B-C2B-C1B	-4.57	102.29	106.29
19	4	1203	CLA	C2A-C1A-CHA	-4.57	114.49	122.58
19	A	1766	CLA	C1D-CHD-C4C	-4.56	115.69	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1748	CLA	C1D-CHD-C4C	-4.56	115.70	122.60
19	B	1770	CLA	CHD-C4C-C3C	-4.56	117.90	124.94
19	A	1775	CLA	C3C-C4C-CHD	-4.55	117.83	125.32
19	2	1221	CLA	C1D-CHD-C4C	-4.55	114.61	126.32
20	A	7048	LMU	C3'-C4'-C5'	-4.55	100.55	110.84
20	A	7017	LMU	O5B-C5B-C4B	-4.55	101.14	109.68
19	2	1219	CLA	C3C-C4C-CHD	-4.55	117.84	125.32
22	B	1776	BCR	C38-C26-C25	-4.55	120.14	124.61
19	A	1771	CLA	CMA-C3A-C2A	-4.55	94.24	114.35
19	1	1146	CLA	C1-C2-C3	-4.54	119.26	126.71
19	3	1213	CLA	C2D-C3D-C4D	-4.54	102.30	106.30
19	2	1218	CLA	C1D-CHD-C4C	-4.54	115.72	122.60
19	4	1205	CLA	C4-C3-C2	-4.54	114.58	123.50
20	A	7027	LMU	C1B-O1B-C4'	-4.54	106.14	118.01
19	3	3008	CLA	O1D-CGD-CBD	-4.54	118.12	124.62
19	B	1768	CLA	CMD-C2D-C3D	-4.53	116.22	125.09
20	A	7038	LMU	C6B-C5B-C4B	-4.53	101.83	113.02
19	3	1213	CLA	C1D-CHD-C4C	-4.53	114.67	126.32
19	A	1783	CLA	C3D-CAD-CBD	-4.53	101.20	107.60
20	1	1200	LMU	O3'-C3'-C4'	-4.52	99.17	109.87
19	2	2010	CLA	C3C-C4C-CHD	-4.52	117.88	125.32
20	A	7042	LMU	C1'-O5'-C5'	-4.52	104.97	113.75
19	B	1759	CLA	C3D-CAD-CBD	-4.52	101.21	107.60
19	B	1736	CLA	CMD-C2D-C3D	-4.52	116.25	125.09
19	4	1208	CLA	C1D-CHD-C4C	-4.52	114.70	126.32
19	B	1752	CLA	O1D-CGD-CBD	-4.51	118.16	124.62
19	J	1043	CLA	CHD-C4C-C3C	-4.51	117.97	124.94
19	A	1795	CLA	CAA-CBA-CGA	-4.50	100.14	113.32
19	B	1744	CLA	C3D-CAD-CBD	-4.50	101.24	107.60
19	3	1219	CLA	CHD-C4C-C3C	-4.48	118.02	124.94
19	1	1010	CLA	C3B-C2B-C1B	-4.48	102.37	106.29
19	A	1797	CLA	C6-C5-C3	-4.47	102.67	112.48
20	B	1783	LMU	C3B-C4B-C5B	-4.47	102.40	110.20
22	I	1032	BCR	C27-C26-C25	-4.47	117.09	122.78
20	A	7036	LMU	C6B-C5B-C4B	-4.45	102.03	113.02
19	A	1784	CLA	O1D-CGD-CBD	-4.45	118.25	124.62
19	B	1773	CLA	CAA-C2A-C3A	-4.44	105.57	116.20
22	B	1781	BCR	C38-C26-C25	-4.43	120.25	124.61
22	A	1802	BCR	C24-C23-C22	-4.43	119.46	126.22
19	3	1224	CLA	CBC-CAC-C3C	-4.43	98.87	112.39
19	4	1203	CLA	C2D-C3D-C4D	-4.43	102.40	106.30
19	B	1763	CLA	O2D-CGD-O1D	-4.43	114.65	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	8061	SUC	C4-C3-C2	-4.42	102.54	110.79
22	A	1807	BCR	C33-C5-C6	-4.42	120.26	124.61
20	A	7035	LMU	C3'-C4'-C5'	-4.42	100.84	110.84
19	B	1735	CLA	C1D-CHD-C4C	-4.42	115.91	122.60
19	3	1212	CLA	C3D-CAD-CBD	-4.42	101.35	107.60
19	R	1054	CLA	CMD-C2D-C3D	-4.42	116.45	125.09
21	B	8062	SUC	O2-C2-C3	-4.41	100.40	110.34
19	B	1760	CLA	CMD-C2D-C3D	-4.41	116.47	125.09
19	3	1215	CLA	C3C-C4C-CHD	-4.40	118.08	125.32
19	4	1196	CLA	C3D-CAD-CBD	-4.40	101.37	107.60
19	A	1765	CLA	CHC-C1C-C2C	-4.40	114.77	126.35
19	B	1742	CLA	CMD-C2D-C3D	-4.40	116.48	125.09
19	B	1757	CLA	CHD-C4C-C3C	-4.40	118.14	124.94
19	1	1309	CLA	C2A-C1A-CHA	-4.39	114.80	122.58
19	B	1747	CLA	CHD-C4C-C3C	-4.39	118.15	124.94
19	A	1793	CLA	O2D-CGD-O1D	-4.39	114.72	123.79
19	3	1212	CLA	CHD-C4C-C3C	-4.39	118.15	124.94
19	1	1191	CLA	C3C-C4C-CHD	-4.39	118.09	125.32
19	B	1756	CLA	CHD-C4C-C3C	-4.39	118.15	124.94
19	2	1216	CLA	C3A-C4A-CHB	-4.39	119.63	124.06
20	A	7032	LMU	O2B-C2B-C3B	-4.38	100.47	110.34
19	4	1201	CLA	O1D-CGD-CBD	-4.38	118.34	124.62
19	A	1792	CLA	CMD-C2D-C3D	-4.38	116.51	125.09
19	1	1303	CLA	C2A-C1A-CHA	-4.38	114.82	122.58
19	1	1190	CLA	CHD-C4C-C3C	-4.38	118.17	124.94
19	4	4014	CLA	CHD-C4C-C3C	-4.38	118.17	124.94
19	2	1223	CLA	CHD-C4C-C3C	-4.38	118.18	124.94
19	2	1218	CLA	C6-C5-C3	-4.37	102.88	112.48
19	2	1223	CLA	O1D-CGD-CBD	-4.37	118.35	124.62
22	A	1807	BCR	C24-C23-C22	-4.37	119.55	126.22
19	1	1142	CLA	C3D-CAD-CBD	-4.37	101.41	107.60
19	A	1763	CLA	O1D-CGD-CBD	-4.37	118.35	124.62
22	A	1803	BCR	C7-C8-C9	-4.37	119.55	126.22
19	A	1773	CLA	O1D-CGD-CBD	-4.37	118.36	124.62
19	B	1740	CLA	CHD-C4C-C3C	-4.37	118.19	124.94
19	4	1207	CLA	C3B-C2B-C1B	-4.37	102.47	106.29
19	A	1763	CLA	CAA-C2A-C3A	-4.37	100.66	113.22
19	B	1754	CLA	CAA-C2A-C1A	-4.36	97.10	112.47
22	B	1779	BCR	C38-C26-C25	-4.36	120.33	124.61
19	A	1770	CLA	O1D-CGD-CBD	-4.35	118.38	124.62
20	A	7048	LMU	C4B-C3B-C2B	-4.35	102.67	110.79
19	2	1212	CLA	CHD-C4C-C3C	-4.35	118.22	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1215	CLA	C2C-C1C-CHC	-4.35	117.42	125.15
19	B	1746	CLA	CHD-C4C-C3C	-4.34	118.23	124.94
19	3	1214	CLA	CHD-C4C-C3C	-4.34	117.56	124.83
22	A	1807	BCR	C7-C8-C9	-4.34	119.60	126.22
19	4	1199	CLA	C3D-CAD-CBD	-4.34	101.46	107.60
19	1	1308	CLA	C3D-CAD-CBD	-4.34	101.47	107.60
19	4	1210	CLA	C1D-CHD-C4C	-4.34	115.17	126.32
22	B	1777	BCR	C30-C25-C26	-4.33	116.30	122.66
22	A	1803	BCR	C24-C23-C22	-4.33	119.61	126.22
22	B	1781	BCR	C7-C8-C9	-4.33	119.62	126.22
22	B	1777	BCR	C37-C22-C21	-4.33	116.51	122.90
19	B	1754	CLA	C3D-CAD-CBD	-4.32	101.48	107.60
19	1	1149	CLA	O2D-CGD-O1D	-4.32	114.87	123.79
19	1	1142	CLA	CHD-C4C-C3C	-4.31	118.27	124.94
19	B	1786	CLA	C3D-CAD-CBD	-4.31	101.50	107.60
20	A	7022	LMU	O2'-C2'-C1'	-4.31	100.57	110.02
19	A	1770	CLA	C3D-CAD-CBD	-4.31	101.50	107.60
19	1	1193	CLA	CHD-C4C-C3C	-4.31	118.28	124.94
19	B	1760	CLA	CHD-C4C-C3C	-4.31	118.28	124.94
19	2	1213	CLA	C4-C3-C2	-4.31	115.04	123.50
19	4	1204	CLA	C3C-C4C-CHD	-4.30	118.24	125.32
20	A	7033	LMU	O1B-C4'-C5'	-4.30	98.02	109.32
19	A	1769	CLA	C3D-CAD-CBD	-4.30	101.52	107.60
19	A	1774	CLA	C3D-CAD-CBD	-4.29	101.53	107.60
22	A	1802	BCR	C38-C26-C25	-4.29	120.39	124.61
22	B	1777	BCR	C34-C9-C10	-4.29	116.57	122.90
19	F	1156	CLA	CHD-C4C-C3C	-4.29	118.32	124.94
19	2	1213	CLA	C3D-CAD-CBD	-4.29	101.54	107.60
20	1	1200	LMU	C1B-O5B-C5B	-4.28	105.43	113.75
19	1	1308	CLA	CHD-C4C-C3C	-4.28	118.33	124.94
19	3	1215	CLA	C1D-CHD-C4C	-4.28	115.32	126.32
22	B	1776	BCR	C24-C23-C22	-4.28	119.70	126.22
22	B	1782	BCR	C37-C22-C23	-4.27	110.98	118.10
19	4	1196	CLA	CHD-C4C-C3C	-4.27	118.34	124.94
19	A	1793	CLA	C3D-CAD-CBD	-4.27	101.56	107.60
19	B	1768	CLA	C3D-CAD-CBD	-4.27	101.56	107.60
19	I	1031	CLA	CHD-C4C-C3C	-4.27	118.34	124.94
22	B	1780	BCR	C27-C26-C25	-4.27	117.34	122.78
19	2	1218	CLA	O2D-CGD-O1D	-4.26	114.99	123.79
20	A	7040	LMU	O2'-C2'-C3'	-4.26	100.75	110.34
19	B	1786	CLA	C1D-CHD-C4C	-4.26	116.16	122.60
19	B	1763	CLA	CHD-C4C-C3C	-4.26	118.36	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1784	CLA	C3D-CAD-CBD	-4.26	101.58	107.60
19	A	1764	CLA	CHD-C4C-C3C	-4.25	118.37	124.94
19	A	1774	CLA	CHD-C4C-C3C	-4.25	118.37	124.94
19	1	1303	CLA	C3C-C4C-CHD	-4.25	118.33	125.32
19	3	1220	CLA	C1D-CHD-C4C	-4.25	115.39	126.32
19	B	1742	CLA	C3D-CAD-CBD	-4.25	101.59	107.60
19	2	1217	CLA	C3D-CAD-CBD	-4.25	101.59	107.60
22	3	1225	BCR	C16-C15-C14	-4.24	114.01	123.39
19	B	1756	CLA	C3D-CAD-CBD	-4.24	101.60	107.60
20	A	7017	LMU	C1B-O5B-C5B	-4.24	105.52	113.75
20	N	1086	LMU	C2'-C3'-C4'	-4.24	100.30	109.60
19	B	1737	CLA	CMD-C2D-C3D	-4.23	116.81	125.09
19	B	1750	CLA	C3D-CAD-CBD	-4.23	101.61	107.60
19	2	1219	CLA	C2A-C1A-CHA	-4.23	115.09	122.58
20	A	7038	LMU	C2'-C3'-C4'	-4.23	100.31	109.60
22	B	1782	BCR	C24-C25-C26	-4.22	111.70	121.37
22	B	1780	BCR	C8-C7-C6	-4.22	114.63	127.32
19	1	1145	CLA	CMD-C2D-C3D	-4.22	116.83	125.09
19	1	1193	CLA	CMD-C2D-C3D	-4.22	116.83	125.09
19	3	3001	CLA	C2A-C1A-CHA	-4.22	115.11	122.58
19	3	1216	CLA	C3C-C4C-CHD	-4.22	118.38	125.32
19	B	1787	CLA	CHD-C4C-C3C	-4.22	118.42	124.94
22	A	1802	BCR	C7-C8-C9	-4.22	119.79	126.22
19	F	1155	CLA	CAB-C3B-C4B	-4.22	121.39	128.36
19	1	1189	CLA	CHD-C4C-C3C	-4.21	118.43	124.94
19	A	1794	CLA	O2D-CGD-O1D	-4.21	115.09	123.79
19	A	1799	CLA	C6-C5-C3	-4.21	103.24	112.48
19	1	1303	CLA	C1D-CHD-C4C	-4.21	115.49	126.32
22	B	1776	BCR	C7-C8-C9	-4.20	119.81	126.22
19	3	1217	CLA	C3C-C4C-CHD	-4.20	118.41	125.32
19	4	1197	CLA	CHD-C4C-C3C	-4.20	117.80	124.83
19	1	1307	CLA	C1D-CHD-C4C	-4.20	115.53	126.32
22	B	1781	BCR	C24-C23-C22	-4.19	119.82	126.22
19	2	1213	CLA	CMD-C2D-C3D	-4.19	116.89	125.09
21	2	1225	SUC	O4'-C4'-C3'	-4.19	98.69	112.01
19	A	1765	CLA	O2D-CGD-O1D	-4.18	115.16	123.79
22	A	1802	BCR	C33-C5-C6	-4.18	120.50	124.61
20	A	7028	LMU	O5'-C1'-C2'	-4.18	101.70	110.28
19	2	1214	CLA	C3C-C4C-CHD	-4.18	118.44	125.32
19	B	1745	CLA	C1D-CHD-C4C	-4.18	116.28	122.60
19	A	1797	CLA	CHC-C1C-C2C	-4.18	115.36	126.35
19	1	1148	CLA	C4B-CHC-C1C	-4.18	120.29	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1043	CLA	C3D-CAD-CBD	-4.17	101.70	107.60
19	B	1754	CLA	C1D-CHD-C4C	-4.17	116.29	122.60
19	2	1222	CLA	C3D-CAD-CBD	-4.17	101.70	107.60
19	A	1777	CLA	CHD-C4C-C3C	-4.17	118.50	124.94
22	A	1804	BCR	C7-C8-C9	-4.17	119.86	126.22
20	A	7023	LMU	O3'-C3'-C2'	-4.17	100.95	110.34
19	1	1189	CLA	CGD-CBD-CAD	-4.17	96.50	110.62
19	2	1216	CLA	C3C-C4C-CHD	-4.16	118.47	125.32
19	B	1743	CLA	C4-C3-C2	-4.16	115.33	123.50
22	B	1778	BCR	C7-C8-C9	-4.16	119.87	126.22
20	A	7036	LMU	O3B-C3B-C4B	-4.16	100.98	110.34
22	B	1782	BCR	C30-C25-C26	-4.16	116.56	122.66
19	L	1166	CLA	C3D-CAD-CBD	-4.15	101.72	107.60
19	F	1155	CLA	CMD-C2D-C3D	-4.15	116.97	125.09
19	1	1190	CLA	O2D-CGD-O1D	-4.15	115.22	123.79
19	A	1811	CLA	C3D-CAD-CBD	-4.15	101.73	107.60
19	B	1767	CLA	CHD-C4C-C3C	-4.15	118.53	124.94
19	2	1216	CLA	C2C-C1C-CHC	-4.15	117.78	125.15
19	B	1771	CLA	C3D-CAD-CBD	-4.14	101.75	107.60
19	A	1782	CLA	C3D-CAD-CBD	-4.14	101.75	107.60
19	A	1760	CLA	CMD-C2D-C3D	-4.14	117.00	125.09
19	2	1214	CLA	C2C-C1C-CHC	-4.13	117.80	125.15
19	I	1031	CLA	O1D-CGD-CBD	-4.13	118.70	124.62
19	4	1207	CLA	C2A-C1A-CHA	-4.13	115.26	122.58
19	2	1222	CLA	O2D-CGD-O1D	-4.13	115.26	123.79
19	4	1211	CLA	CGD-CBD-CAD	-4.13	96.63	110.62
19	B	1736	CLA	C3D-CAD-CBD	-4.13	101.76	107.60
19	3	1219	CLA	C3D-CAD-CBD	-4.13	101.76	107.60
19	A	1790	CLA	C3D-CAD-CBD	-4.13	101.76	107.60
19	B	1742	CLA	O1D-CGD-CBD	-4.13	118.70	124.62
19	A	1798	CLA	O1D-CGD-CBD	-4.13	118.70	124.62
19	2	1213	CLA	CHD-C4C-C3C	-4.13	118.56	124.94
21	B	8056	SUC	O5-C5-C4	-4.12	101.95	109.68
19	A	1760	CLA	CHD-C4C-C3C	-4.11	118.58	124.94
20	A	7042	LMU	C4B-C3B-C2B	-4.11	103.12	110.79
20	A	7032	LMU	O5B-C5B-C4B	-4.11	101.97	109.68
21	B	8052	SUC	C6-C5-C4	-4.11	102.88	113.02
19	B	1753	CLA	C3D-CAD-CBD	-4.11	101.79	107.60
19	A	1766	CLA	CMD-C2D-C3D	-4.11	117.05	125.09
20	A	7022	LMU	C6B-C5B-C4B	-4.11	102.89	113.02
19	A	1766	CLA	O1D-CGD-CBD	-4.11	118.74	124.62
22	A	1805	BCR	C24-C23-C22	-4.10	119.96	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1788	CLA	CHD-C4C-C3C	-4.10	118.60	124.94
20	A	7048	LMU	C3B-C4B-C5B	-4.10	103.05	110.20
19	J	1044	CLA	C3D-CAD-CBD	-4.10	101.81	107.60
19	A	1812	CLA	C3D-CAD-CBD	-4.10	101.81	107.60
19	4	1207	CLA	C3C-C4C-CHD	-4.10	118.58	125.32
19	B	1771	CLA	C1D-CHD-C4C	-4.10	116.40	122.60
19	A	1763	CLA	CAA-C2A-C1A	-4.10	98.03	112.47
19	3	1220	CLA	C2A-C1A-CHA	-4.10	115.33	122.58
19	B	1773	CLA	CMA-C3A-C2A	-4.09	106.39	116.20
19	A	1764	CLA	CAA-C2A-C1A	-4.09	98.06	112.47
19	B	1760	CLA	O1D-CGD-CBD	-4.08	118.77	124.62
19	L	1166	CLA	O1D-CGD-CBD	-4.08	118.78	124.62
19	A	1769	CLA	CHD-C4C-C3C	-4.08	118.64	124.94
19	A	1764	CLA	C6-C5-C3	-4.08	103.54	112.48
19	B	1743	CLA	C3D-CAD-CBD	-4.07	101.84	107.60
19	4	1204	CLA	C2A-C1A-CHA	-4.07	115.37	122.58
22	B	1778	BCR	C24-C23-C22	-4.07	120.01	126.22
19	B	1769	CLA	C3D-CAD-CBD	-4.07	101.84	107.60
19	1	1148	CLA	C3D-CAD-CBD	-4.07	101.84	107.60
19	1	1189	CLA	O2D-CGD-O1D	-4.07	115.39	123.79
19	3	3015	CLA	C2C-C1C-CHC	-4.07	117.93	125.15
19	1	1146	CLA	O2D-CGD-O1D	-4.07	115.40	123.79
22	L	1170	BCR	C37-C22-C21	-4.06	116.90	122.90
19	1	1195	CLA	CHD-C4C-C3C	-4.06	118.02	124.83
22	B	1775	BCR	C7-C8-C9	-4.06	120.02	126.22
22	A	1806	BCR	C24-C23-C22	-4.06	120.03	126.22
19	A	1767	CLA	CAA-C2A-C3A	-4.05	101.56	113.22
22	B	1779	BCR	C7-C8-C9	-4.05	120.04	126.22
19	A	1764	CLA	O2D-CGD-O1D	-4.05	115.43	123.79
19	K	1085	CLA	CHD-C4C-C3C	-4.05	118.68	124.94
19	B	1761	CLA	C1D-CHD-C4C	-4.05	116.48	122.60
19	3	3001	CLA	C2D-C3D-C4D	-4.05	102.74	106.30
22	B	1782	BCR	C38-C26-C25	-4.04	120.64	124.61
19	A	1781	CLA	CHD-C4C-C3C	-4.04	118.70	124.94
19	B	1745	CLA	O1D-CGD-CBD	-4.04	118.83	124.62
19	A	1776	CLA	C3D-CAD-CBD	-4.04	101.89	107.60
20	A	7016	LMU	C1-O1'-C1'	-4.03	106.89	113.94
19	A	1777	CLA	C3D-CAD-CBD	-4.03	101.90	107.60
19	1	1010	CLA	C3C-C4C-CHD	-4.03	118.69	125.32
19	B	1772	CLA	CHD-C4C-C3C	-4.03	118.72	124.94
19	A	1812	CLA	CMD-C2D-C3D	-4.03	117.21	125.09
19	2	1220	CLA	CHD-C4C-C3C	-4.02	118.09	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1167	CLA	C3D-CAD-CBD	-4.02	101.91	107.60
20	A	7036	LMU	C3'-C4'-C5'	-4.02	101.74	110.84
20	A	7032	LMU	C1'-C2'-C3'	-4.02	102.05	109.97
20	A	7022	LMU	O2'-C2'-C3'	-4.02	101.28	110.34
20	A	7037	LMU	O5'-C1'-C2'	-4.01	102.04	110.28
19	3	1216	CLA	C2C-C1C-CHC	-4.01	118.03	125.15
21	B	8059	SUC	C4-C3-C2	-4.00	103.32	110.79
19	4	1206	CLA	CHD-C4C-C3C	-4.00	118.75	124.94
19	1	1187	CLA	CBC-CAC-C3C	-4.00	100.18	112.39
19	1	1145	CLA	O1D-CGD-CBD	-4.00	118.89	124.62
19	B	1736	CLA	CHD-C4C-C3C	-4.00	118.76	124.94
20	A	7032	LMU	C4B-C3B-C2B	-3.99	103.34	110.79
20	A	7024	LMU	C3B-C4B-C5B	-3.99	103.23	110.20
19	A	1765	CLA	C3D-CAD-CBD	-3.99	101.96	107.60
21	B	8054	SUC	C2'-O1-C1	-3.99	107.02	117.53
19	A	1759	CLA	O2D-CGD-O1D	-3.99	115.56	123.79
22	A	1805	BCR	C7-C8-C9	-3.98	120.14	126.22
19	2	1219	CLA	C2D-C3D-C4D	-3.98	102.80	106.30
19	B	1744	CLA	CAA-CBA-CGA	-3.98	101.66	113.32
19	1	1309	CLA	C2D-C3D-C4D	-3.98	102.80	106.30
20	A	7033	LMU	O2B-C2B-C1B	-3.98	101.30	110.02
19	A	1790	CLA	CMD-C2D-C3D	-3.98	117.31	125.09
19	B	1760	CLA	C3D-CAD-CBD	-3.97	101.98	107.60
20	A	7043	LMU	O3'-C3'-C4'	-3.97	100.47	109.87
19	4	1210	CLA	C3C-C4C-CHD	-3.97	118.79	125.32
19	A	1781	CLA	C3D-CAD-CBD	-3.96	101.99	107.60
20	K	1086	LMU	O3'-C3'-C2'	-3.96	101.41	110.34
19	B	1787	CLA	C5-C3-C2	-3.96	113.54	121.05
20	N	1086	LMU	C4B-C3B-C2B	-3.96	103.41	110.79
19	B	1750	CLA	O1D-CGD-CBD	-3.96	118.95	124.62
19	B	1758	CLA	CHD-C4C-C3C	-3.96	118.83	124.94
20	A	7041	LMU	O6B-C6B-C5B	-3.96	98.26	111.33
19	A	1762	CLA	CHD-C4C-C3C	-3.95	118.83	124.94
19	B	1768	CLA	CHD-C4C-C3C	-3.95	118.83	124.94
19	B	1771	CLA	CHD-C4C-C3C	-3.95	118.83	124.94
19	B	1759	CLA	O1D-CGD-CBD	-3.95	118.96	124.62
21	2	1225	SUC	O2-C2-C1	-3.95	101.37	110.02
19	A	1795	CLA	CHD-C4C-C3C	-3.95	118.84	124.94
19	A	1782	CLA	CHD-C4C-C3C	-3.94	118.85	124.94
19	A	1789	CLA	CHC-C1C-C2C	-3.94	115.99	126.35
22	B	1782	BCR	C27-C26-C25	-3.94	117.76	122.78
19	3	3001	CLA	C3B-C2B-C1B	-3.93	102.85	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1217	CLA	C2C-C1C-CHC	-3.93	118.16	125.15
19	A	1765	CLA	CMD-C2D-C3D	-3.93	117.39	125.09
19	4	1201	CLA	CMD-C2D-C3D	-3.93	117.40	125.09
19	K	1085	CLA	C3D-CAD-CBD	-3.93	102.04	107.60
19	A	1793	CLA	O1D-CGD-CBD	-3.93	118.99	124.62
19	R	1055	CLA	C6-C5-C3	-3.93	103.86	112.48
19	L	1168	CLA	O2D-CGD-O1D	-3.93	115.68	123.79
19	2	1216	CLA	C1D-CHD-C4C	-3.92	116.23	126.32
19	1	1188	CLA	O2A-CGA-O1A	-3.92	113.37	123.49
21	B	8059	SUC	O1'-C1'-C2'	-3.92	99.37	111.91
19	3	1223	CLA	C3C-C2C-C1C	-3.92	102.82	107.23
20	A	7036	LMU	C4B-C3B-C2B	-3.92	103.48	110.79
19	1	1197	CLA	C2A-C1A-CHA	-3.92	115.64	122.58
20	A	7013	LMU	C4B-C3B-C2B	-3.92	103.48	110.79
22	3	1225	BCR	C11-C12-C13	-3.91	114.80	126.32
19	A	1790	CLA	C1-C2-C3	-3.91	120.29	126.71
19	B	1755	CLA	O2D-CGD-O1D	-3.91	115.72	123.79
19	A	1800	CLA	C3D-CAD-CBD	-3.91	102.07	107.60
19	A	1762	CLA	C3D-CAD-CBD	-3.90	102.08	107.60
19	A	1783	CLA	CMD-C2D-C3D	-3.90	117.45	125.09
19	1	1241	CLA	O1D-CGD-CBD	-3.90	119.03	124.62
19	A	1768	CLA	CHD-C4C-C3C	-3.90	118.91	124.94
19	A	1767	CLA	C11-C12-C13	-3.90	102.56	115.49
19	B	1759	CLA	O2D-CGD-O1D	-3.90	115.74	123.79
19	4	1198	CLA	C11-C10-C8	-3.90	102.56	115.49
21	2	1225	SUC	C1-O5-C5	-3.90	106.99	113.64
19	B	1761	CLA	C3D-CAD-CBD	-3.90	102.09	107.60
19	2	1221	CLA	C3C-C4C-CHD	-3.89	118.91	125.32
19	2	1222	CLA	CMD-C2D-C3D	-3.89	117.47	125.09
19	B	1753	CLA	CMD-C2D-C3D	-3.89	117.48	125.09
19	4	1208	CLA	C3C-C4C-CHD	-3.89	118.92	125.32
19	4	1199	CLA	O2D-CGD-O1D	-3.88	115.77	123.79
19	B	1735	CLA	C3D-CAD-CBD	-3.88	102.11	107.60
19	1	1010	CLA	C2D-C3D-C4D	-3.88	102.89	106.30
22	B	1780	BCR	C40-C30-C25	-3.88	104.22	110.30
19	4	1206	CLA	O1D-CGD-CBD	-3.87	119.07	124.62
19	1	1196	CLA	CAA-C2A-C1A	-3.87	98.83	112.47
22	A	1806	BCR	C7-C8-C9	-3.87	120.32	126.22
19	1	1198	CLA	C3C-C4C-CHD	-3.86	118.96	125.32
19	1	1188	CLA	CBA-CAA-C2A	-3.86	102.84	113.73
19	1	1505	CLA	CHD-C4C-C3C	-3.86	118.98	124.94
19	A	1780	CLA	OBD-CAD-CBD	-3.86	120.12	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7005	LMU	C3'-C4'-C5'	-3.86	102.12	110.84
19	3	1216	CLA	C2A-C1A-CHA	-3.85	115.76	122.58
19	A	1791	CLA	CMD-C2D-C3D	-3.85	117.56	125.09
19	4	1202	CLA	CHD-C4C-C3C	-3.85	118.38	124.83
19	F	1156	CLA	C3D-CAD-CBD	-3.85	102.16	107.60
19	A	1761	CLA	CHD-C4C-C3C	-3.85	119.00	124.94
19	2	1214	CLA	C2A-C1A-CHA	-3.84	115.77	122.58
19	1	1187	CLA	CGD-CBD-CAD	-3.84	97.60	110.62
20	N	1086	LMU	C3'-C4'-C5'	-3.84	102.15	110.84
19	2	1212	CLA	C3D-CAD-CBD	-3.84	102.17	107.60
19	3	1217	CLA	C2A-C1A-CHA	-3.84	115.78	122.58
20	A	7042	LMU	C1B-O1B-C4'	-3.84	107.98	118.01
19	1	1187	CLA	CAA-C2A-C3A	-3.84	102.18	113.22
19	4	4014	CLA	C3D-CAD-CBD	-3.84	102.17	107.60
19	A	1791	CLA	C3D-CAD-CBD	-3.83	102.18	107.60
20	A	7020	LMU	C3'-C4'-C5'	-3.83	102.17	110.84
20	N	1086	LMU	O2B-C2B-C3B	-3.83	101.72	110.34
19	2	2010	CLA	C2A-C1A-CHA	-3.83	115.80	122.58
22	B	1779	BCR	C24-C23-C22	-3.83	120.39	126.22
19	A	1760	CLA	OBD-CAD-C3D	-3.82	120.55	128.35
19	A	1800	CLA	OBD-CAD-CBD	-3.81	120.19	125.94
19	B	1786	CLA	CBA-CAA-C2A	-3.81	103.00	113.73
19	4	1205	CLA	O1D-CGD-CBD	-3.81	119.17	124.62
19	F	1157	CLA	O2D-CGD-O1D	-3.81	115.93	123.79
20	A	7043	LMU	O5'-C5'-C4'	-3.80	101.71	109.75
19	A	1781	CLA	CMD-C2D-C3D	-3.80	117.65	125.09
19	A	1782	CLA	CMD-C2D-C3D	-3.80	117.66	125.09
19	B	1746	CLA	C4-C3-C2	-3.80	116.05	123.50
22	L	1169	BCR	C11-C10-C9	-3.80	121.72	127.20
20	A	7037	LMU	C1B-O1B-C4'	-3.79	108.09	118.01
19	3	1223	CLA	C1D-CHD-C4C	-3.79	116.56	126.32
19	B	1737	CLA	C3D-CAD-CBD	-3.79	102.24	107.60
19	4	1200	CLA	O2D-CGD-O1D	-3.79	115.96	123.79
19	B	1767	CLA	C3D-CAD-CBD	-3.79	102.24	107.60
19	3	1215	CLA	C3B-C2B-C1B	-3.78	102.98	106.29
22	A	1804	BCR	C24-C23-C22	-3.78	120.45	126.22
19	4	1197	CLA	CAA-C2A-C3A	-3.78	107.14	116.20
20	B	1783	LMU	C3'-C4'-C5'	-3.78	102.30	110.84
19	A	1800	CLA	O2D-CGD-O1D	-3.78	115.99	123.79
20	A	7022	LMU	C3B-C4B-C5B	-3.78	103.62	110.20
20	A	7033	LMU	C3'-C4'-C5'	-3.78	102.30	110.84
19	B	1769	CLA	CMD-C2D-C3D	-3.77	117.70	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1054	CLA	CHD-C4C-C3C	-3.77	119.11	124.94
20	1	1200	LMU	O2'-C2'-C1'	-3.77	101.75	110.02
19	4	4007	CLA	CHC-C1C-C2C	-3.77	116.43	126.35
19	B	1740	CLA	O2A-CGA-O1A	-3.76	113.78	123.49
19	K	1085	CLA	CMD-C2D-C3D	-3.76	117.73	125.09
19	B	1751	CLA	CMD-C2D-C3D	-3.76	117.73	125.09
19	B	1755	CLA	CAA-CBA-CGA	-3.76	102.32	113.32
22	B	1775	BCR	C24-C23-C22	-3.76	120.49	126.22
19	A	1785	CLA	CHD-C4C-C3C	-3.75	119.14	124.94
19	A	1799	CLA	C3D-CAD-CBD	-3.75	102.29	107.60
19	B	1787	CLA	O2D-CGD-O1D	-3.75	116.04	123.79
19	4	1199	CLA	C1D-CHD-C4C	-3.75	116.92	122.60
20	A	7014	LMU	C1B-O1B-C4'	-3.75	108.22	118.01
19	J	1044	CLA	O1D-CGD-CBD	-3.75	119.25	124.62
19	A	1760	CLA	C3D-CAD-CBD	-3.75	102.30	107.60
19	2	1221	CLA	C2D-C3D-C4D	-3.74	103.01	106.30
19	A	1768	CLA	C3D-CAD-CBD	-3.74	102.30	107.60
19	4	4007	CLA	CHD-C4C-C3C	-3.74	119.16	124.94
19	3	1220	CLA	C2C-C1C-CHC	-3.74	118.51	125.15
19	2	1213	CLA	O2D-CGD-O1D	-3.74	116.07	123.79
19	B	1748	CLA	O2D-CGD-O1D	-3.73	116.08	123.79
19	A	1794	CLA	CHD-C4C-C3C	-3.73	119.18	124.94
19	2	1214	CLA	C3B-C2B-C1B	-3.73	103.03	106.29
19	B	1786	CLA	CAA-C2A-C3A	-3.73	102.50	113.22
19	B	1746	CLA	C3D-CAD-CBD	-3.73	102.33	107.60
19	1	1187	CLA	CBA-CAA-C2A	-3.72	103.23	113.73
19	A	1775	CLA	C3B-C2B-C1B	-3.72	103.03	106.29
19	A	1776	CLA	CHD-C4C-C3C	-3.72	119.19	124.94
19	A	1761	CLA	C3D-CAD-CBD	-3.72	102.34	107.60
19	1	1146	CLA	CMD-C2D-C3D	-3.72	117.82	125.09
19	2	1221	CLA	C2A-C1A-CHA	-3.72	116.00	122.58
19	B	1743	CLA	CHD-C4C-C3C	-3.71	119.20	124.94
19	3	1219	CLA	O2D-CGD-O1D	-3.71	116.12	123.79
19	1	1187	CLA	C3D-CAD-CBD	-3.71	102.35	107.60
19	3	1217	CLA	C3B-C2B-C1B	-3.71	103.04	106.29
19	1	1014	CLA	C2A-C1A-CHA	-3.71	117.06	123.89
19	A	1764	CLA	C3D-CAD-CBD	-3.70	102.36	107.60
19	B	1749	CLA	C3D-CAD-CBD	-3.70	102.36	107.60
19	A	1792	CLA	C3D-CAD-CBD	-3.70	102.37	107.60
19	B	1762	CLA	O1D-CGD-CBD	-3.70	119.32	124.62
19	1	1014	CLA	CHC-C1C-C2C	-3.70	116.62	126.35
20	A	7021	LMU	C6B-C5B-C4B	-3.70	103.90	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1222	CLA	C4-C3-C2	-3.69	116.25	123.50
19	3	3001	CLA	C3C-C4C-CHD	-3.69	119.25	125.32
19	B	1744	CLA	CAA-C2A-C3A	-3.69	102.61	113.22
19	B	1762	CLA	C1-C2-C3	-3.69	120.67	126.71
22	B	1780	BCR	C4-C5-C6	-3.68	118.09	122.78
19	2	1215	CLA	CHD-C4C-C3C	-3.68	119.25	124.94
19	L	1167	CLA	O2D-CGD-O1D	-3.68	116.19	123.79
19	4	1203	CLA	C2C-C1C-CHC	-3.68	118.61	125.15
19	1	1014	CLA	O2A-CGA-O1A	-3.68	114.00	123.49
19	A	1812	CLA	CHD-C4C-C3C	-3.68	119.26	124.94
19	K	1085	CLA	C1-C2-C3	-3.68	120.68	126.71
19	4	1196	CLA	CMD-C2D-C3D	-3.68	117.90	125.09
19	1	1195	CLA	CMD-C2D-C3D	-3.67	117.90	125.09
19	A	1780	CLA	CMD-C2D-C3D	-3.67	117.91	125.09
19	A	1812	CLA	O2D-CGD-O1D	-3.67	116.21	123.79
19	1	1188	CLA	CHC-C1C-C2C	-3.67	116.70	126.35
19	4	1208	CLA	C2D-C3D-C4D	-3.67	103.07	106.30
19	A	1796	CLA	O2D-CGD-O1D	-3.66	116.22	123.79
19	4	1202	CLA	CMD-C2D-C3D	-3.66	117.94	125.09
19	B	1755	CLA	C3D-CAD-CBD	-3.66	102.43	107.60
19	2	1218	CLA	C3D-CAD-CBD	-3.66	102.43	107.60
19	2	1216	CLA	C3B-C2B-C1B	-3.65	103.09	106.29
19	4	1198	CLA	C2C-C1C-NC	-3.65	107.52	110.24
19	B	1738	CLA	C3D-CAD-CBD	-3.65	102.43	107.60
19	3	3008	CLA	CHD-C4C-C3C	-3.65	119.30	124.94
20	A	7043	LMU	C3'-C4'-C5'	-3.65	102.59	110.84
22	B	1777	BCR	C33-C5-C6	-3.64	121.03	124.61
19	A	1777	CLA	CMD-C2D-C3D	-3.64	117.97	125.09
19	1	1142	CLA	CMD-C2D-C3D	-3.64	117.97	125.09
19	B	1758	CLA	CMD-C2D-C3D	-3.64	117.98	125.09
19	A	1787	CLA	CHD-C4C-C3C	-3.63	119.33	124.94
19	R	1055	CLA	CMD-C2D-C3D	-3.63	117.98	125.09
19	4	1197	CLA	CMD-C2D-C3D	-3.63	117.99	125.09
19	B	1756	CLA	CMD-C2D-C3D	-3.62	118.00	125.09
19	1	1014	CLA	CMA-C3A-C2A	-3.62	98.33	114.35
19	2	1218	CLA	CHC-C1C-C2C	-3.62	116.83	126.35
19	A	1761	CLA	CHC-C1C-C2C	-3.62	116.83	126.35
19	3	1216	CLA	C2D-C3D-C4D	-3.62	103.12	106.30
19	3	1218	CLA	CMD-C2D-C3D	-3.62	118.01	125.09
19	B	1760	CLA	O2D-CGD-O1D	-3.62	116.32	123.79
19	B	1757	CLA	C3D-CAD-CBD	-3.61	102.49	107.60
19	4	1201	CLA	C2C-C1C-NC	-3.61	107.55	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1741	CLA	CHD-C4C-C3C	-3.61	119.37	124.94
20	A	7050	LMU	C6'-C5'-C4'	-3.61	102.75	113.25
19	4	1198	CLA	O2D-CGD-O1D	-3.60	116.35	123.79
19	4	1199	CLA	CMD-C2D-C3D	-3.60	118.04	125.09
20	B	1783	LMU	O6'-C6'-C5'	-3.60	99.43	111.33
19	L	1167	CLA	CHD-C4C-C3C	-3.60	119.38	124.94
19	2	1215	CLA	C3D-CAD-CBD	-3.60	102.51	107.60
19	A	1762	CLA	O2D-CGD-O1D	-3.60	116.36	123.79
20	A	7005	LMU	O3'-C3'-C4'	-3.60	101.36	109.87
20	A	7028	LMU	O5B-C5B-C4B	-3.60	102.93	109.68
19	A	1771	CLA	C2A-C1A-CHA	-3.60	117.26	123.89
19	1	1197	CLA	C2D-C3D-C4D	-3.59	103.14	106.30
19	4	1210	CLA	C2A-C1A-CHA	-3.59	116.22	122.58
19	1	1308	CLA	CMD-C2D-C3D	-3.59	118.07	125.09
20	A	7016	LMU	O3'-C3'-C4'	-3.59	101.39	109.87
19	A	1792	CLA	CAA-C2A-C3A	-3.58	102.91	113.22
19	1	1145	CLA	CHD-C4C-C3C	-3.58	119.40	124.94
19	1	1303	CLA	C2C-C1C-CHC	-3.58	118.78	125.15
21	B	8059	SUC	O6-C6-C5	-3.58	99.49	111.33
20	A	7025	LMU	C1B-O1B-C4'	-3.58	108.65	118.01
19	4	1204	CLA	C2C-C1C-CHC	-3.58	118.79	125.15
19	1	1307	CLA	C3C-C4C-CHD	-3.58	119.43	125.32
19	F	1156	CLA	CMD-C2D-C3D	-3.58	118.09	125.09
19	3	1217	CLA	C2D-C3D-C4D	-3.58	103.15	106.30
21	B	8062	SUC	C4-C3-C2	-3.58	104.12	110.79
19	3	1220	CLA	C3C-C4C-CHD	-3.57	119.44	125.32
19	1	1241	CLA	C3D-CAD-CBD	-3.57	102.54	107.60
19	2	1219	CLA	C2C-C1C-CHC	-3.57	118.80	125.15
20	A	7028	LMU	O3'-C3'-C4'	-3.57	101.42	109.87
19	1	1191	CLA	C2C-C1C-CHC	-3.57	118.80	125.15
20	A	7023	LMU	O2'-C2'-C3'	-3.57	102.29	110.34
20	A	7020	LMU	C1-O1'-C1'	-3.57	107.70	113.94
22	L	1170	BCR	C7-C6-C5	-3.57	113.19	121.37
21	B	8053	SUC	O3'-C3'-C2'	-3.57	102.51	113.96
19	A	1785	CLA	O2D-CGD-O1D	-3.57	116.42	123.79
19	4	1199	CLA	CHC-C1C-C2C	-3.57	116.97	126.35
19	1	1307	CLA	C2A-C1A-CHA	-3.57	116.26	122.58
19	3	1213	CLA	C3B-C2B-C1B	-3.56	103.17	106.29
21	B	8060	SUC	O6'-C6'-C5'	-3.56	99.56	111.33
19	B	1757	CLA	CMD-C2D-C3D	-3.56	118.13	125.09
20	A	7032	LMU	C1'-O5'-C5'	-3.56	106.84	113.75
19	2	1223	CLA	C3D-CAD-CBD	-3.55	102.57	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1194	CLA	C1D-CHD-C4C	-3.55	117.18	126.32
19	1	1146	CLA	CMB-C2B-C1B	-3.55	122.48	128.36
19	A	1793	CLA	CHD-C4C-C3C	-3.55	119.45	124.94
19	2	2010	CLA	C3B-C2B-C1B	-3.55	103.18	106.29
19	B	1786	CLA	CHD-C4C-C3C	-3.54	119.47	124.94
19	4	1207	CLA	C2C-C1C-CHC	-3.54	118.86	125.15
19	A	1780	CLA	C3D-CAD-CBD	-3.54	102.59	107.60
19	B	1738	CLA	O2D-CGD-O1D	-3.54	116.48	123.79
20	A	7020	LMU	C3B-C4B-C5B	-3.54	104.03	110.20
20	A	7049	LMU	C6B-C5B-C4B	-3.54	104.28	113.02
19	L	1167	CLA	CGD-CBD-CAD	-3.54	98.64	110.62
19	1	1187	CLA	CHC-C1C-C2C	-3.54	117.05	126.35
20	A	7022	LMU	O1B-C1B-O5B	-3.54	101.73	110.68
19	4	1209	CLA	CAA-C2A-C3A	-3.53	107.74	116.20
19	3	1213	CLA	C2C-C1C-CHC	-3.53	118.87	125.15
21	F	1158	SUC	C1'-C2'-C3'	-3.53	102.58	114.49
19	A	1764	CLA	CMD-C2D-C3D	-3.53	118.19	125.09
19	F	1155	CLA	CHD-C4C-C3C	-3.53	118.93	124.83
21	B	8062	SUC	O5-C5-C4	-3.53	103.07	109.68
19	A	1767	CLA	CHC-C1C-C2C	-3.52	117.08	126.35
19	A	1788	CLA	CHD-C4C-C3C	-3.52	119.50	124.94
19	A	1789	CLA	CMA-C3A-C2A	-3.52	98.77	114.35
19	2	1223	CLA	CGD-CBD-CAD	-3.52	98.70	110.62
22	I	1032	BCR	C32-C1-C6	-3.52	104.79	110.30
20	A	7023	LMU	C3B-C4B-C5B	-3.52	104.06	110.20
19	2	1212	CLA	CMD-C2D-C3D	-3.52	118.21	125.09
19	4	4014	CLA	CMD-C2D-C3D	-3.51	118.22	125.09
20	N	1086	LMU	O4'-C4B-C3B	-3.51	102.44	110.34
19	A	1783	CLA	CHD-C4C-C3C	-3.51	119.52	124.94
19	3	1216	CLA	C3B-C2B-C1B	-3.51	103.22	106.29
19	B	1767	CLA	CMD-C2D-C3D	-3.51	118.23	125.09
19	1	1187	CLA	CHD-C4C-C3C	-3.50	119.53	124.94
22	B	1780	BCR	C28-C29-C30	-3.50	101.86	114.83
23	B	1774	PQN	C2M-C2-C3	-3.50	116.61	124.10
19	B	1773	CLA	CHD-C4C-C3C	-3.50	118.97	124.83
19	B	1751	CLA	O1D-CGD-CBD	-3.50	119.60	124.62
19	A	1789	CLA	C3D-CAD-CBD	-3.50	102.65	107.60
19	4	1206	CLA	C3D-CAD-CBD	-3.49	102.66	107.60
19	1	1149	CLA	CHC-C1C-C2C	-3.49	117.17	126.35
19	B	1769	CLA	CHD-C4C-C3C	-3.49	119.55	124.94
19	1	1190	CLA	CMD-C2D-C3D	-3.48	118.27	125.09
19	1	1193	CLA	O2D-CGD-O1D	-3.48	116.60	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1194	CLA	C3C-C4C-CHD	-3.48	119.59	125.32
19	J	1043	CLA	CMD-C2D-C3D	-3.48	118.28	125.09
19	B	1765	CLA	O1D-CGD-CBD	-3.48	119.64	124.62
19	J	1044	CLA	CHD-C4C-C3C	-3.48	119.56	124.94
19	1	1197	CLA	C3C-C4C-CHD	-3.48	119.60	125.32
19	R	1055	CLA	CHC-C1C-C2C	-3.48	117.20	126.35
19	1	1241	CLA	C4-C3-C2	-3.48	116.68	123.50
21	B	8056	SUC	O1-C1-C2	-3.48	96.76	108.36
19	A	1800	CLA	C4-C3-C2	-3.48	116.68	123.50
19	A	1766	CLA	C2A-C1A-CHA	-3.48	117.49	123.89
19	1	1010	CLA	C2A-C1A-CHA	-3.47	116.43	122.58
19	1	1145	CLA	CHC-C1C-C2C	-3.47	117.22	126.35
19	B	1743	CLA	CMD-C2D-C3D	-3.47	118.30	125.09
20	A	7032	LMU	O1B-C1B-C2B	-3.47	99.66	108.10
19	A	1797	CLA	C6-C7-C8	-3.47	103.98	115.49
19	A	1792	CLA	CHD-C4C-C3C	-3.47	119.58	124.94
19	B	1755	CLA	CGD-CBD-CAD	-3.46	98.88	110.62
21	B	8059	SUC	C3-C4-C5	-3.46	104.16	110.20
19	B	1741	CLA	C3D-CAD-CBD	-3.46	102.70	107.60
19	A	1772	CLA	O2A-CGA-O1A	-3.46	114.56	123.49
19	B	1744	CLA	C6-C7-C8	-3.46	104.01	115.49
19	1	1188	CLA	CHD-C4C-C3C	-3.46	119.60	124.94
20	K	1086	LMU	O2B-C2B-C1B	-3.46	102.44	110.02
19	1	1146	CLA	CHD-C4C-C3C	-3.45	119.60	124.94
19	B	1763	CLA	CMD-C2D-C3D	-3.45	118.33	125.09
19	L	1167	CLA	CMD-C2D-C3D	-3.45	118.34	125.09
19	1	1197	CLA	C2C-C1C-CHC	-3.45	119.02	125.15
20	A	7050	LMU	O3B-C3B-C2B	-3.45	102.58	110.34
20	A	7036	LMU	O5'-C1'-C2'	-3.45	103.21	110.28
19	A	1797	CLA	CGD-CBD-CAD	-3.44	98.95	110.62
19	1	1146	CLA	O2A-CGA-O1A	-3.44	114.60	123.49
19	A	1770	CLA	CHD-C4C-C3C	-3.44	119.62	124.94
19	3	3011	CLA	C3D-CAD-CBD	-3.44	102.73	107.60
19	4	1205	CLA	CMD-C2D-C3D	-3.44	118.36	125.09
20	A	7022	LMU	O5B-C1B-C2B	-3.44	103.22	110.28
19	A	1791	CLA	CHD-C4C-C3C	-3.44	119.63	124.94
19	B	1750	CLA	O2D-CGD-O1D	-3.44	116.69	123.79
22	L	1170	BCR	C24-C23-C22	-3.44	120.97	126.22
20	A	7026	LMU	C1B-O5B-C5B	-3.44	107.07	113.75
19	1	1193	CLA	O1D-CGD-CBD	-3.43	119.70	124.62
19	3	3011	CLA	CHD-C4C-C3C	-3.43	119.64	124.94
19	B	1738	CLA	CHC-C1C-C2C	-3.43	117.33	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1220	CLA	C2D-C3D-C4D	-3.42	103.29	106.30
20	A	7048	LMU	O5B-C5B-C4B	-3.42	103.26	109.68
19	3	1220	CLA	C3B-C2B-C1B	-3.41	103.31	106.29
19	A	1779	CLA	CHD-C4C-C3C	-3.41	119.68	124.94
19	A	1780	CLA	CHD-C4C-C3C	-3.40	119.68	124.94
22	B	1780	BCR	C1-C6-C5	-3.40	117.67	122.66
19	2	1215	CLA	CMD-C2D-C3D	-3.40	118.44	125.09
19	2	1221	CLA	C2C-C1C-CHC	-3.40	119.11	125.15
21	B	8062	SUC	O1'-C1'-C2'	-3.40	101.05	111.91
19	A	1759	CLA	C1-C2-C3	-3.40	121.14	126.71
19	B	1759	CLA	C16-C15-C13	-3.39	104.23	115.49
19	F	1157	CLA	CBA-CAA-C2A	-3.39	104.17	113.73
19	A	1791	CLA	CHC-C1C-C2C	-3.39	117.43	126.35
19	1	1010	CLA	C2C-C1C-CHC	-3.39	119.13	125.15
19	A	1776	CLA	CMD-C2D-C3D	-3.39	118.46	125.09
19	A	1790	CLA	CHD-C4C-C3C	-3.39	119.71	124.94
19	B	1752	CLA	CMD-C2D-C3D	-3.38	118.47	125.09
20	A	7048	LMU	C1B-O5B-C5B	-3.38	107.19	113.75
19	A	1778	CLA	CMD-C2D-C3D	-3.38	118.48	125.09
19	3	1224	CLA	O1D-CGD-CBD	-3.37	119.79	124.62
20	A	7020	LMU	C1'-O5'-C5'	-3.37	107.20	113.75
19	4	1211	CLA	C3D-CAD-CBD	-3.37	102.84	107.60
22	B	1782	BCR	C36-C18-C19	-3.36	112.50	118.10
20	A	7041	LMU	O5'-C1'-C2'	-3.36	103.38	110.28
19	B	1744	CLA	C2C-C1C-NC	-3.36	107.74	110.24
19	I	1031	CLA	C3D-CAD-CBD	-3.36	102.85	107.60
19	B	1755	CLA	OBD-CAD-C3D	-3.35	121.51	128.35
19	A	1784	CLA	CHD-C4C-C3C	-3.35	119.76	124.94
19	B	1788	CLA	CMD-C2D-C3D	-3.35	118.53	125.09
22	B	1780	BCR	C37-C22-C21	-3.35	117.95	122.90
21	B	8053	SUC	C1-C2-C3	-3.35	103.36	109.97
22	B	1777	BCR	C35-C13-C14	-3.35	117.95	122.90
19	A	1770	CLA	CMD-C2D-C3D	-3.35	118.54	125.09
19	4	4007	CLA	O2D-CGD-O1D	-3.35	116.88	123.79
20	A	7005	LMU	C3B-C4B-C5B	-3.34	104.37	110.20
19	B	1737	CLA	CHD-C4C-C3C	-3.34	119.78	124.94
19	B	1753	CLA	C5-C3-C2	-3.34	114.71	121.05
19	1	1198	CLA	C2C-C1C-CHC	-3.34	119.21	125.15
19	3	3001	CLA	C2C-C1C-CHC	-3.34	119.21	125.15
19	A	1778	CLA	CHD-C4C-C3C	-3.34	119.78	124.94
21	B	8061	SUC	C1'-C2'-C3'	-3.34	103.22	114.49
20	A	7030	LMU	C1'-O5'-C5'	-3.34	107.27	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1187	CLA	O1D-CGD-CBD	-3.33	119.85	124.62
21	B	8054	SUC	O3'-C3'-C4'	-3.33	101.32	113.29
19	A	1788	CLA	CMD-C2D-C3D	-3.33	118.58	125.09
19	B	1771	CLA	O1D-CGD-CBD	-3.32	119.86	124.62
19	A	1811	CLA	O2A-CGA-O1A	-3.32	114.92	123.49
19	4	1209	CLA	CHD-C4C-C3C	-3.32	119.27	124.83
19	A	1810	CLA	CAA-C2A-C3A	-3.32	103.67	113.22
19	4	1200	CLA	CBC-CAC-C3C	-3.32	102.25	112.39
19	A	1796	CLA	C4-C3-C2	-3.32	116.99	123.50
21	B	8061	SUC	O3'-C3'-C4'	-3.32	101.38	113.29
19	B	1741	CLA	CMD-C2D-C3D	-3.31	118.61	125.09
19	A	1773	CLA	CMD-C2D-C3D	-3.31	118.61	125.09
20	A	7013	LMU	O5B-C1B-C2B	-3.31	103.49	110.28
19	A	1795	CLA	CHC-C1C-C2C	-3.31	117.66	126.35
19	1	1148	CLA	C2A-C1A-CHA	-3.31	117.80	123.89
19	A	1784	CLA	O2D-CGD-O1D	-3.30	116.97	123.79
20	A	7028	LMU	C1B-O1B-C4'	-3.30	109.37	118.01
22	B	1777	BCR	C15-C14-C13	-3.30	122.44	127.20
20	A	7005	LMU	C1B-O1B-C4'	-3.29	109.41	118.01
20	A	7039	LMU	O3'-C3'-C4'	-3.29	102.09	109.87
19	B	1745	CLA	CHD-C4C-C3C	-3.28	119.87	124.94
19	1	1014	CLA	C7-C6-C5	-3.28	103.36	113.06
19	B	1758	CLA	C3D-CAD-CBD	-3.28	102.96	107.60
19	B	1770	CLA	CAA-C2A-C3A	-3.27	103.81	113.22
19	A	1766	CLA	CHD-C4C-C3C	-3.27	119.88	124.94
19	3	1214	CLA	CMD-C2D-C3D	-3.27	118.70	125.09
19	A	1767	CLA	CAA-C2A-C1A	-3.27	100.95	112.47
19	A	1763	CLA	C1D-CHD-C4C	-3.27	117.66	122.60
20	1	1200	LMU	O5B-C5B-C4B	-3.27	103.55	109.68
19	A	1767	CLA	CHD-C4C-C3C	-3.26	119.90	124.94
19	A	1771	CLA	CBC-CAC-C3C	-3.26	102.42	112.39
22	I	1032	BCR	C8-C7-C6	-3.26	117.51	127.32
19	A	1796	CLA	C3D-CAD-CBD	-3.26	102.99	107.60
19	2	2010	CLA	C2C-C1C-CHC	-3.26	119.36	125.15
19	B	1739	CLA	O2A-CGA-O1A	-3.25	115.09	123.49
19	A	1785	CLA	C3D-CAD-CBD	-3.25	103.00	107.60
19	2	1217	CLA	C6-C5-C3	-3.25	105.35	112.48
19	1	1303	CLA	C3B-C2B-C1B	-3.24	103.45	106.29
22	3	1225	BCR	C23-C24-C25	-3.24	117.58	127.32
19	A	1763	CLA	CBC-CAC-C3C	-3.24	102.51	112.39
19	B	1748	CLA	CHD-C4C-C3C	-3.24	119.94	124.94
19	A	1778	CLA	CHC-C1C-C2C	-3.24	117.84	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1775	CLA	C2C-C1C-CHC	-3.23	119.41	125.15
19	A	1792	CLA	O2D-CGD-O1D	-3.23	117.12	123.79
23	A	1801	PQN	C21-C20-C18	-3.22	104.82	115.49
20	A	7037	LMU	O3B-C3B-C4B	-3.22	103.09	110.34
19	F	1157	CLA	CAA-C2A-C3A	-3.22	103.97	113.22
19	2	1220	CLA	CMD-C2D-C3D	-3.21	118.80	125.09
19	2	1217	CLA	CHC-C1C-C2C	-3.21	117.90	126.35
19	3	3008	CLA	C3D-CAD-CBD	-3.21	103.06	107.60
20	A	7033	LMU	O1B-C1B-O5B	-3.21	102.55	110.68
19	1	1014	CLA	C3D-CAD-CBD	-3.21	103.06	107.60
19	A	1766	CLA	CMA-C3A-C2A	-3.21	100.15	114.35
19	B	1742	CLA	CAA-C2A-C3A	-3.21	103.99	113.22
20	A	7032	LMU	C1-O1'-C1'	-3.21	108.34	113.94
20	A	7021	LMU	C1'-O5'-C5'	-3.20	107.53	113.75
20	A	7050	LMU	O3'-C3'-C2'	-3.20	103.14	110.34
19	1	1190	CLA	OBD-CAD-C3D	-3.19	121.84	128.35
19	B	1787	CLA	C3D-CAD-CBD	-3.19	103.08	107.60
20	A	7028	LMU	O5B-C1B-C2B	-3.19	103.73	110.28
19	4	1198	CLA	CHC-C1C-C2C	-3.18	117.97	126.35
19	4	1200	CLA	CGD-CBD-CAD	-3.18	99.86	110.62
19	A	1763	CLA	C3D-CAD-CBD	-3.18	103.11	107.60
19	A	1772	CLA	C3D-CAD-CBD	-3.17	103.11	107.60
19	A	1766	CLA	C3D-CAD-CBD	-3.17	103.11	107.60
19	B	1760	CLA	CMA-C3A-C2A	-3.17	100.31	114.35
19	3	3008	CLA	O2A-CGA-O1A	-3.17	115.31	123.49
21	B	8056	SUC	C1-C2-C3	-3.17	103.72	109.97
19	4	1201	CLA	CHC-C1C-C2C	-3.17	118.01	126.35
19	1	1188	CLA	C4-C3-C2	-3.17	117.28	123.50
19	B	1758	CLA	O2A-CGA-O1A	-3.17	115.32	123.49
20	A	7041	LMU	O2'-C2'-C1'	-3.17	103.08	110.02
19	4	1199	CLA	CAC-C3C-C2C	-3.17	121.96	127.51
19	A	1772	CLA	CMD-C2D-C3D	-3.17	118.90	125.09
19	A	1793	CLA	CHC-C1C-C2C	-3.16	118.03	126.35
22	L	1169	BCR	C15-C16-C17	-3.16	116.40	123.39
19	1	1196	CLA	OBD-CAD-CBD	-3.16	121.17	125.94
19	A	1779	CLA	CMD-C2D-C3D	-3.16	118.91	125.09
19	A	1795	CLA	CAA-C2A-C1A	-3.16	101.34	112.47
20	A	7030	LMU	C3'-C4'-C5'	-3.16	103.70	110.84
19	B	1772	CLA	O2A-CGA-O1A	-3.16	115.35	123.49
19	4	1207	CLA	C2D-C3D-C4D	-3.16	103.52	106.30
19	A	1786	CLA	CHC-C1C-C2C	-3.15	118.05	126.35
19	A	1763	CLA	CMD-C2D-C3D	-3.15	118.92	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1777	BCR	C16-C15-C14	-3.15	116.42	123.39
20	A	1809	LMU	O2B-C2B-C1B	-3.15	103.11	110.02
19	B	1764	CLA	CMD-C2D-C3D	-3.15	118.93	125.09
19	B	1770	CLA	C3D-CAD-CBD	-3.15	103.14	107.60
22	3	1225	BCR	C36-C18-C17	-3.15	118.25	122.90
22	3	1225	BCR	C15-C14-C13	-3.14	122.66	127.20
19	A	1762	CLA	CMD-C2D-C3D	-3.14	118.94	125.09
19	B	1744	CLA	O1D-CGD-CBD	-3.14	120.12	124.62
19	B	1764	CLA	O2A-CGA-O1A	-3.14	115.39	123.49
19	1	1145	CLA	C4-C3-C2	-3.14	117.34	123.50
19	3	1218	CLA	O1D-CGD-CBD	-3.14	120.12	124.62
19	B	1735	CLA	O2D-CGD-O1D	-3.13	117.32	123.79
19	A	1793	CLA	CAA-C2A-C1A	-3.13	101.43	112.47
19	3	1218	CLA	CHC-C1C-C2C	-3.13	118.12	126.35
19	R	1054	CLA	C4-C3-C2	-3.12	117.37	123.50
19	A	1789	CLA	CAC-C3C-C2C	-3.12	122.03	127.51
19	1	1192	CLA	O1D-CGD-CBD	-3.12	120.14	124.62
20	A	7030	LMU	O3'-C3'-C2'	-3.12	103.31	110.34
19	B	1737	CLA	O2D-CGD-O1D	-3.12	117.34	123.79
19	1	1241	CLA	CHD-C4C-C3C	-3.12	120.12	124.94
20	A	7016	LMU	O5'-C1'-O1'	-3.12	102.54	110.05
19	B	1742	CLA	CHD-C4C-C3C	-3.12	120.12	124.94
21	B	8055	SUC	C6'-C5'-C4'	-3.12	107.70	115.08
19	3	1222	CLA	CHC-C1C-C2C	-3.12	118.15	126.35
20	B	1783	LMU	C1'-C2'-C3'	-3.12	103.82	109.97
20	A	7042	LMU	C1'-C2'-C3'	-3.11	103.84	109.97
19	A	1799	CLA	O1D-CGD-CBD	-3.11	120.16	124.62
19	4	1201	CLA	C6-C5-C3	-3.11	109.24	114.43
19	B	1765	CLA	CMD-C2D-C3D	-3.11	119.01	125.09
19	B	1755	CLA	CHD-C4C-C3C	-3.11	120.14	124.94
22	B	1779	BCR	C28-C27-C26	-3.10	108.95	113.87
19	B	1737	CLA	CHC-C1C-C2C	-3.10	118.20	126.35
19	4	1198	CLA	C16-C15-C13	-3.10	105.22	115.49
19	4	1198	CLA	CBC-CAC-C3C	-3.09	102.97	112.39
20	A	7037	LMU	C6'-C5'-C4'	-3.09	104.27	113.25
19	A	1768	CLA	CMD-C2D-C3D	-3.08	119.06	125.09
19	A	1765	CLA	CAC-C3C-C2C	-3.08	122.11	127.51
19	4	1210	CLA	C2D-C3D-C4D	-3.08	103.59	106.30
19	A	1787	CLA	O2D-CGD-O1D	-3.08	117.44	123.79
21	B	8059	SUC	C6-C5-C4	-3.07	105.43	113.02
19	A	1788	CLA	CHC-C1C-C2C	-3.07	118.27	126.35
20	L	1171	LMU	O5'-C5'-C4'	-3.07	103.26	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7037	LMU	C3'-C4'-C5'	-3.07	103.90	110.84
19	A	1776	CLA	O1D-CGD-CBD	-3.07	120.22	124.62
21	F	1158	SUC	O4'-C4'-C3'	-3.07	102.26	112.01
19	A	1761	CLA	O1D-CGD-CBD	-3.07	120.22	124.62
19	L	1167	CLA	CHC-C1C-C2C	-3.06	118.29	126.35
19	4	1206	CLA	CHC-C1C-C2C	-3.06	118.31	126.35
19	4	1199	CLA	O1D-CGD-CBD	-3.06	120.24	124.62
19	3	1219	CLA	C4-C3-C2	-3.06	117.50	123.50
19	A	1761	CLA	CMD-C2D-C3D	-3.06	119.11	125.09
19	A	1793	CLA	C2A-C1A-CHA	-3.05	118.27	123.89
19	A	1796	CLA	CAA-C2A-C3A	-3.05	104.44	113.22
20	K	1086	LMU	C1B-O5B-C5B	-3.05	107.83	113.75
20	A	7024	LMU	C4B-C3B-C2B	-3.05	105.11	110.79
19	3	1212	CLA	CMD-C2D-C3D	-3.04	119.13	125.09
19	B	1738	CLA	CMD-C2D-C3D	-3.04	119.13	125.09
20	A	7030	LMU	O5'-C5'-C4'	-3.04	103.32	109.75
19	A	1780	CLA	O2A-CGA-O1A	-3.04	115.64	123.49
19	A	1769	CLA	CHC-C1C-C2C	-3.04	118.35	126.35
22	B	1781	BCR	C3-C4-C5	-3.04	109.04	113.87
19	3	1224	CLA	CAC-C3C-C2C	-3.04	122.18	127.51
19	1	1307	CLA	C2D-C3D-C4D	-3.04	103.63	106.30
19	4	1201	CLA	C4-C3-C2	-3.03	117.54	123.50
22	L	1169	BCR	C19-C18-C17	-3.03	114.10	118.98
19	A	1771	CLA	C3A-C2A-C1A	-3.03	96.36	101.50
19	B	1760	CLA	CHC-C1C-C2C	-3.03	118.38	126.35
23	B	1774	PQN	C16-C15-C13	-3.03	105.84	112.48
19	B	1764	CLA	CAA-CBA-CGA	-3.03	104.45	113.32
19	4	1211	CLA	CBA-CAA-C2A	-3.03	105.19	113.73
19	B	1760	CLA	C2A-C1A-CHA	-3.03	118.31	123.89
20	A	7027	LMU	O3'-C3'-C4'	-3.03	102.71	109.87
19	B	1764	CLA	CHC-C1C-C2C	-3.03	118.39	126.35
19	A	1783	CLA	C4-C3-C2	-3.03	117.56	123.50
19	B	1786	CLA	CHC-C1C-C2C	-3.02	118.41	126.35
19	3	1222	CLA	C2A-C1A-CHA	-3.01	118.33	123.89
19	B	1769	CLA	CHC-C1C-C2C	-3.01	118.42	126.35
19	A	1810	CLA	C3B-C4B-NB	-3.01	105.32	109.21
20	A	7027	LMU	O5B-C5B-C4B	-3.01	104.03	109.68
20	A	7050	LMU	C3-C2-C1	-3.01	100.04	113.47
21	B	8060	SUC	C4-C3-C2	-3.00	105.19	110.79
19	F	1157	CLA	C2A-C1A-CHA	-3.00	118.36	123.89
19	1	1196	CLA	CHC-C1C-C2C	-2.99	118.47	126.35
19	B	1753	CLA	CHD-C4C-C3C	-2.99	120.31	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1791	CLA	O1D-CGD-CBD	-2.99	120.34	124.62
19	B	1753	CLA	CHC-C1C-C2C	-2.99	118.50	126.35
19	3	1218	CLA	CHD-C4C-C3C	-2.98	120.33	124.94
19	A	1786	CLA	C3D-CAD-CBD	-2.98	103.38	107.60
19	1	1149	CLA	CAC-C3C-C2C	-2.98	122.28	127.51
19	B	1761	CLA	O2D-CGD-O1D	-2.98	117.64	123.79
20	A	7013	LMU	O3'-C3'-C4'	-2.98	102.83	109.87
19	B	1747	CLA	CMD-C2D-C3D	-2.98	119.27	125.09
19	2	1218	CLA	CMD-C2D-C3D	-2.98	119.27	125.09
19	B	1739	CLA	CAA-C2A-C3A	-2.98	104.66	113.22
19	2	1223	CLA	CHC-C1C-C2C	-2.97	118.53	126.35
19	A	1769	CLA	CAA-C2A-C1A	-2.97	101.99	112.47
19	B	1772	CLA	CHC-C1C-C2C	-2.97	118.54	126.35
19	A	1790	CLA	O1D-CGD-CBD	-2.97	120.36	124.62
19	3	1223	CLA	C3C-C4C-CHD	-2.97	120.43	125.32
19	A	1780	CLA	C4-C3-C2	-2.97	117.67	123.50
19	R	1054	CLA	O2A-CGA-O1A	-2.97	115.83	123.49
19	3	3011	CLA	CMD-C2D-C3D	-2.97	119.29	125.09
19	B	1755	CLA	CMD-C2D-C3D	-2.97	119.29	125.09
20	A	7028	LMU	C1B-C2B-C3B	-2.96	104.13	109.97
19	B	1762	CLA	C3D-CAD-CBD	-2.96	103.41	107.60
19	A	1795	CLA	CMD-C2D-C3D	-2.96	119.30	125.09
20	A	7013	LMU	C3B-C4B-C5B	-2.96	105.04	110.20
20	A	7037	LMU	O5'-C5'-C4'	-2.96	103.50	109.75
19	A	1763	CLA	CHC-C1C-C2C	-2.95	118.58	126.35
22	B	1775	BCR	C3-C4-C5	-2.95	109.18	113.87
20	A	7032	LMU	O1B-C4'-C3'	-2.95	99.54	107.17
19	A	1781	CLA	O1D-CGD-CBD	-2.95	120.39	124.62
20	L	1171	LMU	O3B-C3B-C2B	-2.95	103.69	110.34
20	A	7043	LMU	C1'-C2'-C3'	-2.95	104.15	109.97
19	1	1309	CLA	C2C-C1C-CHC	-2.95	119.90	125.15
19	B	1748	CLA	CMD-C2D-C3D	-2.95	119.31	125.09
19	F	1156	CLA	O1D-CGD-CBD	-2.95	120.39	124.62
22	B	1779	BCR	C3-C4-C5	-2.95	109.18	113.87
20	A	7050	LMU	C1B-O5B-C5B	-2.95	108.02	113.75
19	1	1241	CLA	O2D-CGD-O1D	-2.95	117.70	123.79
20	A	7028	LMU	O2'-C2'-C1'	-2.95	103.55	110.02
20	A	7030	LMU	O3'-C3'-C4'	-2.95	102.90	109.87
19	A	1785	CLA	O1D-CGD-CBD	-2.95	120.40	124.62
19	B	1738	CLA	CHD-C4C-C3C	-2.94	120.39	124.94
19	A	1774	CLA	O2D-CGD-O1D	-2.94	117.72	123.79
19	B	1743	CLA	CHC-C1C-C2C	-2.94	118.62	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1198	CLA	C7-C6-C5	-2.94	104.37	113.06
19	F	1155	CLA	CAA-C2A-C1A	-2.94	104.03	112.17
19	4	1210	CLA	C2C-C1C-CHC	-2.94	119.93	125.15
19	B	1739	CLA	CHC-C1C-C2C	-2.93	118.64	126.35
19	A	1789	CLA	O2A-CGA-O1A	-2.93	115.93	123.49
19	B	1771	CLA	CAA-C2A-C3A	-2.93	104.79	113.22
19	A	1800	CLA	CMD-C2D-C3D	-2.93	119.36	125.09
20	A	7028	LMU	O5'-C1'-O1'	-2.92	103.02	110.05
19	B	1738	CLA	CMA-C3A-C2A	-2.92	101.43	114.35
20	A	7041	LMU	O2B-C2B-C1B	-2.92	103.62	110.02
20	A	7023	LMU	C6B-C5B-C4B	-2.92	105.82	113.02
21	B	8056	SUC	C1-O5-C5	-2.91	108.09	113.75
19	A	1770	CLA	CHC-C1C-C2C	-2.91	118.70	126.35
19	J	1044	CLA	O2D-CGD-O1D	-2.91	117.78	123.79
19	B	1755	CLA	CHC-C1C-C2C	-2.91	118.70	126.35
19	A	1762	CLA	CHC-C1C-C2C	-2.91	118.71	126.35
19	B	1786	CLA	CBC-CAC-C3C	-2.90	103.53	112.39
19	A	1810	CLA	C6-C7-C8	-2.90	105.86	115.49
19	1	1146	CLA	C3D-CAD-CBD	-2.90	103.50	107.60
19	A	1762	CLA	C2A-C1A-CHA	-2.90	118.55	123.89
19	J	1044	CLA	CHC-C1C-C2C	-2.90	118.73	126.35
19	3	1219	CLA	CAA-CBA-CGA	-2.89	104.85	113.32
19	A	1812	CLA	C2A-C1A-CHA	-2.89	118.56	123.89
19	2	1218	CLA	O1D-CGD-CBD	-2.89	120.48	124.62
19	B	1748	CLA	CHC-C1C-C2C	-2.89	118.75	126.35
19	A	1764	CLA	O2A-CGA-O1A	-2.89	116.05	123.49
19	A	1787	CLA	C3D-CAD-CBD	-2.88	103.52	107.60
19	3	1224	CLA	CHC-C1C-C2C	-2.88	118.76	126.35
21	B	8059	SUC	C2'-O1-C1	-2.88	109.93	117.53
19	B	1788	CLA	CHC-C1C-C2C	-2.88	118.78	126.35
19	B	1738	CLA	CAA-C2A-C3A	-2.88	104.94	113.22
19	B	1761	CLA	CHC-C1C-C2C	-2.87	118.79	126.35
22	A	1802	BCR	C3-C4-C5	-2.87	109.31	113.87
19	4	1196	CLA	O1D-CGD-CBD	-2.87	120.51	124.62
19	A	1768	CLA	CHC-C1C-C2C	-2.87	118.81	126.35
19	A	1771	CLA	CMD-C2D-C3D	-2.87	119.48	125.09
19	3	1224	CLA	CMD-C2D-C3D	-2.87	119.48	125.09
19	A	1785	CLA	CAA-C2A-C1A	-2.87	102.36	112.47
21	B	8052	SUC	C4-C3-C2	-2.87	105.44	110.79
19	1	1308	CLA	O1D-CGD-CBD	-2.86	120.52	124.62
19	2	1222	CLA	CHD-C4C-C3C	-2.86	120.52	124.94
22	A	1806	BCR	C3-C4-C5	-2.86	109.33	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7039	LMU	O3B-C3B-C2B	-2.86	103.90	110.34
19	B	1756	CLA	O1D-CGD-CBD	-2.86	120.52	124.62
19	A	1787	CLA	CMD-C2D-C3D	-2.86	119.50	125.09
19	B	1759	CLA	CMA-C3A-C2A	-2.86	101.71	114.35
20	B	1783	LMU	O3B-C3B-C2B	-2.85	103.91	110.34
19	B	1755	CLA	CAC-C3C-C2C	-2.85	122.51	127.51
19	4	4007	CLA	C6-C5-C3	-2.85	109.67	114.43
22	B	1781	BCR	C28-C27-C26	-2.85	109.35	113.87
19	1	1505	CLA	CHC-C1C-C2C	-2.85	118.86	126.35
19	B	1750	CLA	C4-C3-C2	-2.85	117.91	123.50
22	B	1780	BCR	C34-C9-C10	-2.85	118.70	122.90
22	L	1170	BCR	C19-C18-C17	-2.84	114.40	118.98
21	B	8061	SUC	O3-C3-C4	-2.84	103.94	110.34
19	A	1782	CLA	CHC-C1C-C2C	-2.84	118.89	126.35
19	A	1771	CLA	CBA-CAA-C2A	-2.84	105.73	113.73
19	R	1054	CLA	O2D-CGD-O1D	-2.83	117.94	123.79
19	2	1212	CLA	O1D-CGD-CBD	-2.83	120.57	124.62
19	2	1222	CLA	CHC-C1C-C2C	-2.83	118.91	126.35
19	A	1784	CLA	CHC-C1C-C2C	-2.83	118.92	126.35
19	1	1505	CLA	O1D-CGD-CBD	-2.83	120.57	124.62
19	4	1206	CLA	CMD-C2D-C3D	-2.82	119.57	125.09
22	A	1805	BCR	C3-C4-C5	-2.82	109.40	113.87
19	A	1787	CLA	C4-C3-C2	-2.81	117.98	123.50
19	3	1221	CLA	C1D-CHD-C4C	-2.81	119.08	126.32
19	B	1754	CLA	C3A-C2A-C1A	-2.81	96.73	101.50
19	A	1782	CLA	O1D-CGD-CBD	-2.81	120.59	124.62
19	3	1212	CLA	CHC-C1C-C2C	-2.81	118.96	126.35
19	A	1776	CLA	CHC-C1C-C2C	-2.81	118.96	126.35
19	B	1771	CLA	O2D-CGD-O1D	-2.81	117.99	123.79
19	A	1797	CLA	C11-C12-C13	-2.81	106.18	115.49
19	A	1765	CLA	O2A-CGA-O1A	-2.80	116.26	123.49
21	B	8056	SUC	O1-C2'-C1'	-2.80	100.71	109.69
19	A	1787	CLA	O1D-CGD-CBD	-2.80	120.61	124.62
19	2	1219	CLA	C3B-C2B-C1B	-2.80	103.84	106.29
19	B	1741	CLA	O2D-CGD-O1D	-2.80	118.01	123.79
20	A	7035	LMU	O5'-C5'-C4'	-2.80	103.83	109.75
19	1	1142	CLA	O1D-CGD-CBD	-2.80	120.61	124.62
19	K	1085	CLA	CHC-C1C-C2C	-2.80	118.99	126.35
20	B	1783	LMU	O1'-C1'-C2'	-2.80	104.51	108.04
22	B	1776	BCR	C28-C27-C26	-2.80	109.43	113.87
19	A	1777	CLA	O1D-CGD-CBD	-2.80	120.62	124.62
23	A	1801	PQN	C2M-C2-C3	-2.79	118.12	124.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7023	LMU	C1'-O5'-C5'	-2.79	108.33	113.75
21	2	1225	SUC	C2'-O1-C1	-2.79	110.18	117.53
19	1	1188	CLA	CAC-C3C-C2C	-2.79	122.62	127.51
20	A	7050	LMU	C3B-C4B-C5B	-2.79	105.34	110.20
19	A	1798	CLA	CHD-C4C-C3C	-2.79	120.63	124.94
21	B	8062	SUC	O1-C2'-C1'	-2.79	100.75	109.69
22	A	1803	BCR	C3-C4-C5	-2.79	109.45	113.87
19	B	1745	CLA	CHC-C1C-C2C	-2.79	119.02	126.35
19	1	1194	CLA	C2C-C1C-CHC	-2.78	120.21	125.15
19	4	1201	CLA	CMA-C3A-C2A	-2.78	102.05	114.35
22	B	1775	BCR	C28-C27-C26	-2.78	109.46	113.87
19	A	1795	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
19	B	1753	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
22	L	1170	BCR	C36-C18-C17	-2.77	118.81	122.90
19	A	1774	CLA	C4-C3-C2	-2.77	118.06	123.50
19	1	1145	CLA	O2A-CGA-O1A	-2.77	116.34	123.49
19	A	1792	CLA	CHC-C1C-C2C	-2.77	119.07	126.35
19	B	1763	CLA	CAA-CBA-CGA	-2.77	105.21	113.32
19	B	1769	CLA	CBC-CAC-C3C	-2.77	103.94	112.39
19	4	1210	CLA	C3B-C2B-C1B	-2.77	103.87	106.29
19	3	3011	CLA	O2D-CGD-O1D	-2.77	118.08	123.79
22	3	1225	BCR	C24-C23-C22	-2.77	122.00	126.22
21	2	1225	SUC	O1-C2'-O2'	-2.77	101.73	110.52
19	A	1781	CLA	CHC-C1C-C2C	-2.76	119.08	126.35
22	I	1032	BCR	C40-C30-C25	-2.76	105.97	110.30
19	B	1757	CLA	O1D-CGD-CBD	-2.76	120.66	124.62
19	B	1748	CLA	C3D-CAD-CBD	-2.76	103.69	107.60
19	B	1749	CLA	CHC-C1C-C2C	-2.76	119.09	126.35
19	B	1738	CLA	C16-C15-C13	-2.76	106.33	115.49
22	A	1802	BCR	C28-C27-C26	-2.76	109.49	113.87
19	B	1760	CLA	OBD-CAD-CBD	-2.76	121.77	125.94
19	B	1749	CLA	CGD-CBD-CAD	-2.76	101.27	110.62
19	4	1200	CLA	CMB-C2B-C1B	-2.76	123.80	128.36
19	A	1792	CLA	C2A-C1A-CHA	-2.76	118.81	123.89
19	A	1763	CLA	O2D-CGD-O1D	-2.75	118.10	123.79
20	1	1200	LMU	C6'-C5'-C4'	-2.75	105.24	113.25
20	A	7025	LMU	O3B-C3B-C2B	-2.75	104.15	110.34
19	A	1790	CLA	CHC-C1C-C2C	-2.75	119.12	126.35
19	A	1791	CLA	O2D-CGD-O1D	-2.75	118.11	123.79
19	A	1769	CLA	CMD-C2D-C3D	-2.75	119.71	125.09
19	A	1786	CLA	CMD-C2D-C3D	-2.75	119.72	125.09
19	B	1762	CLA	O2D-CGD-O1D	-2.74	118.12	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1738	CLA	C11-C12-C13	-2.74	106.40	115.49
22	A	1807	BCR	C3-C4-C5	-2.74	109.52	113.87
22	B	1778	BCR	C28-C27-C26	-2.74	109.52	113.87
22	L	1169	BCR	C28-C27-C26	-2.74	109.53	113.87
19	4	1209	CLA	CHC-C1C-C2C	-2.73	119.16	126.35
19	A	1798	CLA	CHC-C1C-C2C	-2.73	119.16	126.35
21	F	1158	SUC	C4-C3-C2	-2.73	105.69	110.79
22	A	1803	BCR	C28-C27-C26	-2.73	109.53	113.87
19	J	1043	CLA	O1D-CGD-CBD	-2.73	120.71	124.62
20	A	7032	LMU	O6'-C6'-C5'	-2.73	102.31	111.33
20	A	7017	LMU	C6'-C5'-C4'	-2.73	105.30	113.25
19	J	1044	CLA	CBC-CAC-C3C	-2.73	104.06	112.39
19	L	1166	CLA	O2D-CGD-O1D	-2.73	118.16	123.79
19	B	1759	CLA	C11-C12-C13	-2.73	106.44	115.49
19	J	1044	CLA	CAC-C3C-C2C	-2.73	122.73	127.51
21	B	8059	SUC	C1-C2-C3	-2.72	104.61	109.97
19	K	1085	CLA	O1D-CGD-CBD	-2.72	120.72	124.62
19	B	1740	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
20	A	7025	LMU	C4B-C3B-C2B	-2.72	105.71	110.79
19	A	1798	CLA	O2A-CGA-O1A	-2.72	116.47	123.49
19	R	1055	CLA	O2A-CGA-O1A	-2.72	116.47	123.49
19	A	1759	CLA	CAA-C2A-C3A	-2.72	105.39	113.22
19	B	1744	CLA	CHC-C1C-C2C	-2.72	119.20	126.35
19	B	1770	CLA	CMD-C2D-C3D	-2.72	119.77	125.09
22	B	1782	BCR	C32-C1-C31	-2.72	99.66	108.37
19	A	1779	CLA	CAA-C2A-C3A	-2.71	105.42	113.22
20	L	1171	LMU	O3'-C3'-C4'	-2.71	103.45	109.87
19	1	1241	CLA	CHC-C1C-C2C	-2.71	119.22	126.35
19	2	1218	CLA	CHD-C4C-C3C	-2.71	120.75	124.94
22	B	1776	BCR	C3-C4-C5	-2.71	109.57	113.87
19	R	1054	CLA	CHC-C1C-C2C	-2.71	119.23	126.35
19	4	1206	CLA	C4-C3-C2	-2.71	118.19	123.50
20	A	7037	LMU	O6B-C6B-C5B	-2.71	102.39	111.33
22	A	1807	BCR	C28-C27-C26	-2.70	109.58	113.87
19	B	1771	CLA	O2A-CGA-O1A	-2.70	116.51	123.49
19	A	1769	CLA	O2D-CGD-O1D	-2.70	118.21	123.79
19	3	1222	CLA	O2A-CGA-O1A	-2.70	116.52	123.49
19	A	1759	CLA	CMD-C2D-C3D	-2.70	119.81	125.09
19	B	1747	CLA	CHC-C1C-C2C	-2.70	119.25	126.35
19	A	1766	CLA	O2D-CGD-O1D	-2.70	118.22	123.79
21	B	8052	SUC	C2'-O1-C1	-2.69	110.43	117.53
20	A	7043	LMU	C1-O1'-C1'	-2.69	109.24	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7037	LMU	O2B-C2B-C3B	-2.69	104.28	110.34
20	A	7014	LMU	C1'-O5'-C5'	-2.69	108.52	113.75
19	A	1799	CLA	C6-C7-C8	-2.69	106.57	115.49
19	B	1751	CLA	CHC-C1C-C2C	-2.69	119.28	126.35
20	A	7036	LMU	O3'-C3'-C4'	-2.69	103.51	109.87
19	F	1156	CLA	CHC-C1C-C2C	-2.69	119.28	126.35
19	B	1741	CLA	CHC-C1C-C2C	-2.69	119.28	126.35
19	1	1148	CLA	O2A-CGA-O1A	-2.69	116.56	123.49
22	3	1225	BCR	C34-C9-C10	-2.68	118.94	122.90
20	A	7041	LMU	C1B-O5B-C5B	-2.68	108.53	113.75
20	A	7039	LMU	O5'-C1'-C2'	-2.68	104.77	110.28
20	A	7030	LMU	O2'-C2'-C1'	-2.68	104.15	110.02
19	A	1780	CLA	CHC-C1C-C2C	-2.68	119.31	126.35
21	B	8055	SUC	C2'-O1-C1	-2.68	110.47	117.53
19	B	1771	CLA	CHC-C1C-C2C	-2.68	119.31	126.35
19	A	1782	CLA	C2A-C1A-CHA	-2.68	118.96	123.89
19	A	1769	CLA	CAA-CBA-CGA	-2.68	105.48	113.32
19	A	1759	CLA	CHC-C1C-C2C	-2.67	119.32	126.35
19	A	1785	CLA	CHC-C1C-C2C	-2.67	119.32	126.35
19	1	1146	CLA	CHC-C1C-C2C	-2.67	119.33	126.35
19	A	1773	CLA	CHC-C1C-C2C	-2.67	119.33	126.35
19	3	1222	CLA	C3D-CAD-CBD	-2.67	103.82	107.60
19	B	1749	CLA	O2A-CGA-O1A	-2.66	116.61	123.49
19	A	1760	CLA	CHC-C1C-C2C	-2.66	119.34	126.35
19	B	1742	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
19	F	1155	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
19	B	1738	CLA	O2A-CGA-O1A	-2.66	116.64	123.49
22	3	1225	BCR	C28-C27-C26	-2.66	109.65	113.87
19	1	1187	CLA	O2D-CGD-O1D	-2.65	118.31	123.79
19	L	1168	CLA	C1-C2-C3	-2.65	122.36	126.71
21	B	8062	SUC	O3'-C3'-C2'	-2.65	105.47	113.96
20	A	7023	LMU	O5'-C5'-C6'	-2.65	99.66	106.36
19	B	1757	CLA	CHC-C1C-C2C	-2.65	119.39	126.35
19	B	1739	CLA	CMD-C2D-C3D	-2.64	119.92	125.09
19	4	1202	CLA	CHC-C1C-C2C	-2.64	119.40	126.35
19	R	1055	CLA	O2D-CGD-O1D	-2.64	118.33	123.79
21	F	1158	SUC	O2-C2-C3	-2.64	104.39	110.34
19	B	1759	CLA	CHC-C1C-C2C	-2.64	119.40	126.35
24	B	1784	LMG	C8-O7-C10	-2.64	111.56	117.89
19	4	1209	CLA	CAC-C3C-C2C	-2.64	121.39	126.81
19	1	1145	CLA	CAC-C3C-C2C	-2.63	122.89	127.51
19	B	1739	CLA	CHD-C4C-C3C	-2.63	120.87	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7033	LMU	O5'-C5'-C4'	-2.63	104.19	109.75
19	4	1196	CLA	CHC-C1C-C2C	-2.63	119.43	126.35
19	A	1762	CLA	CAA-C2A-C1A	-2.63	103.21	112.47
19	B	1766	CLA	CMD-C2D-C3D	-2.62	119.95	125.09
20	A	7023	LMU	C8-C7-C6	-2.62	100.98	114.53
19	2	1217	CLA	C11-C12-C13	-2.62	106.79	115.49
19	B	1786	CLA	C7-C6-C5	-2.62	105.31	113.06
20	A	7040	LMU	C4B-C3B-C2B	-2.62	105.90	110.79
19	1	1014	CLA	OBD-CAD-CBD	-2.62	121.99	125.94
20	A	7016	LMU	O5B-C5B-C4B	-2.62	104.77	109.68
20	K	1086	LMU	O2'-C2'-C3'	-2.61	104.46	110.34
19	B	1737	CLA	O1D-CGD-CBD	-2.61	120.88	124.62
19	A	1794	CLA	CHC-C1C-C2C	-2.61	119.49	126.35
21	B	8059	SUC	O3'-C3'-C2'	-2.61	105.59	113.96
19	2	1215	CLA	O2D-CGD-O1D	-2.61	118.41	123.79
19	B	1756	CLA	CHC-C1C-C2C	-2.61	119.49	126.35
19	B	1758	CLA	CAA-C2A-C3A	-2.61	105.72	113.22
20	B	1783	LMU	O3'-C3'-C4'	-2.61	103.70	109.87
19	A	1795	CLA	CAA-C2A-C3A	-2.61	105.72	113.22
19	3	1222	CLA	CMD-C2D-C3D	-2.61	119.99	125.09
19	K	1085	CLA	C2A-C1A-CHA	-2.61	119.09	123.89
19	B	1735	CLA	CMD-C2D-C3D	-2.60	119.99	125.09
20	A	7034	LMU	O2B-C2B-C3B	-2.60	104.48	110.34
19	2	1212	CLA	CHC-C1C-C2C	-2.60	119.51	126.35
19	B	1736	CLA	CHC-C1C-C2C	-2.60	119.51	126.35
20	1	1199	LMU	C1B-O1B-C4'	-2.60	111.22	118.01
19	I	1031	CLA	CHC-C1C-C2C	-2.60	119.52	126.35
19	A	1783	CLA	O2A-CGA-O1A	-2.60	116.79	123.49
19	4	4007	CLA	CMB-C2B-C1B	-2.60	124.07	128.36
20	A	7028	LMU	O4'-C4B-C5B	-2.60	102.36	109.24
19	B	1743	CLA	O2D-CGD-O1D	-2.60	118.43	123.79
19	J	1044	CLA	C11-C12-C13	-2.59	106.89	115.49
22	A	1802	BCR	C23-C24-C25	-2.59	119.53	127.32
22	B	1778	BCR	C3-C4-C5	-2.59	109.75	113.87
19	A	1785	CLA	CMD-C2D-C3D	-2.59	120.03	125.09
19	A	1774	CLA	CMD-C2D-C3D	-2.58	120.03	125.09
19	B	1742	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
19	2	1217	CLA	CAA-CBA-CGA	-2.58	105.75	113.32
22	A	1803	BCR	C8-C7-C6	-2.58	119.56	127.32
19	3	1218	CLA	CAC-C3C-C2C	-2.58	122.99	127.51
19	A	1800	CLA	C2A-C1A-CHA	-2.58	119.14	123.89
19	1	1142	CLA	CHC-C1C-C2C	-2.58	119.57	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7010	LMU	C1B-O1B-C4'	-2.58	111.27	118.01
20	A	7023	LMU	C4B-C3B-C2B	-2.58	105.98	110.79
19	4	4014	CLA	CHC-C1C-C2C	-2.58	119.57	126.35
19	4	1208	CLA	C2C-C1C-CHC	-2.58	120.57	125.15
21	F	1158	SUC	O1'-C1'-C2'	-2.57	103.69	111.91
19	B	1788	CLA	CAA-C2A-C3A	-2.57	105.82	113.22
19	B	1761	CLA	C1-C2-C3	-2.57	122.50	126.71
19	A	1771	CLA	O2A-CGA-O1A	-2.57	116.86	123.49
20	A	7032	LMU	C1B-O1B-C4'	-2.57	111.30	118.01
19	B	1773	CLA	CHC-C1C-C2C	-2.57	119.60	126.35
19	3	1214	CLA	CHC-C1C-C2C	-2.57	119.60	126.35
19	3	1222	CLA	CBC-CAC-C3C	-2.57	104.56	112.39
22	A	1807	BCR	C23-C24-C25	-2.57	119.61	127.32
19	1	1190	CLA	O1D-CGD-CBD	-2.56	120.95	124.62
22	A	1803	BCR	C23-C24-C25	-2.56	119.62	127.32
20	A	7042	LMU	C1-O1'-C1'	-2.56	109.47	113.94
22	B	1776	BCR	C23-C24-C25	-2.56	119.64	127.32
20	A	7041	LMU	C6'-C5'-C4'	-2.55	105.81	113.25
23	B	1774	PQN	C14-C13-C12	-2.55	118.49	123.50
19	1	1149	CLA	O2A-CGA-O1A	-2.55	116.90	123.49
19	B	1768	CLA	CHC-C1C-C2C	-2.55	119.64	126.35
19	B	1786	CLA	C16-C17-C18	-2.55	103.01	115.87
19	2	1217	CLA	CMD-C2D-C3D	-2.55	120.10	125.09
19	3	1215	CLA	C2D-C3D-C4D	-2.55	104.06	106.30
19	A	1795	CLA	O2D-CGD-O1D	-2.55	118.53	123.79
19	I	1031	CLA	CMD-C2D-C3D	-2.55	120.11	125.09
22	B	1781	BCR	C8-C7-C6	-2.54	119.67	127.32
22	A	1806	BCR	C28-C27-C26	-2.54	109.83	113.87
19	3	1219	CLA	C6-C7-C8	-2.54	107.06	115.49
19	2	1213	CLA	CHC-C1C-C2C	-2.54	119.67	126.35
19	B	1737	CLA	CAA-C2A-C1A	-2.54	103.52	112.47
20	A	7026	LMU	C1B-O1B-C4'	-2.54	111.37	118.01
19	B	1744	CLA	C9-C8-C7	-2.54	101.31	111.08
22	B	1780	BCR	C32-C1-C6	-2.54	106.32	110.30
22	A	1807	BCR	C8-C7-C6	-2.54	119.70	127.32
20	1	1200	LMU	C1'-O5'-C5'	-2.54	108.82	113.75
19	A	1774	CLA	CHC-C1C-C2C	-2.53	119.69	126.35
19	A	1787	CLA	O2A-CGA-O1A	-2.53	116.96	123.49
19	3	1219	CLA	CMD-C2D-C3D	-2.53	120.14	125.09
19	A	1783	CLA	C6-C7-C8	-2.53	107.09	115.49
19	A	1781	CLA	C2A-C1A-CHA	-2.53	119.22	123.89
22	A	1802	BCR	C27-C26-C25	-2.53	119.56	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1781	BCR	C23-C24-C25	-2.53	119.72	127.32
20	A	7032	LMU	O3'-C3'-C4'	-2.53	103.90	109.87
19	B	1735	CLA	CAA-C2A-C1A	-2.52	103.57	112.47
20	A	7015	LMU	O5B-C5B-C4B	-2.52	104.95	109.68
22	B	1782	BCR	C34-C9-C8	-2.52	113.90	118.10
19	L	1168	CLA	CAA-CBA-CGA	-2.52	105.94	113.32
19	F	1157	CLA	C3D-CAD-CBD	-2.52	104.03	107.60
19	B	1738	CLA	O1D-CGD-CBD	-2.52	121.01	124.62
19	1	1190	CLA	CHC-C1C-C2C	-2.52	119.73	126.35
22	L	1169	BCR	C37-C22-C21	-2.52	119.18	122.90
22	B	1777	BCR	C39-C30-C25	-2.52	106.36	110.30
19	1	1308	CLA	CHC-C1C-C2C	-2.51	119.74	126.35
19	1	1145	CLA	CMA-C3A-C2A	-2.51	103.24	114.35
19	J	1044	CLA	O2A-CGA-O1A	-2.51	117.01	123.49
20	A	1808	LMU	O6'-C6'-C5'	-2.51	103.04	111.33
20	A	7050	LMU	C1-O1'-C1'	-2.51	109.56	113.94
19	4	1206	CLA	O2A-CGA-O1A	-2.51	117.02	123.49
20	A	7028	LMU	O5'-C5'-C6'	-2.51	100.02	106.36
20	A	7027	LMU	C4B-C3B-C2B	-2.51	106.11	110.79
19	B	1761	CLA	CMD-C2D-C3D	-2.51	120.19	125.09
22	A	1802	BCR	C8-C7-C6	-2.50	119.80	127.32
19	B	1752	CLA	CHC-C1C-C2C	-2.50	119.77	126.35
19	B	1763	CLA	CHC-C1C-C2C	-2.50	119.77	126.35
19	3	3008	CLA	CMD-C2D-C3D	-2.50	120.20	125.09
21	B	8052	SUC	O4'-C4'-C5'	-2.50	103.56	111.05
19	A	1794	CLA	OBD-CAD-CBD	-2.50	122.17	125.94
22	A	1805	BCR	C28-C27-C26	-2.49	109.91	113.87
22	A	1804	BCR	C28-C27-C26	-2.49	109.91	113.87
19	A	1796	CLA	O2A-CGA-O1A	-2.49	117.06	123.49
19	1	1303	CLA	C2D-C3D-C4D	-2.49	104.11	106.30
19	A	1787	CLA	CHC-C1C-C2C	-2.49	119.81	126.35
20	A	7042	LMU	C3B-C4B-C5B	-2.49	105.86	110.20
22	3	1225	BCR	C37-C22-C21	-2.49	119.23	122.90
19	A	1785	CLA	C5-C3-C2	-2.49	116.34	121.05
19	A	1811	CLA	CHC-C1C-C2C	-2.48	119.82	126.35
21	B	8062	SUC	O5-C1-O1	-2.48	101.63	109.96
19	A	1765	CLA	C5-C3-C2	-2.48	116.35	121.05
19	A	1789	CLA	CAA-C2A-C3A	-2.48	106.09	113.22
19	A	1763	CLA	CBA-CAA-C2A	-2.48	106.74	113.73
20	A	7023	LMU	C1-O1'-C1'	-2.48	109.61	113.94
19	2	1213	CLA	CAA-C2A-C1A	-2.48	103.74	112.47
19	A	1768	CLA	O2D-CGD-O1D	-2.47	118.68	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1740	CLA	CHC-C1C-C2C	-2.47	119.85	126.35
19	4	1208	CLA	C2D-C1D-ND	-2.47	107.93	110.13
20	A	7028	LMU	C3B-C4B-C5B	-2.47	105.89	110.20
19	3	3011	CLA	CHC-C1C-C2C	-2.47	119.86	126.35
20	L	1171	LMU	C1B-O1B-C4'	-2.46	111.57	118.01
19	1	1505	CLA	CGD-CBD-CAD	-2.46	102.27	110.62
19	3	1221	CLA	C3C-C4C-CHD	-2.46	121.27	125.32
19	B	1772	CLA	CMD-C2D-C3D	-2.46	120.27	125.09
22	B	1776	BCR	C8-C7-C6	-2.46	119.92	127.32
19	2	1217	CLA	C2A-C1A-CHA	-2.46	119.35	123.89
19	A	1810	CLA	CMA-C3A-C2A	-2.46	103.47	114.35
21	B	8056	SUC	O3'-C3'-C4'	-2.46	104.45	113.29
19	4	1202	CLA	C2A-C1A-CHA	-2.46	119.36	123.89
19	1	1192	CLA	O2A-CGA-O1A	-2.46	117.15	123.49
19	A	1810	CLA	CMD-C2D-C3D	-2.46	120.28	125.09
19	R	1055	CLA	C6-C7-C8	-2.46	107.34	115.49
22	B	1778	BCR	C8-C7-C6	-2.46	119.94	127.32
19	A	1788	CLA	O2D-CGD-O1D	-2.46	118.72	123.79
21	B	8053	SUC	C1-O5-C5	-2.46	108.98	113.75
22	A	1804	BCR	C8-C7-C6	-2.45	119.96	127.32
19	1	1193	CLA	CHC-C1C-C2C	-2.45	119.92	126.35
19	B	1772	CLA	CMA-C3A-C2A	-2.45	103.53	114.35
19	B	1763	CLA	CAA-C2A-C1A	-2.45	103.85	112.47
21	B	8052	SUC	O3-C3-C4	-2.45	104.83	110.34
19	J	1043	CLA	CHC-C1C-C2C	-2.44	119.92	126.35
19	A	1777	CLA	O2D-CGD-O1D	-2.44	118.74	123.79
19	2	1217	CLA	C4-C3-C2	-2.44	118.70	123.50
19	B	1755	CLA	O1D-CGD-CBD	-2.44	121.12	124.62
19	B	1745	CLA	CAC-C3C-C2C	-2.44	123.23	127.51
20	A	7050	LMU	C1'-C2'-C3'	-2.44	105.17	109.97
19	B	1767	CLA	O1D-CGD-CBD	-2.44	121.13	124.62
19	A	1776	CLA	CAA-C2A-C3A	-2.44	106.21	113.22
19	A	1764	CLA	CHC-C1C-C2C	-2.43	119.95	126.35
22	A	1807	BCR	C27-C26-C25	-2.43	119.68	122.78
19	2	1212	CLA	O2D-CGD-O1D	-2.43	118.77	123.79
19	3	3008	CLA	CHC-C1C-C2C	-2.43	119.96	126.35
22	B	1775	BCR	C8-C7-C6	-2.43	120.02	127.32
19	A	1812	CLA	CHC-C1C-C2C	-2.43	119.96	126.35
19	A	1789	CLA	C5-C3-C2	-2.43	116.45	121.05
19	4	1196	CLA	C2A-C1A-CHA	-2.43	119.41	123.89
20	A	7050	LMU	C2'-C3'-C4'	-2.43	104.27	109.60
19	1	1188	CLA	CMB-C2B-C1B	-2.43	124.35	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1778	BCR	C23-C24-C25	-2.43	120.03	127.32
19	A	1764	CLA	CAA-C2A-C3A	-2.43	106.24	113.22
22	A	1807	BCR	C4-C5-C6	-2.42	119.69	122.78
19	A	1766	CLA	CHC-C1C-C2C	-2.42	119.98	126.35
19	2	1215	CLA	CHC-C1C-C2C	-2.42	119.98	126.35
22	A	1805	BCR	C23-C24-C25	-2.42	120.04	127.32
22	L	1169	BCR	C8-C7-C6	-2.42	120.05	127.32
19	A	1786	CLA	CHD-C4C-C3C	-2.42	121.21	124.94
20	A	7038	LMU	C4B-C3B-C2B	-2.42	106.28	110.79
19	A	1791	CLA	C2A-C1A-CHA	-2.42	119.44	123.89
19	B	1759	CLA	O2A-CGA-O1A	-2.42	117.26	123.49
19	J	1043	CLA	O2D-CGD-O1D	-2.41	118.80	123.79
22	A	1805	BCR	C8-C7-C6	-2.41	120.06	127.32
20	1	1200	LMU	O5'-C1'-C2'	-2.41	105.32	110.28
19	1	1014	CLA	O1D-CGD-CBD	-2.41	121.16	124.62
19	B	1770	CLA	CHC-C1C-C2C	-2.41	120.01	126.35
19	B	1787	CLA	CBA-CAA-C2A	-2.41	106.93	113.73
19	B	1767	CLA	O2D-CGD-O1D	-2.41	118.81	123.79
19	A	1771	CLA	C2C-C1C-NC	-2.41	108.45	110.24
22	A	1802	BCR	C4-C5-C6	-2.41	119.71	122.78
19	4	4014	CLA	O1D-CGD-CBD	-2.40	121.18	124.62
20	L	1171	LMU	C1'-C2'-C3'	-2.40	105.24	109.97
22	A	1804	BCR	C3-C4-C5	-2.40	110.06	113.87
20	A	7006	LMU	C1B-O1B-C4'	-2.40	111.73	118.01
20	1	1200	LMU	O5B-C1B-C2B	-2.40	105.35	110.28
21	B	8062	SUC	O4-C4-C3	-2.40	104.93	110.34
19	B	1787	CLA	CMD-C2D-C3D	-2.40	120.39	125.09
21	2	1225	SUC	O4-C4-C5	-2.40	104.21	109.84
22	B	1779	BCR	C8-C7-C6	-2.40	120.11	127.32
19	1	1241	CLA	O2A-CGA-O1A	-2.40	117.31	123.49
19	I	1031	CLA	O2D-CGD-O1D	-2.39	118.85	123.79
19	2	1222	CLA	CAC-C3C-C2C	-2.39	123.31	127.51
22	A	1806	BCR	C23-C24-C25	-2.39	120.13	127.32
20	A	7005	LMU	C2'-C3'-C4'	-2.39	104.35	109.60
20	A	7051	LMU	C1B-O1B-C4'	-2.39	111.76	118.01
19	A	1761	CLA	C6-C7-C8	-2.38	107.58	115.49
19	B	1770	CLA	O2D-CGD-O1D	-2.38	118.87	123.79
20	A	7036	LMU	C6'-C5'-C4'	-2.38	106.31	113.25
20	A	7004	LMU	C1B-O1B-C4'	-2.38	111.78	118.01
19	A	1791	CLA	CAC-C3C-C2C	-2.38	123.33	127.51
19	1	1308	CLA	C2A-C1A-CHA	-2.38	119.50	123.89
19	F	1156	CLA	C2A-C1A-CHA	-2.38	119.50	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1756	CLA	C2A-C1A-CHA	-2.38	119.50	123.89
19	1	1145	CLA	CAA-C2A-C3A	-2.38	106.37	113.22
19	A	1785	CLA	C2A-C1A-CHA	-2.38	119.50	123.89
19	B	1750	CLA	CHC-C1C-C2C	-2.38	120.10	126.35
19	B	1769	CLA	C4-C3-C2	-2.38	118.83	123.50
22	A	1803	BCR	C27-C26-C25	-2.38	119.75	122.78
19	1	1241	CLA	CMD-C2D-C3D	-2.37	120.45	125.09
19	R	1055	CLA	O1A-CGA-CBA	-2.37	114.24	123.72
19	1	1014	CLA	C4-C3-C2	-2.37	118.85	123.50
19	A	1786	CLA	O1D-CGD-CBD	-2.37	121.23	124.62
22	B	1780	BCR	C2-C3-C4	-2.37	105.56	111.53
19	2	1212	CLA	C2A-C1A-CHA	-2.37	119.53	123.89
20	A	7035	LMU	C2'-C3'-C4'	-2.37	104.41	109.60
19	1	1142	CLA	C2A-C1A-CHA	-2.36	119.54	123.89
20	A	7009	LMU	C1B-O1B-C4'	-2.36	111.84	118.01
19	B	1758	CLA	CHC-C1C-C2C	-2.36	120.15	126.35
22	I	1032	BCR	C4-C5-C6	-2.36	119.78	122.78
19	4	1205	CLA	C2A-C1A-CHA	-2.36	119.54	123.89
19	A	1760	CLA	O2A-CGA-O1A	-2.36	117.41	123.49
19	3	1221	CLA	C3C-C4C-NC	-2.36	108.03	110.09
19	1	1196	CLA	CMB-C2B-C3B	-2.35	120.48	125.09
20	A	7048	LMU	C2'-C3'-C4'	-2.35	104.43	109.60
19	A	1796	CLA	C6-C7-C8	-2.35	107.69	115.49
19	A	1761	CLA	O1A-CGA-CBA	-2.35	114.32	123.72
19	4	4014	CLA	O2D-CGD-O1D	-2.35	118.94	123.79
19	B	1746	CLA	O2D-CGD-O1D	-2.35	118.94	123.79
19	1	1190	CLA	C2A-C1A-CHA	-2.35	119.56	123.89
19	A	1767	CLA	O2D-CGD-O1D	-2.35	118.94	123.79
20	A	7043	LMU	O5B-C5B-C4B	-2.35	105.28	109.68
19	1	1149	CLA	CHD-C4C-C3C	-2.35	121.31	124.94
19	A	1797	CLA	O2A-CGA-O1A	-2.35	117.44	123.49
19	A	1783	CLA	C11-C10-C8	-2.34	107.71	115.49
19	G	1099	CLA	CBC-CAC-C3C	-2.34	105.24	112.39
20	A	7005	LMU	C1'-C2'-C3'	-2.34	105.36	109.97
20	A	7041	LMU	O5B-C1B-C2B	-2.34	105.47	110.28
19	A	1782	CLA	O2D-CGD-O1D	-2.34	118.96	123.79
20	A	7019	LMU	O2'-C2'-C3'	-2.34	105.07	110.34
19	B	1758	CLA	CAA-C2A-C1A	-2.34	104.22	112.47
19	A	1786	CLA	CAA-C2A-C3A	-2.34	106.50	113.22
19	G	1099	CLA	CHC-C1C-C2C	-2.34	120.21	126.35
19	B	1737	CLA	CBC-CAC-C3C	-2.33	105.26	112.39
19	B	1771	CLA	C2A-C1A-CHA	-2.33	119.59	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1806	BCR	C8-C7-C6	-2.33	120.31	127.32
19	A	1774	CLA	CAA-CBA-CGA	-2.33	106.49	113.32
19	L	1166	CLA	CMD-C2D-C3D	-2.33	120.53	125.09
21	B	8055	SUC	O1-C2'-O2'	-2.33	103.12	110.52
21	B	8062	SUC	C6'-C5'-C4'	-2.33	109.58	115.08
22	A	1803	BCR	C11-C12-C13	-2.33	119.47	126.32
22	A	1806	BCR	C35-C13-C14	-2.33	119.47	122.90
20	A	7030	LMU	O2B-C2B-C3B	-2.32	105.11	110.34
19	B	1786	CLA	C11-C10-C8	-2.32	107.78	115.49
20	A	7003	LMU	C1B-O1B-C4'	-2.32	111.94	118.01
22	3	1225	BCR	C8-C7-C6	-2.32	120.35	127.32
22	A	1806	BCR	C20-C19-C18	-2.32	119.49	126.32
22	B	1782	BCR	C29-C30-C25	-2.32	106.69	110.36
21	B	8052	SUC	O1-C2'-O2'	-2.32	103.15	110.52
20	A	7021	LMU	C3B-C4B-C5B	-2.32	106.16	110.20
21	B	8054	SUC	O4'-C4'-C3'	-2.31	104.66	112.01
19	B	1766	CLA	CHC-C1C-C2C	-2.31	120.27	126.35
19	B	1738	CLA	CBC-CAC-C3C	-2.31	105.33	112.39
19	B	1788	CLA	C6-C7-C8	-2.31	107.82	115.49
19	3	1212	CLA	C4-C3-C2	-2.31	115.17	122.61
19	B	1773	CLA	CMD-C2D-C3D	-2.31	120.57	125.09
19	1	1196	CLA	C3A-C2A-C1A	-2.31	97.58	101.50
19	B	1757	CLA	C2A-C1A-CHA	-2.31	119.63	123.89
19	A	1785	CLA	O2A-CGA-O1A	-2.31	117.53	123.49
19	4	1200	CLA	CAC-C3C-C2C	-2.31	123.46	127.51
19	A	1793	CLA	CAA-C2A-C3A	-2.31	106.58	113.22
19	B	1771	CLA	C2C-C1C-NC	-2.31	108.53	110.24
19	B	1765	CLA	CHC-C1C-C2C	-2.31	120.29	126.35
20	A	7050	LMU	O1'-C1-C2	-2.31	100.71	109.88
19	G	1099	CLA	CAC-C3C-C4C	-2.30	121.48	124.83
19	B	1741	CLA	CAC-C3C-C2C	-2.30	123.47	127.51
22	A	1805	BCR	C35-C13-C14	-2.30	119.50	122.90
19	1	1149	CLA	O1D-CGD-CBD	-2.30	121.32	124.62
19	K	1085	CLA	O2D-CGD-O1D	-2.30	119.04	123.79
22	B	1779	BCR	C23-C24-C25	-2.30	120.42	127.32
22	L	1170	BCR	C32-C1-C31	-2.30	101.01	108.37
22	A	1804	BCR	C23-C24-C25	-2.30	120.42	127.32
19	4	4014	CLA	C2A-C1A-CHA	-2.30	119.66	123.89
19	F	1156	CLA	O2D-CGD-O1D	-2.30	119.05	123.79
19	2	1218	CLA	CAA-CBA-CGA	-2.29	106.60	113.32
19	L	1166	CLA	CHC-C1C-C2C	-2.29	120.32	126.35
22	A	1804	BCR	C4-C5-C6	-2.29	119.86	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1763	CLA	C2A-C1A-CHA	-2.29	119.66	123.89
20	A	7040	LMU	O5'-C5'-C4'	-2.29	104.91	109.75
19	A	1799	CLA	O2D-CGD-O1D	-2.29	119.06	123.79
19	2	1220	CLA	CHC-C1C-C2C	-2.29	120.33	126.35
21	B	8054	SUC	O1-C2'-C1'	-2.29	102.36	109.69
19	B	1788	CLA	CMA-C3A-C2A	-2.29	104.23	114.35
19	4	1200	CLA	O1D-CGD-CBD	-2.29	121.34	124.62
22	B	1781	BCR	C11-C12-C13	-2.29	119.59	126.32
19	B	1751	CLA	CMA-C3A-C2A	-2.29	104.24	114.35
22	A	1803	BCR	C20-C19-C18	-2.29	119.59	126.32
19	B	1764	CLA	CAA-C2A-C1A	-2.28	104.42	112.47
19	B	1735	CLA	C2A-C1A-CHA	-2.28	119.69	123.89
19	B	1762	CLA	CHC-C1C-C2C	-2.28	120.36	126.35
22	B	1775	BCR	C23-C24-C25	-2.28	120.48	127.32
22	B	1782	BCR	C10-C11-C12	-2.28	116.19	123.13
22	B	1778	BCR	C37-C22-C21	-2.28	119.54	122.90
22	I	1032	BCR	C28-C27-C26	-2.27	110.26	113.87
19	A	1771	CLA	O1D-CGD-CBD	-2.27	121.37	124.62
19	4	1206	CLA	O2D-CGD-O1D	-2.27	119.10	123.79
19	A	1776	CLA	O2D-CGD-O1D	-2.27	119.11	123.79
19	A	1772	CLA	C4-C3-C2	-2.27	119.05	123.50
19	4	4007	CLA	CMA-C3A-C2A	-2.27	104.32	114.35
19	B	1761	CLA	CHD-C4C-C3C	-2.27	121.44	124.94
19	2	1215	CLA	CAA-C2A-C3A	-2.27	106.70	113.22
19	B	1769	CLA	O1D-CGD-CBD	-2.26	121.39	124.62
19	B	1737	CLA	C6-C7-C8	-2.26	108.00	115.49
19	1	1014	CLA	C11-C12-C13	-2.26	108.00	115.49
22	I	1032	BCR	C31-C1-C6	-2.26	106.77	110.30
19	A	1774	CLA	CAA-C2A-C1A	-2.26	104.52	112.47
19	J	1044	CLA	CMD-C2D-C3D	-2.26	120.68	125.09
19	A	1771	CLA	CHC-C1C-C2C	-2.25	120.42	126.35
20	A	7023	LMU	O5B-C5B-C4B	-2.25	105.45	109.68
20	A	7030	LMU	O5B-C5B-C4B	-2.25	105.45	109.68
19	A	1788	CLA	C4-C3-C2	-2.25	119.08	123.50
20	A	7028	LMU	C1-O1'-C1'	-2.25	110.00	113.94
19	A	1786	CLA	O2A-CGA-O1A	-2.25	117.68	123.49
19	B	1757	CLA	O2D-CGD-O1D	-2.25	119.14	123.79
19	1	1192	CLA	CHC-C1C-C2C	-2.25	120.43	126.35
22	A	1802	BCR	C11-C12-C13	-2.25	119.69	126.32
22	A	1807	BCR	C11-C12-C13	-2.25	119.70	126.32
20	A	7038	LMU	C1'-C2'-C3'	-2.25	105.54	109.97
20	A	7026	LMU	C4B-C3B-C2B	-2.24	106.60	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1505	CLA	C4-C3-C2	-2.24	119.10	123.50
19	A	1769	CLA	O1D-CGD-CBD	-2.24	121.41	124.62
19	J	1043	CLA	C2A-C1A-CHA	-2.24	119.76	123.89
20	A	7014	LMU	O5B-C1B-C2B	-2.24	105.68	110.28
19	B	1744	CLA	C5-C3-C2	-2.24	116.81	121.05
22	B	1778	BCR	C4-C5-C6	-2.24	119.93	122.78
21	B	8053	SUC	O3-C3-C2	-2.24	105.30	110.34
21	B	8053	SUC	C6'-C5'-C4'	-2.24	109.79	115.08
19	1	1190	CLA	CAA-C2A-C3A	-2.24	106.79	113.22
20	1	1200	LMU	O4'-C4B-C3B	-2.24	105.30	110.34
22	B	1776	BCR	C11-C12-C13	-2.24	119.74	126.32
20	1	1200	LMU	O6B-C6B-C5B	-2.23	103.95	111.33
22	B	1781	BCR	C20-C19-C18	-2.23	119.74	126.32
21	3	1226	SUC	C1'-C2'-C3'	-2.23	106.95	114.49
19	B	1735	CLA	C5-C3-C2	-2.23	116.82	121.05
19	B	1739	CLA	C11-C12-C13	-2.23	108.09	115.49
22	B	1776	BCR	C4-C5-C6	-2.23	119.94	122.78
20	A	7022	LMU	O2B-C2B-C3B	-2.23	105.32	110.34
21	B	8059	SUC	C1'-C2'-C3'	-2.23	106.97	114.49
19	A	1779	CLA	CAC-C3C-C2C	-2.23	123.61	127.51
19	3	1219	CLA	C2A-C1A-CHA	-2.23	119.79	123.89
19	B	1762	CLA	C2A-C1A-CHA	-2.23	119.79	123.89
19	A	1779	CLA	CHC-C1C-C2C	-2.22	120.50	126.35
20	A	7042	LMU	C5-C4-C3	-2.22	103.05	114.53
20	B	1783	LMU	O2'-C2'-C1'	-2.22	105.15	110.02
20	4	1212	LMU	C4B-C3B-C2B	-2.22	106.65	110.79
22	A	1806	BCR	C34-C9-C10	-2.22	119.62	122.90
19	B	1760	CLA	C7-C6-C5	-2.22	106.51	113.06
22	B	1778	BCR	C35-C13-C14	-2.22	119.63	122.90
20	A	7037	LMU	C6-C5-C4	-2.21	103.10	114.53
22	B	1775	BCR	C27-C26-C25	-2.21	119.96	122.78
22	A	1805	BCR	C37-C22-C21	-2.21	119.64	122.90
19	B	1786	CLA	C12-C11-C10	-2.21	102.02	112.99
19	B	1742	CLA	CAC-C3C-C2C	-2.21	123.63	127.51
22	B	1778	BCR	C36-C18-C17	-2.21	119.64	122.90
19	4	1197	CLA	CHC-C1C-C2C	-2.21	120.54	126.35
22	A	1807	BCR	C20-C19-C18	-2.21	119.82	126.32
20	A	7021	LMU	O5'-C5'-C6'	-2.21	100.78	106.36
19	A	1812	CLA	O2A-CGA-O1A	-2.21	117.80	123.49
19	A	1788	CLA	O2A-CGA-O1A	-2.20	117.80	123.49
22	B	1780	BCR	C20-C19-C18	-2.20	119.83	126.32
21	F	1158	SUC	O1-C2'-C1'	-2.20	102.63	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1776	BCR	C27-C26-C25	-2.20	119.97	122.78
20	A	7021	LMU	C1-O1'-C1'	-2.20	110.10	113.94
19	G	1099	CLA	CAA-CBA-CGA	-2.20	106.88	113.32
19	1	1148	CLA	CMC-C2C-C1C	-2.20	121.62	125.02
19	B	1772	CLA	C4-C3-C2	-2.20	119.19	123.50
22	I	1032	BCR	C3-C2-C1	-2.20	106.70	114.83
19	3	3011	CLA	C5-C3-C2	-2.20	116.89	121.05
19	1	1014	CLA	C11-C10-C8	-2.19	108.21	115.49
21	B	8052	SUC	C6'-C5'-C4'	-2.19	109.90	115.08
19	G	1099	CLA	O2A-CGA-O1A	-2.19	117.84	123.49
20	R	1056	LMU	C1B-O1B-C4'	-2.19	112.28	118.01
20	A	7020	LMU	C8-C7-C6	-2.19	103.23	114.53
19	A	1799	CLA	CHC-C1C-C2C	-2.19	120.60	126.35
20	A	7020	LMU	O2B-C2B-C3B	-2.18	105.42	110.34
19	F	1157	CLA	CHC-C1C-C2C	-2.18	120.61	126.35
22	A	1804	BCR	C27-C26-C25	-2.18	120.00	122.78
19	A	1797	CLA	CAA-C2A-C3A	-2.18	106.95	113.22
22	A	1803	BCR	C4-C5-C6	-2.18	120.00	122.78
21	B	8053	SUC	O4'-C4'-C5'	-2.18	104.52	111.05
19	A	1783	CLA	CHC-C1C-C2C	-2.18	120.62	126.35
19	3	1224	CLA	C5-C3-C2	-2.18	116.92	121.05
22	B	1775	BCR	C11-C12-C13	-2.18	119.91	126.32
22	B	1776	BCR	C20-C19-C18	-2.18	119.91	126.32
19	B	1742	CLA	C5-C3-C2	-2.17	116.93	121.05
21	B	8053	SUC	C4-C3-C2	-2.17	106.73	110.79
20	A	7039	LMU	O5B-C5B-C4B	-2.17	105.60	109.68
19	4	1198	CLA	CHA-C1A-NA	-2.17	120.71	126.06
19	B	1743	CLA	O2A-CGA-O1A	-2.17	117.89	123.49
19	A	1793	CLA	O2A-CGA-O1A	-2.17	117.89	123.49
19	1	1307	CLA	C1C-NC-C4C	-2.17	103.58	106.07
19	B	1746	CLA	O2A-CGA-O1A	-2.17	117.89	123.49
22	L	1170	BCR	C27-C26-C25	-2.17	120.02	122.78
20	A	7042	LMU	O1B-C1B-C2B	-2.17	102.83	108.10
19	B	1749	CLA	CAA-C2A-C3A	-2.17	106.99	113.22
20	A	7020	LMU	O6B-C6B-C5B	-2.17	104.17	111.33
20	A	7028	LMU	O2B-C2B-C1B	-2.17	105.27	110.02
22	B	1778	BCR	C11-C12-C13	-2.17	119.94	126.32
20	N	1086	LMU	C6B-C5B-C4B	-2.16	107.68	113.02
19	R	1054	CLA	CGD-CBD-CAD	-2.16	103.30	110.62
19	A	1764	CLA	C2A-C1A-CHA	-2.16	119.91	123.89
19	1	1307	CLA	C2C-C1C-CHC	-2.16	121.31	125.15
21	B	8053	SUC	C1'-C2'-C3'	-2.16	107.19	114.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1802	BCR	C20-C19-C18	-2.16	119.96	126.32
22	A	1805	BCR	C34-C9-C10	-2.16	119.71	122.90
19	B	1761	CLA	CAA-CBA-CGA	-2.16	106.99	113.32
19	3	1218	CLA	O2D-CGD-O1D	-2.16	119.33	123.79
19	A	1812	CLA	C16-C15-C13	-2.16	108.33	115.49
21	B	8056	SUC	O3-C3-C2	-2.16	105.48	110.34
19	A	1772	CLA	C2A-C1A-CHA	-2.16	119.91	123.89
19	4	1196	CLA	O2D-CGD-O1D	-2.16	119.34	123.79
20	B	1783	LMU	O2'-C2'-C3'	-2.16	105.48	110.34
22	A	1805	BCR	C27-C26-C25	-2.15	120.03	122.78
22	B	1779	BCR	C11-C12-C13	-2.15	119.98	126.32
19	1	1146	CLA	O1D-CGD-CBD	-2.15	121.53	124.62
19	A	1790	CLA	O2A-CGA-O1A	-2.15	117.93	123.49
19	A	1766	CLA	C3B-C4B-NB	-2.15	106.43	109.21
22	A	1805	BCR	C36-C18-C17	-2.15	119.72	122.90
22	B	1775	BCR	C20-C19-C18	-2.15	119.98	126.32
19	1	1189	CLA	C2A-C1A-CHA	-2.15	119.92	123.89
19	B	1735	CLA	O2A-CGA-O1A	-2.15	117.94	123.49
19	A	1787	CLA	CMB-C2B-C1B	-2.15	124.81	128.36
19	1	1195	CLA	CHC-C1C-C2C	-2.15	120.70	126.35
19	B	1753	CLA	C2A-C1A-CHA	-2.15	119.93	123.89
20	B	1783	LMU	O5'-C5'-C6'	-2.15	100.93	106.36
20	A	7043	LMU	C1B-C2B-C3B	-2.14	105.75	109.97
20	A	7049	LMU	O3B-C3B-C4B	-2.14	105.51	110.34
20	A	7036	LMU	O5'-C1'-O1'	-2.14	104.89	110.05
19	4	1200	CLA	C2C-C1C-NC	-2.14	108.65	110.24
20	1	1200	LMU	C1B-C2B-C3B	-2.14	105.75	109.97
19	A	1794	CLA	CBC-CAC-C3C	-2.14	105.86	112.39
20	A	7023	LMU	O4'-C4B-C5B	-2.14	103.57	109.24
19	A	1762	CLA	O2A-CGA-O1A	-2.14	117.97	123.49
22	A	1806	BCR	C37-C22-C21	-2.14	119.74	122.90
19	1	1191	CLA	C2D-C1D-ND	-2.14	108.23	110.13
19	A	1772	CLA	CAA-C2A-C1A	-2.14	104.93	112.47
22	A	1805	BCR	C30-C25-C26	-2.14	119.52	122.66
19	A	1800	CLA	O1D-CGD-CBD	-2.14	121.56	124.62
19	B	1772	CLA	C2A-C1A-CHA	-2.14	119.95	123.89
19	1	1142	CLA	O2D-CGD-O1D	-2.14	119.38	123.79
20	A	7037	LMU	O2'-C2'-C3'	-2.14	105.53	110.34
22	L	1169	BCR	C24-C23-C22	-2.13	122.96	126.22
19	B	1735	CLA	CHC-C1C-C2C	-2.13	120.74	126.35
19	J	1044	CLA	C6-C5-C3	-2.13	107.81	112.48
22	A	1806	BCR	C1-C6-C5	-2.13	119.53	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	8056	SUC	C2'-O1-C1	-2.13	111.92	117.53
22	B	1778	BCR	C20-C19-C18	-2.13	120.05	126.32
19	B	1746	CLA	CHC-C1C-C2C	-2.13	120.75	126.35
22	A	1804	BCR	C20-C19-C18	-2.13	120.06	126.32
19	B	1761	CLA	CAA-C2A-C3A	-2.12	107.11	113.22
22	B	1782	BCR	C16-C15-C14	-2.12	118.69	123.39
19	B	1743	CLA	C2A-C1A-CHA	-2.12	119.97	123.89
20	A	7041	LMU	O1'-C1-C2	-2.12	101.43	109.88
19	1	1189	CLA	CHC-C1C-C2C	-2.12	120.77	126.35
22	A	1806	BCR	C27-C26-C25	-2.12	120.08	122.78
19	A	1768	CLA	C2A-C1A-CHA	-2.12	119.98	123.89
20	A	7016	LMU	C4-C3-C2	-2.12	103.58	114.53
20	A	7037	LMU	O5B-C1B-C2B	-2.12	105.93	110.28
19	B	1786	CLA	O2D-CGD-O1D	-2.12	119.42	123.79
19	B	1750	CLA	CMD-C2D-C3D	-2.12	120.95	125.09
20	A	7050	LMU	O5B-C5B-C6B	-2.11	101.01	106.36
22	B	1781	BCR	C27-C26-C25	-2.11	120.09	122.78
20	A	7022	LMU	C6'-C5'-C4'	-2.11	107.10	113.25
19	A	1811	CLA	CMD-C2D-C3D	-2.11	120.96	125.09
19	A	1772	CLA	CHC-C1C-C2C	-2.11	120.80	126.35
20	A	7048	LMU	C1B-C2B-C3B	-2.11	105.82	109.97
19	B	1787	CLA	CAC-C3C-C2C	-2.11	123.82	127.51
22	A	1804	BCR	C1-C6-C5	-2.10	119.57	122.66
19	2	1218	CLA	C11-C10-C8	-2.10	108.51	115.49
19	1	1196	CLA	C6-C5-C3	-2.10	101.92	112.89
19	2	1222	CLA	CAA-C2A-C3A	-2.10	107.17	113.22
19	A	1781	CLA	O2D-CGD-O1D	-2.10	119.45	123.79
19	4	1200	CLA	C3D-CAD-CBD	-2.10	104.62	107.60
22	L	1169	BCR	C23-C24-C25	-2.10	121.00	127.32
19	A	1794	CLA	CAA-CBA-CGA	-2.10	107.17	113.32
22	A	1804	BCR	C11-C12-C13	-2.10	120.13	126.32
19	B	1748	CLA	CMB-C2B-C1B	-2.10	124.89	128.36
22	B	1778	BCR	C1-C6-C5	-2.10	119.58	122.66
22	A	1806	BCR	C30-C25-C26	-2.10	119.58	122.66
19	A	1786	CLA	CAC-C3C-C2C	-2.10	123.83	127.51
22	B	1779	BCR	C20-C19-C18	-2.10	120.14	126.32
19	B	1745	CLA	C2A-C1A-CHA	-2.09	120.03	123.89
19	A	1794	CLA	OBD-CAD-C3D	-2.09	124.09	128.35
19	A	1763	CLA	CHD-C4C-C3C	-2.09	121.71	124.94
20	A	7013	LMU	O5'-C1'-C2'	-2.09	105.99	110.28
19	2	1218	CLA	C6-C7-C8	-2.09	108.56	115.49
20	L	1171	LMU	C1B-C2B-C3B	-2.09	105.86	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7049	LMU	O2B-C2B-C1B	-2.09	105.45	110.02
19	B	1761	CLA	CAC-C3C-C2C	-2.08	123.86	127.51
19	A	1810	CLA	C2A-C1A-CHA	-2.08	120.05	123.89
22	B	1778	BCR	C34-C9-C10	-2.08	119.82	122.90
22	B	1781	BCR	C35-C13-C14	-2.08	119.83	122.90
22	3	1225	BCR	C39-C30-C25	-2.08	107.04	110.30
20	A	7016	LMU	C6B-C5B-C4B	-2.08	107.88	113.02
22	B	1779	BCR	C27-C26-C25	-2.08	120.13	122.78
19	B	1744	CLA	CAC-C3C-C4C	-2.08	121.81	124.83
19	B	1787	CLA	C2C-C1C-NC	-2.08	108.70	110.24
20	A	7035	LMU	O1B-C1B-O5B	-2.07	105.43	110.68
20	A	7024	LMU	C1'-O5'-C5'	-2.07	109.72	113.75
19	1	1192	CLA	CMD-C2D-C3D	-2.07	121.03	125.09
19	A	1777	CLA	CHC-C1C-C2C	-2.07	120.90	126.35
19	F	1155	CLA	CAA-C2A-C3A	-2.07	111.24	116.20
19	2	1220	CLA	CAA-C2A-C3A	-2.07	111.25	116.20
19	B	1736	CLA	C2A-C1A-CHA	-2.07	120.08	123.89
19	1	1505	CLA	CBA-CAA-C2A	-2.07	107.91	113.73
19	A	1796	CLA	C2A-C1A-CHA	-2.07	120.08	123.89
22	B	1781	BCR	C37-C22-C21	-2.06	119.85	122.90
19	A	1767	CLA	C4-C3-C2	-2.06	119.45	123.50
19	A	1810	CLA	CBC-CAC-C3C	-2.06	106.09	112.39
20	A	7048	LMU	C6-C5-C4	-2.06	103.87	114.53
19	B	1767	CLA	CHC-C1C-C2C	-2.06	120.93	126.35
19	B	1747	CLA	CBA-CAA-C2A	-2.06	107.92	113.73
22	B	1776	BCR	C37-C22-C21	-2.06	119.86	122.90
22	B	1780	BCR	C15-C16-C17	-2.06	118.84	123.39
19	2	1217	CLA	C16-C17-C18	-2.06	105.51	115.87
19	A	1769	CLA	CBC-CAC-C3C	-2.05	106.12	112.39
19	1	1307	CLA	C3B-C4B-NB	-2.05	108.25	110.09
19	B	1759	CLA	C12-C11-C10	-2.05	102.80	112.99
19	L	1167	CLA	O2A-CGA-O1A	-2.05	118.19	123.49
19	L	1166	CLA	CAA-CBA-CGA	-2.05	107.31	113.32
22	B	1775	BCR	C36-C18-C17	-2.05	119.87	122.90
22	A	1804	BCR	C35-C13-C14	-2.05	119.87	122.90
19	B	1738	CLA	C2A-C1A-CHA	-2.05	120.11	123.89
19	A	1766	CLA	CAA-C2A-C1A	-2.05	105.25	112.47
22	B	1776	BCR	C35-C13-C14	-2.04	119.88	122.90
