



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2WSC
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-04
Resolution : 3.30 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

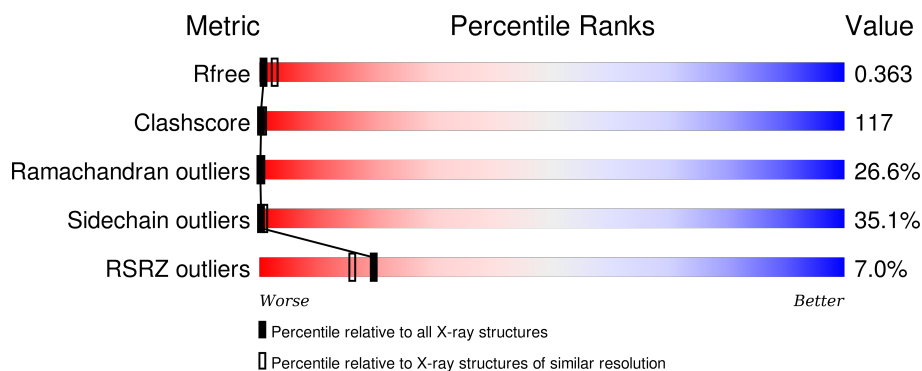
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 ≥ 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>10%</div> <div>30% 25% 11% 32%</div> </div>
2	2	269	<div> <div>6%</div> <div>24% 30% 10% 35%</div> </div>
3	3	276	<div> <div>8%</div> <div>16% 21% 16% 6% 41%</div> </div>
4	4	251	<div> <div>10%</div> <div>22% 27% 14% 34%</div> </div>
5	A	758	<div> <div>4%</div> <div>6% 48% 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	1187	X	-	-	-
19	CLA	1	1188	X	-	-	-
19	CLA	1	1189	X	-	-	-
19	CLA	1	1190	X	-	-	-
19	CLA	1	1191	X	-	-	X
19	CLA	1	1192	X	-	-	-
19	CLA	1	1193	X	-	-	-
19	CLA	1	1194	X	-	-	-
19	CLA	1	1195	X	-	-	-
19	CLA	1	1196	X	-	-	-
19	CLA	1	1197	X	-	-	X
19	CLA	1	1198	X	-	-	-
19	CLA	1	1199	X	-	-	-
19	CLA	1	1200	X	-	-	-
19	CLA	1	1201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	1212	X	-	-	-
19	CLA	2	1213	X	-	-	-
19	CLA	2	1214	X	-	-	-
19	CLA	2	1215	X	-	X	-
19	CLA	2	1216	X	-	-	-
19	CLA	2	1217	X	-	-	X
19	CLA	2	1218	X	-	-	-
19	CLA	2	1219	X	-	-	-
19	CLA	2	1220	X	-	X	-
19	CLA	2	1221	X	-	-	-
19	CLA	2	1222	X	-	-	-
19	CLA	2	1223	X	-	-	-
19	CLA	2	1224	X	-	-	-
19	CLA	2	1227	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	3	1212	X	-	-	-
19	CLA	3	1213	X	-	-	-
19	CLA	3	1214	X	-	-	-
19	CLA	3	1215	X	-	-	-
19	CLA	3	1216	X	-	-	-
19	CLA	3	1217	X	-	-	-
19	CLA	3	1218	X	-	X	-
19	CLA	3	1219	X	-	-	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3002	X	-	-	-
19	CLA	3	3007	X	-	-	-
19	CLA	3	3008	X	-	-	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3014	X	-	-	-
19	CLA	3	3015	X	-	-	-
19	CLA	4	1196	X	-	X	-
19	CLA	4	1197	X	-	-	-
19	CLA	4	1198	X	-	X	-
19	CLA	4	1199	X	-	X	-
19	CLA	4	1200	X	-	-	X
19	CLA	4	1201	X	-	X	-
19	CLA	4	1202	X	-	-	X
19	CLA	4	1203	X	-	-	-
19	CLA	4	1204	X	-	-	-
19	CLA	4	1205	X	-	-	-
19	CLA	4	1206	X	-	-	-
19	CLA	4	1207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	1208	X	-	-	-
19	CLA	4	1209	X	-	-	-
19	CLA	4	4003	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	-	-	-
19	CLA	A	1763	X	-	X	-
19	CLA	A	1764	X	-	X	-
19	CLA	A	1765	X	-	X	-
19	CLA	A	1766	X	-	-	-
19	CLA	A	1767	X	-	X	-
19	CLA	A	1768	X	-	-	-
19	CLA	A	1769	X	-	X	-
19	CLA	A	1770	X	-	X	-
19	CLA	A	1771	X	-	-	-
19	CLA	A	1772	X	-	X	-
19	CLA	A	1773	X	-	-	-
19	CLA	A	1774	X	-	X	-
19	CLA	A	1775	X	-	-	-
19	CLA	A	1776	X	-	X	-
19	CLA	A	1777	X	-	-	X
19	CLA	A	1778	X	-	-	-
19	CLA	A	1779	X	-	X	-
19	CLA	A	1780	X	-	-	-
19	CLA	A	1781	X	-	X	-
19	CLA	A	1782	X	-	X	-
19	CLA	A	1783	X	-	X	-
19	CLA	A	1784	X	-	-	-
19	CLA	A	1785	X	-	-	-
19	CLA	A	1786	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	-	X	-
19	CLA	A	1792	X	-	X	-
19	CLA	A	1793	X	-	X	X
19	CLA	A	1794	X	-	X	-
19	CLA	A	1795	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1796	X	-	X	-
19	CLA	A	1797	X	-	X	-
19	CLA	A	1798	X	-	X	-
19	CLA	A	1799	X	-	-	-
19	CLA	A	1800	X	-	X	-
19	CLA	A	1801	X	-	-	X
19	CLA	A	1811	X	-	-	-
19	CLA	A	1812	X	-	X	-
19	CLA	A	1813	X	-	X	-
19	CLA	A	1815	X	-	-	-
19	CLA	A	1816	X	-	X	-
19	CLA	A	1817	X	-	-	-
19	CLA	B	1735	X	-	X	-
19	CLA	B	1736	X	-	-	-
19	CLA	B	1737	X	-	X	-
19	CLA	B	1738	X	-	-	-
19	CLA	B	1739	X	-	X	-
19	CLA	B	1740	X	-	-	-
19	CLA	B	1741	X	-	-	-
19	CLA	B	1742	X	-	-	-
19	CLA	B	1743	X	-	X	-
19	CLA	B	1744	X	-	-	-
19	CLA	B	1745	X	-	-	-
19	CLA	B	1746	X	-	X	X
19	CLA	B	1747	X	-	X	-
19	CLA	B	1748	X	-	-	-
19	CLA	B	1749	X	-	-	-
19	CLA	B	1750	X	-	-	-
19	CLA	B	1751	X	-	-	-
19	CLA	B	1752	X	-	-	-
19	CLA	B	1753	X	-	X	-
19	CLA	B	1754	X	-	X	-
19	CLA	B	1755	X	-	X	X
19	CLA	B	1756	X	-	X	-
19	CLA	B	1757	X	-	X	-
19	CLA	B	1758	X	-	X	-
19	CLA	B	1759	X	-	X	-
19	CLA	B	1760	X	-	-	-
19	CLA	B	1761	X	-	-	-
19	CLA	B	1762	X	-	X	-
19	CLA	B	1763	X	-	-	-
19	CLA	B	1764	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1765	X	-	-	-
19	CLA	B	1766	X	-	-	-
19	CLA	B	1767	X	-	-	-
19	CLA	B	1768	X	-	X	-
19	CLA	B	1769	X	-	X	-
19	CLA	B	1770	X	-	X	-
19	CLA	B	1771	X	-	X	-
19	CLA	B	1772	X	-	-	-
19	CLA	B	1785	X	-	X	-
19	CLA	B	1786	X	-	X	-
19	CLA	B	1787	X	-	X	-
19	CLA	F	1155	X	-	-	-
19	CLA	F	1156	X	-	-	-
19	CLA	F	1157	X	-	-	-
19	CLA	G	1099	X	-	-	-
19	CLA	H	1079	X	-	-	-
19	CLA	I	1031	X	-	-	-
19	CLA	I	1033	X	-	-	-
19	CLA	J	1043	X	-	X	-
19	CLA	J	1044	X	-	X	-
19	CLA	J	1045	X	-	X	-
19	CLA	J	1046	X	-	-	-
19	CLA	K	1085	X	-	X	-
19	CLA	K	1142	X	-	X	-
19	CLA	K	1146	X	-	-	-
19	CLA	K	3009	X	-	-	-
19	CLA	L	1166	X	-	-	-
19	CLA	L	1167	X	-	-	-
19	CLA	L	1168	X	-	-	-
19	CLA	L	1505	X	-	-	-
19	CLA	R	1054	X	-	-	-
19	CLA	R	1055	X	-	-	-
20	LMU	A	7016	-	-	X	-
20	LMU	A	7020	-	-	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	R	1057	X	-	-	-
21	SUC	2	1226	X	-	X	-
21	SUC	3	1221	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	SUC	B	8051	X	-	-	-
21	SUC	B	8052	X	-	X	-
21	SUC	B	8053	X	-	-	-
21	SUC	B	8054	X	-	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	H	1080	X	-	-	-
22	BCR	3	1220	-	-	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	-
22	BCR	A	1808	-	-	X	X
22	BCR	B	1775	-	-	-	X
22	BCR	B	1777	-	-	X	-
22	BCR	B	1778	-	-	X	-
22	BCR	B	1779	-	-	X	-
22	BCR	B	1780	-	-	X	-
22	BCR	B	1781	-	-	-	X
22	BCR	I	1032	-	-	X	X
22	BCR	L	1169	-	-	X	X
23	PQN	A	1802	X	-	-	-
23	PQN	B	1773	X	-	X	-
24	LMG	B	1783	-	-	X	-
25	SF4	B	1784	-	-	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 36379 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	165	Total	C	N	O	S	0	0	0
			1264	822	208	230	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
			1374	899	226	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	162	Total	C	N	O	S	0	0	0
			1254	826	203	220	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
			1319	861	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			