19	A	1776	CLA	C5-C3-C2	-2.04	117.17	121.05
21	B	8056	SUC	O4'-C4'-C3'	-2.04	105.52	112.01
20	A	7036	LMU	O2'-C2'-C1'	-2.04	105.54	110.02
22	A	1805	BCR	C11-C12-C13	-2.04	120.31	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	1170	BCR	C23-C24-C25	-2.04	121.19	127.32
20	A	1809	LMU	O6'-C6'-C5'	-2.04	104.59	111.33
19	3	1218	CLA	C2A-C1A-CHA	-2.04	120.13	123.89
20	A	1809	LMU	O3'-C3'-C2'	-2.04	105.75	110.34
19	B	1754	CLA	C2C-C1C-NC	-2.03	108.73	110.24
19	A	1812	CLA	O1D-CGD-CBD	-2.03	121.71	124.62
20	A	7036	LMU	O1B-C4'-C3'	-2.03	101.92	107.17
19	4	1197	CLA	CAA-C2A-C1A	-2.03	106.55	112.17
19	B	1738	CLA	CBA-CAA-C2A	-2.03	108.01	113.73
22	B	1777	BCR	C28-C27-C26	-2.03	110.65	113.87
22	B	1777	BCR	C8-C7-C6	-2.02	121.24	127.32
19	1	1308	CLA	O2D-CGD-O1D	-2.02	119.62	123.79
22	A	1805	BCR	C20-C19-C18	-2.02	120.38	126.32
19	F	1156	CLA	CMA-C3A-C2A	-2.02	111.37	116.20
19	A	1783	CLA	O2D-CGD-O1D	-2.02	119.62	123.79
20	A	7016	LMU	O6'-C6'-C5'	-2.02	104.67	111.33
23	A	1801	PQN	O1-C1-C10	-2.02	118.16	121.55
22	A	1804	BCR	C36-C18-C17	-2.01	119.93	122.90
19	F	1156	CLA	CAA-C2A-C3A	-2.01	111.38	116.20
22	B	1775	BCR	C34-C9-C10	-2.01	119.93	122.90
20	A	7036	LMU	O5'-C5'-C4'	-2.01	105.50	109.75
22	B	1780	BCR	C8-C9-C10	-2.01	115.75	118.98
21	B	8061	SUC	O1'-C1'-C2'	-2.01	105.49	111.91
22	B	1778	BCR	C27-C26-C25	-2.01	120.22	122.78
22	B	1778	BCR	C30-C25-C26	-2.01	119.71	122.66
20	A	7005	LMU	O2B-C2B-C3B	-2.01	105.82	110.34
19	B	1735	CLA	C3B-C4B-NB	-2.01	106.62	109.21
22	B	1776	BCR	C36-C18-C17	-2.01	119.94	122.90
22	A	1806	BCR	C11-C12-C13	-2.01	120.42	126.32
19	B	1749	CLA	O2D-CGD-O1D	-2.00	119.65	123.79
19	B	1788	CLA	O1D-CGD-CBD	-2.00	121.75	124.62
20	A	7037	LMU	C4-C3-C2	-2.00	104.20	114.53
21	B	8060	SUC	O2'-C2'-C3'	2.00	110.13	105.58
19	A	1785	CLA	CHB-C4A-NA	2.00	127.28	124.51
19	1	1193	CLA	CMC-C2C-C1C	2.00	128.12	125.02
19	B	1735	CLA	C6-C5-C3	2.01	116.89	112.48
19	L	1167	CLA	CMC-C2C-C1C	2.01	128.12	125.02
20	A	7016	LMU	C4B-C3B-C2B	2.01	114.54	110.79
21	B	8061	SUC	C2'-C3'-C4'	2.01	107.05	102.00
19	A	1769	CLA	C4A-NA-C1A	2.01	108.96	106.36
19	B	1764	CLA	CBA-CAA-C2A	2.01	119.41	113.73
19	1	1191	CLA	C2B-C3B-C4B	2.01	108.05	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1764	CLA	CAC-C3C-C4C	2.01	127.75	124.83
20	A	7017	LMU	C3B-C4B-C5B	2.01	113.71	110.20
19	B	1743	CLA	CAA-CBA-CGA	2.01	119.21	113.32
19	1	1187	CLA	CAA-C2A-C1A	2.01	119.58	112.47
21	F	1158	SUC	O1-C2'-O2'	2.01	116.91	110.52
20	A	7015	LMU	O4'-C4B-C5B	2.02	114.58	109.24
20	A	7021	LMU	O5B-C5B-C6B	2.02	111.46	106.36
19	K	1085	CLA	C5-C3-C4	2.02	119.61	114.64
19	A	1765	CLA	CHB-C4A-NA	2.02	127.31	124.51
19	B	1760	CLA	CMB-C2B-C1B	2.02	131.71	128.36
19	2	1220	CLA	CMB-C2B-C1B	2.03	131.72	128.36
19	R	1055	CLA	CAA-CBA-CGA	2.03	119.26	113.32
19	3	1212	CLA	C3B-C4B-NB	2.03	111.83	109.21
19	J	1044	CLA	C4-C3-C5	2.03	118.51	115.41
19	A	1791	CLA	C4A-NA-C1A	2.04	108.99	106.36
19	2	1215	CLA	CMB-C2B-C3B	2.04	129.08	125.09
19	B	1752	CLA	O2A-CGA-CBA	2.04	120.88	112.36
19	B	1739	CLA	C3A-C2A-C1A	2.04	104.97	101.50
19	B	1758	CLA	CAC-C3C-C2C	2.04	131.09	127.51
19	3	1217	CLA	C2B-C3B-C4B	2.05	108.08	106.29
19	3	1212	CLA	C2C-C1C-NC	2.05	111.77	110.24
19	B	1748	CLA	C4-C3-C5	2.05	118.53	115.41
19	B	1770	CLA	CHB-C4A-NA	2.05	127.35	124.51
19	B	1787	CLA	C4A-NA-C1A	2.05	109.01	106.36
19	4	1200	CLA	CAA-C2A-C3A	2.05	119.11	113.22
19	3	3015	CLA	C2B-C3B-C4B	2.05	108.08	106.29
19	B	1750	CLA	CHB-C4A-NA	2.05	127.35	124.51
19	4	1204	CLA	C2A-C1A-NA	2.05	115.16	110.36
20	A	7014	LMU	O4'-C4B-C3B	2.06	114.97	110.34
19	4	1197	CLA	CMC-C2C-C1C	2.06	128.20	125.02
19	A	1796	CLA	C5-C3-C2	2.06	124.95	121.05
20	L	1171	LMU	O2B-C2B-C1B	2.06	114.54	110.02
19	1	1196	CLA	C3B-C4B-NB	2.06	111.88	109.21
19	A	1799	CLA	C4A-NA-C1A	2.06	109.03	106.36
20	A	7047	LMU	C1B-C2B-C3B	2.07	114.04	109.97
19	A	1767	CLA	O2A-CGA-CBA	2.07	118.20	111.90
19	2	1213	CLA	CED-O2D-CGD	2.07	120.84	115.99
19	B	1772	CLA	C6-C5-C3	2.07	117.03	112.48
19	B	1743	CLA	O2A-CGA-CBA	2.07	118.21	111.90
22	L	1170	BCR	C23-C22-C21	2.07	122.32	118.98
19	L	1168	CLA	CHB-C4A-NA	2.07	127.38	124.51
19	2	1219	CLA	C3B-C4B-NB	2.07	111.95	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1749	CLA	CED-O2D-CGD	2.08	120.87	115.99
19	1	1014	CLA	C2C-C1C-NC	2.08	111.79	110.24
19	A	1767	CLA	C4-C3-C5	2.08	118.59	115.41
19	B	1748	CLA	CAC-C3C-C4C	2.08	127.85	124.83
20	A	7024	LMU	C3'-C4'-C5'	2.08	115.55	110.84
19	R	1055	CLA	CHB-C4A-NA	2.09	127.40	124.51
19	A	1779	CLA	CGD-CBD-CAD	2.09	117.70	110.62
20	A	7019	LMU	C4B-C3B-C2B	2.09	114.69	110.79
20	N	1086	LMU	O1B-C4'-C5'	2.09	114.81	109.32
20	A	7014	LMU	O5B-C5B-C4B	2.09	113.60	109.68
20	A	7049	LMU	O3B-C3B-C2B	2.09	115.04	110.34
19	A	1777	CLA	CED-O2D-CGD	2.09	120.89	115.99
19	A	1799	CLA	O2A-CGA-CBA	2.09	118.27	111.90
19	L	1167	CLA	CMB-C2B-C3B	2.09	129.18	125.09
19	2	1215	CLA	CED-O2D-CGD	2.10	120.91	115.99
19	A	1760	CLA	C6-C5-C3	2.10	117.08	112.48
20	A	7014	LMU	O1B-C4'-C3'	2.10	112.58	107.17
19	B	1751	CLA	CMB-C2B-C3B	2.10	129.19	125.09
19	3	1224	CLA	CGD-CBD-CAD	2.10	117.74	110.62
19	1	1145	CLA	C4-C3-C5	2.10	118.61	115.41
19	B	1736	CLA	CMB-C2B-C3B	2.10	129.19	125.09
20	A	7025	LMU	C3'-C4'-C5'	2.10	115.59	110.84
21	B	8061	SUC	O1-C2'-C3'	2.10	115.37	108.04
19	2	1216	CLA	C2A-C1A-NA	2.10	115.28	110.36
19	1	1148	CLA	CHB-C4A-NA	2.11	127.42	124.51
20	4	1212	LMU	C1B-C2B-C3B	2.11	114.12	109.97
20	A	7033	LMU	C1'-C2'-C3'	2.11	114.12	109.97
19	B	1757	CLA	CHB-C4A-NA	2.11	127.43	124.51
19	B	1742	CLA	CHB-C4A-NA	2.11	127.43	124.51
19	4	1203	CLA	C3B-C4B-NB	2.11	111.98	110.09
20	A	7027	LMU	O6B-C6B-C5B	2.11	118.31	111.33
19	A	1791	CLA	C3B-C4B-NB	2.11	111.94	109.21
19	B	1763	CLA	CBA-CAA-C2A	2.12	119.70	113.73
19	B	1764	CLA	C3A-C2A-C1A	2.12	105.09	101.50
19	B	1735	CLA	O2A-CGA-CBA	2.12	118.37	111.90
20	A	7031	LMU	O5'-C5'-C6'	2.12	111.72	106.36
19	1	1197	CLA	C2B-C3B-C4B	2.12	108.14	106.29
19	L	1166	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	A	1783	CLA	CMB-C2B-C3B	2.13	129.25	125.09
19	1	1198	CLA	C2B-C3B-C4B	2.13	108.15	106.29
19	2	1220	CLA	CAC-C3C-C4C	2.13	128.32	125.02
19	B	1773	CLA	CAC-C3C-C4C	2.14	128.32	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1741	CLA	CHB-C4A-NA	2.14	127.47	124.51
19	A	1776	CLA	CMB-C2B-C3B	2.14	129.28	125.09
19	A	1772	CLA	CMB-C2B-C3B	2.14	129.28	125.09
20	A	7013	LMU	O2B-C2B-C1B	2.14	114.72	110.02
19	B	1766	CLA	CMB-C2B-C3B	2.14	129.28	125.09
19	2	1217	CLA	CHB-C4A-NA	2.15	127.48	124.51
19	B	1754	CLA	CHC-C1C-NC	2.15	127.71	123.67
20	A	7047	LMU	O5B-C5B-C6B	2.15	111.78	106.36
19	A	1769	CLA	CMB-C2B-C3B	2.15	129.29	125.09
19	1	1146	CLA	CED-O2D-CGD	2.16	121.05	115.99
19	A	1771	CLA	C5-C3-C4	2.16	119.94	114.64
19	B	1752	CLA	CMB-C2B-C3B	2.16	129.31	125.09
19	A	1800	CLA	CED-O2D-CGD	2.16	121.06	115.99
19	B	1747	CLA	CED-O2D-CGD	2.16	121.06	115.99
19	B	1766	CLA	CHB-C4A-NA	2.17	127.51	124.51
21	B	8056	SUC	C6'-C5'-C4'	2.17	120.21	115.08
19	4	1206	CLA	CAC-C3C-C4C	2.17	127.98	124.83
20	A	7039	LMU	O2B-C2B-C1B	2.17	114.78	110.02
19	B	1738	CLA	C4-C3-C5	2.17	118.73	115.41
21	B	8062	SUC	O1-C2'-C3'	2.18	115.63	108.04
19	2	1222	CLA	O2A-CGA-CBA	2.18	118.53	111.90
19	A	1792	CLA	CHB-C4A-NA	2.18	127.52	124.51
19	4	1205	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	R	1055	CLA	CMB-C2B-C1B	2.18	131.97	128.36
19	A	1811	CLA	CMB-C2B-C3B	2.18	129.36	125.09
20	A	7041	LMU	C1'-O5'-C5'	2.18	117.98	113.75
20	A	7042	LMU	O4'-C4B-C5B	2.18	115.03	109.24
19	2	1213	CLA	C3A-C2A-C1A	2.19	105.21	101.50
19	3	1212	CLA	CED-O2D-CGD	2.19	121.12	115.99
19	A	1774	CLA	CHB-C4A-NA	2.19	127.54	124.51
19	1	1505	CLA	CHB-C4A-NA	2.19	127.54	124.51
19	1	1191	CLA	C2A-C1A-NA	2.19	115.48	110.36
19	A	1797	CLA	CAC-C3C-C2C	2.19	131.35	127.51
19	2	1215	CLA	O2A-CGA-CBA	2.19	118.58	111.90
20	A	7040	LMU	O4'-C4B-C3B	2.19	115.28	110.34
20	A	7020	LMU	O5B-C5B-C4B	2.20	113.80	109.68
19	3	1218	CLA	C3B-C4B-NB	2.20	112.05	109.21
19	1	1187	CLA	CMA-C3A-C2A	2.20	124.08	114.35
20	A	7023	LMU	O3'-C3'-C4'	2.20	115.08	109.87
20	A	7038	LMU	O1'-C1'-C2'	2.20	110.82	108.04
19	A	1786	CLA	CGD-CBD-CAD	2.21	118.10	110.62
19	4	1202	CLA	CHB-C4A-NA	2.21	127.56	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3008	CLA	CMB-C2B-C3B	2.21	129.41	125.09
20	A	1809	LMU	C1B-C2B-C3B	2.21	114.33	109.97
19	B	1771	CLA	CBA-CAA-C2A	2.21	119.98	113.73
19	2	1218	CLA	C2C-C1C-NC	2.21	111.89	110.24
19	A	1811	CLA	CED-O2D-CGD	2.22	121.19	115.99
19	2	1222	CLA	C5-C3-C4	2.22	120.09	114.64
19	B	1754	CLA	O1D-CGD-CBD	2.22	127.80	124.62
19	4	1201	CLA	C4A-NA-C1A	2.22	109.22	106.36
20	A	7025	LMU	O1'-C1'-C2'	2.22	110.84	108.04
19	4	1206	CLA	CED-O2D-CGD	2.22	121.19	115.99
19	3	1223	CLA	C2C-C3C-C4C	2.22	109.73	107.23
19	B	1737	CLA	CMB-C2B-C1B	2.22	132.03	128.36
21	3	1226	SUC	C6-C5-C4	2.22	118.48	113.02
20	A	1809	LMU	C1'-C2'-C3'	2.22	114.34	109.97
19	4	1211	CLA	C3A-C2A-C1A	2.22	105.26	101.50
22	B	1777	BCR	C2-C1-C6	2.22	113.88	110.36
19	A	1766	CLA	CED-O2D-CGD	2.22	121.20	115.99
19	1	1010	CLA	C2B-C3B-C4B	2.22	108.23	106.29
19	B	1739	CLA	CAC-C3C-C4C	2.22	128.06	124.83
21	B	8056	SUC	O5-C5-C6	2.23	111.98	106.36
19	B	1768	CLA	CAC-C3C-C4C	2.23	128.06	124.83
19	A	1778	CLA	CED-O2D-CGD	2.23	121.21	115.99
19	2	1212	CLA	CHB-C4A-NA	2.23	127.59	124.51
19	2	1214	CLA	C3B-C4B-NB	2.23	112.09	110.09
19	B	1753	CLA	CHB-C4A-NA	2.23	127.59	124.51
19	1	1192	CLA	CMB-C2B-C3B	2.23	129.45	125.09
19	A	1786	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	F	1157	CLA	CMC-C2C-C1C	2.23	128.47	125.02
20	A	7022	LMU	C1'-C2'-C3'	2.23	114.37	109.97
19	L	1167	CLA	CAC-C3C-C4C	2.23	128.07	124.83
20	A	7015	LMU	O1B-C1B-C2B	2.24	113.54	108.10
23	A	1801	PQN	C8-C7-C6	2.24	123.46	120.19
20	A	7024	LMU	C1B-O5B-C5B	2.24	118.09	113.75
20	A	7022	LMU	O5'-C5'-C4'	2.24	114.47	109.75
22	L	1170	BCR	C11-C10-C9	2.24	130.43	127.20
19	B	1763	CLA	C9-C8-C10	2.24	119.68	111.08
19	B	1735	CLA	C3A-C2A-C1A	2.24	105.30	101.50
19	4	1204	CLA	C2B-C3B-C4B	2.24	108.25	106.29
22	3	1225	BCR	C35-C13-C12	2.24	121.83	118.10
19	4	1206	CLA	CMB-C2B-C3B	2.24	129.48	125.09
19	1	1145	CLA	CED-O2D-CGD	2.25	121.26	115.99
19	A	1792	CLA	O2A-CGA-CBA	2.25	118.75	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1770	CLA	CED-O2D-CGD	2.25	121.27	115.99
19	K	1085	CLA	CHB-C4A-NA	2.25	127.63	124.51
19	A	1795	CLA	CGD-CBD-CAD	2.26	118.27	110.62
21	B	8053	SUC	C2'-O1-C1	2.26	123.48	117.53
19	B	1770	CLA	O2A-CGA-CBA	2.26	118.78	111.90
19	B	1760	CLA	O2A-CGA-CBA	2.26	118.79	111.90
20	A	7026	LMU	O5B-C1B-C2B	2.26	114.92	110.28
19	B	1761	CLA	CHB-C4A-NA	2.27	127.65	124.51
20	A	7043	LMU	O2B-C2B-C3B	2.27	115.44	110.34
22	B	1782	BCR	C15-C14-C13	2.27	130.47	127.20
20	2	1224	LMU	O5'-C5'-C6'	2.27	112.10	106.36
20	A	7027	LMU	C1'-O5'-C5'	2.27	118.16	113.75
19	4	1200	CLA	CED-O2D-CGD	2.28	121.33	115.99
19	A	1771	CLA	CED-O2D-CGD	2.28	121.33	115.99
20	A	1808	LMU	C3B-C4B-C5B	2.28	114.17	110.20
19	F	1156	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	B	1750	CLA	CAA-C2A-C1A	2.28	120.52	112.47
19	A	1769	CLA	C4-C3-C5	2.28	118.90	115.41
19	A	1797	CLA	CHB-C4A-NA	2.29	127.67	124.51
20	A	7022	LMU	C1B-O1B-C4'	2.29	123.98	118.01
19	A	1798	CLA	C5-C3-C4	2.29	120.27	114.64
19	1	1307	CLA	C3D-C4D-ND	2.29	112.16	110.13
20	A	7027	LMU	C3B-C4B-C5B	2.29	114.19	110.20
19	2	1217	CLA	CAA-C2A-C3A	2.29	119.81	113.22
19	1	1303	CLA	C3D-C4D-ND	2.29	112.17	110.13
19	B	1767	CLA	CED-O2D-CGD	2.29	121.37	115.99
19	A	1796	CLA	CHC-C1C-NC	2.30	127.99	123.67
19	A	1811	CLA	C4-C3-C5	2.30	118.91	115.41
20	A	1808	LMU	O1'-C1'-C2'	2.30	110.94	108.04
19	A	1762	CLA	CED-O2D-CGD	2.30	121.38	115.99
22	B	1782	BCR	C8-C9-C10	2.30	122.69	118.98
22	L	1170	BCR	C2-C1-C6	2.30	114.00	110.36
20	A	7048	LMU	O3'-C3'-C4'	2.30	115.31	109.87
22	B	1777	BCR	C35-C13-C12	2.30	121.93	118.10
19	4	1201	CLA	C4C-C3C-C2C	2.31	110.69	106.94
19	A	1782	CLA	CHB-C4A-NA	2.31	127.70	124.51
20	1	1200	LMU	O1B-C4'-C3'	2.31	113.12	107.17
22	B	1782	BCR	C20-C19-C18	2.31	133.11	126.32
19	B	1787	CLA	O2A-CGA-CBA	2.31	118.94	111.90
19	A	1771	CLA	CMC-C2C-C1C	2.31	128.60	125.02
19	A	1798	CLA	O2A-CGA-CBA	2.31	118.94	111.90
21	B	8060	SUC	O2'-C5'-C6'	2.31	115.57	108.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1210	CLA	C3D-C4D-ND	2.31	112.18	110.13
21	B	8061	SUC	O5-C1-O1	2.31	117.73	109.96
19	1	1148	CLA	CMB-C2B-C3B	2.32	129.62	125.09
19	B	1766	CLA	CED-O2D-CGD	2.32	121.43	115.99
19	A	1785	CLA	CAA-CBA-CGA	2.32	120.11	113.32
19	A	1761	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	B	1758	CLA	C4-C3-C5	2.32	118.95	115.41
21	B	8054	SUC	O5-C1-C2	2.32	115.05	110.28
19	B	1772	CLA	O2D-CGD-CBD	2.33	114.49	111.30
19	4	4014	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	A	7027	LMU	O5'-C1'-C2'	2.33	115.06	110.28
20	A	7043	LMU	O5B-C5B-C6B	2.33	112.25	106.36
19	A	1796	CLA	CMB-C2B-C3B	2.33	129.65	125.09
19	4	1197	CLA	CAC-C3C-C4C	2.33	128.63	125.02
19	A	1780	CLA	C14-C13-C12	2.34	120.05	111.08
20	A	7017	LMU	O5'-C5'-C4'	2.34	114.68	109.75
21	F	1158	SUC	O5-C5-C6	2.34	112.26	106.36
19	A	1776	CLA	CHB-C4A-NA	2.34	127.75	124.51
20	A	7038	LMU	O5'-C1'-C2'	2.34	115.08	110.28
19	B	1738	CLA	C4A-NA-C1A	2.34	109.38	106.36
19	G	1099	CLA	CED-O2D-CGD	2.34	121.48	115.99
20	A	7022	LMU	O4'-C4B-C5B	2.34	115.44	109.24
20	A	7049	LMU	C1B-O5B-C5B	2.34	118.29	113.75
19	1	1187	CLA	C2C-C1C-NC	2.34	111.99	110.24
19	3	1222	CLA	C6-C5-C3	2.35	117.63	112.48
21	B	8053	SUC	O2'-C5'-C6'	2.35	115.68	108.57
19	A	1761	CLA	C4-C3-C5	2.35	118.99	115.41
20	A	7023	LMU	C1'-C2'-C3'	2.35	114.60	109.97
22	B	1780	BCR	C12-C13-C14	2.35	122.77	118.98
22	B	1777	BCR	C1-C6-C7	2.35	122.40	115.82
19	B	1739	CLA	C4A-NA-C1A	2.35	109.40	106.36
19	A	1767	CLA	C3A-C2A-C1A	2.35	105.48	101.50
20	A	7042	LMU	O5B-C5B-C6B	2.35	112.30	106.36
19	2	1221	CLA	C2B-C3B-C4B	2.36	108.35	106.29
19	A	1788	CLA	C4-C3-C5	2.36	119.00	115.41
19	3	1218	CLA	CED-O2D-CGD	2.36	121.53	115.99
20	A	7028	LMU	O1B-C4'-C5'	2.36	115.53	109.32
19	A	1773	CLA	C4-C3-C5	2.36	119.02	115.41
19	A	1784	CLA	CGD-CBD-CAD	2.37	118.65	110.62
19	L	1168	CLA	CMC-C2C-C1C	2.37	128.69	125.02
22	B	1777	BCR	C33-C5-C4	2.37	117.92	113.43
19	A	1770	CLA	CHB-C4A-NA	2.37	127.79	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	1171	LMU	O1B-C1B-O5B	2.37	116.69	110.68
19	A	1778	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	A	1764	CLA	CMB-C2B-C3B	2.37	129.73	125.09
19	1	1148	CLA	CHC-C1C-NC	2.37	128.14	123.67
20	A	7013	LMU	O1'-C1'-C2'	2.38	111.04	108.04
19	A	1795	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	4	1198	CLA	C1C-C2C-C3C	2.38	109.75	106.91
19	B	1747	CLA	CAC-C3C-C4C	2.38	128.28	124.83
19	3	3008	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	A	1810	CLA	CHC-C1C-NC	2.38	128.15	123.67
19	A	1789	CLA	CHB-C4A-NA	2.38	127.81	124.51
20	A	7025	LMU	O2B-C2B-C1B	2.39	115.25	110.02
19	1	1190	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	2	1223	CLA	C4A-NA-C1A	2.39	109.45	106.36
19	R	1055	CLA	C4A-NA-C1A	2.39	109.45	106.36
20	A	7019	LMU	C3'-C4'-C5'	2.40	116.26	110.84
19	A	1760	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	B	1745	CLA	CAC-C3C-C4C	2.40	128.31	124.83
19	3	1215	CLA	C3D-C2D-C1D	2.40	108.42	106.30
19	A	1774	CLA	CED-O2D-CGD	2.40	121.62	115.99
21	B	8054	SUC	C3-C4-C5	2.40	114.39	110.20
19	B	1786	CLA	CMB-C2B-C3B	2.40	129.79	125.09
19	A	1783	CLA	C4-C3-C5	2.40	119.08	115.41
21	B	8062	SUC	O1-C1-C2	2.41	116.39	108.36
19	4	1207	CLA	C3D-C2D-C1D	2.41	108.42	106.30
19	3	1219	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	B	1788	CLA	CED-O2D-CGD	2.41	121.64	115.99
19	A	1799	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	A	7025	LMU	O4'-C4B-C3B	2.41	115.76	110.34
21	2	1225	SUC	O3-C3-C4	2.41	115.76	110.34
19	1	1189	CLA	CAC-C3C-C4C	2.42	128.34	124.83
19	I	1031	CLA	C4-C3-C5	2.42	119.10	115.41
19	A	1786	CLA	CBA-CAA-C2A	2.42	120.56	113.73
19	3	1214	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	B	8062	SUC	O1-C2'-O2'	2.42	118.20	110.52
20	A	7026	LMU	O1B-C1B-O5B	2.42	116.81	110.68
19	4	1211	CLA	CMB-C2B-C3B	2.42	129.82	125.09
20	A	7028	LMU	O3'-C3'-C2'	2.42	115.79	110.34
20	A	7041	LMU	O4'-C4B-C3B	2.42	115.79	110.34
20	A	7041	LMU	O5'-C5'-C4'	2.42	114.87	109.75
19	A	1764	CLA	O2A-CGA-CBA	2.42	119.29	111.90
21	2	1225	SUC	O1'-C1'-C2'	2.43	119.68	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1781	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	A	1787	CLA	CBA-CAA-C2A	2.43	120.60	113.73
19	A	1765	CLA	C2C-C1C-NC	2.44	112.06	110.24
19	B	1759	CLA	C4A-NA-C1A	2.44	109.51	106.36
19	L	1168	CLA	O2A-CGA-CBA	2.44	119.33	111.90
19	B	1787	CLA	CAA-C2A-C1A	2.44	121.08	112.47
19	A	1785	CLA	CMC-C2C-C1C	2.44	128.80	125.02
20	A	7048	LMU	O2'-C2'-C1'	2.44	115.38	110.02
19	3	1215	CLA	C3D-C4D-ND	2.45	112.30	110.13
19	B	1740	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	A	1759	CLA	C5-C3-C4	2.45	120.67	114.64
20	A	7028	LMU	O4'-C4B-C3B	2.45	115.86	110.34
20	A	7015	LMU	C6B-C5B-C4B	2.45	119.07	113.02
21	F	1158	SUC	O2'-C2'-C1'	2.45	114.66	107.98
19	1	1189	CLA	CHC-C1C-NC	2.46	128.29	123.67
19	A	1778	CLA	CAA-C2A-C3A	2.46	120.31	114.13
19	4	1197	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	B	1786	CLA	CAC-C3C-C4C	2.46	128.41	124.83
19	A	1791	CLA	CED-O2D-CGD	2.47	121.77	115.99
19	3	1214	CLA	CMB-C2B-C3B	2.47	130.18	125.14
21	B	8061	SUC	O2'-C2'-C1'	2.47	114.69	107.98
19	A	1774	CLA	CMB-C2B-C3B	2.47	129.91	125.09
19	1	1190	CLA	OBD-CAD-CBD	2.47	129.66	125.94
19	1	1307	CLA	C3D-C2D-C1D	2.47	108.48	106.30
20	A	7033	LMU	O5'-C5'-C6'	2.47	112.60	106.36
19	B	1758	CLA	CMB-C2B-C3B	2.47	129.92	125.09
19	L	1168	CLA	CAA-C2A-C1A	2.47	121.19	112.47
19	4	1198	CLA	C1C-NC-C4C	2.48	109.28	106.27
19	L	1167	CLA	CED-O2D-CGD	2.48	121.80	115.99
19	B	1767	CLA	O2A-CGA-CBA	2.48	119.45	111.90
19	R	1055	CLA	C3B-C4B-NB	2.48	112.42	109.21
19	A	1800	CLA	CHC-C1C-NC	2.48	128.34	123.67
19	3	1213	CLA	C2A-C1A-NA	2.49	116.18	110.36
19	1	1149	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	L	1168	CLA	CHC-C1C-NC	2.49	128.36	123.67
20	A	7026	LMU	O5'-C5'-C4'	2.49	115.01	109.75
19	B	1749	CLA	CAC-C3C-C4C	2.49	128.45	124.83
19	A	1799	CLA	CMC-C2C-C1C	2.49	128.88	125.02
22	L	1169	BCR	C30-C25-C24	2.50	122.81	115.82
19	B	1748	CLA	CED-O2D-CGD	2.50	121.85	115.99
22	3	1225	BCR	C33-C5-C4	2.50	118.17	113.43
19	A	1812	CLA	O2A-CGA-CBA	2.50	119.51	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7017	LMU	O1B-C1B-C2B	2.50	114.19	108.10
19	1	1189	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	B	1740	CLA	O2A-CGA-CBA	2.50	119.52	111.90
19	2	1220	CLA	CMC-C2C-C1C	2.50	128.89	125.02
19	3	1212	CLA	O2A-CGA-CBA	2.50	119.53	111.90
19	A	1770	CLA	CED-O2D-CGD	2.51	121.87	115.99
19	2	1213	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	A	1784	CLA	C4-C3-C5	2.51	119.25	115.41
20	A	7022	LMU	O5B-C5B-C4B	2.51	114.40	109.68
19	A	1761	CLA	CAC-C3C-C4C	2.52	128.48	124.83
20	A	7035	LMU	O1B-C4'-C5'	2.52	115.94	109.32
19	A	1784	CLA	O2A-CGA-CBA	2.52	119.58	111.90
19	3	3011	CLA	CAC-C3C-C4C	2.52	128.49	124.83
19	B	1741	CLA	C4-C3-C5	2.52	119.26	115.41
19	B	1768	CLA	O2A-CGA-CBA	2.52	119.59	111.90
20	A	7034	LMU	C1B-C2B-C3B	2.53	114.95	109.97
20	A	7048	LMU	O4'-C4B-C3B	2.53	116.03	110.34
19	3	1224	CLA	CAC-C3C-C4C	2.53	128.50	124.83
19	B	1772	CLA	C4A-NA-C1A	2.53	109.63	106.36
19	A	1764	CLA	CAA-CBA-CGA	2.53	120.73	113.32
19	A	1788	CLA	CHB-C4A-NA	2.53	128.02	124.51
21	B	8052	SUC	O2'-C5'-C6'	2.53	116.24	108.57
19	B	1738	CLA	CAC-C3C-C4C	2.54	128.51	124.83
19	A	1772	CLA	O2A-CGA-CBA	2.54	119.65	111.90
19	B	1745	CLA	O2A-CGA-CBA	2.54	119.65	111.90
19	B	1737	CLA	C4-C3-C5	2.55	119.30	115.41
19	A	1785	CLA	CED-O2D-CGD	2.55	121.96	115.99
19	4	1201	CLA	C5-C3-C2	2.55	125.89	121.05
19	J	1044	CLA	CMB-C2B-C3B	2.55	130.09	125.09
19	1	1505	CLA	C6-C5-C3	2.55	118.09	112.48
19	B	1746	CLA	CED-O2D-CGD	2.56	121.98	115.99
19	2	1213	CLA	CAC-C3C-C4C	2.56	128.54	124.83
20	A	7049	LMU	O5B-C5B-C4B	2.56	114.48	109.68
20	A	7014	LMU	O5B-C5B-C6B	2.56	112.82	106.36
23	A	1801	PQN	O1-C1-C2	2.56	123.46	120.27
19	B	1751	CLA	CMC-C2C-C1C	2.56	128.98	125.02
19	1	1146	CLA	C5-C3-C4	2.56	120.94	114.64
19	B	1767	CLA	CHB-C4A-NA	2.56	128.06	124.51
19	A	1759	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	A	1761	CLA	CED-O2D-CGD	2.57	122.01	115.99
19	A	1780	CLA	CAC-C3C-C4C	2.57	128.56	124.83
19	A	1770	CLA	CMB-C2B-C1B	2.57	132.61	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1790	CLA	O2A-CGA-CBA	2.57	119.72	111.90
21	B	8059	SUC	O2-C2-C3	2.57	116.12	110.34
19	B	1762	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	1	1014	CLA	C4-C3-C5	2.57	119.34	115.41
20	A	7048	LMU	C1'-O5'-C5'	2.58	118.75	113.75
19	4	1199	CLA	O2A-CGA-CBA	2.58	119.75	111.90
19	B	1753	CLA	CAC-C3C-C4C	2.58	128.57	124.83
19	B	1756	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	3	1212	CLA	CAC-C3C-C4C	2.59	128.58	124.83
20	A	7013	LMU	O1B-C4'-C5'	2.59	116.12	109.32
19	A	1812	CLA	CGD-CBD-CAD	2.59	119.39	110.62
20	A	7036	LMU	C1B-O5B-C5B	2.59	118.77	113.75
19	1	1188	CLA	CHB-C4A-NA	2.59	128.09	124.51
20	A	7033	LMU	C6B-C5B-C4B	2.59	119.40	113.02
19	B	1787	CLA	CMC-C2C-C1C	2.59	129.03	125.02
19	B	1750	CLA	O2A-CGA-CBA	2.60	119.81	111.90
19	B	1762	CLA	O2A-CGA-CBA	2.60	119.81	111.90
22	B	1780	BCR	C35-C13-C12	2.60	122.42	118.10
19	J	1044	CLA	CED-O2D-CGD	2.60	122.08	115.99
19	K	1085	CLA	O2A-CGA-CBA	2.60	119.83	111.90
19	A	1771	CLA	CAC-C3C-C4C	2.60	128.61	124.83
19	B	1772	CLA	CMB-C2B-C1B	2.60	132.67	128.36
19	1	1149	CLA	CAA-C2A-C1A	2.61	121.66	112.47
19	4	1205	CLA	O2A-CGA-CBA	2.61	119.84	111.90
21	B	8059	SUC	O4-C4-C3	2.61	116.20	110.34
22	B	1777	BCR	C32-C1-C6	2.61	114.39	110.30
19	1	1145	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	4	1201	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	4	1210	CLA	C3D-C2D-C1D	2.61	108.60	106.30
20	A	7032	LMU	C3'-C4'-C5'	2.61	116.74	110.84
20	A	7039	LMU	C1'-O5'-C5'	2.61	118.82	113.75
19	B	1745	CLA	CED-O2D-CGD	2.61	122.12	115.99
20	L	1171	LMU	O5B-C5B-C4B	2.61	114.59	109.68
19	B	1771	CLA	CHB-C4A-NA	2.62	128.13	124.51
19	A	1780	CLA	CMB-C2B-C3B	2.62	130.21	125.09
19	A	1799	CLA	CMB-C2B-C1B	2.62	132.70	128.36
19	3	3011	CLA	C4-C3-C5	2.62	119.41	115.41
19	B	1755	CLA	CMC-C2C-C1C	2.62	129.08	125.02
19	1	1193	CLA	O2A-CGA-CBA	2.63	119.90	111.90
19	B	1743	CLA	CAC-C3C-C4C	2.63	128.64	124.83
20	A	7015	LMU	C4B-C3B-C2B	2.63	115.69	110.79
21	3	1226	SUC	O2-C2-C3	2.63	116.25	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	8054	SUC	O2-C2-C1	2.63	115.78	110.02
19	B	1773	CLA	CMC-C2C-C1C	2.63	129.09	125.02
20	A	7038	LMU	O1B-C1B-C2B	2.63	114.51	108.10
22	B	1780	BCR	C7-C8-C9	2.63	130.23	126.22
20	N	1086	LMU	O1B-C4'-C3'	2.64	113.97	107.17
19	3	1215	CLA	C3B-C4B-NB	2.64	112.46	110.09
20	A	7038	LMU	O3'-C3'-C2'	2.64	116.27	110.34
19	A	1760	CLA	CMB-C2B-C3B	2.64	130.25	125.09
19	4	1200	CLA	CHC-C1C-NC	2.64	128.64	123.67
19	B	1741	CLA	CAC-C3C-C4C	2.64	128.67	124.83
20	A	7027	LMU	O5'-C5'-C6'	2.65	113.04	106.36
19	3	1219	CLA	CMC-C2C-C1C	2.65	129.12	125.02
19	A	1797	CLA	CED-O2D-CGD	2.66	122.22	115.99
19	4	4007	CLA	CGD-CBD-CAD	2.66	119.63	110.62
19	1	1307	CLA	C3C-C4C-NC	2.66	112.43	110.09
19	2	1218	CLA	CHB-C4A-NA	2.66	128.19	124.51
19	B	1786	CLA	CGD-CBD-CAD	2.66	119.65	110.62
19	B	1743	CLA	CHB-C4A-NA	2.66	128.20	124.51
19	3	1219	CLA	CHC-C1C-NC	2.67	128.69	123.67
19	B	1746	CLA	CHB-C4A-NA	2.67	128.20	124.51
19	B	1773	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	1	1308	CLA	O2A-CGA-CBA	2.67	120.04	111.90
19	3	3008	CLA	CAA-CBA-CGA	2.67	121.14	113.32
19	4	1196	CLA	O2A-CGA-CBA	2.67	120.05	111.90
19	4	4007	CLA	O2A-CGA-CBA	2.68	120.06	111.90
20	A	7027	LMU	C3'-C4'-C5'	2.68	116.90	110.84
20	A	7048	LMU	O5'-C5'-C6'	2.68	113.13	106.36
19	A	1810	CLA	O2A-CGA-CBA	2.68	120.07	111.90
19	3	1224	CLA	CMC-C2C-C1C	2.68	129.17	125.02
19	1	1193	CLA	CMB-C2B-C3B	2.68	130.34	125.09
19	A	1772	CLA	CHC-C1C-NC	2.69	128.72	123.67
19	G	1099	CLA	O2A-CGA-CBA	2.69	120.08	111.90
19	J	1043	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	B	1743	CLA	C6-C5-C3	2.69	118.39	112.48
19	4	1196	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	I	1032	BCR	C23-C22-C21	2.69	123.32	118.98
19	A	1788	CLA	CMB-C2B-C3B	2.69	130.36	125.09
19	A	1793	CLA	CHB-C4A-NA	2.70	128.24	124.51
20	N	1086	LMU	C1'-O5'-C5'	2.70	118.99	113.75
20	A	7017	LMU	O2B-C2B-C3B	2.70	116.42	110.34
20	A	7035	LMU	O5'-C5'-C6'	2.70	113.18	106.36
19	A	1772	CLA	CHB-C4A-NA	2.70	128.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1205	CLA	CHC-C1C-NC	2.70	128.75	123.67
19	J	1043	CLA	O2A-CGA-CBA	2.71	120.14	111.90
19	B	1738	CLA	CMB-C2B-C1B	2.71	132.84	128.36
19	A	1773	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	3	1220	CLA	C3D-C4D-ND	2.71	112.54	110.13
20	A	7042	LMU	O6'-C6'-C5'	2.71	120.30	111.33
19	A	1767	CLA	CAA-CBA-CGA	2.71	121.26	113.32
19	4	1205	CLA	CED-O2D-CGD	2.71	122.36	115.99
19	A	1759	CLA	CMB-C2B-C3B	2.72	130.40	125.09
19	B	1762	CLA	CED-O2D-CGD	2.73	122.38	115.99
22	B	1780	BCR	C39-C30-C25	2.73	114.58	110.30
19	A	1759	CLA	O2A-CGA-CBA	2.73	120.21	111.90
19	4	4014	CLA	O2A-CGA-CBA	2.73	120.22	111.90
19	B	1762	CLA	CMC-C2C-C1C	2.73	129.25	125.02
20	A	1809	LMU	O3B-C3B-C2B	2.74	116.50	110.34
20	A	7013	LMU	O5'-C5'-C6'	2.74	113.27	106.36
19	J	1044	CLA	C3A-C2A-C1A	2.74	106.14	101.50
22	B	1780	BCR	C23-C22-C21	2.74	123.39	118.98
20	A	1808	LMU	C3'-C4'-C5'	2.74	117.03	110.84
19	B	1748	CLA	O2A-CGA-CBA	2.74	120.25	111.90
20	K	1086	LMU	O3B-C3B-C2B	2.74	116.51	110.34
19	1	1189	CLA	O2A-CGA-CBA	2.74	120.26	111.90
19	B	1771	CLA	CMB-C2B-C3B	2.74	130.46	125.09
19	B	1765	CLA	CHC-C1C-NC	2.74	128.84	123.67
20	A	7025	LMU	O5'-C5'-C4'	2.74	115.54	109.75
19	2	1212	CLA	O2A-CGA-CBA	2.74	120.26	111.90
19	4	1201	CLA	C1C-NC-C4C	2.74	109.60	106.27
19	B	1755	CLA	C2C-C1C-NC	2.75	112.29	110.24
19	A	1781	CLA	O2A-CGA-CBA	2.75	120.27	111.90
19	2	1218	CLA	O2A-CGA-CBA	2.75	120.27	111.90
19	3	1218	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	1	1308	CLA	CHB-C4A-NA	2.75	128.31	124.51
20	A	7021	LMU	O1B-C1B-C2B	2.75	114.79	108.10
19	A	1763	CLA	CED-O2D-CGD	2.75	122.44	115.99
19	B	1764	CLA	CMB-C2B-C3B	2.75	130.48	125.09
19	B	1750	CLA	CMC-C2C-C1C	2.76	129.29	125.02
19	A	1810	CLA	CMB-C2B-C3B	2.76	130.48	125.09
19	A	1776	CLA	CED-O2D-CGD	2.76	122.46	115.99
19	2	1220	CLA	CHB-C4A-NA	2.76	128.33	124.51
19	1	1145	CLA	CGD-CBD-CAD	2.76	119.98	110.62
21	2	1225	SUC	O3-C3-C2	2.76	116.55	110.34
19	A	1768	CLA	O2A-CGA-CBA	2.76	120.32	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1055	CLA	CAC-C3C-C4C	2.76	128.84	124.83
19	4	1203	CLA	C3D-C2D-C1D	2.76	108.73	106.30
21	2	1225	SUC	O5-C1-C2	2.76	115.95	110.28
22	B	1780	BCR	C24-C25-C26	2.77	127.71	121.37
20	A	7033	LMU	C4B-C3B-C2B	2.77	115.95	110.79
20	A	7050	LMU	O5'-C1'-O1'	2.77	116.72	110.05
19	A	1812	CLA	CHC-C1C-NC	2.78	128.89	123.67
20	A	7034	LMU	C3B-C4B-C5B	2.78	115.04	110.20
19	B	1742	CLA	CAC-C3C-C4C	2.78	128.86	124.83
24	B	1784	LMG	O8-C28-C29	2.78	120.37	111.90
19	A	1789	CLA	CED-O2D-CGD	2.78	122.51	115.99
21	B	8054	SUC	O1-C2'-C3'	2.78	117.73	108.04
19	3	3008	CLA	O2A-CGA-CBA	2.78	120.37	111.90
22	B	1777	BCR	C36-C18-C19	2.78	122.73	118.10
19	B	1757	CLA	O2A-CGA-CBA	2.79	120.39	111.90
19	A	1792	CLA	CMB-C2B-C3B	2.79	130.55	125.09
19	A	1779	CLA	CMC-C2C-C1C	2.80	129.35	125.02
19	1	1193	CLA	CAA-CBA-CGA	2.80	121.52	113.32
22	B	1782	BCR	C15-C16-C17	2.81	129.60	123.39
21	B	8056	SUC	O1-C2'-C3'	2.81	117.83	108.04
19	3	1222	CLA	CMC-C2C-C1C	2.81	129.37	125.02
19	L	1167	CLA	O2A-CGA-CBA	2.81	120.47	111.90
19	3	1212	CLA	CMB-C2B-C3B	2.81	130.59	125.09
19	1	1145	CLA	CAC-C3C-C4C	2.81	128.92	124.83
19	A	1779	CLA	CAC-C3C-C4C	2.82	128.92	124.83
19	B	1762	CLA	CHC-C1C-NC	2.82	128.97	123.67
19	A	1782	CLA	O2A-CGA-CBA	2.82	120.48	111.90
19	A	1762	CLA	CHB-C4A-NA	2.82	128.41	124.51
19	A	1760	CLA	O2D-CGD-CBD	2.82	115.17	111.30
20	A	7023	LMU	O5B-C5B-C6B	2.82	113.49	106.36
19	B	1750	CLA	CHC-C1C-NC	2.82	128.98	123.67
19	B	1748	CLA	CMB-C2B-C3B	2.82	130.61	125.09
19	1	1196	CLA	C4A-NA-C1A	2.82	110.01	106.36
19	3	1223	CLA	C2B-C3B-C4B	2.83	108.76	106.29
19	B	1747	CLA	CHB-C4A-NA	2.83	128.42	124.51
19	1	1192	CLA	C4-C3-C5	2.83	119.72	115.41
19	B	1772	CLA	C4-C3-C5	2.83	119.73	115.41
20	A	7019	LMU	O5'-C5'-C4'	2.83	115.72	109.75
20	A	7023	LMU	O1B-C1B-C2B	2.83	114.99	108.10
19	A	1798	CLA	CHB-C4A-NA	2.83	128.43	124.51
19	B	1737	CLA	O2A-CGA-CBA	2.84	120.54	111.90
19	4	1206	CLA	C4-C3-C5	2.84	119.74	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1755	CLA	CHC-C1C-NC	2.84	129.01	123.67
19	B	1763	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	B	1782	BCR	C40-C30-C25	2.84	114.76	110.30
19	F	1157	CLA	C2C-C1C-NC	2.85	112.36	110.24
19	2	1221	CLA	C3D-C2D-C1D	2.85	108.81	106.30
19	2	1222	CLA	CHB-C4A-NA	2.85	128.45	124.51
19	B	1735	CLA	CHB-C4A-NA	2.85	128.46	124.51
20	A	7048	LMU	O5'-C1'-C2'	2.85	116.13	110.28
19	1	1241	CLA	O2A-CGA-CBA	2.86	120.60	111.90
20	A	7024	LMU	O5B-C5B-C6B	2.86	113.58	106.36
22	B	1780	BCR	C33-C5-C4	2.86	118.85	113.43
19	1	1196	CLA	CHB-C4A-NA	2.86	128.47	124.51
19	1	1142	CLA	CHB-C4A-NA	2.86	128.47	124.51
19	B	1751	CLA	O2A-CGA-CBA	2.86	120.62	111.90
19	A	1781	CLA	C4-C3-C5	2.87	119.78	115.41
19	B	1741	CLA	O2A-CGA-CBA	2.87	120.64	111.90
20	A	7014	LMU	O2B-C2B-C1B	2.87	116.31	110.02
19	A	1794	CLA	CHB-C4A-NA	2.87	128.48	124.51
19	B	1745	CLA	CMC-C2C-C1C	2.87	129.46	125.02
19	B	1746	CLA	CHC-C1C-NC	2.87	129.08	123.67
20	A	7043	LMU	O1B-C4'-C5'	2.87	116.87	109.32
19	4	1196	CLA	C4-C3-C5	2.87	119.80	115.41
19	B	1740	CLA	O2D-CGD-CBD	2.88	115.24	111.30
19	A	1791	CLA	CHB-C4A-NA	2.88	128.49	124.51
20	A	7031	LMU	O1B-C4'-C3'	2.88	114.60	107.17
19	4	1201	CLA	C3B-C4B-NB	2.88	112.94	109.21
19	A	1799	CLA	CAC-C3C-C4C	2.89	129.02	124.83
19	B	1757	CLA	C4-C3-C5	2.89	119.82	115.41
19	B	1768	CLA	CHC-C1C-NC	2.89	129.11	123.67
19	4	1208	CLA	C2B-C3B-C4B	2.89	108.82	106.29
19	I	1031	CLA	CHB-C4A-NA	2.89	128.51	124.51
20	B	1783	LMU	C1'-O5'-C5'	2.90	119.37	113.75
19	B	1756	CLA	O2A-CGA-CBA	2.90	120.75	111.90
19	A	1786	CLA	CAC-C3C-C4C	2.91	129.05	124.83
21	B	8061	SUC	O6'-C6'-C5'	2.91	120.94	111.33
19	A	1780	CLA	CHB-C4A-NA	2.91	128.54	124.51
19	A	1784	CLA	CHB-C4A-NA	2.91	128.54	124.51
19	1	1192	CLA	CAC-C3C-C4C	2.91	129.06	124.83
19	A	1768	CLA	CHB-C4A-NA	2.91	128.54	124.51
19	A	1787	CLA	O2A-CGA-CBA	2.91	120.78	111.90
19	F	1157	CLA	O2A-CGA-CBA	2.92	120.78	111.90
20	L	1171	LMU	O5'-C5'-C6'	2.92	113.73	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1744	CLA	CHB-C4A-NA	2.92	128.55	124.51
20	A	7026	LMU	O3'-C3'-C2'	2.92	116.91	110.34
19	4	1200	CLA	CMB-C2B-C3B	2.92	130.80	125.09
19	B	1744	CLA	O2A-CGA-CBA	2.92	120.80	111.90
19	A	1795	CLA	CMB-C2B-C3B	2.92	130.80	125.09
19	A	1783	CLA	CHC-C1C-NC	2.92	129.17	123.67
19	1	1198	CLA	C3D-C2D-C1D	2.92	108.88	106.30
19	A	1800	CLA	CMC-C2C-C1C	2.92	129.54	125.02
19	4	1199	CLA	C4-C3-C5	2.93	119.88	115.41
20	A	7030	LMU	O1B-C4'-C3'	2.93	114.72	107.17
19	B	1756	CLA	C4-C3-C5	2.93	119.88	115.41
20	A	7048	LMU	O1B-C4'-C3'	2.93	114.72	107.17
19	A	1762	CLA	O2A-CGA-CBA	2.93	120.82	111.90
19	B	1736	CLA	CHB-C4A-NA	2.93	128.57	124.51
20	A	7024	LMU	O5'-C5'-C6'	2.94	113.78	106.36
21	B	8060	SUC	O5-C1-C2	2.94	116.31	110.28
19	B	1742	CLA	O2A-CGA-CBA	2.94	120.87	111.90
20	A	7033	LMU	O2'-C2'-C1'	2.95	116.48	110.02
19	A	1798	CLA	CAC-C3C-C4C	2.95	129.11	124.83
19	A	1793	CLA	O2A-CGA-CBA	2.95	120.88	111.90
19	B	1749	CLA	CHB-C4A-NA	2.95	128.59	124.51
19	2	1219	CLA	C3D-C2D-C1D	2.95	108.90	106.30
19	B	1786	CLA	O2A-CGA-CBA	2.96	120.90	111.90
20	A	7042	LMU	O2'-C2'-C1'	2.96	116.50	110.02
19	4	1211	CLA	CHC-C1C-NC	2.96	129.24	123.67
20	A	7017	LMU	O5'-C5'-C6'	2.96	113.84	106.36
19	3	3011	CLA	CMB-C2B-C3B	2.96	130.88	125.09
20	A	7035	LMU	O5'-C1'-C2'	2.96	116.35	110.28
19	2	1215	CLA	CHB-C4A-NA	2.96	128.61	124.51
19	A	1777	CLA	O2A-CGA-CBA	2.96	120.93	111.90
19	1	1194	CLA	C3D-C2D-C1D	2.97	108.92	106.30
19	1	1190	CLA	CGD-CBD-CAD	2.97	120.69	110.62
19	B	1772	CLA	CAA-CBA-CGA	2.97	122.01	113.32
20	A	7023	LMU	C1B-C2B-C3B	2.97	115.83	109.97
19	A	1774	CLA	O2A-CGA-CBA	2.97	120.95	111.90
20	A	7005	LMU	O4'-C4B-C3B	2.97	117.03	110.34
19	B	1746	CLA	CMB-C2B-C3B	2.98	130.91	125.09
19	3	1212	CLA	CHC-C1C-NC	2.98	129.27	123.67
20	A	7030	LMU	C1B-O5B-C5B	2.98	119.53	113.75
19	B	1741	CLA	CMC-C2C-C1C	2.98	129.63	125.02
19	3	1212	CLA	C5-C3-C4	2.99	121.98	114.64
20	A	7030	LMU	O1'-C1'-C2'	2.99	111.82	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1786	CLA	CHB-C4A-NA	2.99	128.65	124.51
19	A	1799	CLA	CHC-C1C-NC	2.99	129.30	123.67
22	L	1169	BCR	C15-C14-C13	2.99	131.52	127.20
19	1	1149	CLA	C3A-C2A-C1A	2.99	106.58	101.50
20	A	7040	LMU	C1'-C2'-C3'	3.00	115.88	109.97
19	3	3008	CLA	CHC-C1C-NC	3.00	129.31	123.67
20	B	1783	LMU	O1B-C4'-C5'	3.00	117.20	109.32
19	1	1197	CLA	C3D-C2D-C1D	3.00	108.94	106.30
19	1	1505	CLA	O2A-CGA-CBA	3.00	121.04	111.90
21	B	8056	SUC	O4'-C4'-C5'	3.00	120.06	111.05
19	1	1188	CLA	C3A-C2A-C1A	3.01	106.59	101.50
19	B	1750	CLA	C4-C3-C5	3.01	120.00	115.41
19	B	1767	CLA	CHC-C1C-NC	3.01	129.34	123.67
20	A	7040	LMU	O2B-C2B-C1B	3.01	116.62	110.02
20	A	7026	LMU	C6B-C5B-C4B	3.01	120.45	113.02
20	A	7038	LMU	O3B-C3B-C2B	3.02	117.13	110.34
20	A	7017	LMU	O5'-C1'-C2'	3.02	116.46	110.28
19	B	1773	CLA	CHC-C1C-NC	3.02	129.35	123.67
19	4	1204	CLA	CHC-C1C-NC	3.02	129.18	123.78
20	A	7026	LMU	O5'-C5'-C6'	3.02	113.99	106.36
19	B	1754	CLA	CMC-C2C-C1C	3.03	129.71	125.02
19	3	1219	CLA	O2A-CGA-CBA	3.03	121.13	111.90
19	B	1788	CLA	O2A-CGA-CBA	3.04	121.15	111.90
19	1	1010	CLA	C3D-C4D-ND	3.04	112.83	110.13
19	2	1218	CLA	CGD-CBD-CAD	3.04	120.93	110.62
20	A	7024	LMU	C2'-C3'-C4'	3.05	116.29	109.60
22	L	1170	BCR	C29-C30-C25	3.05	115.19	110.36
19	B	1768	CLA	CMC-C2C-C1C	3.05	129.74	125.02
19	A	1773	CLA	CED-O2D-CGD	3.05	123.14	115.99
20	A	7019	LMU	C1'-C2'-C3'	3.05	115.99	109.97
19	A	1782	CLA	C4-C3-C5	3.05	120.07	115.41
20	A	7037	LMU	O1B-C4'-C3'	3.06	115.06	107.17
19	1	1192	CLA	CHC-C1C-NC	3.06	129.43	123.67
19	B	1741	CLA	CMB-C2B-C3B	3.06	131.08	125.09
21	B	8056	SUC	O2'-C2'-C1'	3.06	116.32	107.98
20	A	7028	LMU	O5B-C5B-C6B	3.06	114.10	106.36
19	A	1760	CLA	CBA-CAA-C2A	3.06	122.38	113.73
20	A	7022	LMU	O1B-C4'-C3'	3.07	115.08	107.17
19	A	1767	CLA	CHB-C4A-NA	3.07	128.75	124.51
20	A	7019	LMU	O5B-C5B-C6B	3.07	114.12	106.36
19	B	1755	CLA	O2A-CGA-CBA	3.07	121.26	111.90
19	A	1783	CLA	CHB-C4A-NA	3.07	128.76	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1208	CLA	CHC-C1C-NC	3.08	129.28	123.78
21	3	1226	SUC	O4-C4-C5	3.08	117.39	109.24
19	4	1209	CLA	CMC-C2C-C1C	3.08	129.79	125.02
19	A	1777	CLA	CHB-C4A-NA	3.09	128.78	124.51
20	A	7014	LMU	O5'-C1'-O1'	3.09	117.49	110.05
20	A	7021	LMU	O1'-C1'-C2'	3.09	111.94	108.04
19	2	1221	CLA	C3D-C4D-ND	3.09	112.87	110.13
19	A	1797	CLA	CBA-CAA-C2A	3.09	122.46	113.73
19	B	1772	CLA	CHB-C4A-NA	3.09	128.79	124.51
20	A	7014	LMU	C1B-C2B-C3B	3.09	116.07	109.97
19	A	1761	CLA	O2A-CGA-CBA	3.10	121.34	111.90
20	2	1224	LMU	O1B-C4'-C3'	3.10	115.16	107.17
20	A	7013	LMU	O1B-C4'-C3'	3.10	115.17	107.17
19	A	1789	CLA	O2A-CGA-CBA	3.10	121.35	111.90
19	4	1206	CLA	O2A-CGA-CBA	3.10	121.36	111.90
19	1	1241	CLA	CED-O2D-CGD	3.10	123.27	115.99
19	1	1195	CLA	CHC-C1C-NC	3.11	129.51	123.67
22	I	1032	BCR	C19-C18-C17	3.11	123.99	118.98
19	3	1224	CLA	C4-C3-C5	3.11	120.15	115.41
19	A	1779	CLA	CHB-C4A-NA	3.11	128.81	124.51
20	A	1809	LMU	C1B-O5B-C5B	3.11	119.78	113.75
19	B	1751	CLA	CHC-C1C-NC	3.11	129.53	123.67
20	A	7021	LMU	O5B-C5B-C4B	3.11	115.53	109.68
19	A	1787	CLA	CHC-C1C-NC	3.12	129.53	123.67
19	B	1764	CLA	CED-O2D-CGD	3.12	123.30	115.99
19	B	1745	CLA	CHB-C4A-NA	3.12	128.82	124.51
19	B	1759	CLA	CHC-C1C-NC	3.12	129.54	123.67
20	A	7026	LMU	O1B-C1B-C2B	3.13	115.72	108.10
19	1	1505	CLA	CED-O2D-CGD	3.14	123.35	115.99
22	I	1032	BCR	C24-C25-C26	3.14	128.57	121.37
19	A	1771	CLA	CGD-CBD-CAD	3.15	121.29	110.62
20	A	7020	LMU	C1B-O5B-C5B	3.15	119.85	113.75
22	L	1169	BCR	C33-C5-C4	3.15	119.40	113.43
19	4	1209	CLA	CHC-C1C-NC	3.15	129.60	123.67
19	3	1219	CLA	C4-C3-C5	3.15	120.22	115.41
20	A	7035	LMU	O3'-C3'-C4'	3.15	117.33	109.87
19	1	1189	CLA	CMC-C2C-C1C	3.15	129.90	125.02
19	2	1223	CLA	O2A-CGA-CBA	3.16	121.52	111.90
20	A	7025	LMU	O1B-C1B-C2B	3.16	115.79	108.10
20	A	7023	LMU	O1'-C1'-C2'	3.16	112.03	108.04
19	B	1754	CLA	CBA-CAA-C2A	3.17	122.66	113.73
22	B	1780	BCR	C38-C26-C27	3.17	119.44	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1779	CLA	CHC-C1C-NC	3.17	129.65	123.67
20	A	1808	LMU	C2'-C3'-C4'	3.18	116.58	109.60
19	A	1762	CLA	CMB-C2B-C3B	3.18	131.31	125.09
19	4	1201	CLA	CED-O2D-CGD	3.18	123.45	115.99
19	2	1220	CLA	CHC-C1C-NC	3.18	129.66	123.67
19	A	1776	CLA	CGD-CBD-CAD	3.19	121.42	110.62
19	4	4007	CLA	CMB-C2B-C3B	3.19	131.33	125.09
23	A	1801	PQN	C2M-C2-C1	3.19	121.45	116.27
19	A	1779	CLA	C4-C3-C5	3.20	120.29	115.41
19	2	1213	CLA	C4-C3-C5	3.20	120.29	115.41
20	A	7030	LMU	O5B-C5B-C6B	3.20	114.44	106.36
22	B	1777	BCR	C23-C22-C21	3.20	124.14	118.98
19	B	1766	CLA	CHC-C1C-NC	3.20	129.70	123.67
19	B	1758	CLA	CHB-C4A-NA	3.21	128.95	124.51
21	B	8061	SUC	O2'-C5'-C6'	3.21	118.28	108.57
19	1	1149	CLA	CGD-CBD-CAD	3.21	121.50	110.62
19	B	1740	CLA	CHC-C1C-NC	3.21	129.72	123.67
19	R	1054	CLA	CED-O2D-CGD	3.22	123.53	115.99
19	2	1223	CLA	CAA-C2A-C1A	3.22	123.83	112.47
19	3	3001	CLA	C3D-C4D-ND	3.22	112.99	110.13
22	B	1779	BCR	C38-C26-C27	3.22	119.54	113.43
19	A	1790	CLA	CHC-C1C-NC	3.22	129.74	123.67
19	1	1190	CLA	CHC-C1C-NC	3.23	129.75	123.67
19	3	3011	CLA	CHC-C1C-NC	3.23	129.75	123.67
19	A	1774	CLA	C4-C3-C5	3.23	120.34	115.41
19	1	1145	CLA	O2D-CGD-CBD	3.23	115.73	111.30
19	3	1216	CLA	C3D-C4D-ND	3.23	113.00	110.13
19	A	1797	CLA	CMC-C2C-C3C	3.24	135.35	125.94
20	A	7013	LMU	O4'-C4B-C5B	3.24	117.83	109.24
19	I	1031	CLA	O2A-CGA-CBA	3.24	121.78	111.90
19	A	1777	CLA	CHC-C1C-NC	3.24	129.77	123.67
19	4	1197	CLA	CHC-C1C-NC	3.24	129.78	123.67
19	4	1207	CLA	C3D-C4D-ND	3.25	113.01	110.13
19	4	1210	CLA	CHC-C1C-NC	3.25	129.59	123.78
22	B	1779	BCR	C33-C5-C4	3.25	119.59	113.43
19	B	1769	CLA	O2A-CGA-CBA	3.25	121.80	111.90
20	A	1809	LMU	C2'-C3'-C4'	3.25	116.74	109.60
19	J	1043	CLA	C4-C3-C5	3.25	120.37	115.41
19	3	1217	CLA	C3D-C4D-ND	3.25	113.02	110.13
20	A	7017	LMU	C4B-C3B-C2B	3.26	116.88	110.79
19	3	1220	CLA	C3D-C2D-C1D	3.26	109.17	106.30
19	3	1224	CLA	O2A-CGA-CBA	3.26	121.84	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1223	CLA	CHC-C1C-NC	3.27	129.82	123.67
20	A	7027	LMU	C2'-C3'-C4'	3.27	116.77	109.60
19	A	1765	CLA	C4-C3-C5	3.27	120.40	115.41
19	B	1771	CLA	C4-C3-C5	3.27	120.40	115.41
19	B	1755	CLA	CHB-C4A-NA	3.27	129.04	124.51
20	A	7037	LMU	O3'-C3'-C4'	3.27	117.62	109.87
19	1	1188	CLA	CMB-C2B-C3B	3.27	131.49	125.09
19	2	1222	CLA	CHC-C1C-NC	3.28	129.84	123.67
20	A	7005	LMU	C1B-O5B-C5B	3.28	120.11	113.75
20	A	7031	LMU	O5'-C1'-O1'	3.28	117.95	110.05
20	A	7043	LMU	O3B-C3B-C2B	3.28	117.73	110.34
22	B	1781	BCR	C38-C26-C27	3.28	119.66	113.43
19	B	1752	CLA	CHC-C1C-NC	3.29	129.85	123.67
19	1	1196	CLA	CMB-C2B-C1B	3.29	133.80	128.36
20	A	7017	LMU	O5B-C5B-C6B	3.29	114.67	106.36
19	B	1761	CLA	CED-O2D-CGD	3.29	123.70	115.99
19	B	1761	CLA	CGD-CBD-CAD	3.29	121.78	110.62
19	3	1217	CLA	C3D-C2D-C1D	3.30	109.20	106.30
19	B	1746	CLA	O2A-CGA-CBA	3.30	121.95	111.90
19	1	1014	CLA	CAA-C2A-C1A	3.30	124.11	112.47
20	A	7025	LMU	C1'-O5'-C5'	3.30	120.15	113.75
19	A	1783	CLA	O2A-CGA-CBA	3.30	121.96	111.90
19	A	1790	CLA	CHB-C4A-NA	3.30	129.08	124.51
19	1	1303	CLA	CHC-C1C-NC	3.30	129.69	123.78
19	4	1200	CLA	CMC-C2C-C1C	3.30	130.13	125.02
19	A	1764	CLA	CHC-C1C-NC	3.31	129.89	123.67
19	3	1213	CLA	C3D-C2D-C1D	3.31	109.21	106.30
22	B	1781	BCR	C33-C5-C4	3.31	119.70	113.43
19	4	1208	CLA	C3D-C4D-ND	3.32	113.08	110.13
19	B	1765	CLA	CED-O2D-CGD	3.32	123.78	115.99
22	3	1225	BCR	C38-C26-C27	3.32	119.73	113.43
19	B	1761	CLA	CHC-C1C-NC	3.32	129.93	123.67
19	3	1216	CLA	C3D-C2D-C1D	3.33	109.23	106.30
20	A	7037	LMU	O5'-C5'-C6'	3.33	114.76	106.36
19	B	1745	CLA	CHC-C1C-NC	3.33	129.93	123.67
19	R	1054	CLA	CHC-C1C-NC	3.33	129.94	123.67
19	B	1761	CLA	CAC-C3C-C4C	3.33	129.67	124.83
19	A	1800	CLA	O2A-CGA-CBA	3.33	122.06	111.90
20	A	1808	LMU	C1B-O5B-C5B	3.34	120.22	113.75
19	B	1765	CLA	CHB-C4A-NA	3.34	129.12	124.51
19	R	1054	CLA	C4-C3-C5	3.34	120.50	115.41
19	B	1772	CLA	CHC-C1C-NC	3.34	129.95	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1197	CLA	CMB-C2B-C3B	3.34	131.97	125.14
19	B	1741	CLA	CHC-C1C-NC	3.34	129.96	123.67
19	A	1794	CLA	O2A-CGA-CBA	3.34	122.08	111.90
20	A	7020	LMU	O5B-C1B-C2B	3.34	117.13	110.28
19	1	1149	CLA	CBA-CAA-C2A	3.34	123.16	113.73
19	G	1099	CLA	CHB-C4A-NA	3.34	129.14	124.51
19	A	1773	CLA	CHC-C1C-NC	3.35	129.97	123.67
19	B	1763	CLA	CHC-C1C-NC	3.35	129.97	123.67
20	A	7037	LMU	C1'-C2'-C3'	3.35	116.57	109.97
22	L	1170	BCR	C32-C1-C6	3.35	115.55	110.30
20	A	7005	LMU	O3B-C3B-C4B	3.35	117.88	110.34
21	B	8061	SUC	O3-C3-C2	3.35	117.89	110.34
22	A	1802	BCR	C33-C5-C4	3.35	119.79	113.43
19	1	1190	CLA	CED-O2D-CGD	3.36	123.88	115.99
19	A	1796	CLA	O2A-CGA-CBA	3.36	122.15	111.90
20	A	7027	LMU	O1B-C1B-C2B	3.37	116.29	108.10
19	B	1764	CLA	O2A-CGA-CBA	3.37	122.16	111.90
19	1	1192	CLA	O2A-CGA-CBA	3.37	122.16	111.90
19	1	1194	CLA	C2B-C3B-C4B	3.37	109.23	106.29
19	A	1786	CLA	O2A-CGA-CBA	3.37	122.17	111.90
22	B	1775	BCR	C33-C5-C4	3.37	119.82	113.43
19	B	1764	CLA	CHC-C1C-NC	3.38	130.03	123.67
19	G	1099	CLA	CHC-C1C-NC	3.38	130.03	123.67
19	A	1796	CLA	CHB-C4A-NA	3.38	129.19	124.51
19	A	1792	CLA	CHC-C1C-NC	3.39	130.04	123.67
19	2	1223	CLA	CHB-C4A-NA	3.39	129.20	124.51
19	B	1758	CLA	CHC-C1C-NC	3.39	130.05	123.67
22	A	1805	BCR	C33-C5-C4	3.40	119.88	113.43
22	B	1776	BCR	C38-C26-C27	3.40	119.88	113.43
19	1	1193	CLA	CHC-C1C-NC	3.41	130.08	123.67
19	A	1775	CLA	CHC-C1C-NC	3.41	129.87	123.78
19	A	1763	CLA	CHC-C1C-NC	3.41	130.08	123.67
19	2	1217	CLA	C4-C3-C5	3.41	120.61	115.41
19	L	1166	CLA	CHC-C1C-NC	3.41	130.09	123.67
20	A	7005	LMU	O5B-C5B-C6B	3.41	114.98	106.36
19	B	1743	CLA	C5-C3-C2	3.42	127.53	121.05
19	I	1031	CLA	CHC-C1C-NC	3.42	130.11	123.67
19	J	1044	CLA	CHB-C4A-NA	3.42	129.25	124.51
20	A	7032	LMU	O5B-C5B-C6B	3.43	115.01	106.36
19	A	1810	CLA	CHB-C4A-NA	3.43	129.25	124.51
19	B	1743	CLA	CHC-C1C-NC	3.43	130.12	123.67
19	A	1780	CLA	O2A-CGA-CBA	3.43	122.36	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1785	CLA	CHC-C1C-NC	3.43	130.13	123.67
19	A	1776	CLA	C4-C3-C5	3.44	120.66	115.41
19	A	1777	CLA	C4-C3-C5	3.44	119.58	115.68
19	J	1044	CLA	CHC-C1C-NC	3.44	130.15	123.67
19	B	1735	CLA	CED-O2D-CGD	3.44	124.07	115.99
22	B	1782	BCR	C19-C18-C17	3.45	124.54	118.98
19	3	1222	CLA	O2A-CGA-CBA	3.45	122.42	111.90
20	4	1212	LMU	O1'-C1'-C2'	3.46	112.41	108.04
19	A	1780	CLA	CHC-C1C-NC	3.46	130.18	123.67
19	A	1789	CLA	C2C-C1C-NC	3.46	112.82	110.24
19	B	1760	CLA	CHC-C1C-NC	3.46	130.19	123.67
19	3	1214	CLA	CHC-C1C-NC	3.46	130.19	123.67
19	B	1787	CLA	CHC-C1C-NC	3.46	130.19	123.67
19	2	1221	CLA	CHC-C1C-NC	3.47	129.98	123.78
22	L	1170	BCR	C1-C6-C7	3.47	125.53	115.82
19	A	1794	CLA	CHC-C1C-NC	3.47	130.20	123.67
20	A	7036	LMU	O3'-C3'-C2'	3.47	118.15	110.34
22	A	1803	BCR	C33-C5-C4	3.47	120.01	113.43
19	B	1742	CLA	CHC-C1C-NC	3.47	130.20	123.67
19	1	1010	CLA	CHC-C1C-NC	3.47	129.99	123.78
22	A	1806	BCR	C33-C5-C4	3.47	120.01	113.43
19	A	1759	CLA	CHC-C1C-NC	3.47	130.21	123.67
19	B	1755	CLA	CAC-C3C-C4C	3.47	129.87	124.83
19	A	1766	CLA	CMB-C2B-C3B	3.47	131.88	125.09
20	A	7027	LMU	C1'-C2'-C3'	3.48	116.82	109.97
19	A	1771	CLA	CMB-C2B-C3B	3.48	131.89	125.09
19	3	3001	CLA	CHC-C1C-NC	3.48	130.00	123.78
22	B	1775	BCR	C38-C26-C27	3.48	120.03	113.43
19	B	1735	CLA	CHC-C1C-NC	3.48	130.22	123.67
19	B	1757	CLA	CHC-C1C-NC	3.48	130.22	123.67
19	J	1044	CLA	O2A-CGA-CBA	3.48	122.52	111.90
19	3	1218	CLA	CAC-C3C-C4C	3.49	129.89	124.83
22	A	1807	BCR	C33-C5-C4	3.49	120.05	113.43
19	2	1213	CLA	CHC-C1C-NC	3.49	130.24	123.67
19	2	1215	CLA	CHC-C1C-NC	3.49	130.24	123.67
22	A	1802	BCR	C38-C26-C27	3.49	120.05	113.43
19	B	1746	CLA	C4-C3-C5	3.49	120.74	115.41
20	A	7033	LMU	O1'-C1'-C2'	3.50	112.46	108.04
20	A	7016	LMU	C2'-C3'-C4'	3.50	117.28	109.60
19	A	1811	CLA	CHC-C1C-NC	3.50	130.25	123.67
19	A	1798	CLA	CHC-C1C-NC	3.50	130.26	123.67
19	4	1200	CLA	CAC-C3C-C4C	3.51	129.92	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1166	CLA	CED-O2D-CGD	3.51	124.22	115.99
19	B	1740	CLA	CMB-C2B-C3B	3.51	131.96	125.09
19	1	1241	CLA	CHC-C1C-NC	3.51	130.28	123.67
19	B	1749	CLA	O2A-CGA-CBA	3.51	122.61	111.90
20	A	7017	LMU	C1'-C2'-C3'	3.52	116.91	109.97
19	A	1788	CLA	CHC-C1C-NC	3.52	130.30	123.67
22	B	1778	BCR	C38-C26-C27	3.52	120.11	113.43
19	A	1812	CLA	CHB-C4A-NA	3.52	129.38	124.51
19	A	1788	CLA	O2A-CGA-CBA	3.53	122.65	111.90
19	4	1206	CLA	CHC-C1C-NC	3.53	130.31	123.67
19	B	1747	CLA	CHC-C1C-NC	3.53	130.31	123.67
22	B	1776	BCR	C33-C5-C4	3.53	120.12	113.43
20	A	7024	LMU	C1'-C2'-C3'	3.54	116.96	109.97
19	A	1768	CLA	CHC-C1C-NC	3.54	130.34	123.67
19	A	1776	CLA	CHC-C1C-NC	3.55	130.34	123.67
20	A	7049	LMU	O1'-C1'-C2'	3.55	112.53	108.04
19	A	1811	CLA	CHB-C4A-NA	3.56	129.43	124.51
19	A	1810	CLA	CMC-C2C-C1C	3.56	130.53	125.02
19	2	1212	CLA	CHC-C1C-NC	3.56	130.37	123.67
20	K	1086	LMU	O1B-C4'-C5'	3.56	118.68	109.32
19	A	1779	CLA	O2D-CGD-CBD	3.56	116.19	111.30
19	4	1199	CLA	CHB-C4A-NA	3.56	129.44	124.51
19	4	4014	CLA	CHC-C1C-NC	3.56	130.38	123.67
19	1	1014	CLA	CAA-C2A-C3A	3.57	123.47	113.22
19	1	1194	CLA	CHC-C1C-NC	3.57	130.16	123.78
19	1	1146	CLA	CHB-C4A-NA	3.57	129.44	124.51
19	3	1222	CLA	CED-O2D-CGD	3.57	124.37	115.99
19	4	1202	CLA	CHC-C1C-NC	3.57	130.40	123.67
19	B	1753	CLA	CED-O2D-CGD	3.58	124.38	115.99
19	4	1209	CLA	CHB-C4A-NA	3.58	129.46	124.51
19	A	1800	CLA	C4-C3-C5	3.58	120.87	115.41
19	A	1762	CLA	CHC-C1C-NC	3.58	130.41	123.67
19	B	1739	CLA	O2A-CGA-CBA	3.58	122.82	111.90
20	A	7048	LMU	O5B-C5B-C6B	3.59	115.42	106.36
19	4	1211	CLA	CHB-C4A-NA	3.59	129.48	124.51
19	K	1085	CLA	CHC-C1C-NC	3.59	130.43	123.67
19	1	1197	CLA	C3D-C4D-ND	3.59	113.32	110.13
19	B	1738	CLA	O2A-CGA-CBA	3.59	122.84	111.90
22	B	1777	BCR	C38-C26-C27	3.60	120.25	113.43
22	A	1807	BCR	C38-C26-C27	3.60	120.25	113.43
19	B	1740	CLA	C4-C3-C5	3.61	120.92	115.41
19	A	1767	CLA	CMB-C2B-C1B	3.61	134.34	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1167	CLA	CHC-C1C-NC	3.62	130.48	123.67
22	A	1806	BCR	C38-C26-C27	3.62	120.29	113.43
19	B	1740	CLA	CGD-CBD-CAD	3.62	122.91	110.62
19	F	1156	CLA	CHC-C1C-NC	3.63	130.49	123.67
22	A	1805	BCR	C38-C26-C27	3.63	120.30	113.43
22	B	1782	BCR	C33-C5-C4	3.63	120.31	113.43
19	A	1775	CLA	C3D-C4D-ND	3.63	113.36	110.13
20	A	7036	LMU	O5B-C5B-C6B	3.63	115.54	106.36
19	B	1787	CLA	CAC-C3C-C4C	3.64	130.11	124.83
20	A	7038	LMU	C1'-O5'-C5'	3.64	120.81	113.75
19	3	1224	CLA	O2D-CGD-CBD	3.64	116.29	111.30
22	A	1803	BCR	C38-C26-C27	3.64	120.33	113.43
19	J	1044	CLA	CAC-C3C-C4C	3.64	130.12	124.83
19	2	2010	CLA	CHC-C1C-NC	3.65	130.30	123.78
20	A	7026	LMU	O3'-C3'-C4'	3.65	118.51	109.87
19	2	1213	CLA	O2A-CGA-CBA	3.65	123.03	111.90
19	F	1155	CLA	CHB-C4A-NA	3.65	129.56	124.51
20	N	1086	LMU	C3B-C4B-C5B	3.65	116.57	110.20
19	J	1043	CLA	CHC-C1C-NC	3.65	130.55	123.67
20	A	7038	LMU	O5B-C5B-C6B	3.65	115.59	106.36
19	A	1781	CLA	CHC-C1C-NC	3.66	130.56	123.67
19	1	1187	CLA	CMC-C2C-C1C	3.66	130.69	125.02
19	4	1201	CLA	CGD-CBD-CAD	3.67	123.08	110.62
19	B	1759	CLA	CHB-C4A-NA	3.68	129.60	124.51
19	1	1197	CLA	CHC-C1C-NC	3.68	130.35	123.78
19	B	1763	CLA	C4-C3-C5	3.69	121.04	115.41
19	A	1789	CLA	CAC-C3C-C4C	3.69	130.19	124.83
19	B	1748	CLA	CHC-C1C-NC	3.69	130.62	123.67
19	1	1148	CLA	O2A-CGA-CBA	3.69	123.15	111.90
19	4	4007	CLA	CHB-C4A-NA	3.70	129.62	124.51
19	A	1784	CLA	CHC-C1C-NC	3.70	130.63	123.67
19	B	1753	CLA	CHC-C1C-NC	3.70	130.63	123.67
20	A	7037	LMU	O1B-C1B-O5B	3.70	120.05	110.68
19	A	1778	CLA	CHC-C1C-NC	3.70	130.64	123.67
19	1	1149	CLA	CED-O2D-CGD	3.71	124.68	115.99
19	A	1766	CLA	CHC-C1C-NC	3.71	130.64	123.67
22	A	1804	BCR	C33-C5-C4	3.71	120.45	113.43
22	A	1804	BCR	C38-C26-C27	3.71	120.45	113.43
19	B	1786	CLA	CHC-C1C-NC	3.71	130.66	123.67
20	A	1809	LMU	O5B-C1B-C2B	3.71	117.90	110.28
21	B	8051	SUC	O5-C5-C4	3.72	116.67	109.68
19	A	1774	CLA	CHC-C1C-NC	3.72	130.68	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1778	BCR	C33-C5-C4	3.73	120.49	113.43
19	3	3011	CLA	CHB-C4A-NA	3.73	129.67	124.51
19	A	1770	CLA	CHC-C1C-NC	3.74	130.71	123.67
20	A	7039	LMU	O1B-C1B-O5B	3.74	120.16	110.68
19	3	1222	CLA	CHC-C1C-NC	3.74	130.72	123.67
20	A	7031	LMU	O1B-C1B-C2B	3.75	117.22	108.10
19	A	1764	CLA	CHB-C4A-NA	3.75	129.70	124.51
19	A	1782	CLA	CHC-C1C-NC	3.75	130.73	123.67
19	A	1786	CLA	CHC-C1C-NC	3.76	130.75	123.67
19	4	1199	CLA	CAC-C3C-C4C	3.77	130.30	124.83
19	1	1188	CLA	O2A-CGA-CBA	3.77	123.39	111.90
20	A	7043	LMU	C1B-O5B-C5B	3.77	121.07	113.75
19	4	1205	CLA	C4-C3-C5	3.78	121.18	115.41
19	3	3008	CLA	CED-O2D-CGD	3.78	124.86	115.99
19	B	1739	CLA	CHB-C4A-NA	3.78	129.74	124.51
19	3	1213	CLA	C3D-C4D-ND	3.79	113.49	110.13
19	B	1739	CLA	CHC-C1C-NC	3.80	130.82	123.67
19	B	1786	CLA	O2D-CGD-CBD	3.80	116.52	111.30
19	B	1756	CLA	CHC-C1C-NC	3.80	130.83	123.67
19	A	1769	CLA	CHB-C4A-NA	3.80	129.77	124.51
19	4	1196	CLA	CHC-C1C-NC	3.80	130.83	123.67
20	B	1783	LMU	O2B-C2B-C1B	3.81	118.38	110.02
19	1	1308	CLA	CHC-C1C-NC	3.81	130.84	123.67
20	K	1086	LMU	O5B-C5B-C6B	3.81	115.99	106.36
19	A	1796	CLA	CMC-C2C-C1C	3.81	130.92	125.02
19	1	1505	CLA	CHC-C1C-NC	3.82	130.85	123.67
19	B	1769	CLA	C4-C3-C5	3.82	121.24	115.41
19	3	1220	CLA	CHC-C1C-NC	3.82	130.61	123.78
19	1	1010	CLA	C3D-C2D-C1D	3.83	109.67	106.30
20	N	1086	LMU	O2'-C2'-C1'	3.83	118.42	110.02
19	1	1142	CLA	CHC-C1C-NC	3.84	130.89	123.67
20	A	7033	LMU	O5'-C1'-C2'	3.84	118.16	110.28
19	B	1752	CLA	CHB-C4A-NA	3.84	129.83	124.51
20	A	7033	LMU	C3B-C4B-C5B	3.85	116.91	110.20
20	A	1808	LMU	O5'-C5'-C4'	3.85	117.88	109.75
20	A	7020	LMU	C1B-C2B-C3B	3.85	117.56	109.97
19	B	1753	CLA	O2D-CGD-CBD	3.85	116.59	111.30
19	F	1155	CLA	CMB-C2B-C3B	3.86	133.02	125.14
19	A	1810	CLA	CED-O2D-CGD	3.86	125.03	115.99
19	3	1218	CLA	CHC-C1C-NC	3.86	130.93	123.67
19	B	1735	CLA	CMB-C2B-C3B	3.86	132.64	125.09
20	A	7015	LMU	C1B-C2B-C3B	3.86	117.59	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1736	CLA	CHC-C1C-NC	3.87	130.94	123.67
23	B	1774	PQN	C2M-C2-C1	3.87	122.55	116.27
19	1	1187	CLA	CHC-C1C-NC	3.87	130.96	123.67
19	B	1771	CLA	O2A-CGA-CBA	3.88	123.72	111.90
19	B	1769	CLA	CHC-C1C-NC	3.89	130.99	123.67
19	A	1811	CLA	O2A-CGA-CBA	3.90	123.77	111.90
19	1	1187	CLA	C4A-NA-C1A	3.90	111.41	106.36
19	B	1759	CLA	O2A-CGA-CBA	3.91	123.81	111.90
19	4	1198	CLA	O2A-CGA-CBA	3.91	123.83	111.90
19	4	1201	CLA	O2D-CGD-CBD	3.92	116.67	111.30
19	A	1811	CLA	CAA-C2A-C1A	3.93	126.32	112.47
20	A	7027	LMU	C6B-C5B-C4B	3.93	122.70	113.02
20	A	7025	LMU	O3B-C3B-C4B	3.93	119.19	110.34
20	A	7021	LMU	C1B-O5B-C5B	3.93	121.38	113.75
19	A	1767	CLA	O2D-CGD-CBD	3.93	116.70	111.30
19	B	1770	CLA	CHC-C1C-NC	3.94	131.08	123.67
19	B	1735	CLA	C4-C3-C5	3.94	121.43	115.41
19	A	1780	CLA	O2D-CGD-CBD	3.94	116.71	111.30
19	A	1765	CLA	O2A-CGA-CBA	3.94	123.92	111.90
19	B	1787	CLA	C6-C5-C3	3.95	121.14	112.48
19	1	1241	CLA	CHB-C4A-NA	3.95	129.97	124.51
19	A	1771	CLA	CHC-C1C-NC	3.96	131.12	123.67
20	A	7016	LMU	C1B-C2B-C3B	3.96	117.78	109.97
20	A	7038	LMU	O5B-C5B-C4B	3.96	117.12	109.68
19	4	1208	CLA	C3D-C2D-C1D	3.97	109.79	106.30
19	2	1219	CLA	C3D-C4D-ND	3.97	113.65	110.13
19	2	1214	CLA	C3D-C2D-C1D	3.97	109.80	106.30
20	A	7038	LMU	C1B-O5B-C5B	3.97	121.45	113.75
19	3	3015	CLA	CHC-C1C-NC	3.98	130.89	123.78
20	A	7026	LMU	O5B-C5B-C6B	3.98	116.41	106.36
20	4	1212	LMU	C1B-O5B-C5B	3.98	121.47	113.75
20	A	7022	LMU	O2B-C2B-C1B	3.99	118.77	110.02
19	A	1789	CLA	CHC-C1C-NC	4.00	131.19	123.67
20	B	1783	LMU	O5B-C5B-C6B	4.00	116.48	106.36
19	A	1772	CLA	C4-C3-C5	4.00	121.52	115.41
19	A	1773	CLA	O2A-CGA-CBA	4.01	124.12	111.90
22	I	1032	BCR	C30-C25-C24	4.03	127.09	115.82
19	B	1788	CLA	CHC-C1C-NC	4.03	131.25	123.67
19	2	1218	CLA	CHC-C1C-NC	4.04	131.28	123.67
22	B	1782	BCR	C31-C1-C6	4.05	116.65	110.30
19	1	1198	CLA	CHC-C1C-NC	4.05	131.03	123.78
19	A	1785	CLA	C4-C3-C5	4.05	121.60	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1212	CLA	CAA-C2A-C1A	4.06	126.78	112.47
19	3	1223	CLA	CHC-C1C-NC	4.07	131.05	123.78
19	B	1749	CLA	CHC-C1C-NC	4.07	131.32	123.67
19	B	1753	CLA	C4-C3-C5	4.07	121.63	115.41
19	4	1207	CLA	CHC-C1C-NC	4.07	131.06	123.78
19	1	1149	CLA	CHC-C1C-NC	4.08	131.34	123.67
19	4	1210	CLA	C2B-C1B-NB	4.08	113.75	110.09
19	2	1222	CLA	CAC-C3C-C4C	4.08	130.75	124.83
19	A	1760	CLA	CHC-C1C-NC	4.08	131.35	123.67
19	2	1214	CLA	CHC-C1C-NC	4.08	131.08	123.78
20	K	1086	LMU	O2'-C2'-C1'	4.08	118.97	110.02
19	2	1212	CLA	C4-C3-C5	4.09	120.31	115.68
19	4	4007	CLA	C4-C3-C5	4.09	121.65	115.41
19	A	1798	CLA	O2D-CGD-CBD	4.09	116.91	111.30
19	F	1155	CLA	CHC-C1C-NC	4.10	131.38	123.67
19	1	1146	CLA	O2A-CGA-CBA	4.12	124.45	111.90
24	B	1784	LMG	O7-C10-C11	4.13	120.51	111.53
19	A	1771	CLA	O2A-CGA-CBA	4.14	124.50	111.90
20	A	7021	LMU	O2B-C2B-C1B	4.14	119.10	110.02
19	1	1191	CLA	CHC-C1C-NC	4.15	131.20	123.78
19	L	1167	CLA	CHB-C4A-NA	4.15	130.25	124.51
19	A	1787	CLA	CMB-C2B-C3B	4.16	133.22	125.09
19	A	1778	CLA	CAA-C2A-C1A	4.19	121.41	112.14
22	B	1777	BCR	C8-C9-C10	4.19	125.73	118.98
19	1	1145	CLA	O2A-CGA-CBA	4.20	124.68	111.90
20	A	7023	LMU	C2'-C3'-C4'	4.20	118.83	109.60
19	1	1014	CLA	CHC-C1C-NC	4.21	131.58	123.67
21	3	1226	SUC	O5-C1-C2	4.21	118.91	110.28
19	1	1146	CLA	CHC-C1C-NC	4.22	131.61	123.67
19	1	1187	CLA	CED-O2D-CGD	4.24	125.94	115.99
19	3	1221	CLA	C3D-C2D-C1D	4.25	110.04	106.30
20	A	7040	LMU	O1B-C1B-C2B	4.26	118.47	108.10
19	B	1788	CLA	CGD-CBD-CAD	4.26	125.06	110.62
19	2	1217	CLA	CHC-C1C-NC	4.26	131.69	123.67
20	A	7020	LMU	O1'-C1'-C2'	4.27	113.43	108.04
19	3	1213	CLA	CHC-C1C-NC	4.27	131.41	123.78
20	A	7037	LMU	O3B-C3B-C2B	4.30	120.02	110.34
22	B	1782	BCR	C38-C26-C27	4.31	121.59	113.43
19	B	1758	CLA	O2A-CGA-CBA	4.31	125.05	111.90
20	A	7047	LMU	O1B-C4'-C5'	4.32	120.66	109.32
19	4	1199	CLA	CHC-C1C-NC	4.32	131.80	123.67
19	2	1219	CLA	CHC-C1C-NC	4.32	131.51	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7026	LMU	O4'-C4B-C5B	4.33	120.71	109.24
19	4	1201	CLA	O2A-CGA-CBA	4.33	125.10	111.90
19	1	1241	CLA	C4-C3-C5	4.34	122.03	115.41
20	A	7037	LMU	O1B-C1B-C2B	4.34	118.67	108.10
20	A	7019	LMU	C2'-C3'-C4'	4.34	119.14	109.60
19	A	1795	CLA	CHC-C1C-NC	4.35	131.85	123.67
19	A	1783	CLA	O2D-CGD-CBD	4.35	117.27	111.30
20	A	7050	LMU	O1B-C4'-C3'	4.36	118.43	107.17
20	A	7026	LMU	O4'-C4B-C3B	4.36	120.16	110.34
20	A	7024	LMU	O5B-C1B-C2B	4.37	119.25	110.28
19	B	1787	CLA	CHB-C4A-NA	4.37	130.56	124.51
19	4	1209	CLA	CAC-C3C-C4C	4.38	131.80	125.02
22	L	1169	BCR	C36-C18-C19	4.39	125.40	118.10
19	3	3001	CLA	C3D-C2D-C1D	4.40	110.17	106.30
19	1	1149	CLA	CAC-C3C-C4C	4.40	131.22	124.83
21	B	8061	SUC	O5-C5-C6	4.40	117.48	106.36
19	A	1771	CLA	CHB-C4A-NA	4.41	130.61	124.51
21	B	8061	SUC	C1-O5-C5	4.41	122.31	113.75
19	3	1221	CLA	CHC-C1C-NC	4.42	131.68	123.78
19	1	1149	CLA	O2A-CGA-CBA	4.43	125.39	111.90
19	1	1307	CLA	C2B-C3B-C4B	4.44	110.17	106.29
19	3	1216	CLA	CHC-C1C-NC	4.44	131.72	123.78
19	1	1196	CLA	CHC-C1C-NC	4.46	132.05	123.67
22	B	1780	BCR	C34-C9-C8	4.46	125.51	118.10
19	A	1811	CLA	O2D-CGD-CBD	4.46	117.41	111.30
19	1	1188	CLA	CAA-C2A-C1A	4.46	128.19	112.47
20	L	1171	LMU	C3B-C4B-C5B	4.46	117.97	110.20
19	1	1146	CLA	CMB-C2B-C3B	4.47	133.82	125.09
19	B	1749	CLA	O2D-CGD-CBD	4.47	117.43	111.30
20	A	7032	LMU	C2'-C3'-C4'	4.47	119.42	109.60
19	A	1780	CLA	C4-C3-C5	4.48	122.25	115.41
20	A	7049	LMU	C1B-C2B-C3B	4.49	118.81	109.97
19	3	1217	CLA	CHC-C1C-NC	4.50	131.83	123.78
20	N	1086	LMU	O5B-C5B-C4B	4.50	118.13	109.68
19	B	1771	CLA	CHC-C1C-NC	4.51	132.16	123.67
19	A	1761	CLA	O2D-CGD-CBD	4.51	117.49	111.30
23	A	1801	PQN	C14-C13-C15	4.52	122.31	115.41
19	B	1788	CLA	CHB-C4A-NA	4.52	130.77	124.51
20	A	7050	LMU	O5'-C5'-C6'	4.55	117.84	106.36
19	1	1193	CLA	CAA-C2A-C3A	4.55	126.29	113.22
20	A	7021	LMU	C1B-O1B-C4'	4.55	129.89	118.01
19	3	1224	CLA	CHC-C1C-NC	4.55	132.23	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	1169	BCR	C38-C26-C27	4.55	122.06	113.43
19	A	1767	CLA	CHC-C1C-NC	4.55	132.24	123.67
19	A	1791	CLA	CHC-C1C-NC	4.56	132.24	123.67
19	B	1737	CLA	CHB-C4A-NA	4.56	130.82	124.51
19	R	1054	CLA	O2A-CGA-CBA	4.57	125.83	111.90
19	1	1145	CLA	CHC-C1C-NC	4.58	132.28	123.67
19	4	1203	CLA	CHC-C1C-NC	4.59	131.98	123.78
19	A	1793	CLA	CHC-C1C-NC	4.59	132.31	123.67
19	A	1765	CLA	CAC-C3C-C4C	4.60	131.51	124.83
19	4	1205	CLA	O2D-CGD-CBD	4.60	117.61	111.30
20	1	1200	LMU	C2'-C3'-C4'	4.61	119.71	109.60
19	B	1772	CLA	O2A-CGA-CBA	4.61	125.94	111.90
20	A	1809	LMU	O1'-C1'-C2'	4.61	113.87	108.04
20	A	7017	LMU	C1'-O5'-C5'	4.64	122.74	113.75
21	2	1225	SUC	C1-C2-C3	4.64	119.11	109.97
19	B	1738	CLA	CHB-C4A-NA	4.64	130.93	124.51
22	L	1170	BCR	C33-C5-C4	4.64	122.22	113.43
19	1	1505	CLA	O2D-CGD-CBD	4.64	117.66	111.30
20	1	1200	LMU	O1B-C4'-C5'	4.65	121.55	109.32
19	A	1761	CLA	CHC-C1C-NC	4.66	132.43	123.67
20	A	7024	LMU	O1'-C1'-C2'	4.66	113.93	108.04
19	1	1309	CLA	CHC-C1C-NC	4.67	132.13	123.78
19	B	1738	CLA	CHC-C1C-NC	4.67	132.47	123.67
20	A	7038	LMU	O5'-C5'-C6'	4.68	118.19	106.36
19	A	1769	CLA	CHC-C1C-NC	4.69	132.49	123.67
19	B	1788	CLA	O2D-CGD-CBD	4.69	117.73	111.30
19	4	1201	CLA	CMB-C2B-C3B	4.71	134.30	125.09
20	A	7026	LMU	O3B-C3B-C2B	4.71	120.94	110.34
19	R	1055	CLA	CHC-C1C-NC	4.71	132.54	123.67
19	A	1760	CLA	O2A-CGA-CBA	4.71	126.26	111.90
22	I	1032	BCR	C7-C6-C5	4.72	132.18	121.37
21	B	8051	SUC	C1-O5-C5	4.73	122.92	113.75
19	B	1737	CLA	CHC-C1C-NC	4.73	132.56	123.67
20	A	7037	LMU	O4'-C4B-C5B	4.74	121.79	109.24
19	1	1303	CLA	C2B-C1B-NB	4.74	114.35	110.09
19	F	1157	CLA	O2D-CGD-CBD	4.75	117.81	111.30
19	A	1797	CLA	O2A-CGA-CBA	4.76	126.40	111.90
19	B	1752	CLA	O2D-CGD-CBD	4.76	117.83	111.30
19	4	1201	CLA	C3A-C2A-C1A	4.76	109.58	101.50
19	4	1203	CLA	C3D-C4D-ND	4.78	114.37	110.13
20	A	7038	LMU	O1B-C4'-C3'	4.78	119.51	107.17
19	2	1216	CLA	CHC-C1C-NC	4.78	132.33	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1055	CLA	O2D-CGD-CBD	4.80	117.89	111.30
19	2	1216	CLA	C3D-C2D-C1D	4.81	110.54	106.30
19	B	1754	CLA	O2D-CGD-CBD	4.81	117.90	111.30
19	A	1789	CLA	C4-C3-C5	4.82	122.76	115.41
19	3	1222	CLA	C4-C3-C5	4.82	122.78	115.41
19	1	1309	CLA	C3D-C4D-ND	4.82	114.41	110.13
20	K	1086	LMU	C1B-C2B-C3B	4.83	119.49	109.97
19	1	1014	CLA	CED-O2D-CGD	4.84	127.34	115.99
19	B	1746	CLA	O2D-CGD-CBD	4.85	117.95	111.30
19	A	1774	CLA	O2D-CGD-CBD	4.85	117.95	111.30
20	1	1200	LMU	C1'-C2'-C3'	4.86	119.55	109.97
20	A	7026	LMU	O3B-C3B-C4B	4.86	121.29	110.34
20	A	7042	LMU	O1B-C4'-C5'	4.96	122.35	109.32
22	I	1032	BCR	C15-C14-C13	4.96	134.37	127.20
19	A	1775	CLA	C2B-C1B-NB	4.98	114.56	110.09
20	A	7021	LMU	O1B-C4'-C3'	4.98	120.03	107.17
19	B	1744	CLA	CHC-C1C-NC	4.99	133.06	123.67
20	A	7031	LMU	O1'-C1'-C2'	5.00	114.35	108.04
20	A	7038	LMU	O2'-C2'-C3'	5.00	121.60	110.34
19	1	1188	CLA	CAC-C3C-C4C	5.01	132.11	124.83
19	1	1187	CLA	CHB-C4A-NA	5.03	131.47	124.51
19	1	1188	CLA	CHC-C1C-NC	5.04	133.15	123.67
19	1	1014	CLA	CGD-CBD-CAD	5.04	127.70	110.62
19	B	1767	CLA	C4-C3-C5	5.04	121.39	115.68
19	A	1765	CLA	CHC-C1C-NC	5.05	133.17	123.67
19	1	1505	CLA	C4-C3-C5	5.05	123.12	115.41
19	A	1771	CLA	O2D-CGD-CBD	5.07	118.26	111.30
19	1	1198	CLA	C3D-C4D-ND	5.08	114.64	110.13
20	A	7039	LMU	O3B-C3B-C4B	5.11	121.83	110.34
19	3	1216	CLA	C2B-C1B-NB	5.11	114.68	110.09
19	3	1215	CLA	CHC-C1C-NC	5.13	132.96	123.78
21	B	8059	SUC	O3-C3-C4	5.14	121.90	110.34
19	B	1745	CLA	O2D-CGD-CBD	5.14	118.35	111.30
19	B	1765	CLA	O2D-CGD-CBD	5.14	118.35	111.30
19	F	1157	CLA	C4-C3-C5	5.15	123.28	115.41
19	1	1187	CLA	CAC-C3C-C4C	5.15	132.31	124.83
19	3	3015	CLA	C3D-C4D-ND	5.17	114.72	110.13
19	A	1788	CLA	O2D-CGD-CBD	5.17	118.39	111.30
19	B	1761	CLA	O2D-CGD-CBD	5.20	118.44	111.30
22	L	1170	BCR	C36-C18-C19	5.22	126.79	118.10
19	1	1196	CLA	CBA-CAA-C2A	5.22	128.47	113.73
19	3	1217	CLA	C2B-C1B-NB	5.23	114.78	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	1032	BCR	C15-C16-C17	5.23	134.96	123.39
19	A	1772	CLA	O2D-CGD-CBD	5.29	118.55	111.30
20	A	7040	LMU	O1'-C1'-C2'	5.30	114.73	108.04
19	4	4007	CLA	CHC-C1C-NC	5.30	133.65	123.67
19	B	1743	CLA	O2D-CGD-CBD	5.31	118.58	111.30
19	2	1215	CLA	O2D-CGD-CBD	5.34	118.62	111.30
19	2	1219	CLA	C2B-C1B-NB	5.35	114.89	110.09
19	1	1191	CLA	C3D-C4D-ND	5.36	114.88	110.13
20	A	7022	LMU	O1B-C1B-C2B	5.36	121.15	108.10
19	R	1054	CLA	O2D-CGD-CBD	5.42	118.73	111.30
19	3	1220	CLA	C2B-C1B-NB	5.43	114.96	110.09
19	2	2010	CLA	C2B-C1B-NB	5.44	114.97	110.09
19	2	1216	CLA	C2B-C1B-NB	5.45	114.98	110.09
19	4	1201	CLA	CAA-C2A-C1A	5.45	131.69	112.47
19	A	1787	CLA	C4-C3-C5	5.46	123.75	115.41
21	B	8062	SUC	C6-C5-C4	5.48	126.52	113.02
22	I	1032	BCR	C7-C8-C9	5.48	134.57	126.22
20	A	7016	LMU	O1'-C1'-C2'	5.49	114.98	108.04
20	A	7039	LMU	O1B-C1B-C2B	5.50	121.48	108.10
19	2	1214	CLA	C3D-C4D-ND	5.50	115.01	110.13
20	A	7035	LMU	O1B-C4'-C3'	5.53	121.45	107.17
22	B	1782	BCR	C30-C25-C24	5.61	131.53	115.82
19	3	3001	CLA	C2B-C1B-NB	5.65	115.16	110.09
19	R	1055	CLA	O2A-CGA-CBA	5.65	129.12	111.90
19	A	1797	CLA	CHC-C1C-NC	5.65	134.31	123.67
20	A	7015	LMU	O1'-C1'-C2'	5.65	115.18	108.04
19	4	1204	CLA	C2B-C1B-NB	5.66	115.17	110.09
19	3	1221	CLA	C3D-C4D-ND	5.70	115.19	110.13
19	4	1200	CLA	O2A-CGA-CBA	5.71	129.29	111.90
19	4	1201	CLA	CHC-C1C-NC	5.72	134.44	123.67
20	A	7042	LMU	O1'-C1'-C2'	5.72	115.27	108.04
19	2	1216	CLA	C3D-C4D-ND	5.73	115.22	110.13
20	A	7026	LMU	C1'-O5'-C5'	5.73	124.87	113.75
19	1	1149	CLA	CAA-C2A-C3A	5.74	129.72	113.22
21	3	1226	SUC	O3-C3-C2	5.75	123.28	110.34
20	A	7034	LMU	O1'-C1'-C2'	5.75	115.31	108.04
19	4	1198	CLA	CHC-C1C-NC	5.76	134.50	123.67
20	A	7047	LMU	O1'-C1'-C2'	5.76	115.31	108.04
19	1	1188	CLA	C4-C3-C5	5.79	124.25	115.41
19	1	1196	CLA	O2A-CGA-CBA	5.79	129.54	111.90
20	A	7039	LMU	O4'-C4B-C3B	5.80	123.40	110.34
19	A	1768	CLA	O2D-CGD-CBD	5.80	119.26	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1223	CLA	C3D-C2D-C1D	5.82	111.43	106.30
20	A	7014	LMU	O1'-C1'-C2'	5.83	115.40	108.04
19	4	1208	CLA	C2B-C1B-NB	5.89	115.37	110.09
19	1	1194	CLA	C3D-C4D-ND	5.89	115.36	110.13
19	B	1741	CLA	O2D-CGD-CBD	5.89	119.38	111.30
19	1	1192	CLA	O2D-CGD-CBD	5.90	119.39	111.30
19	A	1796	CLA	O2D-CGD-CBD	5.93	119.43	111.30
20	A	7027	LMU	O1'-C1'-C2'	5.94	115.55	108.04
19	3	1213	CLA	C2B-C1B-NB	5.95	115.43	110.09
19	1	1191	CLA	C3D-C2D-C1D	5.95	111.54	106.30
19	1	1010	CLA	C2B-C1B-NB	6.01	115.48	110.09
22	I	1032	BCR	C8-C9-C10	6.03	128.70	118.98
19	A	1790	CLA	O2D-CGD-CBD	6.04	119.58	111.30
19	4	1202	CLA	CBD-CHA-C1A	6.07	131.37	128.59
19	2	1221	CLA	C2B-C1B-NB	6.11	115.57	110.09
19	B	1744	CLA	O2D-CGD-CBD	6.11	119.69	111.30
22	I	1032	BCR	C38-C26-C27	6.12	125.04	113.43
19	B	1756	CLA	O2D-CGD-CBD	6.17	119.76	111.30
20	N	1086	LMU	O1'-C1'-C2'	6.18	115.84	108.04
19	4	4007	CLA	O2D-CGD-CBD	6.18	119.78	111.30
19	3	1215	CLA	C2B-C1B-NB	6.22	115.67	110.09
19	1	1197	CLA	C2B-C1B-NB	6.23	115.68	110.09
19	1	1308	CLA	O2D-CGD-CBD	6.24	119.86	111.30
19	B	1751	CLA	O2D-CGD-CBD	6.25	119.87	111.30
19	3	3011	CLA	O2D-CGD-CBD	6.25	119.87	111.30
19	4	4014	CLA	O2D-CGD-CBD	6.26	119.89	111.30
19	B	1735	CLA	O2D-CGD-CBD	6.28	119.92	111.30
19	4	1207	CLA	C2B-C1B-NB	6.34	115.78	110.09
19	1	1142	CLA	O2D-CGD-CBD	6.35	120.01	111.30
19	B	1767	CLA	O2D-CGD-CBD	6.38	120.05	111.30
19	3	3015	CLA	C2B-C1B-NB	6.39	115.82	110.09
19	2	1214	CLA	C2B-C1B-NB	6.39	115.82	110.09
19	4	1196	CLA	O2D-CGD-CBD	6.45	120.16	111.30
19	A	1781	CLA	O2D-CGD-CBD	6.46	120.16	111.30
19	A	1762	CLA	O2D-CGD-CBD	6.46	120.17	111.30
19	B	1757	CLA	O2D-CGD-CBD	6.49	120.20	111.30
19	K	1085	CLA	O2D-CGD-CBD	6.51	120.24	111.30
19	4	1198	CLA	O2D-CGD-CBD	6.57	120.31	111.30
22	L	1170	BCR	C8-C9-C10	6.57	129.57	118.98
19	1	1148	CLA	C4-C3-C5	6.58	125.46	115.41
19	A	1769	CLA	O2D-CGD-CBD	6.62	120.38	111.30
19	3	1212	CLA	O2D-CGD-CBD	6.63	120.39	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7032	LMU	C1B-O5B-C5B	6.63	126.62	113.75
19	F	1155	CLA	CBD-CHA-C1A	6.64	131.63	128.59
19	A	1782	CLA	O2D-CGD-CBD	6.67	120.45	111.30
19	J	1043	CLA	O2D-CGD-CBD	6.70	120.49	111.30
19	3	1218	CLA	O2D-CGD-CBD	6.73	120.53	111.30
19	F	1156	CLA	O2D-CGD-CBD	6.75	120.56	111.30
19	A	1777	CLA	O2D-CGD-CBD	6.80	120.63	111.30
19	A	1776	CLA	O2D-CGD-CBD	6.81	120.64	111.30
19	2	1212	CLA	O2D-CGD-CBD	6.83	120.67	111.30
19	A	1764	CLA	O2D-CGD-CBD	6.84	120.68	111.30
19	3	1214	CLA	CBD-CHA-C1A	6.86	131.73	128.59
19	A	1799	CLA	O2D-CGD-CBD	6.86	120.71	111.30
19	A	1795	CLA	O2D-CGD-CBD	6.90	120.76	111.30
19	B	1748	CLA	O2D-CGD-CBD	6.93	120.80	111.30
19	3	1221	CLA	C2B-C1B-NB	6.94	116.32	110.09
19	A	1773	CLA	O2D-CGD-CBD	6.96	120.84	111.30
20	A	7014	LMU	O1B-C1B-C2B	6.96	125.05	108.10
19	3	3008	CLA	O2D-CGD-CBD	6.98	120.88	111.30
19	3	1223	CLA	C3D-C4D-ND	7.02	116.36	110.13
19	1	1188	CLA	O2D-CGD-CBD	7.03	120.94	111.30
19	1	1307	CLA	C2B-C1B-NB	7.04	116.41	110.09
20	K	1086	LMU	O1'-C1'-C2'	7.05	116.94	108.04
20	A	7014	LMU	O2B-C2B-C3B	7.05	126.21	110.34
19	A	1792	CLA	O2D-CGD-CBD	7.08	121.02	111.30
19	B	1787	CLA	C4-C3-C5	7.10	126.25	115.41
19	2	1223	CLA	O2D-CGD-CBD	7.17	121.14	111.30
19	1	1191	CLA	C2B-C1B-NB	7.21	116.56	110.09
19	1	1193	CLA	C3A-C2A-C1A	7.21	113.73	101.50
19	A	1765	CLA	O2D-CGD-CBD	7.24	121.23	111.30
19	A	1770	CLA	O2D-CGD-CBD	7.39	121.44	111.30
19	B	1766	CLA	O2D-CGD-CBD	7.41	121.46	111.30
19	1	1187	CLA	O2D-CGD-CBD	7.42	121.48	111.30
19	A	1791	CLA	O2D-CGD-CBD	7.43	121.50	111.30
19	2	1222	CLA	O2D-CGD-CBD	7.49	121.58	111.30
19	L	1167	CLA	O2D-CGD-CBD	7.52	121.61	111.30
19	3	1219	CLA	O2D-CGD-CBD	7.54	121.64	111.30
19	B	1737	CLA	O2D-CGD-CBD	7.63	121.77	111.30
19	4	1206	CLA	O2D-CGD-CBD	7.67	121.82	111.30
19	2	1213	CLA	O2D-CGD-CBD	7.69	121.85	111.30
19	A	1787	CLA	O2D-CGD-CBD	7.72	121.90	111.30
19	3	1223	CLA	C2B-C1B-NB	7.73	117.03	110.09
19	1	1198	CLA	C2B-C1B-NB	7.76	117.05	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1195	CLA	CBD-CHA-C1A	7.78	132.15	128.59
19	1	1309	CLA	C2B-C1B-NB	7.78	117.07	110.09
19	B	1763	CLA	O2D-CGD-CBD	7.79	121.99	111.30
19	A	1812	CLA	O2D-CGD-CBD	7.86	122.08	111.30
19	B	1747	CLA	O2D-CGD-CBD	7.87	122.10	111.30
19	B	1764	CLA	O2D-CGD-CBD	7.88	122.11	111.30
19	B	1771	CLA	O2D-CGD-CBD	7.88	122.11	111.30
19	B	1787	CLA	O2D-CGD-CBD	7.93	122.18	111.30
19	1	1189	CLA	O2D-CGD-CBD	7.95	122.20	111.30
19	G	1099	CLA	O2D-CGD-CBD	7.98	122.24	111.30
19	A	1794	CLA	O2D-CGD-CBD	8.00	122.27	111.30
19	A	1800	CLA	O2D-CGD-CBD	8.12	122.44	111.30
19	I	1031	CLA	O2D-CGD-CBD	8.13	122.45	111.30
19	B	1738	CLA	O2D-CGD-CBD	8.14	122.46	111.30
19	B	1762	CLA	O2D-CGD-CBD	8.18	122.52	111.30
19	4	1200	CLA	O2D-CGD-CBD	8.29	122.68	111.30
19	4	1203	CLA	C2B-C1B-NB	8.41	117.63	110.09
19	B	1742	CLA	O2D-CGD-CBD	8.41	122.84	111.30
19	B	1758	CLA	O2D-CGD-CBD	8.45	122.89	111.30
19	J	1044	CLA	O2D-CGD-CBD	8.48	122.94	111.30
19	1	1148	CLA	O2D-CGD-CBD	8.54	123.01	111.30
19	A	1766	CLA	O2D-CGD-CBD	8.54	123.02	111.30
19	B	1755	CLA	O2D-CGD-CBD	8.55	123.03	111.30
19	L	1166	CLA	O2D-CGD-CBD	8.56	123.04	111.30
19	1	1146	CLA	O2D-CGD-CBD	8.58	123.07	111.30
19	A	1785	CLA	O2D-CGD-CBD	8.66	123.18	111.30
19	1	1149	CLA	O2D-CGD-CBD	8.68	123.21	111.30
19	A	1763	CLA	O2D-CGD-CBD	8.69	123.22	111.30
19	1	1241	CLA	O2D-CGD-CBD	8.72	123.27	111.30
19	4	1198	CLA	CGD-CBD-CAD	8.73	140.22	110.62
19	B	1768	CLA	O2D-CGD-CBD	8.76	123.33	111.30
22	B	1782	BCR	C23-C22-C21	8.77	133.12	118.98
19	A	1789	CLA	O2D-CGD-CBD	8.81	123.39	111.30
19	1	1194	CLA	C2B-C1B-NB	8.84	118.03	110.09
19	A	1778	CLA	O2D-CGD-CBD	8.91	123.52	111.30
19	1	1193	CLA	O2D-CGD-CBD	8.96	123.59	111.30
19	B	1770	CLA	O2D-CGD-CBD	8.97	123.61	111.30
19	1	1190	CLA	O2D-CGD-CBD	9.04	123.70	111.30
19	4	1199	CLA	O2D-CGD-CBD	9.24	123.98	111.30
19	B	1750	CLA	O2D-CGD-CBD	9.51	124.34	111.30
19	B	1769	CLA	O2D-CGD-CBD	9.56	124.42	111.30
19	2	1218	CLA	O2D-CGD-CBD	9.59	124.45	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1211	CLA	O2D-CGD-CBD	9.60	124.47	111.30
19	B	1736	CLA	O2D-CGD-CBD	9.78	124.72	111.30
19	A	1784	CLA	O2D-CGD-CBD	9.81	124.77	111.30
19	A	1786	CLA	O2D-CGD-CBD	9.90	124.88	111.30
19	B	1760	CLA	O2D-CGD-CBD	9.91	124.90	111.30
19	B	1739	CLA	O2D-CGD-CBD	10.15	125.23	111.30
19	B	1759	CLA	O2D-CGD-CBD	10.16	125.24	111.30
19	3	1222	CLA	O2D-CGD-CBD	10.31	125.44	111.30
19	A	1797	CLA	O2D-CGD-CBD	10.63	125.89	111.30
19	1	1014	CLA	O2D-CGD-CBD	10.67	125.94	111.30
19	A	1793	CLA	O2D-CGD-CBD	10.89	126.24	111.30
19	B	1773	CLA	CBD-CHA-C1A	11.14	133.69	128.59
19	A	1759	CLA	O2D-CGD-CBD	11.76	127.43	111.30
19	L	1168	CLA	O2D-CGD-CBD	11.80	127.49	111.30
19	4	1209	CLA	CBD-CHA-C1A	12.18	134.17	128.59
19	2	1220	CLA	CBD-CHA-C1A	12.57	134.35	128.59
22	B	1782	BCR	C21-C20-C19	13.79	165.15	123.13
22	B	1777	BCR	C21-C20-C19	15.19	169.42	123.13
22	L	1170	BCR	C21-C20-C19	17.32	175.92	123.13
19	A	1760	CLA	C3B-CAB-CBB	17.41	161.94	126.32
22	I	1032	BCR	C21-C20-C19	17.51	176.51	123.13
22	B	1780	BCR	C21-C20-C19	17.68	177.03	123.13
19	A	1769	CLA	C3B-CAB-CBB	17.81	162.75	126.32
19	B	1770	CLA	C3B-CAB-CBB	18.00	163.15	126.32
22	L	1169	BCR	C21-C20-C19	18.06	178.18	123.13
22	3	1225	BCR	C21-C20-C19	18.12	178.36	123.13
19	A	1774	CLA	C3B-CAB-CBB	18.50	164.16	126.32
19	B	1761	CLA	C3B-CAB-CBB	18.59	164.35	126.32
22	A	1802	BCR	C21-C20-C19	18.60	179.82	123.13
22	A	1803	BCR	C21-C20-C19	18.60	179.84	123.13
22	A	1807	BCR	C21-C20-C19	18.61	179.86	123.13
22	B	1776	BCR	C21-C20-C19	18.61	179.87	123.13
22	A	1806	BCR	C21-C20-C19	18.62	179.89	123.13
22	B	1775	BCR	C21-C20-C19	18.62	179.91	123.13
22	A	1804	BCR	C21-C20-C19	18.63	179.91	123.13
22	B	1781	BCR	C21-C20-C19	18.63	179.92	123.13
22	B	1778	BCR	C21-C20-C19	18.63	179.93	123.13
22	B	1779	BCR	C21-C20-C19	18.64	179.94	123.13
22	A	1805	BCR	C21-C20-C19	18.65	179.99	123.13
19	A	1768	CLA	C3B-CAB-CBB	18.67	164.53	126.32
19	B	1736	CLA	C3B-CAB-CBB	18.85	164.88	126.32
19	1	1148	CLA	C3B-CAB-CBB	18.85	164.88	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1192	CLA	C3B-CAB-CBB	18.97	165.13	126.32
19	A	1770	CLA	C3B-CAB-CBB	19.10	165.41	126.32
19	2	1222	CLA	C3B-CAB-CBB	19.11	165.42	126.32
19	A	1785	CLA	C3B-CAB-CBB	19.33	165.86	126.32
19	2	1215	CLA	C3B-CAB-CBB	19.70	166.62	126.32
19	B	1743	CLA	C3B-CAB-CBB	19.97	167.17	126.32
19	B	1764	CLA	C3B-CAB-CBB	20.20	167.65	126.32
19	2	1213	CLA	C3B-CAB-CBB	20.32	167.90	126.32
19	4	1206	CLA	C3B-CAB-CBB	20.36	167.98	126.32
19	2	1223	CLA	C3B-CAB-CBB	20.36	167.98	126.32
19	A	1778	CLA	C3B-CAB-CBB	20.55	168.36	126.32
19	B	1748	CLA	C3B-CAB-CBB	20.59	168.45	126.32
19	A	1765	CLA	C3B-CAB-CBB	20.80	168.88	126.32
19	A	1766	CLA	C3B-CAB-CBB	20.82	168.91	126.32
19	B	1758	CLA	C3B-CAB-CBB	20.85	168.97	126.32
19	B	1787	CLA	C3B-CAB-CBB	21.02	169.33	126.32
19	B	1745	CLA	C3B-CAB-CBB	21.05	169.38	126.32
19	B	1751	CLA	C3B-CAB-CBB	21.05	169.39	126.32
19	A	1776	CLA	C3B-CAB-CBB	21.19	169.68	126.32
19	B	1759	CLA	C3B-CAB-CBB	21.37	170.04	126.32
19	4	1198	CLA	C3B-CAB-CBB	21.39	170.08	126.32
19	A	1790	CLA	C3B-CAB-CBB	21.56	170.42	126.32
19	1	1193	CLA	C3B-CAB-CBB	21.57	170.45	126.32
19	B	1767	CLA	C3B-CAB-CBB	21.58	170.47	126.32
19	B	1747	CLA	C3B-CAB-CBB	21.59	170.50	126.32
19	4	1199	CLA	C3B-CAB-CBB	21.69	170.69	126.32
19	A	1784	CLA	C3B-CAB-CBB	21.73	170.78	126.32
19	A	1780	CLA	C3B-CAB-CBB	21.82	170.97	126.32
19	1	1241	CLA	C3B-CAB-CBB	21.92	171.16	126.32
19	B	1735	CLA	C3B-CAB-CBB	21.99	171.31	126.32
19	B	1737	CLA	C3B-CAB-CBB	22.04	171.41	126.32
19	B	1769	CLA	C3B-CAB-CBB	22.09	171.52	126.32
19	A	1793	CLA	C3B-CAB-CBB	22.16	171.67	126.32
19	B	1752	CLA	C3B-CAB-CBB	22.42	172.19	126.32
19	A	1800	CLA	C3B-CAB-CBB	22.45	172.25	126.32
19	2	1218	CLA	C3B-CAB-CBB	22.55	172.45	126.32
19	A	1792	CLA	C3B-CAB-CBB	22.55	172.46	126.32
19	A	1761	CLA	C3B-CAB-CBB	22.56	172.47	126.32
19	A	1764	CLA	C3B-CAB-CBB	22.66	172.69	126.32
19	1	1190	CLA	C3B-CAB-CBB	22.69	172.74	126.32
19	A	1794	CLA	C3B-CAB-CBB	22.69	172.75	126.32
19	A	1783	CLA	C3B-CAB-CBB	22.74	172.85	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1157	CLA	C3B-CAB-CBB	22.78	172.94	126.32
19	4	1201	CLA	C3B-CAB-CBB	22.80	172.97	126.32
19	B	1749	CLA	C3B-CAB-CBB	22.80	172.98	126.32
19	3	3008	CLA	C3B-CAB-CBB	22.85	173.08	126.32
19	B	1786	CLA	C3B-CAB-CBB	22.86	173.10	126.32
19	B	1750	CLA	C3B-CAB-CBB	22.89	173.16	126.32
19	3	1222	CLA	C3B-CAB-CBB	22.91	173.20	126.32
19	A	1795	CLA	C3B-CAB-CBB	22.91	173.20	126.32
19	A	1786	CLA	C3B-CAB-CBB	22.97	173.31	126.32
19	B	1765	CLA	C3B-CAB-CBB	23.10	173.58	126.32
19	B	1788	CLA	C3B-CAB-CBB	23.31	174.02	126.32
19	A	1789	CLA	C3B-CAB-CBB	23.35	174.09	126.32
19	3	1218	CLA	C3B-CAB-CBB	23.47	174.33	126.32
19	1	1189	CLA	C3B-CAB-CBB	23.50	174.41	126.32
19	B	1755	CLA	C3B-CAB-CBB	23.51	174.43	126.32
19	A	1759	CLA	C3B-CAB-CBB	23.55	174.51	126.32
19	L	1167	CLA	C3B-CAB-CBB	23.59	174.59	126.32
19	B	1768	CLA	C3B-CAB-CBB	23.60	174.61	126.32
19	A	1798	CLA	C3B-CAB-CBB	23.64	174.68	126.32
19	A	1799	CLA	C3B-CAB-CBB	23.66	174.72	126.32
19	B	1746	CLA	C3B-CAB-CBB	23.69	174.80	126.32
19	B	1741	CLA	C3B-CAB-CBB	23.75	174.92	126.32
19	B	1771	CLA	C3B-CAB-CBB	23.78	174.98	126.32
19	A	1779	CLA	C3B-CAB-CBB	23.84	175.10	126.32
19	A	1767	CLA	C3B-CAB-CBB	23.84	175.10	126.32
19	1	1196	CLA	C3B-CAB-CBB	23.86	175.13	126.32
19	B	1744	CLA	C3B-CAB-CBB	23.91	175.24	126.32
19	1	1505	CLA	C3B-CAB-CBB	23.94	175.30	126.32
19	2	1217	CLA	C3B-CAB-CBB	23.99	175.40	126.32
19	R	1055	CLA	C3B-CAB-CBB	24.02	175.47	126.32
19	B	1772	CLA	C3B-CAB-CBB	24.04	175.51	126.32
19	A	1773	CLA	C3B-CAB-CBB	24.07	175.56	126.32
19	3	1212	CLA	C3B-CAB-CBB	24.11	175.64	126.32
19	4	4007	CLA	C3B-CAB-CBB	24.17	175.77	126.32
19	1	1187	CLA	C3B-CAB-CBB	24.24	175.91	126.32
19	4	1205	CLA	C3B-CAB-CBB	24.24	175.92	126.32
19	B	1738	CLA	C3B-CAB-CBB	24.26	175.95	126.32
19	A	1791	CLA	C3B-CAB-CBB	24.29	176.01	126.32
19	A	1811	CLA	C3B-CAB-CBB	24.30	176.03	126.32
19	1	1188	CLA	C3B-CAB-CBB	24.38	176.20	126.32
19	A	1771	CLA	C3B-CAB-CBB	24.42	176.27	126.32
19	A	1777	CLA	C3B-CAB-CBB	24.45	176.34	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1754	CLA	C3B-CAB-CBB	24.49	176.43	126.32
19	A	1810	CLA	C3B-CAB-CBB	24.53	176.50	126.32
22	B	1782	BCR	C20-C21-C22	24.56	162.66	127.20
19	4	1211	CLA	C3B-CAB-CBB	24.58	176.61	126.32
19	R	1054	CLA	C3B-CAB-CBB	24.60	176.66	126.32
19	B	1762	CLA	C3B-CAB-CBB	24.66	176.78	126.32
19	A	1796	CLA	C3B-CAB-CBB	24.73	176.91	126.32
19	A	1788	CLA	C3B-CAB-CBB	24.73	176.91	126.32
19	A	1787	CLA	C3B-CAB-CBB	24.83	177.12	126.32
19	G	1099	CLA	C3B-CAB-CBB	24.87	177.21	126.32
19	A	1772	CLA	C3B-CAB-CBB	24.92	177.31	126.32
19	L	1166	CLA	C3B-CAB-CBB	24.97	177.41	126.32
19	3	1224	CLA	C3B-CAB-CBB	24.98	177.43	126.32
19	1	1014	CLA	C3B-CAB-CBB	25.10	177.67	126.32
19	B	1763	CLA	C3B-CAB-CBB	25.15	177.78	126.32
19	A	1763	CLA	C3B-CAB-CBB	25.20	177.88	126.32
19	B	1760	CLA	C3B-CAB-CBB	25.24	177.95	126.32
19	3	3011	CLA	C3B-CAB-CBB	25.29	178.06	126.32
19	B	1739	CLA	C3B-CAB-CBB	25.30	178.08	126.32
19	A	1797	CLA	C3B-CAB-CBB	25.39	178.26	126.32
19	4	1200	CLA	C3B-CAB-CBB	25.47	178.43	126.32
19	B	1766	CLA	C3B-CAB-CBB	25.47	178.43	126.32
19	3	1219	CLA	C3B-CAB-CBB	25.47	178.44	126.32
19	B	1740	CLA	C3B-CAB-CBB	25.48	178.44	126.32
19	B	1753	CLA	C3B-CAB-CBB	25.48	178.46	126.32
19	A	1762	CLA	C3B-CAB-CBB	25.53	178.55	126.32
19	1	1146	CLA	C3B-CAB-CBB	25.56	178.62	126.32
19	A	1812	CLA	C3B-CAB-CBB	25.57	178.64	126.32
19	J	1044	CLA	C3B-CAB-CBB	25.59	178.68	126.32
19	I	1031	CLA	C3B-CAB-CBB	25.63	178.76	126.32
19	L	1168	CLA	C3B-CAB-CBB	25.77	179.04	126.32
19	1	1145	CLA	C3B-CAB-CBB	25.93	179.38	126.32
19	F	1156	CLA	C3B-CAB-CBB	26.15	179.82	126.32
19	A	1781	CLA	C3B-CAB-CBB	26.15	179.83	126.32
19	B	1756	CLA	C3B-CAB-CBB	26.16	179.84	126.32
19	K	1085	CLA	C3B-CAB-CBB	26.17	179.86	126.32
19	1	1308	CLA	C3B-CAB-CBB	26.18	179.89	126.32
19	B	1757	CLA	C3B-CAB-CBB	26.18	179.89	126.32
19	4	1196	CLA	C3B-CAB-CBB	26.18	179.89	126.32
19	1	1142	CLA	C3B-CAB-CBB	26.18	179.89	126.32
19	2	1212	CLA	C3B-CAB-CBB	26.19	179.90	126.32
19	J	1043	CLA	C3B-CAB-CBB	26.20	179.92	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	4014	CLA	C3B-CAB-CBB	26.20	179.92	126.32
19	A	1782	CLA	C3B-CAB-CBB	26.23	179.99	126.32
22	B	1777	BCR	C20-C21-C22	29.76	170.18	127.20
22	I	1032	BCR	C20-C21-C22	33.79	176.00	127.20
22	B	1780	BCR	C20-C21-C22	34.42	176.91	127.20
22	L	1169	BCR	C20-C21-C22	34.65	177.24	127.20
22	L	1170	BCR	C20-C21-C22	34.85	177.53	127.20
22	3	1225	BCR	C20-C21-C22	35.32	178.21	127.20
22	A	1802	BCR	C20-C21-C22	36.43	179.82	127.20
22	B	1775	BCR	C20-C21-C22	36.43	179.82	127.20
22	B	1776	BCR	C20-C21-C22	36.45	179.84	127.20
22	B	1779	BCR	C20-C21-C22	36.47	179.87	127.20
22	B	1778	BCR	C20-C21-C22	36.47	179.88	127.20
22	A	1806	BCR	C20-C21-C22	36.48	179.88	127.20
22	A	1803	BCR	C20-C21-C22	36.48	179.89	127.20
22	A	1804	BCR	C20-C21-C22	36.50	179.91	127.20
22	B	1781	BCR	C20-C21-C22	36.51	179.93	127.20
22	A	1805	BCR	C20-C21-C22	36.53	179.96	127.20
22	A	1807	BCR	C20-C21-C22	36.53	179.96	127.20