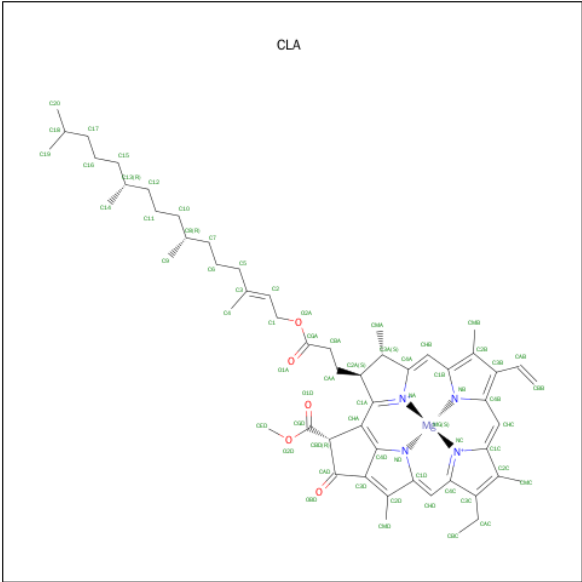
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	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
			36	30	1	4	1		
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
			51	41	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
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	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
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 56	C 46	Mg 1	N 4 O 5	0	0
19	2	1	Total 25	C 20	Mg 1	N 4	0	0
19	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	2	1	Total 25	C 20	Mg 1	N 4	0	0
19	2	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	2	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	2	1	Total 25	C 20	Mg 1	N 4	0	0
19	2	1	Total 56	C 46	Mg 1	N 4 O 5	0	0
19	2	1	Total 25	C 20	Mg 1	N 4	0	0
19	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	2	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	3	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			46	36	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
			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
			57	47	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		

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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
			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
			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
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
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		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			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
			45	35	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
			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
			51	41	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
			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		
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		

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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
			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
			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
			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
			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		
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		

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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
			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
			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	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		

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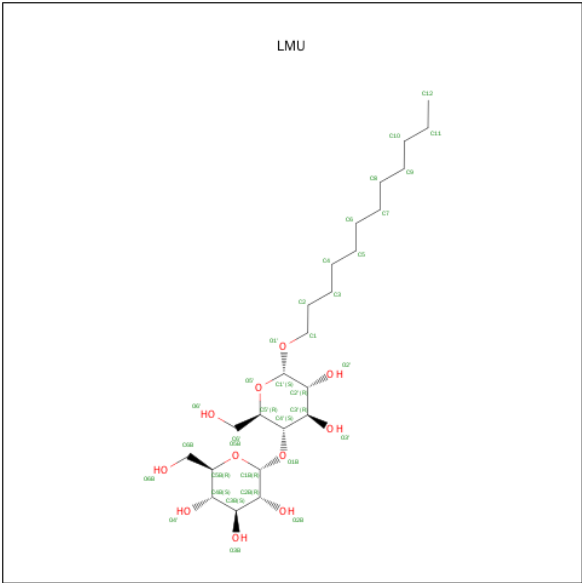
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
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
			65	55	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	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
			46	36	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	J	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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
			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
			50	40	1	4		
19	K	1	Total	C	Mg	N	0	0
			65	55	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	4	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: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
			25	14	11		
20	K	1	Total	C	O	0	0
			35	24	11		
20	L	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	1	1	Total	C	O	0	0
			35	24	11		
20	3	1	Total	C	O	0	0
			35	24	11		
20	2	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		
20	A	1	Total	C	O	0	0
			35	24	11		

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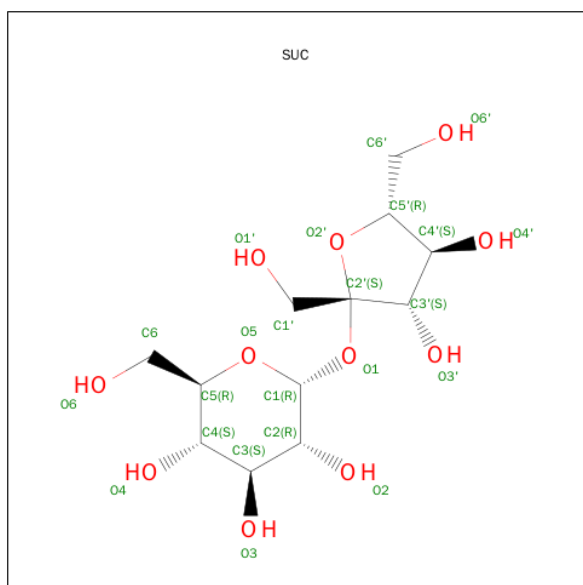
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

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



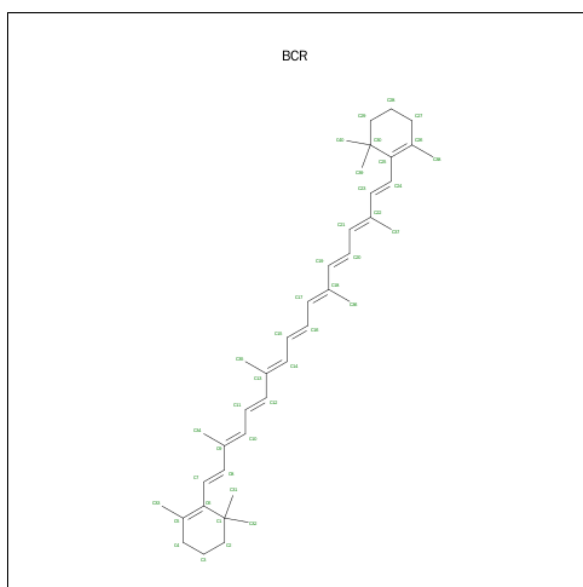
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			22	12	10		
21	3	1	Total	C	O	0	0
			23	12	11		
21	H	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total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

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

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



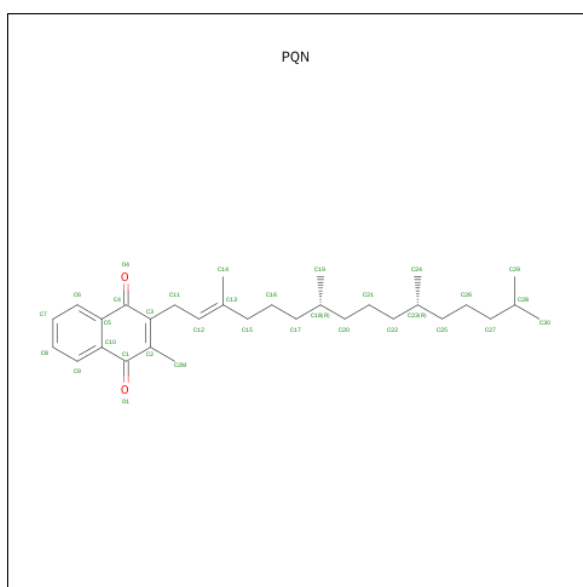
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	3	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		

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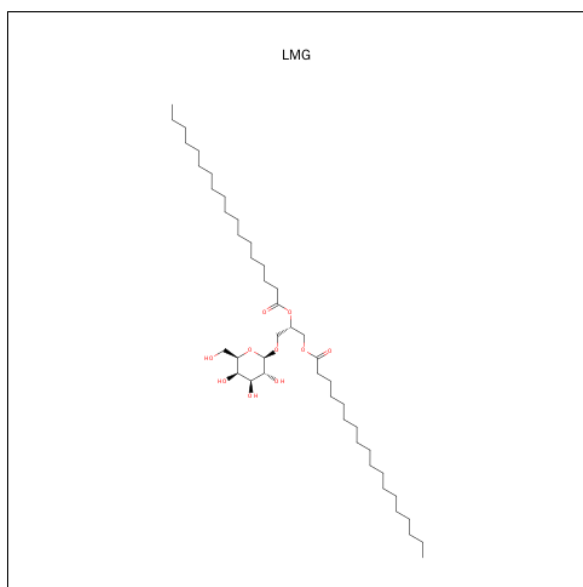
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total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

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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: $C_{45}H_{86}O_{10}$).



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: Fe_4S_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		

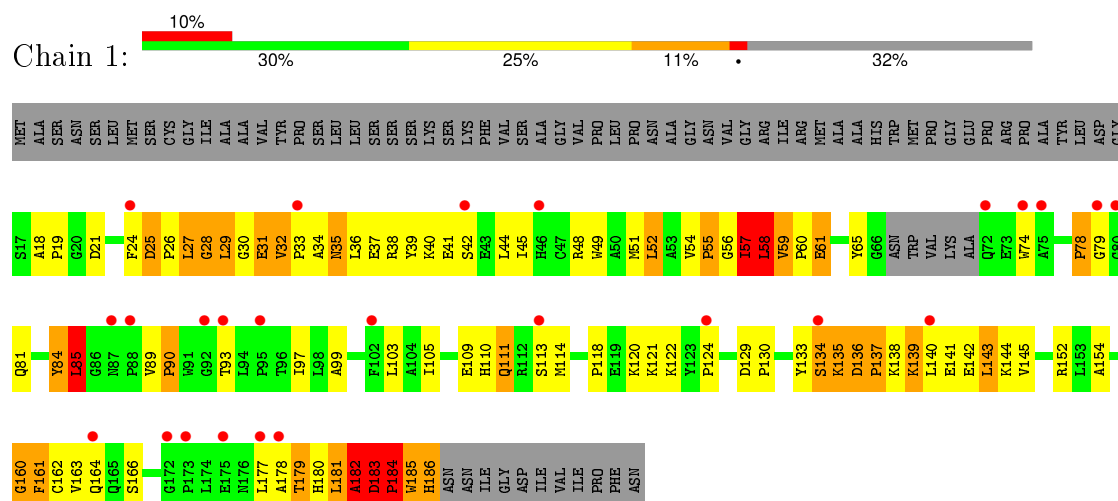
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