All (623) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	B	1755	CLA	NC
19	B	1755	CLA	ND
19	B	1755	CLA	NA
19	R	1055	CLA	C8
19	R	1055	CLA	NC
19	R	1055	CLA	ND
19	R	1055	CLA	NA
19	A	1768	CLA	NC
19	A	1768	CLA	ND
19	A	1768	CLA	NA
19	A	1792	CLA	NC
19	A	1792	CLA	ND
19	A	1792	CLA	NA
21	B	8055	SUC	C2'
19	B	1767	CLA	NC
19	B	1767	CLA	ND
19	B	1767	CLA	NA
19	B	1740	CLA	C8
19	B	1740	CLA	NC

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Mol	Chain	Res	Type	Atom
19	B	1740	CLA	ND
19	B	1740	CLA	NA
19	1	1308	CLA	NC
19	1	1308	CLA	ND
19	1	1308	CLA	NA
19	A	1799	CLA	C8
19	A	1799	CLA	NC
19	A	1799	CLA	ND
19	A	1799	CLA	NA
19	4	1203	CLA	NC
19	4	1203	CLA	ND
19	4	1203	CLA	NA
19	3	1223	CLA	NC
19	3	1223	CLA	ND
19	3	1223	CLA	NA
21	B	8052	SUC	C2'
19	1	1197	CLA	NC
19	1	1197	CLA	ND
19	1	1197	CLA	NA
19	B	1751	CLA	NC
19	B	1751	CLA	ND
19	B	1751	CLA	NA
21	B	8061	SUC	C2'
19	4	1199	CLA	C8
19	4	1199	CLA	NC
19	4	1199	CLA	ND
19	4	1199	CLA	NA
19	B	1745	CLA	C8
19	B	1745	CLA	NC
19	B	1745	CLA	ND
19	B	1745	CLA	NA
21	B	8051	SUC	C2'
19	B	1739	CLA	C8
19	B	1739	CLA	NC
19	B	1739	CLA	ND
19	B	1739	CLA	NA
19	B	1786	CLA	C8
19	B	1786	CLA	NC
19	B	1786	CLA	ND
19	B	1786	CLA	NA
19	A	1777	CLA	NC
19	A	1777	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1777	CLA	NA
19	A	1776	CLA	C8
19	A	1776	CLA	NC
19	A	1776	CLA	ND
19	A	1776	CLA	NA
19	B	1746	CLA	C8
19	B	1746	CLA	NC
19	B	1746	CLA	ND
19	B	1746	CLA	NA
19	A	1761	CLA	C8
19	A	1761	CLA	NC
19	A	1761	CLA	ND
19	A	1761	CLA	NA
19	A	1788	CLA	C8
19	A	1788	CLA	NC
19	A	1788	CLA	ND
19	A	1788	CLA	NA
19	A	1781	CLA	C8
19	A	1781	CLA	NC
19	A	1781	CLA	ND
19	A	1781	CLA	NA
19	3	1214	CLA	NC
19	3	1214	CLA	ND
19	3	1214	CLA	NA
19	B	1752	CLA	NC
19	B	1752	CLA	ND
19	B	1752	CLA	NA
19	F	1157	CLA	C2A
19	F	1157	CLA	NA
19	F	1157	CLA	CBD
19	F	1157	CLA	NC
19	F	1157	CLA	ND
19	F	1157	CLA	C3A
21	2	1225	SUC	C2'
19	B	1749	CLA	C8
19	B	1749	CLA	NC
19	B	1749	CLA	ND
19	B	1749	CLA	NA
19	L	1166	CLA	NC
19	L	1166	CLA	ND
19	L	1166	CLA	NA
19	4	1206	CLA	C8