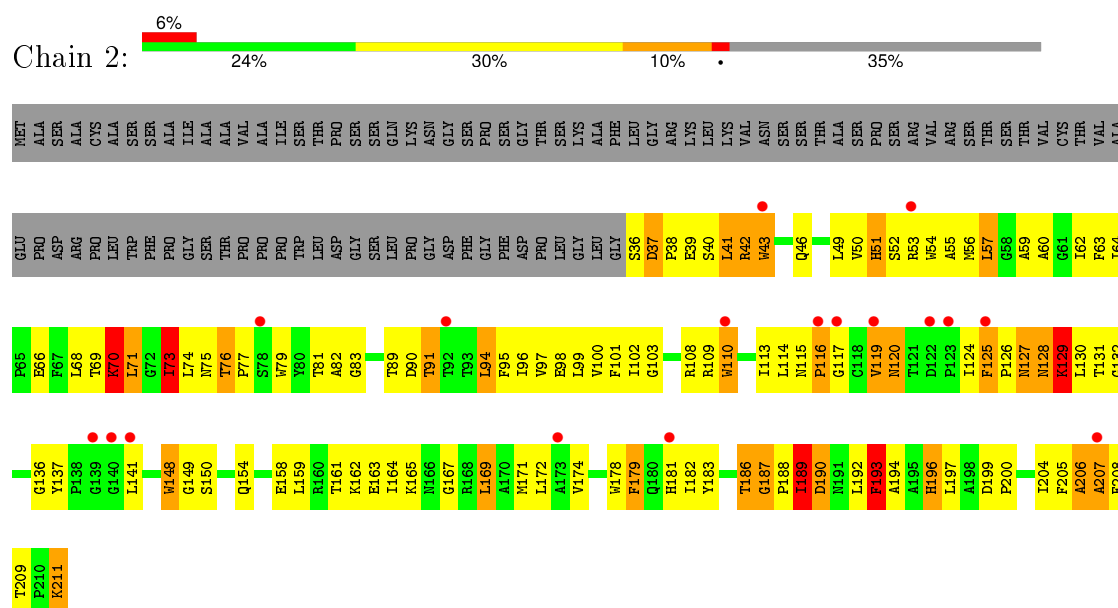
3 Residue-property plots

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.

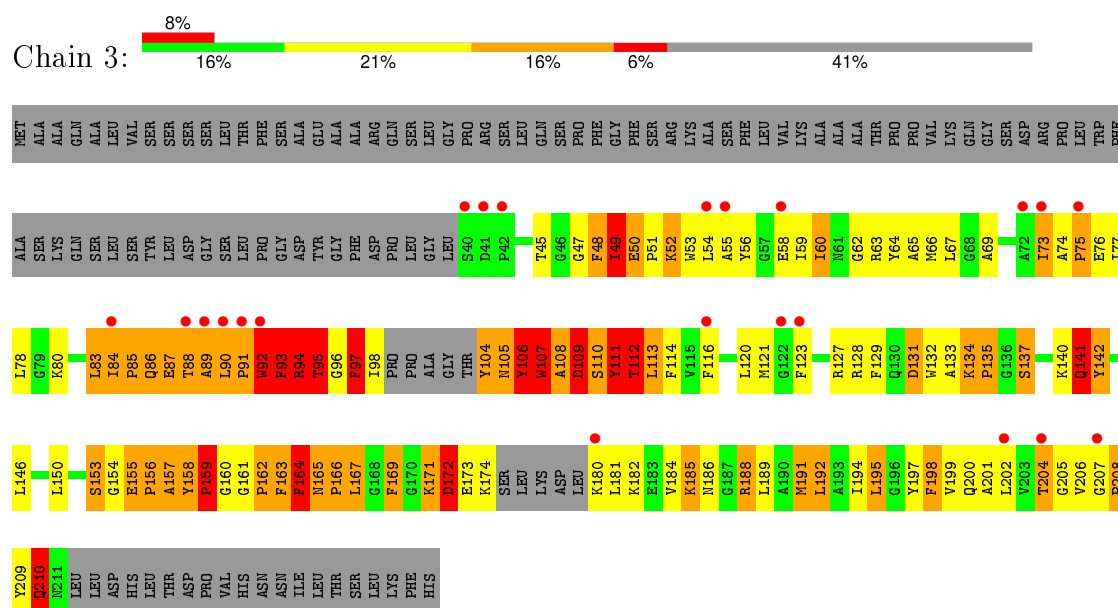
• Molecule 1: AT3G54890



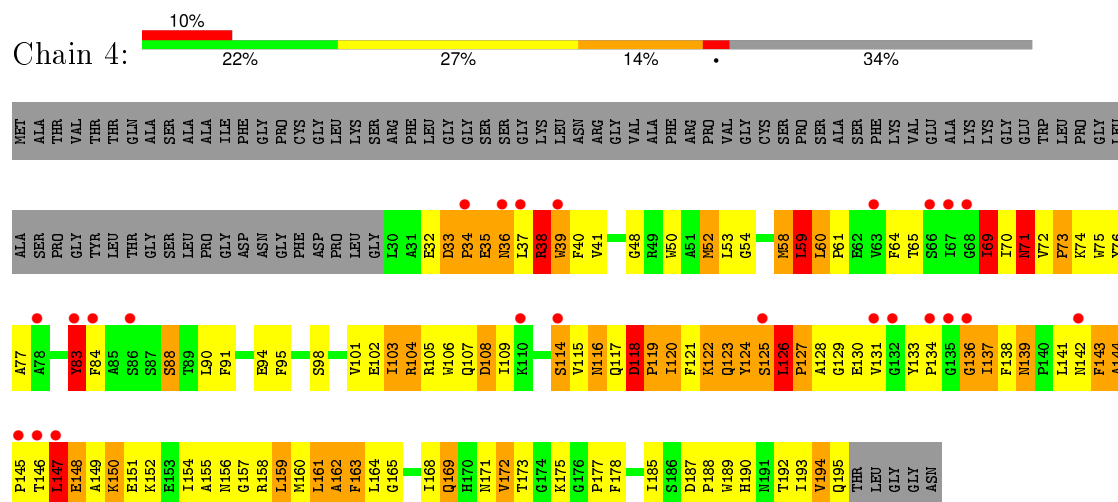
• Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I