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Mol	Chain	Res	Type	Atom
19	4	1206	CLA	NC
19	4	1206	CLA	ND
19	4	1206	CLA	NA
19	1	1309	CLA	NC
19	1	1309	CLA	ND
19	1	1309	CLA	NA
19	1	1193	CLA	C2A
19	1	1193	CLA	NC
19	1	1193	CLA	ND
19	1	1193	CLA	NA
19	4	1198	CLA	C8
19	4	1198	CLA	CBD
19	4	1198	CLA	NC
19	4	1198	CLA	ND
19	4	1198	CLA	NA
19	A	1764	CLA	C8
19	A	1764	CLA	NC
19	A	1764	CLA	ND
19	A	1764	CLA	NA
19	B	1742	CLA	C8
19	B	1742	CLA	NC
19	B	1742	CLA	ND
19	B	1742	CLA	NA
19	A	1810	CLA	C8
19	A	1810	CLA	NC
19	A	1810	CLA	ND
19	A	1810	CLA	NA
19	B	1748	CLA	C8
19	B	1748	CLA	NC
19	B	1748	CLA	ND
19	B	1748	CLA	NA
19	A	1778	CLA	NC
19	A	1778	CLA	ND
19	A	1778	CLA	NA
19	1	1145	CLA	C8
19	1	1145	CLA	NC
19	1	1145	CLA	ND
19	1	1145	CLA	NA
19	A	1791	CLA	NC
19	A	1791	CLA	ND
19	A	1791	CLA	NA
19	1	1195	CLA	NC