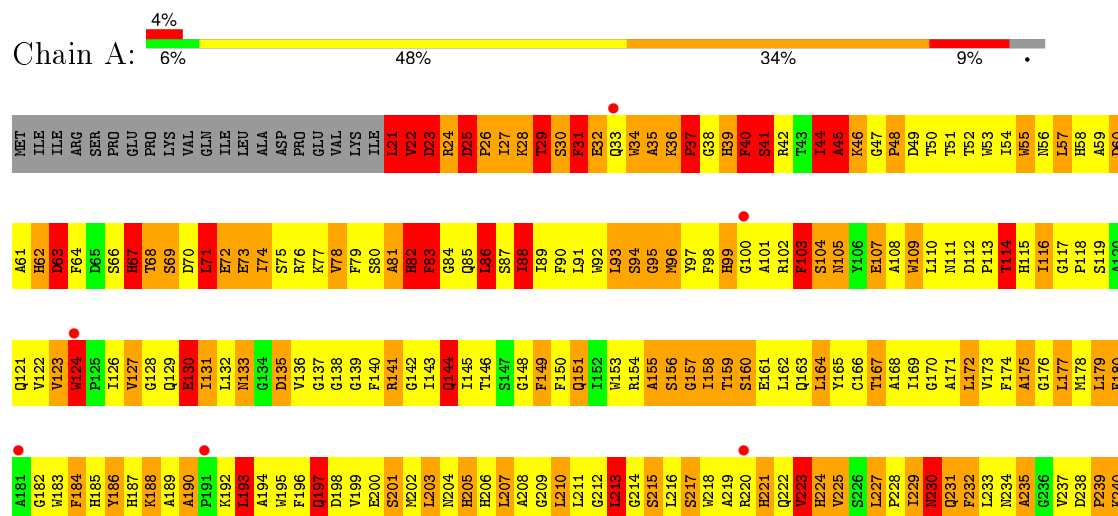
• Molecule 3: LHCA3



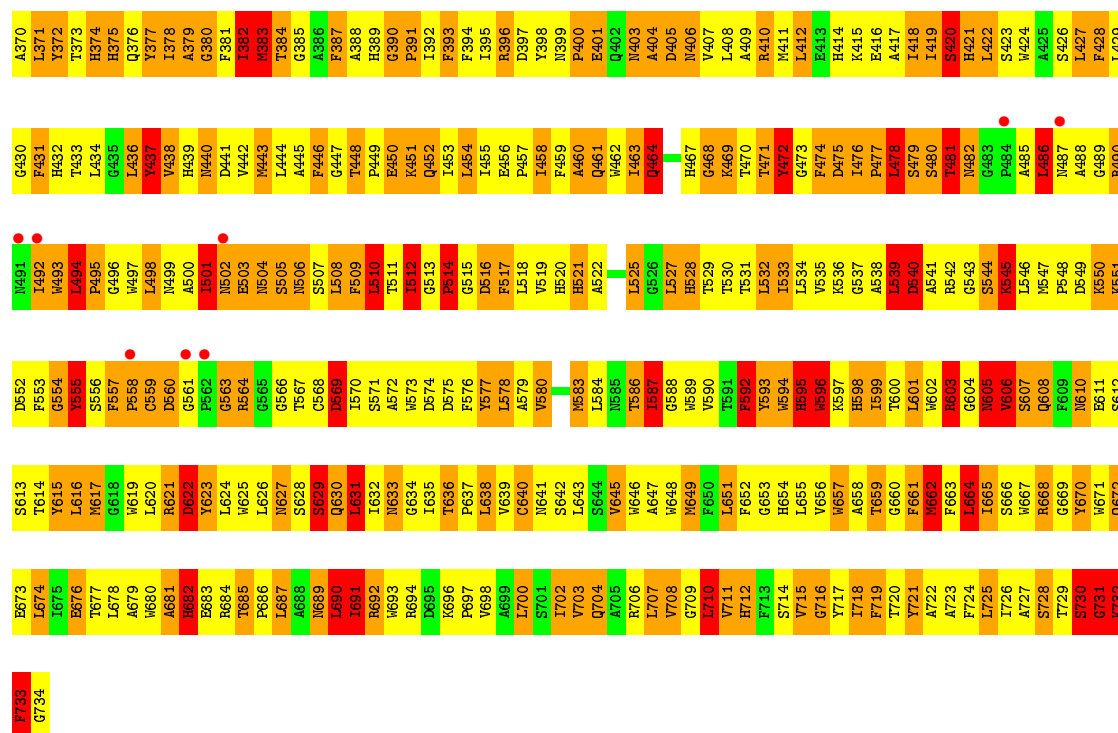
- Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC



- Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



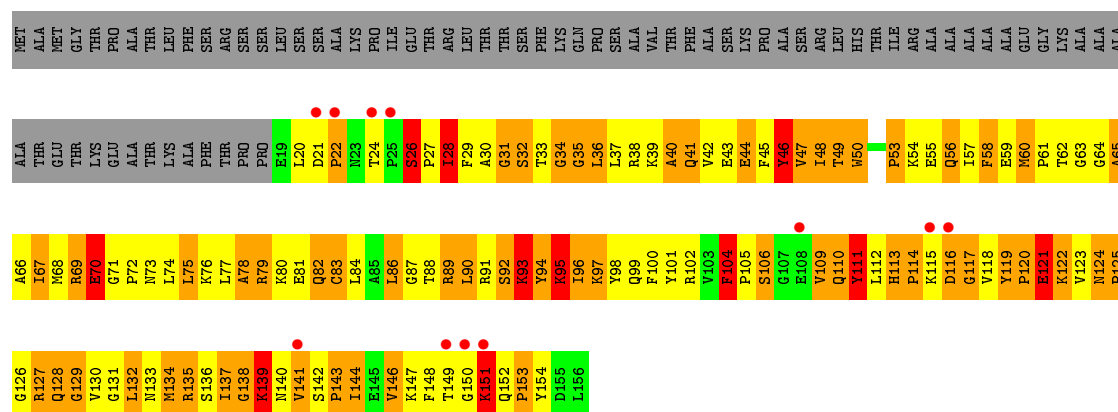




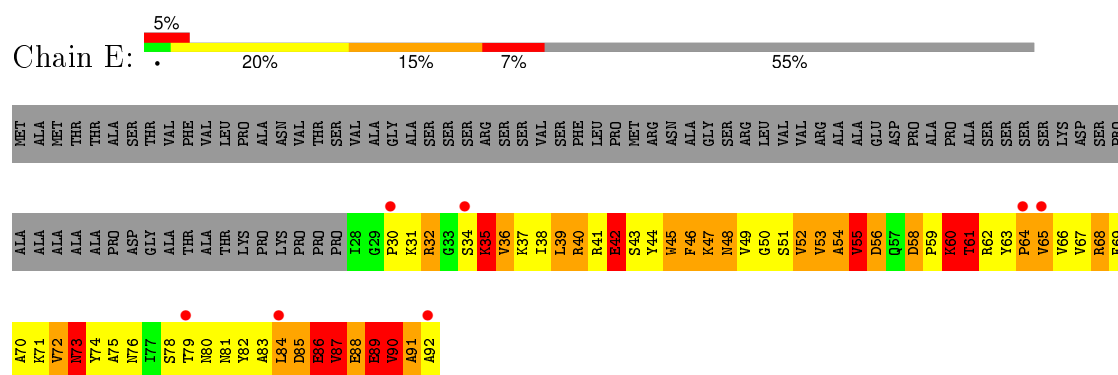
• Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