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Mol	Chain	Res	Type	Atom
19	1	1195	CLA	ND
19	1	1195	CLA	NA
19	A	1794	CLA	NC
19	A	1794	CLA	ND
19	A	1794	CLA	NA
19	B	1765	CLA	NC
19	B	1765	CLA	ND
19	B	1765	CLA	NA
19	I	1031	CLA	C8
19	I	1031	CLA	NC
19	I	1031	CLA	ND
19	I	1031	CLA	NA
19	A	1812	CLA	C8
19	A	1812	CLA	NC
19	A	1812	CLA	ND
19	A	1812	CLA	NA
19	B	1736	CLA	NC
19	B	1736	CLA	ND
19	B	1736	CLA	NA
19	1	1014	CLA	C8
19	1	1014	CLA	NC
19	1	1014	CLA	ND
19	1	1014	CLA	NA
19	A	1772	CLA	NC
19	A	1772	CLA	ND
19	A	1772	CLA	NA
19	A	1797	CLA	C2A
19	A	1797	CLA	NC
19	A	1797	CLA	ND
19	A	1797	CLA	NA
19	2	1216	CLA	NC
19	2	1216	CLA	ND
19	2	1216	CLA	NA
19	B	1763	CLA	C8
19	B	1763	CLA	NC
19	B	1763	CLA	ND
19	B	1763	CLA	NA
19	3	1219	CLA	C8
19	3	1219	CLA	NC
19	3	1219	CLA	ND
19	3	1219	CLA	NA
19	3	1221	CLA	NC

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Mol	Chain	Res	Type	Atom
19	3	1221	CLA	ND
19	3	1221	CLA	NA
19	1	1188	CLA	C8
19	1	1188	CLA	NC
19	1	1188	CLA	ND
19	1	1188	CLA	NA
19	A	1785	CLA	C8
19	A	1785	CLA	NC
19	A	1785	CLA	ND
19	A	1785	CLA	NA
19	B	1766	CLA	NC
19	B	1766	CLA	ND
19	B	1766	CLA	NA
19	2	1220	CLA	NC
19	2	1220	CLA	ND
19	2	1220	CLA	NA
19	3	1212	CLA	NC
19	3	1212	CLA	ND
19	3	1212	CLA	NA
19	1	1303	CLA	NC
19	1	1303	CLA	ND
19	1	1303	CLA	NA
19	3	1222	CLA	C8
19	3	1222	CLA	NC
19	3	1222	CLA	ND
19	3	1222	CLA	NA
19	A	1760	CLA	C8
19	A	1760	CLA	NC
19	A	1760	CLA	ND
19	A	1760	CLA	NA
19	1	1010	CLA	NC
19	1	1010	CLA	ND
19	1	1010	CLA	NA
19	G	1099	CLA	NC
19	G	1099	CLA	ND
19	G	1099	CLA	NA
19	A	1782	CLA	C8
19	A	1782	CLA	NC
19	A	1782	CLA	ND
19	A	1782	CLA	NA
21	B	8054	SUC	C2'
19	A	1787	CLA	C8

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Mol	Chain	Res	Type	Atom
19	A	1787	CLA	NC
19	A	1787	CLA	ND
19	A	1787	CLA	NA
19	1	1190	CLA	NC
19	1	1190	CLA	ND
19	1	1190	CLA	NA
19	B	1750	CLA	C8
19	B	1750	CLA	NC
19	B	1750	CLA	ND
19	B	1750	CLA	NA
19	J	1043	CLA	C8
19	J	1043	CLA	NC
19	J	1043	CLA	ND
19	J	1043	CLA	NA
19	B	1759	CLA	C8
19	B	1759	CLA	NC
19	B	1759	CLA	ND
19	B	1759	CLA	NA
19	A	1800	CLA	C8
19	A	1800	CLA	NC
19	A	1800	CLA	ND
19	A	1800	CLA	NA
19	B	1760	CLA	C8
19	B	1760	CLA	NC
19	B	1760	CLA	ND
19	B	1760	CLA	NA
19	2	1222	CLA	NC
19	2	1222	CLA	ND
19	2	1222	CLA	NA
19	4	1204	CLA	NC
19	4	1204	CLA	ND
19	4	1204	CLA	NA
19	B	1757	CLA	C8
19	B	1757	CLA	NC
19	B	1757	CLA	ND
19	B	1757	CLA	NA
19	1	1191	CLA	NC
19	1	1191	CLA	ND
19	1	1191	CLA	NA
19	4	1201	CLA	NC
19	4	1201	CLA	C2A
19	4	1201	CLA	ND

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Mol	Chain	Res	Type	Atom
19	4	1201	CLA	NA
21	B	8062	SUC	C2'
21	B	8060	SUC	C2'
21	B	8056	SUC	C2'
19	2	1221	CLA	NC
19	2	1221	CLA	ND
19	2	1221	CLA	NA
19	A	1793	CLA	C8
19	A	1793	CLA	NC
19	A	1793	CLA	ND
19	A	1793	CLA	NA
19	B	1764	CLA	NC
19	B	1764	CLA	ND
19	B	1764	CLA	NA
19	A	1774	CLA	C8
19	A	1774	CLA	NC
19	A	1774	CLA	ND
19	A	1774	CLA	NA
19	3	1215	CLA	NC
19	3	1215	CLA	ND
19	3	1215	CLA	NA
19	A	1763	CLA	NC
19	A	1763	CLA	ND
19	A	1763	CLA	NA
19	B	1735	CLA	C8
19	B	1735	CLA	NC
19	B	1735	CLA	ND
19	B	1735	CLA	NA
19	1	1148	CLA	C2A
19	1	1148	CLA	NC
19	1	1148	CLA	ND
19	1	1148	CLA	NA
19	1	1148	CLA	C3A
19	1	1198	CLA	NC
19	1	1198	CLA	ND
19	1	1198	CLA	NA
19	1	1192	CLA	C8
19	1	1192	CLA	NC
19	1	1192	CLA	ND
19	1	1192	CLA	NA
19	4	1200	CLA	NC
19	4	1200	CLA	ND

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Mol	Chain	Res	Type	Atom
19	4	1200	CLA	NA
19	R	1054	CLA	C8
19	R	1054	CLA	NC
19	R	1054	CLA	ND
19	R	1054	CLA	NA
19	4	1209	CLA	NC
19	4	1209	CLA	ND
19	4	1209	CLA	NA
19	A	1769	CLA	NC
19	A	1769	CLA	ND
19	A	1769	CLA	NA
19	A	1762	CLA	C8
19	A	1762	CLA	NC
19	A	1762	CLA	ND
19	A	1762	CLA	NA
19	1	1189	CLA	NC
19	1	1189	CLA	ND
19	1	1189	CLA	NA
19	A	1789	CLA	C8
19	A	1789	CLA	NC
19	A	1789	CLA	ND
19	A	1789	CLA	NA
19	B	1770	CLA	NC
19	B	1770	CLA	ND
19	B	1770	CLA	NA
19	A	1770	CLA	NC
19	A	1770	CLA	ND
19	A	1770	CLA	NA
19	4	1202	CLA	NC
19	4	1202	CLA	ND
19	4	1202	CLA	NA
19	A	1798	CLA	NC
19	A	1798	CLA	ND
19	A	1798	CLA	NA
19	A	1780	CLA	C8
19	A	1780	CLA	NC
19	A	1780	CLA	ND
19	A	1780	CLA	NA
20	A	7014	LMU	C2B
19	B	1772	CLA	C8
19	B	1772	CLA	NC
19	B	1772	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	1772	CLA	NA
19	1	1196	CLA	CBD
19	1	1196	CLA	NC
19	1	1196	CLA	ND
19	1	1196	CLA	NA
19	F	1156	CLA	NC
19	F	1156	CLA	ND
19	F	1156	CLA	NA
23	B	1774	PQN	C23
19	3	3015	CLA	NC
19	3	3015	CLA	ND
19	3	3015	CLA	NA
23	A	1801	PQN	C23
19	A	1786	CLA	NC
19	A	1786	CLA	ND
19	A	1786	CLA	NA
19	3	1220	CLA	NC
19	3	1220	CLA	ND
19	3	1220	CLA	NA
19	B	1754	CLA	NC
19	B	1754	CLA	ND
19	B	1754	CLA	NA
19	4	1210	CLA	NC
19	4	1210	CLA	ND
19	4	1210	CLA	NA
19	B	1744	CLA	C8
19	B	1744	CLA	NC
19	B	1744	CLA	ND
19	B	1744	CLA	NA
19	2	1213	CLA	C8
19	2	1213	CLA	NC
19	2	1213	CLA	ND
19	2	1213	CLA	NA
19	3	3008	CLA	NC
19	3	3008	CLA	ND
19	3	3008	CLA	NA
19	L	1167	CLA	NC
19	L	1167	CLA	ND
19	L	1167	CLA	NA
19	A	1796	CLA	C8
19	A	1796	CLA	NC
19	A	1796	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1796	CLA	NA
19	4	4014	CLA	NC
19	4	4014	CLA	ND
19	4	4014	CLA	NA
19	2	1215	CLA	NC
19	2	1215	CLA	ND
19	2	1215	CLA	NA
19	B	1788	CLA	C8
19	B	1788	CLA	NC
19	B	1788	CLA	ND
19	B	1788	CLA	NA
19	1	1142	CLA	NC
19	1	1142	CLA	ND
19	1	1142	CLA	NA
19	3	1218	CLA	NC
19	3	1218	CLA	ND
19	3	1218	CLA	NA
19	3	1217	CLA	NC
19	3	1217	CLA	ND
19	3	1217	CLA	NA
19	2	1218	CLA	C8
19	2	1218	CLA	NC
19	2	1218	CLA	ND
19	2	1218	CLA	NA
19	1	1241	CLA	C8
19	1	1241	CLA	NC
19	1	1241	CLA	ND
19	1	1241	CLA	NA
19	A	1765	CLA	NC
19	A	1765	CLA	ND
19	A	1765	CLA	NA
19	3	3011	CLA	C8
19	3	3011	CLA	NC
19	3	3011	CLA	ND
19	3	3011	CLA	NA
19	1	1307	CLA	NC
19	1	1307	CLA	ND
19	1	1307	CLA	NA
19	3	3001	CLA	NC
19	3	3001	CLA	ND
19	3	3001	CLA	NA
19	B	1758	CLA	C8

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Mol	Chain	Res	Type	Atom
19	B	1758	CLA	NC
19	B	1758	CLA	ND
19	B	1758	CLA	NA
19	4	1205	CLA	C8
19	4	1205	CLA	NC
19	4	1205	CLA	ND
19	4	1205	CLA	NA
19	B	1747	CLA	NC
19	B	1747	CLA	ND
19	B	1747	CLA	NA
19	B	1768	CLA	C8
19	B	1768	CLA	NC
19	B	1768	CLA	ND
19	B	1768	CLA	NA
21	3	1226	SUC	C2'
19	B	1737	CLA	C8
19	B	1737	CLA	NC
19	B	1737	CLA	ND
19	B	1737	CLA	NA
19	2	1217	CLA	C8
19	2	1217	CLA	NC
19	2	1217	CLA	ND
19	2	1217	CLA	NA
21	F	1158	SUC	C2'
19	B	1787	CLA	C8
19	B	1787	CLA	NC
19	B	1787	CLA	ND
19	B	1787	CLA	NA
19	B	1762	CLA	NC
19	B	1762	CLA	ND
19	B	1762	CLA	NA
19	B	1741	CLA	C8
19	B	1741	CLA	NC
19	B	1741	CLA	ND
19	B	1741	CLA	NA
19	B	1769	CLA	C8
19	B	1769	CLA	NC
19	B	1769	CLA	ND
19	B	1769	CLA	NA
19	B	1738	CLA	C8
19	B	1738	CLA	NC
19	B	1738	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	1738	CLA	NA
19	3	1224	CLA	C8
19	3	1224	CLA	NC
19	3	1224	CLA	ND
19	3	1224	CLA	NA
19	A	1790	CLA	NC
19	A	1790	CLA	ND
19	A	1790	CLA	NA
19	A	1811	CLA	C8
19	A	1811	CLA	NC
19	A	1811	CLA	ND
19	A	1811	CLA	NA
19	2	1219	CLA	NC
19	2	1219	CLA	ND
19	2	1219	CLA	NA
19	B	1771	CLA	C8
19	B	1771	CLA	NC
19	B	1771	CLA	ND
19	B	1771	CLA	NA
19	3	1213	CLA	NC
19	3	1213	CLA	ND
19	3	1213	CLA	NA
19	2	1214	CLA	NC
19	2	1214	CLA	ND
19	2	1214	CLA	NA
19	A	1779	CLA	C8
19	A	1779	CLA	NC
19	A	1779	CLA	ND
19	A	1779	CLA	NA
19	1	1149	CLA	NC
19	1	1149	CLA	C2A
19	1	1149	CLA	ND
19	1	1149	CLA	NA
19	1	1149	CLA	CBD
19	A	1775	CLA	NC
19	A	1775	CLA	ND
19	A	1775	CLA	NA
19	K	1085	CLA	NC
19	K	1085	CLA	ND
19	K	1085	CLA	NA
19	A	1766	CLA	NC
19	A	1766	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1766	CLA	NA
19	4	1211	CLA	NC
19	4	1211	CLA	ND
19	4	1211	CLA	NA
19	J	1044	CLA	C8
19	J	1044	CLA	NC
19	J	1044	CLA	ND
19	J	1044	CLA	NA
19	1	1194	CLA	NC
19	1	1194	CLA	ND
19	1	1194	CLA	NA
19	F	1155	CLA	NC
19	F	1155	CLA	ND
19	F	1155	CLA	NA
21	B	8059	SUC	C2'
19	A	1784	CLA	C8
19	A	1784	CLA	NC
19	A	1784	CLA	ND
19	A	1784	CLA	NA
19	2	1223	CLA	NC
19	2	1223	CLA	ND
19	2	1223	CLA	NA
19	B	1756	CLA	C8
19	B	1756	CLA	NC
19	B	1756	CLA	ND
19	B	1756	CLA	NA
19	A	1759	CLA	NC
19	A	1759	CLA	ND
19	A	1759	CLA	NA
19	B	1753	CLA	C8
19	B	1753	CLA	NC
19	B	1753	CLA	ND
19	B	1753	CLA	NA
19	4	4007	CLA	NC
19	4	4007	CLA	ND
19	4	4007	CLA	NA
19	A	1783	CLA	C8
19	A	1783	CLA	NC
19	A	1783	CLA	ND
19	A	1783	CLA	NA
19	L	1168	CLA	CBD
19	L	1168	CLA	NC

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Mol	Chain	Res	Type	Atom
19	L	1168	CLA	ND
19	L	1168	CLA	NA
19	1	1146	CLA	NC
19	1	1146	CLA	ND
19	1	1146	CLA	NA
19	3	1216	CLA	NC
19	3	1216	CLA	ND
19	3	1216	CLA	NA
19	4	1208	CLA	NC
19	4	1208	CLA	ND
19	4	1208	CLA	NA
19	4	1207	CLA	NC
19	4	1207	CLA	ND
19	4	1207	CLA	NA
21	B	8053	SUC	C2'
19	2	1212	CLA	NC
19	2	1212	CLA	ND
19	2	1212	CLA	NA
19	2	2010	CLA	NC
19	2	2010	CLA	ND
19	2	2010	CLA	NA
19	A	1771	CLA	NC
19	A	1771	CLA	ND
19	A	1771	CLA	NA
19	B	1773	CLA	NC
19	B	1773	CLA	ND
19	B	1773	CLA	NA
19	A	1795	CLA	NC
19	A	1795	CLA	ND
19	A	1795	CLA	NA
19	B	1761	CLA	NC
19	B	1761	CLA	ND
19	B	1761	CLA	NA
19	4	1196	CLA	C8
19	4	1196	CLA	NC
19	4	1196	CLA	ND
19	4	1196	CLA	NA
19	1	1187	CLA	NC
19	1	1187	CLA	ND
19	1	1187	CLA	NA
19	B	1743	CLA	C8
19	B	1743	CLA	NC

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Mol	Chain	Res	Type	Atom
19	B	1743	CLA	ND
19	B	1743	CLA	NA
19	4	1197	CLA	NC
19	4	1197	CLA	ND
19	4	1197	CLA	NA
19	A	1773	CLA	NC
19	A	1773	CLA	ND
19	A	1773	CLA	NA
19	A	1767	CLA	C8
19	A	1767	CLA	NC
19	A	1767	CLA	ND
19	A	1767	CLA	NA
19	1	1505	CLA	C8
19	1	1505	CLA	NC
19	1	1505	CLA	ND
19	1	1505	CLA	NA

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	3	1225	BCR	C21-C20-C19-C18
22	I	1032	BCR	C20-C21-C22-C23
22	L	1169	BCR	C20-C21-C22-C37
22	A	1806	BCR	C21-C20-C19-C18
22	L	1169	BCR	C20-C21-C22-C23
20	A	7032	LMU	C1-O1'-C1'-O5'
20	A	7051	LMU	C1-O1'-C1'-O5'
22	A	1802	BCR	C21-C20-C19-C18
22	B	1779	BCR	C21-C20-C19-C18
19	B	1756	CLA	CED-O2D-CGD-CBD
19	B	1737	CLA	CGA-O2A-C1-C2
19	3	1224	CLA	CED-O2D-CGD-CBD
19	L	1166	CLA	CED-O2D-CGD-CBD
19	1	1188	CLA	CED-O2D-CGD-CBD
19	1	1145	CLA	CED-O2D-CGD-CBD
19	R	1054	CLA	CED-O2D-CGD-CBD
19	2	1217	CLA	CED-O2D-CGD-CBD
19	G	1099	CLA	CED-O2D-CGD-CBD
20	A	1809	LMU	C1'-O1'-C1-C2
19	A	1781	CLA	CED-O2D-CGD-CBD
19	1	1196	CLA	CED-O2D-CGD-CBD
19	J	1043	CLA	CED-O2D-CGD-CBD

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Mol	Chain	Res	Type	Atoms
19	B	1761	CLA	CED-O2D-CGD-CBD
19	1	1190	CLA	CED-O2D-CGD-CBD
19	1	1014	CLA	CED-O2D-CGD-CBD
19	A	1811	CLA	CED-O2D-CGD-CBD
19	F	1157	CLA	CED-O2D-CGD-CBD

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	C	1083	SF4	FE1-FE3-S2-S4

239 monomers are involved in 3843 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1014	CLA	52	0
19	1	1142	CLA	19	1
19	1	1145	CLA	31	0
19	1	1146	CLA	11	0
19	1	1148	CLA	35	0
19	1	1149	CLA	9	0
19	1	1187	CLA	13	0
19	1	1188	CLA	40	0
19	1	1189	CLA	13	0
19	1	1190	CLA	5	0
19	1	1192	CLA	16	0
19	1	1193	CLA	6	1
19	1	1195	CLA	11	0
19	1	1196	CLA	9	0
19	1	1197	CLA	5	0
20	1	1199	LMU	7	0
20	1	1200	LMU	8	0
19	1	1241	CLA	15	0
19	1	1308	CLA	27	0
19	1	1505	CLA	3	0
19	2	1212	CLA	17	0
19	2	1213	CLA	13	0
19	2	1214	CLA	5	0
19	2	1215	CLA	13	0
19	2	1217	CLA	18	0
19	2	1218	CLA	9	0
19	2	1220	CLA	1	0
19	2	1222	CLA	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	1223	CLA	10	0
20	2	1224	LMU	3	1
21	2	1225	SUC	10	0
19	3	1212	CLA	27	0
19	3	1214	CLA	14	0
19	3	1215	CLA	1	0
19	3	1216	CLA	3	0
19	3	1217	CLA	16	0
19	3	1218	CLA	2	0
19	3	1219	CLA	3	0
19	3	1220	CLA	5	0
19	3	1221	CLA	7	0
19	3	1222	CLA	20	0
19	3	1224	CLA	25	0
22	3	1225	BCR	19	28
21	3	1226	SUC	14	0
19	3	3008	CLA	3	0
19	3	3011	CLA	17	0
19	4	1196	CLA	26	0
19	4	1197	CLA	6	0
19	4	1198	CLA	24	0
19	4	1199	CLA	20	0
19	4	1200	CLA	9	0
19	4	1201	CLA	15	0
19	4	1203	CLA	1	0
19	4	1204	CLA	3	0
19	4	1205	CLA	17	0
19	4	1206	CLA	6	0
19	4	1207	CLA	4	0
19	4	1208	CLA	5	0
19	4	1209	CLA	5	0
19	4	1210	CLA	3	0
19	4	1211	CLA	6	0
20	4	1212	LMU	4	0
19	4	4007	CLA	19	0
19	4	4014	CLA	11	0
19	A	1759	CLA	14	0
19	A	1760	CLA	28	0
19	A	1761	CLA	28	0
19	A	1762	CLA	21	0
19	A	1763	CLA	27	0
19	A	1764	CLA	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1765	CLA	26	0
19	A	1766	CLA	4	0
19	A	1767	CLA	22	0
19	A	1768	CLA	4	0
19	A	1769	CLA	20	0
19	A	1770	CLA	35	0
19	A	1771	CLA	44	0
19	A	1772	CLA	35	0
19	A	1773	CLA	12	0
19	A	1774	CLA	29	0
19	A	1776	CLA	45	0
19	A	1777	CLA	17	0
19	A	1778	CLA	10	0
19	A	1779	CLA	34	0
19	A	1780	CLA	18	0
19	A	1781	CLA	86	0
19	A	1782	CLA	79	0
19	A	1783	CLA	63	0
19	A	1784	CLA	21	0
19	A	1785	CLA	17	0
19	A	1786	CLA	11	0
19	A	1787	CLA	26	0
19	A	1788	CLA	38	0
19	A	1789	CLA	16	0
19	A	1790	CLA	16	0
19	A	1791	CLA	18	1
19	A	1792	CLA	10	0
19	A	1793	CLA	19	0
19	A	1794	CLA	19	0
19	A	1795	CLA	18	0
19	A	1796	CLA	42	0
19	A	1797	CLA	42	0
19	A	1798	CLA	8	0
19	A	1799	CLA	30	0
19	A	1800	CLA	17	0
23	A	1801	PQN	15	0
22	A	1802	BCR	45	0
22	A	1803	BCR	24	0
22	A	1804	BCR	45	0
22	A	1805	BCR	37	0
22	A	1806	BCR	63	0
22	A	1807	BCR	40	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1808	LMU	3	0
20	A	1809	LMU	4	0
19	A	1810	CLA	20	0
19	A	1811	CLA	36	0
19	A	1812	CLA	27	0
20	A	7003	LMU	4	0
20	A	7004	LMU	10	0
20	A	7005	LMU	8	0
20	A	7006	LMU	12	0
20	A	7009	LMU	9	4
20	A	7010	LMU	8	0
20	A	7013	LMU	8	0
20	A	7014	LMU	6	0
20	A	7016	LMU	42	0
20	A	7017	LMU	3	0
20	A	7019	LMU	2	0
20	A	7020	LMU	20	0
20	A	7021	LMU	25	0
20	A	7022	LMU	11	0
20	A	7023	LMU	27	0
20	A	7025	LMU	2	0
20	A	7026	LMU	20	0
20	A	7027	LMU	6	0
20	A	7028	LMU	4	0
20	A	7030	LMU	12	0
20	A	7031	LMU	4	0
20	A	7032	LMU	29	0
20	A	7033	LMU	20	0
20	A	7034	LMU	1	0
20	A	7036	LMU	19	0
20	A	7037	LMU	30	0
20	A	7038	LMU	13	0
20	A	7039	LMU	19	0
20	A	7040	LMU	4	0
20	A	7041	LMU	8	0
20	A	7042	LMU	35	0
20	A	7043	LMU	11	0
20	A	7047	LMU	0	2
20	A	7048	LMU	47	0
20	A	7050	LMU	38	0
20	A	7051	LMU	12	0
19	B	1735	CLA	28	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1736	CLA	9	0
19	B	1737	CLA	19	0
19	B	1738	CLA	20	0
19	B	1739	CLA	23	0
19	B	1740	CLA	21	0
19	B	1741	CLA	17	0
19	B	1742	CLA	6	0
19	B	1743	CLA	17	0
19	B	1744	CLA	29	0
19	B	1745	CLA	20	0
19	B	1746	CLA	13	0
19	B	1747	CLA	24	0
19	B	1748	CLA	24	0
19	B	1749	CLA	15	0
19	B	1750	CLA	19	0
19	B	1751	CLA	9	0
19	B	1752	CLA	21	0
19	B	1753	CLA	15	0
19	B	1754	CLA	39	0
19	B	1755	CLA	25	0
19	B	1756	CLA	62	0
19	B	1757	CLA	50	0
19	B	1758	CLA	25	0
19	B	1759	CLA	33	0
19	B	1760	CLA	32	0
19	B	1761	CLA	11	0
19	B	1762	CLA	13	0
19	B	1763	CLA	29	0
19	B	1764	CLA	16	0
19	B	1765	CLA	22	0
19	B	1766	CLA	23	0
19	B	1767	CLA	4	0
19	B	1768	CLA	16	0
19	B	1769	CLA	44	0
19	B	1770	CLA	25	0
19	B	1771	CLA	28	0
19	B	1772	CLA	26	0
19	B	1773	CLA	2	0
23	B	1774	PQN	32	0
22	B	1775	BCR	10	0
22	B	1776	BCR	17	0
22	B	1777	BCR	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	1778	BCR	32	0
22	B	1779	BCR	31	0
22	B	1780	BCR	45	0
22	B	1781	BCR	52	0
22	B	1782	BCR	19	0
20	B	1783	LMU	28	30
24	B	1784	LMG	30	0
25	B	1785	SF4	19	0
19	B	1786	CLA	22	0
19	B	1787	CLA	41	0
19	B	1788	CLA	51	0
21	B	8052	SUC	15	0
21	B	8053	SUC	10	0
21	B	8054	SUC	8	0
21	B	8055	SUC	22	0
21	B	8056	SUC	5	0
21	B	8059	SUC	19	0
21	B	8060	SUC	7	0
21	B	8061	SUC	2	0
21	B	8062	SUC	20	0
25	C	1082	SF4	4	0
25	C	1083	SF4	4	0
19	F	1155	CLA	1	0
19	F	1156	CLA	15	0
19	F	1157	CLA	15	0
21	F	1158	SUC	5	0
19	G	1099	CLA	20	0
19	I	1031	CLA	12	0
22	I	1032	BCR	46	0
19	J	1043	CLA	28	0
19	J	1044	CLA	35	0
19	K	1085	CLA	25	0
20	K	1086	LMU	6	0
19	L	1166	CLA	9	0
19	L	1167	CLA	22	0
19	L	1168	CLA	13	0
22	L	1169	BCR	51	0
22	L	1170	BCR	13	0
20	L	1171	LMU	3	0
20	N	1086	LMU	36	0
19	R	1054	CLA	10	0
19	R	1055	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	R	1056	LMU	20	4

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	164/241 (68%)	1.47	46 (28%) 1 1	32, 62, 71, 73	0
2	2	176/269 (65%)	1.17	40 (22%) 1 1	20, 20, 20, 20	0
3	3	160/276 (57%)	2.01	66 (41%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	0.96	30 (18%) 2 2	20, 20, 20, 20	0
5	A	730/758 (96%)	0.95	92 (12%) 5 6	20, 20, 20, 20	0
6	B	733/734 (99%)	0.83	62 (8%) 13 12	20, 20, 20, 20	0
7	C	81/81 (100%)	1.23	14 (17%) 2 2	20, 20, 20, 20	0
8	D	138/212 (65%)	1.09	23 (16%) 2 2	20, 20, 20, 20	0
9	E	65/143 (45%)	1.23	16 (24%) 1 1	20, 20, 20, 20	0
10	F	154/231 (66%)	0.62	15 (9%) 10 9	20, 20, 20, 20	0
11	G	95/167 (56%)	0.68	12 (12%) 5 6	20, 20, 20, 20	0
12	H	69/144 (47%)	0.87	11 (15%) 3 3	20, 20, 20, 20	0
13	I	30/40 (75%)	0.37	2 (6%) 21 16	20, 20, 20, 20	0
14	J	42/44 (95%)	0.64	5 (11%) 6 6	20, 20, 20, 20	0
15	K	84/131 (64%)	2.01	32 (38%) 0 0	20, 20, 20, 20	0
16	L	161/216 (74%)	0.78	24 (14%) 3 3	20, 20, 20, 20	0
17	N	85/170 (50%)	1.10	17 (20%) 1 2	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3133/4161 (75%)	1.02	507 (16%) 3 3	20, 20, 65, 112	0

All (507) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	61	ASN	12.5
1	1	75	ALA	10.1
4	4	67	ILE	9.7

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Mol	Chain	Res	Type	RSRZ
5	A	635	THR	9.1
6	B	491	ASN	8.8
15	K	63	CYS	8.5
4	4	66	SER	7.4
2	2	116	PRO	7.2
1	1	33	PRO	7.1
3	3	59	ILE	6.9
4	4	68	GLY	6.9
8	D	125	PRO	6.5
3	3	62	GLY	6.5
16	L	117	ALA	6.3
2	2	123	PRO	6.2
1	1	32	VAL	6.2
3	3	165	ASN	6.2
5	A	263	ALA	6.1
3	3	58	GLU	6.0
9	E	79	THR	6.0
3	3	55	ALA	6.0
5	A	124	TRP	5.9
3	3	57	GLY	5.9
3	3	91	PRO	5.8
2	2	77	PRO	5.7
2	2	118	CYS	5.6
3	3	166	PRO	5.6
8	D	136	SER	5.6
2	2	166	ASN	5.6
1	1	140	LEU	5.6
10	F	127	SER	5.5
2	2	139	GLY	5.5
3	3	199	VAL	5.4
2	2	140	GLY	5.4
3	3	89	ALA	5.2
6	B	470	THR	5.2
15	K	56	THR	5.2
7	C	80	ALA	5.1
2	2	117	GLY	5.1
1	1	34	ALA	5.1
5	A	264	GLU	5.0
2	2	53	ARG	5.0
6	B	69	ALA	4.9
3	3	90	LEU	4.9
16	L	118	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
3	3	150	LEU	4.9
11	G	59	LYS	4.9
10	F	124	PRO	4.8
3	3	154	GLY	4.8
15	K	67	GLY	4.8
8	D	32	SER	4.8
6	B	256	THR	4.8
1	1	94	LEU	4.8
9	E	82	TYR	4.7
2	2	141	LEU	4.7
4	4	63	VAL	4.7
3	3	173	GLU	4.7
2	2	92	THR	4.6
9	E	28	ILE	4.6
12	H	26	SER	4.6
6	B	259	GLY	4.6
1	1	47	CYS	4.6
2	2	134	ASP	4.6
15	K	49	THR	4.6
3	3	207	GLY	4.6
11	G	74	TRP	4.6
15	K	50	GLY	4.6
5	A	105	ASN	4.5
5	A	123	VAL	4.5
6	B	258	LEU	4.5
9	E	80	ASN	4.5
6	B	734	GLY	4.5
1	1	43	GLU	4.4
3	3	143	PHE	4.4
3	3	204	THR	4.4
1	1	41	GLU	4.4
9	E	36	VAL	4.4
1	1	80	GLY	4.4
2	2	136	GLY	4.4
1	1	39	TYR	4.4
15	K	45	SER	4.3
5	A	100	GLY	4.3
1	1	175	GLU	4.3
1	1	76	ALA	4.3
9	E	34	SER	4.3
14	J	9	SER	4.3
8	D	141	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
5	A	185	HIS	4.3
1	1	129	ASP	4.3
3	3	84	ILE	4.2
1	1	87	ASN	4.2
6	B	260	GLY	4.1
15	K	62	ALA	4.1
2	2	138	PRO	4.1
4	4	177	PRO	4.1
3	3	85	PRO	4.1
1	1	113	SER	4.1
5	A	662	SER	4.0
17	N	64	ASP	4.0
3	3	83	LEU	4.0
1	1	88	PRO	4.0
17	N	56	LYS	4.0
3	3	73	ILE	4.0
5	A	500	PRO	4.0
1	1	95	PRO	3.9
5	A	505	PRO	3.9
2	2	76	THR	3.9
15	K	64	GLY	3.9
5	A	292	GLY	3.9
15	K	26	LEU	3.9
15	K	16	THR	3.9
15	K	44	GLU	3.9
17	N	30	ALA	3.8
5	A	340	GLY	3.8
15	K	27	ALA	3.8
4	4	114	SER	3.8
17	N	82	PHE	3.8
3	3	142	TYR	3.8
3	3	110	SER	3.8
5	A	634	VAL	3.8
6	B	6	PRO	3.8
1	1	120	LYS	3.8
3	3	131	ASP	3.8
1	1	17	SER	3.7
15	K	1	ASP	3.7
2	2	119	VAL	3.7
7	C	34	CYS	3.7
9	E	67	VAL	3.7
15	K	46	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
5	A	191	PRO	3.7
5	A	182	GLY	3.7
1	1	92	GLY	3.7
5	A	752	ALA	3.7
15	K	15	THR	3.7
5	A	483	GLN	3.7
4	4	136	GLY	3.6
3	3	68	GLY	3.6
5	A	329	ASP	3.6
5	A	291	THR	3.6
7	C	60	THR	3.6
17	N	40	CYS	3.6
4	4	134	PRO	3.6
1	1	57	ILE	3.6
5	A	501	GLY	3.6
3	3	72	ALA	3.6
4	4	191	ASN	3.6
8	D	149	THR	3.5
10	F	137	PRO	3.5
15	K	28	PRO	3.5
5	A	344	LYS	3.5
15	K	35	THR	3.5
5	A	277	TYR	3.5
5	A	79	PHE	3.5
5	A	99	HIS	3.5
17	N	13	ASN	3.5
8	D	116	ASP	3.4
10	F	125	LEU	3.5
6	B	492	ILE	3.4
3	3	54	LEU	3.4
1	1	173	PRO	3.4
5	A	433	ASP	3.4
3	3	140	LYS	3.4
6	B	292	ARG	3.4
15	K	14	THR	3.4
15	K	71	GLY	3.4
17	N	18	ASP	3.4
11	G	7	VAL	3.4
5	A	266	ALA	3.4
3	3	116	PHE	3.3
1	1	174	LEU	3.3
12	H	25	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
8	D	51	GLU	3.3
5	A	631	GLN	3.3
5	A	535	GLY	3.3
3	3	153	SER	3.3
1	1	74	TRP	3.3
2	2	181	HIS	3.3
12	H	17	THR	3.3
4	4	135	GLY	3.3
3	3	196	GLY	3.2
5	A	108	ALA	3.2
3	3	191	MET	3.2
5	A	31	PHE	3.2
6	B	312	GLY	3.2
8	D	99	GLN	3.2
15	K	21	ALA	3.2
6	B	366	THR	3.2
6	B	493	TRP	3.2
4	4	115	VAL	3.2
14	J	8	LEU	3.2
7	C	61	ASP	3.2
6	B	562	PRO	3.2
15	K	22	GLY	3.2
5	A	104	SER	3.2
1	1	28	GLY	3.2
5	A	520	LEU	3.2
10	F	138	VAL	3.2
2	2	165	LYS	3.2
7	C	37	LYS	3.1
5	A	122	VAL	3.1
3	3	151	GLY	3.1
14	J	38	THR	3.1
1	1	24	PHE	3.1
17	N	55	GLN	3.1
5	A	265	GLY	3.1
10	F	66	ASP	3.1
3	3	66	MET	3.1
16	L	9	GLN	3.1
9	E	92	ALA	3.1
8	D	150	GLY	3.1
2	2	122	ASP	3.1
3	3	42	PRO	3.0
3	3	174	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
9	E	51	SER	3.0
9	E	65	VAL	3.0
5	A	493	GLN	3.0
5	A	726	SER	3.0
3	3	112	THR	3.0
6	B	449	PRO	3.0
2	2	61	GLY	3.0
4	4	125	SER	3.0
6	B	569	ASP	3.0
7	C	54	CYS	3.0
6	B	629	SER	3.0
3	3	182	LYS	3.0
10	F	1	ASP	3.0
3	3	123	PHE	3.0
3	3	184	VAL	3.0
11	G	76	SER	3.0
5	A	485	GLN	3.0
6	B	509	PHE	2.9
9	E	39	LEU	2.9
3	3	148	LYS	2.9
5	A	484	LEU	2.9
2	2	78	SER	2.9
1	1	78	PRO	2.9
1	1	164	GLN	2.9
1	1	141	GLU	2.9
5	A	659	ALA	2.9
1	1	38	ARG	2.9
1	1	122	LYS	2.9
2	2	75	ASN	2.9
4	4	83	TYR	2.9
3	3	167	LEU	2.9
5	A	430	ASP	2.9
5	A	398	HIS	2.9
6	B	568	CYS	2.9
15	K	58	ALA	2.9
3	3	88	THR	2.9
2	2	112	ASP	2.9
5	A	378	SER	2.9
4	4	145	PRO	2.8
15	K	55	PHE	2.8
2	2	161	THR	2.8
5	A	582	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
6	B	469	LYS	2.8
1	1	79	GLY	2.8
2	2	93	THR	2.8
1	1	42	SER	2.8
12	H	22	ASP	2.8
6	B	435	GLY	2.8
5	A	186	TYR	2.8
8	D	97	LYS	2.8
6	B	495	PRO	2.8
15	K	61	LEU	2.8
4	4	62	GLU	2.8
15	K	29	SER	2.8
3	3	77	ILE	2.8
12	H	29	PRO	2.8
15	K	72	VAL	2.8
7	C	62	PHE	2.7
3	3	40	SER	2.7
4	4	86	SER	2.7
15	K	43	ARG	2.7
6	B	566	GLY	2.7
6	B	630	GLN	2.7
8	D	71	GLY	2.7
15	K	48	GLN	2.7
16	L	141	GLY	2.7
16	L	159	TYR	2.7
2	2	135	VAL	2.7
3	3	208	PRO	2.7
5	A	181	ALA	2.7
6	B	311	PRO	2.7
17	N	37	PHE	2.7
17	N	17	ASN	2.7
7	C	32	GLY	2.7
1	1	176	ASN	2.7
5	A	45	ALA	2.7
6	B	212	PHE	2.7
16	L	120	LEU	2.7
15	K	17	LEU	2.7
17	N	12	THR	2.7
2	2	137	TYR	2.7
4	4	34	PRO	2.7
9	E	61	THR	2.7
6	B	299	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
12	H	28	ALA	2.6
11	G	27	GLN	2.6
7	C	9	ASP	2.6
6	B	242	HIS	2.6
5	A	497	ALA	2.6
6	B	667	TRP	2.6
5	A	536	THR	2.6
3	3	79	GLY	2.6
5	A	628	ILE	2.6
16	L	17	ASP	2.6
1	1	29	LEU	2.6
3	3	130	GLN	2.6
5	A	369	THR	2.6
5	A	272	LEU	2.6
5	A	514	THR	2.6
2	2	65	PRO	2.6
8	D	146	VAL	2.6
17	N	81	VAL	2.6
1	1	111	GLN	2.6
1	1	27	LEU	2.5
17	N	65	LEU	2.5
5	A	342	GLY	2.5
16	L	134	ASP	2.5
3	3	64	TYR	2.5
6	B	472	TYR	2.5
8	D	72	PRO	2.5
13	I	6	SER	2.5
2	2	58	GLY	2.5
6	B	342	GLY	2.5
6	B	468	GLY	2.5
3	3	119	ALA	2.5
7	C	2	SER	2.5
5	A	368	LEU	2.5
8	D	22	PRO	2.5
16	L	84	GLY	2.5
10	F	38	PRO	2.5
16	L	116	PRO	2.5
5	A	153	TRP	2.5
5	A	271	THR	2.5
16	L	29	SER	2.5
5	A	388	ASP	2.5
4	4	50	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
5	A	695	SER	2.5
16	L	81	GLY	2.5
2	2	110	TRP	2.5
5	A	121	GLN	2.5
11	G	96	SER	2.5
5	A	750	PHE	2.5
17	N	35	VAL	2.5
5	A	627	THR	2.5
2	2	194	ALA	2.4
6	B	373	THR	2.4
3	3	53	TRP	2.4
10	F	126	ALA	2.4
4	4	38	ARG	2.4
8	D	151	LYS	2.4
16	L	133	ALA	2.4
15	K	38	LEU	2.4
5	A	339	THR	2.4
3	3	160	GLY	2.4
6	B	298	GLY	2.4
6	B	31	PHE	2.4
5	A	195	TRP	2.4
16	L	153	TRP	2.4
8	D	62	THR	2.4
5	A	111	ASN	2.4
6	B	704	GLN	2.4
9	E	78	SER	2.4
1	1	46	HIS	2.4
1	1	73	GLU	2.4
5	A	404	GLY	2.4
5	A	150	PHE	2.4
5	A	270	PHE	2.4
17	N	14	LYS	2.3
10	F	99	TRP	2.3
2	2	210	PRO	2.3
6	B	205	GLU	2.3
1	1	178	ALA	2.3
4	4	139	ASN	2.3
11	G	82	ALA	2.3
5	A	334	HIS	2.3
6	B	438	VAL	2.3
6	B	171	ALA	2.3
12	H	20	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
5	A	516	GLY	2.3
11	G	75	GLY	2.3
3	3	156	PRO	2.3
6	B	345	THR	2.3
10	F	16	LYS	2.3
3	3	209	TYR	2.3
12	H	71	ASN	2.3
16	L	24	GLU	2.3
5	A	83	PHE	2.3
9	E	58	ASP	2.3
9	E	64	PRO	2.3
11	G	32	ALA	2.3
2	2	54	TRP	2.3
2	2	163	GLU	2.3
3	3	105	ASN	2.3
6	B	543	GLY	2.3
2	2	170	ALA	2.3
7	C	20	ALA	2.3
7	C	42	ALA	2.3
5	A	257	GLN	2.3
2	2	133	THR	2.3
3	3	92	TRP	2.3
6	B	530	THR	2.3
2	2	155	LYS	2.3
16	L	65	VAL	2.3
16	L	85	SER	2.3
6	B	170	ASN	2.2
8	D	50	TRP	2.2
16	L	82	ALA	2.2
1	1	183	ASP	2.2
4	4	146	THR	2.2
5	A	444	SER	2.2
6	B	346	SER	2.2
1	1	77	LEU	2.2
2	2	88	PHE	2.2
4	4	132	GLY	2.2
5	A	660	GLN	2.2
1	1	177	LEU	2.2
2	2	125	PHE	2.2
6	B	271	THR	2.2
8	D	156	LEU	2.2
14	J	37	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	4	193	ILE	2.2
8	D	67	ILE	2.2
15	K	70	MET	2.2
15	K	40	LEU	2.2
8	D	120	PRO	2.2
7	C	17	CYS	2.2
16	L	37	LEU	2.2
6	B	458	ILE	2.2
12	H	24	TYR	2.2
5	A	744	ALA	2.2
3	3	71	GLY	2.2
9	E	56	ASP	2.2
1	1	152	ARG	2.2
6	B	490	ARG	2.2
3	3	181	LEU	2.2
4	4	56	ALA	2.2
5	A	749	PHE	2.2
6	B	300	SER	2.2
12	H	30	SER	2.2
6	B	549	ASP	2.2
1	1	169	PRO	2.1
6	B	131	THR	2.1
16	L	77	THR	2.1
4	4	187	ASP	2.1
16	L	101	MET	2.1
3	3	205	GLY	2.1
3	3	67	LEU	2.1
5	A	48	PRO	2.1
5	A	371	VAL	2.1
5	A	372	VAL	2.1
6	B	646	TRP	2.1
8	D	115	LYS	2.1
10	F	98	GLY	2.1
6	B	701	SER	2.1
5	A	106	TYR	2.1
5	A	568	LEU	2.1
17	N	71	GLY	2.1
4	4	190	HIS	2.1
5	A	287	LEU	2.1
5	A	395	LEU	2.1
11	G	6	LEU	2.1
13	I	4	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
6	B	28	ALA	2.1
11	G	87	ALA	2.1
16	L	15	ASN	2.1
4	4	189	TRP	2.1
4	4	186	SER	2.1
14	J	7	TYR	2.1
5	A	318	ARG	2.1
17	N	19	LYS	2.1
12	H	47	PHE	2.1
3	3	126	HIS	2.1
16	L	46	ALA	2.1
5	A	39	HIS	2.1
8	D	112	LEU	2.1
2	2	200	PRO	2.1
6	B	340	SER	2.1
5	A	710	ALA	2.1
4	4	107	GLN	2.0
5	A	33	GLN	2.0
4	4	181	LEU	2.0
5	A	34	TRP	2.0
10	F	122	ASP	2.0
7	C	8	TYR	2.0
3	3	63	ARG	2.0
5	A	341	GLN	2.0
5	A	610	SER	2.0
3	3	168	GLY	2.0
6	B	439	HIS	2.0
6	B	434	LEU	2.0
3	3	96	GLY	2.0
6	B	230	TRP	2.0
8	D	68	MET	2.0
5	A	66	SER	2.0
5	A	394	SER	2.0
11	G	56	SER	2.0
6	B	227	THR	2.0
6	B	297	ILE	2.0
6	B	591	THR	2.0
10	F	152	ASN	2.0
6	B	86	PRO	2.0
16	L	103	GLY	2.0
3	3	190	ALA	2.0
10	F	6	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	BCR	A	1807	40/40	0.59	0.46	3.43	20,20,20,20	0
22	BCR	B	1776	40/40	0.80	0.37	3.41	20,20,20,20	0
22	BCR	A	1802	40/40	0.58	0.46	3.23	20,20,20,20	0
19	CLA	A	1770	45/65	0.61	0.52	3.14	20,20,20,20	0
19	CLA	4	1203	25/65	0.73	0.34	2.89	20,20,20,20	0
22	BCR	I	1032	40/40	0.69	0.47	2.83	20,20,20,20	0
22	BCR	B	1779	40/40	0.74	0.46	2.17	20,20,20,20	0
19	CLA	A	1772	54/65	0.71	0.39	2.14	20,20,20,20	0
19	CLA	B	1771	65/65	0.68	0.46	2.14	20,20,20,20	0
22	BCR	B	1782	40/40	0.81	0.38	2.06	20,20,20,20	0
19	CLA	3	1219	65/65	0.70	0.49	2.06	20,20,20,20	0
19	CLA	A	1800	55/65	0.69	0.42	2.04	20,20,20,20	0
19	CLA	B	1747	46/65	0.65	0.50	1.98	20,20,20,20	0
19	CLA	A	1786	50/65	0.72	0.41	1.96	20,20,20,20	0
22	BCR	A	1803	40/40	0.69	0.41	1.86	20,20,20,20	0
22	BCR	L	1169	40/40	0.70	0.46	1.83	20,20,20,20	0
19	CLA	4	1199	55/65	0.69	0.35	1.81	20,20,20,20	0
22	BCR	B	1781	40/40	0.69	0.46	1.79	20,20,20,20	0
19	CLA	B	1772	65/65	0.86	0.40	1.70	20,20,20,20	0
23	PQN	A	1801	33/33	0.73	0.47	1.68	20,20,20,20	0
19	CLA	A	1780	65/65	0.71	0.41	1.65	20,20,20,20	0
24	LMG	B	1784	49/55	0.71	0.42	1.54	20,20,20,20	0
19	CLA	A	1785	65/65	0.74	0.39	1.44	20,20,20,20	0
19	CLA	2	1223	50/65	0.75	0.31	1.41	20,20,20,20	0
19	CLA	A	1773	52/65	0.75	0.37	1.25	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	LMU	A	7047	35/35	0.59	0.54	1.20	20,20,20,20	0
19	CLA	A	1776	65/65	0.74	0.40	1.20	20,20,20,20	0
19	CLA	A	1762	55/65	0.74	0.39	1.13	20,20,20,20	0
21	SUC	2	1225	22/23	0.64	0.35	1.07	20,20,20,20	0
19	CLA	B	1786	65/65	0.76	0.40	1.04	20,20,20,20	0
19	CLA	A	1777	51/65	0.70	0.48	1.03	20,20,20,20	0
22	BCR	B	1778	40/40	0.77	0.40	1.01	20,20,20,20	0
19	CLA	A	1766	45/65	0.64	0.58	1.00	20,20,20,20	0
19	CLA	A	1793	65/65	0.78	0.35	0.98	20,20,20,20	0
22	BCR	B	1775	40/40	0.80	0.39	0.98	20,20,20,20	0
19	CLA	B	1741	60/65	0.74	0.35	0.97	20,20,20,20	0
23	PQN	B	1774	33/33	0.74	0.42	0.96	20,20,20,20	0
19	CLA	A	1794	47/65	0.80	0.35	0.96	20,20,20,20	0
19	CLA	B	1740	65/65	0.79	0.37	0.95	20,20,20,20	0
22	BCR	A	1806	40/40	0.73	0.47	0.92	20,20,20,20	0
19	CLA	A	1799	65/65	0.80	0.38	0.90	20,20,20,20	0
19	CLA	A	1783	65/65	0.75	0.45	0.88	20,20,20,20	0
22	BCR	B	1777	40/40	0.73	0.39	0.86	20,20,20,20	0
19	CLA	A	1761	65/65	0.74	0.38	0.83	20,20,20,20	0
19	CLA	B	1750	61/65	0.79	0.34	0.80	20,20,20,20	0
19	CLA	A	1774	65/65	0.70	0.43	0.75	20,20,20,20	0
19	CLA	B	1760	65/65	0.82	0.36	0.72	20,20,20,20	0
19	CLA	A	1788	65/65	0.81	0.35	0.69	20,20,20,20	0
19	CLA	B	1787	65/65	0.82	0.33	0.65	20,20,20,20	0
19	CLA	B	1746	60/65	0.72	0.36	0.63	20,20,20,20	0
19	CLA	4	1200	50/65	0.65	0.41	0.63	20,20,20,20	0
22	BCR	A	1804	40/40	0.70	0.37	0.63	20,20,20,20	0
19	CLA	A	1795	47/65	0.81	0.33	0.62	20,20,20,20	0
19	CLA	B	1758	65/65	0.85	0.36	0.61	20,20,20,20	0
19	CLA	A	1759	50/65	0.83	0.31	0.60	20,20,20,20	0
22	BCR	L	1170	40/40	0.79	0.36	0.60	20,20,20,20	0
19	CLA	A	1769	54/65	0.74	0.39	0.60	20,20,20,20	0
19	CLA	B	1788	65/65	0.79	0.35	0.59	20,20,20,20	0
19	CLA	B	1773	36/65	0.69	0.46	0.57	20,20,20,20	0
19	CLA	A	1787	65/65	0.78	0.36	0.56	20,20,20,20	0
19	CLA	L	1166	50/65	0.76	0.35	0.56	20,20,20,20	0
19	CLA	2	1214	25/65	0.71	0.36	0.55	20,20,20,20	0
19	CLA	A	1812	65/65	0.78	0.37	0.52	20,20,20,20	0
19	CLA	B	1745	65/65	0.79	0.34	0.50	20,20,20,20	0
19	CLA	B	1763	65/65	0.81	0.33	0.46	20,20,20,20	0
19	CLA	A	1796	65/65	0.81	0.34	0.45	20,20,20,20	0
19	CLA	1	1241	55/65	0.56	0.39	0.44	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	A	1767	65/65	0.70	0.43	0.44	20,20,20,20	0
19	CLA	2	1217	65/65	0.70	0.38	0.42	20,20,20,20	0
19	CLA	B	1762	50/65	0.79	0.36	0.41	20,20,20,20	0
19	CLA	B	1737	60/65	0.81	0.34	0.41	20,20,20,20	0
19	CLA	B	1752	46/65	0.73	0.39	0.40	20,20,20,20	0
19	CLA	B	1735	65/65	0.75	0.40	0.39	20,20,20,20	0
19	CLA	F	1155	36/65	0.77	0.35	0.38	20,20,20,20	0
19	CLA	B	1761	50/65	0.84	0.30	0.38	20,20,20,20	0
19	CLA	B	1751	50/65	0.82	0.35	0.36	20,20,20,20	0
19	CLA	A	1789	55/65	0.84	0.32	0.33	20,20,20,20	0
19	CLA	3	1222	65/65	0.63	0.38	0.33	20,20,20,20	0
19	CLA	B	1748	59/65	0.79	0.37	0.33	20,20,20,20	0
19	CLA	B	1738	65/65	0.83	0.35	0.33	20,20,20,20	0
19	CLA	1	1192	61/65	0.77	0.33	0.32	20,20,20,20	0
20	LMU	A	1809	35/35	0.65	0.41	0.31	20,20,20,20	0
19	CLA	A	1790	50/65	0.76	0.36	0.30	20,20,20,20	0
19	CLA	A	1811	65/65	0.77	0.37	0.30	20,20,20,20	0
19	CLA	4	1205	55/65	0.69	0.37	0.30	20,20,20,20	0
19	CLA	B	1736	45/65	0.80	0.34	0.26	20,20,20,20	0
19	CLA	B	1765	45/65	0.78	0.32	0.26	20,20,20,20	0
19	CLA	A	1781	65/65	0.77	0.36	0.24	20,20,20,20	0
19	CLA	A	1810	65/65	0.82	0.36	0.23	20,20,20,20	0
19	CLA	4	1196	55/65	0.65	0.35	0.23	20,20,20,20	0
19	CLA	A	1760	55/65	0.76	0.33	0.22	20,20,20,20	0
19	CLA	I	1031	60/65	0.84	0.28	0.22	20,20,20,20	0
20	LMU	L	1171	35/35	0.66	0.33	0.22	20,20,20,20	0
19	CLA	A	1784	55/65	0.80	0.40	0.19	20,20,20,20	0
19	CLA	B	1759	65/65	0.86	0.32	0.19	20,20,20,20	0
19	CLA	B	1764	50/65	0.75	0.39	0.19	20,20,20,20	0
19	CLA	B	1742	54/65	0.81	0.29	0.17	20,20,20,20	0
19	CLA	L	1167	47/65	0.83	0.30	0.16	20,20,20,20	0
19	CLA	B	1756	58/65	0.78	0.36	0.15	20,20,20,20	0
19	CLA	3	1213	25/65	0.76	0.36	0.14	20,20,20,20	0
19	CLA	B	1749	60/65	0.87	0.32	0.14	20,20,20,20	0
19	CLA	A	1764	65/65	0.87	0.34	0.12	20,20,20,20	0
19	CLA	B	1743	55/65	0.81	0.29	0.12	20,20,20,20	0
19	CLA	A	1763	46/65	0.79	0.47	0.10	20,20,20,20	0
19	CLA	A	1779	55/65	0.79	0.34	0.02	20,20,20,20	0
19	CLA	3	1214	36/65	0.76	0.34	0.00	20,20,20,20	0
19	CLA	B	1766	45/65	0.57	0.44	-0.01	20,20,20,20	0
19	CLA	B	1739	65/65	0.88	0.33	-0.01	20,20,20,20	0
19	CLA	2	1222	50/65	0.81	0.27	-0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	BCR	A	1805	40/40	0.83	0.32	-0.06	20,20,20,20	0
19	CLA	4	1209	36/65	0.81	0.29	-0.06	20,20,20,20	0
19	CLA	2	1215	50/65	0.73	0.34	-0.10	20,20,20,20	0
19	CLA	A	1778	42/65	0.72	0.37	-0.11	20,20,20,20	0
19	CLA	B	1768	60/65	0.80	0.34	-0.12	20,20,20,20	0
19	CLA	A	1782	65/65	0.79	0.35	-0.14	20,20,20,20	0
19	CLA	F	1156	41/65	0.73	0.30	-0.17	20,20,20,20	0
19	CLA	B	1744	58/65	0.84	0.28	-0.18	20,20,20,20	0
19	CLA	L	1168	50/65	0.74	0.31	-0.19	20,20,20,20	0
19	CLA	B	1755	54/65	0.83	0.32	-0.19	20,20,20,20	0
19	CLA	3	1217	25/65	0.65	0.38	-0.22	20,20,20,20	0
19	CLA	2	1221	25/65	0.70	0.41	-0.26	20,20,20,20	0
19	CLA	B	1757	65/65	0.73	0.38	-0.29	20,20,20,20	0
20	LMU	A	1808	35/35	0.60	0.46	-0.30	20,20,20,20	0
19	CLA	B	1753	55/65	0.84	0.30	-0.31	20,20,20,20	0
22	BCR	B	1780	40/40	0.77	0.32	-0.33	20,20,20,20	0
19	CLA	A	1765	52/65	0.80	0.34	-0.34	20,20,20,20	0
19	CLA	4	1201	52/65	0.79	0.26	-0.37	20,20,20,20	0
19	CLA	B	1769	65/65	0.88	0.28	-0.40	20,20,20,20	0
19	CLA	3	1212	50/65	0.67	0.34	-0.47	20,20,20,20	0
19	CLA	A	1792	49/65	0.84	0.29	-0.47	20,20,20,20	0
19	CLA	B	1770	47/65	0.86	0.30	-0.50	20,20,20,20	0
19	CLA	G	1099	51/65	0.75	0.31	-0.51	20,20,20,20	0
19	CLA	1	1194	25/65	0.81	0.34	-0.57	20,20,20,20	0
19	CLA	1	1197	25/65	0.66	0.36	-0.62	20,20,20,20	0
19	CLA	B	1754	65/65	0.82	0.28	-0.65	20,20,20,20	0
19	CLA	A	1771	50/65	0.79	0.31	-0.75	20,20,20,20	0
19	CLA	3	1216	25/65	0.55	0.41	-0.79	20,20,20,20	0
19	CLA	4	1197	36/65	0.86	0.33	-0.83	20,20,20,20	0
19	CLA	1	1195	36/65	0.85	0.27	-0.85	20,20,20,20	0
19	CLA	1	1189	47/65	0.75	0.27	-0.97	20,20,20,20	0
19	CLA	4	1208	25/65	0.86	0.29	-1.12	20,20,20,20	0
19	CLA	1	1190	46/65	0.80	0.27	-1.15	20,20,20,20	0
25	SF4	C	1082	8/8	0.86	0.17	-2.16	20,20,20,20	0
25	SF4	C	1083	8/8	0.91	0.14	-2.21	20,20,20,20	0
25	SF4	B	1785	8/8	0.94	0.14	-2.48	20,20,20,20	0
20	LMU	N	1086	35/35	0.69	0.33	-	2,39,60,60	0
20	LMU	A	7014	35/35	0.61	0.33	-	20,20,20,20	0
19	CLA	4	1198	65/65	0.70	0.30	-	20,20,20,20	0
20	LMU	A	7040	35/35	0.74	0.24	-	20,20,20,20	0
19	CLA	1	1196	51/65	0.66	0.40	-	20,20,20,20	0
20	LMU	R	1056	35/35	0.64	0.32	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	1	1010	25/65	0.79	0.20	-	20,20,20,20	0
19	CLA	3	3015	25/65	0.67	0.31	-	20,20,20,20	0
22	BCR	3	1225	40/40	0.64	0.37	-	20,20,20,20	0
20	LMU	A	7026	35/35	0.67	0.38	-	20,20,20,20	0
26	UNL	B	8057	23/-	0.78	0.24	-	20,20,20,20	0
19	CLA	3	1220	25/65	0.62	0.44	-	20,20,20,20	0
19	CLA	B	1767	51/65	0.55	0.47	-	20,20,20,20	0
19	CLA	4	1210	25/65	0.90	0.21	-	20,20,20,20	0
20	LMU	A	7006	35/35	0.68	0.31	-	20,20,20,20	0
20	LMU	A	7035	35/35	0.72	0.29	-	20,20,20,20	0
20	LMU	A	7041	35/35	0.66	0.43	-	20,20,20,20	0
21	SUC	B	8061	23/23	0.64	0.29	-	20,20,20,20	0
19	CLA	2	1213	65/65	0.70	0.35	-	20,20,20,20	0
20	LMU	A	7031	35/35	0.74	0.24	-	20,20,20,20	0
20	LMU	A	7009	34/35	0.66	0.41	-	20,20,20,20	0
19	CLA	3	3008	50/65	0.63	0.38	-	20,20,20,20	0
20	LMU	A	7021	35/35	0.67	0.29	-	20,20,20,20	0
21	SUC	B	8054	23/23	0.68	0.30	-	20,20,20,20	0
20	LMU	2	1224	35/35	0.63	0.40	-	20,20,20,20	0
20	LMU	A	7024	35/35	0.67	0.26	-	20,20,20,20	0
19	CLA	4	4014	47/65	0.69	0.29	-	20,20,20,20	0
19	CLA	1	1145	55/65	0.72	0.39	-	20,20,20,20	0
19	CLA	A	1791	45/65	0.70	0.40	-	20,20,20,20	0
20	LMU	A	7036	34/35	0.72	0.27	-	20,20,20,20	0
19	CLA	1	1142	45/65	0.60	0.37	-	20,20,20,20	0
19	CLA	J	1043	61/65	0.69	0.29	-	20,20,20,20	0
19	CLA	3	1218	42/65	0.63	0.37	-	20,20,20,20	0
20	LMU	A	7048	35/35	0.66	0.36	-	2,38,60,60	0
19	CLA	2	1218	65/65	0.60	0.43	-	20,20,20,20	0
20	LMU	A	7022	35/35	0.68	0.36	-	20,20,20,20	0
19	CLA	1	1308	48/65	0.82	0.24	-	20,20,20,20	0
19	CLA	3	3011	65/65	0.71	0.32	-	20,20,20,20	0
19	CLA	1	1307	25/65	0.61	0.68	-	20,20,20,20	0
19	CLA	3	3001	25/65	0.78	0.37	-	20,20,20,20	0
20	LMU	A	7020	35/35	0.48	0.49	-	20,20,20,20	0
20	LMU	A	7027	35/35	0.69	0.26	-	20,20,20,20	0
20	LMU	K	1086	35/35	0.66	0.39	-	20,20,20,20	0
21	SUC	B	8051	23/23	0.63	0.47	-	20,20,20,20	0
19	CLA	4	1204	25/65	0.79	0.27	-	20,20,20,20	0
19	CLA	A	1768	54/65	0.76	0.33	-	20,20,20,20	0
20	LMU	A	7043	35/35	0.64	0.33	-	20,20,20,20	0
21	SUC	3	1226	23/23	0.52	0.71	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	1	1191	25/65	0.72	0.31	-	20,20,20,20	0
19	CLA	R	1055	58/65	0.69	0.34	-	20,20,20,20	0
19	CLA	F	1157	53/65	0.70	0.34	-	20,20,20,20	0
21	SUC	F	1158	23/23	0.76	0.25	-	20,20,20,20	0
20	LMU	A	7032	35/35	0.80	0.33	-	20,20,20,20	0
21	SUC	B	8062	23/23	0.72	0.30	-	20,20,20,20	0
20	LMU	A	7017	35/35	0.56	0.51	-	20,20,20,20	0
21	SUC	B	8060	23/23	0.77	0.23	-	20,20,20,20	0
21	SUC	B	8056	23/23	0.62	0.38	-	20,20,20,20	0
20	LMU	A	7037	35/35	0.81	0.23	-	20,20,20,20	0
20	LMU	A	7042	35/35	0.78	0.27	-	20,20,20,20	0
19	CLA	3	1224	65/65	0.62	0.56	-	20,20,20,20	0
19	CLA	1	1014	61/65	0.68	0.29	-	2,35,60,60	0
21	SUC	B	8055	23/23	0.79	0.29	-	2,29,60,60	0
19	CLA	2	1219	25/65	0.79	0.31	-	20,20,20,20	0
20	LMU	A	7003	35/35	0.63	0.33	-	20,20,20,20	0
19	CLA	A	1797	65/65	0.55	0.47	-	20,20,20,20	0
20	LMU	A	7015	35/35	0.73	0.27	-	20,20,20,20	0
19	CLA	2	1216	25/65	0.64	0.36	-	20,20,20,20	0
19	CLA	1	1149	46/65	0.74	0.24	-	20,20,20,20	0
20	LMU	B	1783	35/35	0.77	0.28	-	2,35,60,60	0
19	CLA	A	1775	25/65	0.72	0.30	-	20,20,20,20	0
20	LMU	4	1212	35/35	0.62	0.32	-	20,20,20,20	0
19	CLA	K	1085	50/65	0.67	0.59	-	20,20,20,20	0
20	LMU	A	7050	35/35	0.60	0.37	-	2,41,60,60	0
19	CLA	4	1211	46/65	0.78	0.26	-	20,20,20,20	0
19	CLA	J	1044	61/65	0.57	0.36	-	20,20,20,20	0
20	LMU	A	7023	35/35	0.79	0.30	-	20,20,20,20	0
19	CLA	3	1223	25/65	0.74	0.26	-	20,20,20,20	0
20	LMU	A	7005	35/35	0.72	0.27	-	20,20,20,20	0
20	LMU	A	7010	35/35	0.55	0.51	-	20,20,20,20	0
20	LMU	A	7051	35/35	0.63	0.31	-	2,30,60,60	0
19	CLA	3	1215	25/65	0.74	0.34	-	20,20,20,20	0
20	LMU	A	7019	35/35	0.72	0.22	-	20,20,20,20	0
21	SUC	B	8059	23/23	0.71	0.38	-	20,20,20,20	0
21	SUC	B	8052	23/23	0.68	0.50	-	20,20,20,20	0
20	LMU	A	7030	35/35	0.60	0.32	-	20,20,20,20	0
20	LMU	A	7034	35/35	0.68	0.26	-	20,20,20,20	0
20	LMU	A	7013	35/35	0.46	0.44	-	20,20,20,20	0
20	LMU	A	7025	35/35	0.51	0.39	-	20,20,20,20	0
19	CLA	3	1221	25/65	0.45	0.43	-	20,20,20,20	0
19	CLA	1	1148	55/65	0.65	0.40	-	20,20,20,20	0

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*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	4	4007	52/65	0.68	0.32	-	20,20,20,20	0
19	CLA	1	1198	25/65	0.80	0.45	-	20,20,20,20	0
20	LMU	A	7016	35/35	0.74	0.28	-	20,20,20,20	0
19	CLA	1	1188	57/65	0.80	0.22	-	2,38,60,60	0
19	CLA	1	1146	50/65	0.60	0.50	-	20,20,20,20	0
19	CLA	4	1206	65/65	0.76	0.30	-	20,20,20,20	0
19	CLA	R	1054	57/65	0.67	0.50	-	20,20,20,20	0
19	CLA	4	1207	25/65	0.80	0.27	-	20,20,20,20	0
21	SUC	B	8053	23/23	0.77	0.20	-	2,41,60,60	0
19	CLA	2	1212	51/65	0.60	0.37	-	20,20,20,20	0
20	LMU	A	7038	35/35	0.56	0.49	-	20,20,20,20	0
19	CLA	1	1309	25/65	0.60	0.45	-	20,20,20,20	0
19	CLA	2	2010	25/65	0.77	0.33	-	20,20,20,20	0
20	LMU	A	7033	35/35	0.70	0.31	-	20,20,20,20	0
19	CLA	2	1220	36/65	0.57	0.49	-	20,20,20,20	0
20	LMU	1	1200	35/35	0.65	0.35	-	2,45,60,60	0
20	LMU	A	7004	35/35	0.65	0.48	-	20,20,20,20	0
20	LMU	A	7049	35/35	0.64	0.30	-	2,51,60,60	0
20	LMU	A	7028	35/35	0.75	0.24	-	20,20,20,20	0
20	LMU	A	7039	35/35	0.77	0.24	-	20,20,20,20	0
20	LMU	1	1199	35/35	0.58	0.36	-	20,20,20,20	0
19	CLA	1	1187	46/65	0.68	0.31	-	20,20,20,20	0
19	CLA	1	1193	51/65	0.75	0.33	-	20,20,20,20	0
19	CLA	4	1202	36/65	0.64	0.40	-	20,20,20,20	0
19	CLA	A	1798	50/65	0.62	0.34	-	20,20,20,20	0
19	CLA	1	1303	25/65	0.73	0.36	-	20,20,20,20	0
19	CLA	1	1505	55/65	0.60	0.50	-	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.