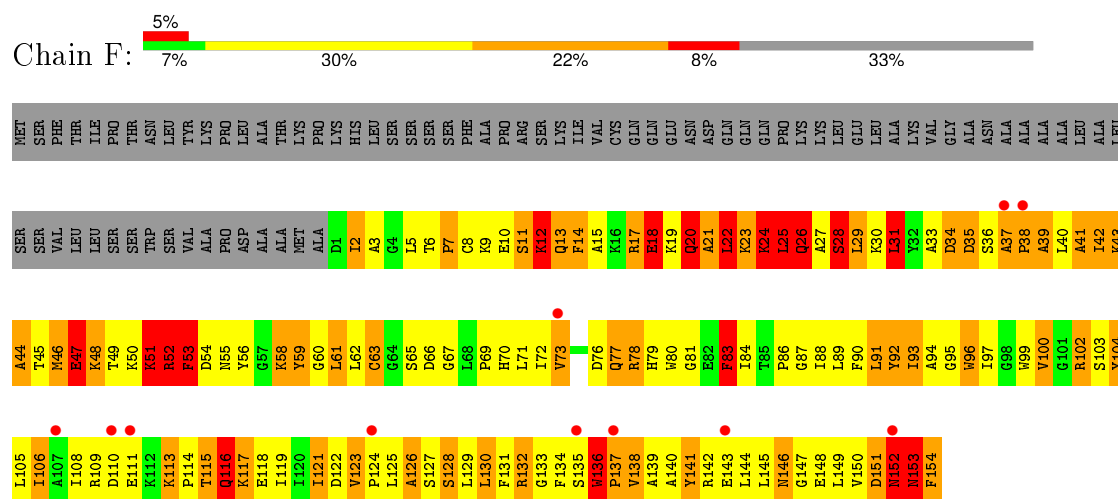
• Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC



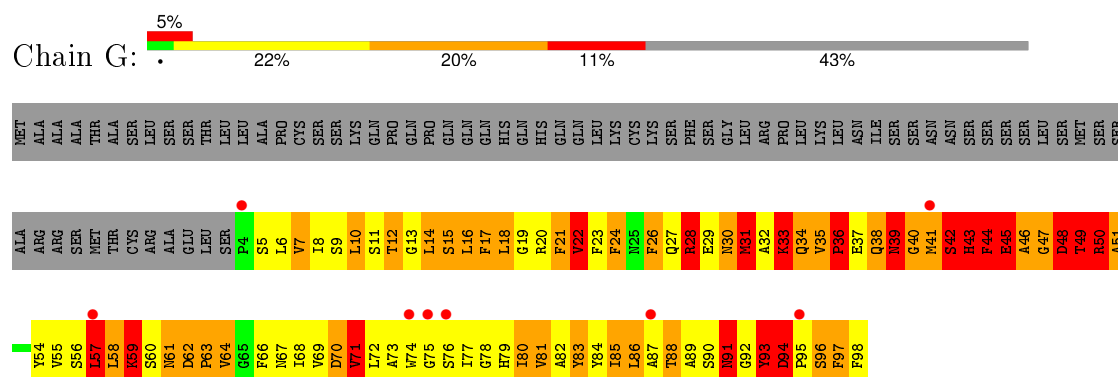
• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC



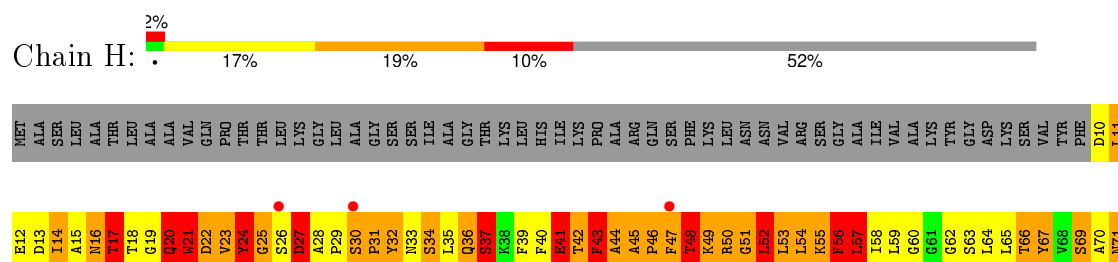
- Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

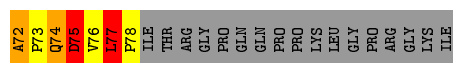


- Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

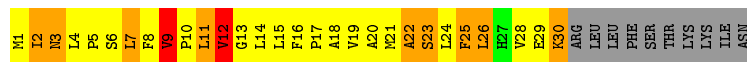


- Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC





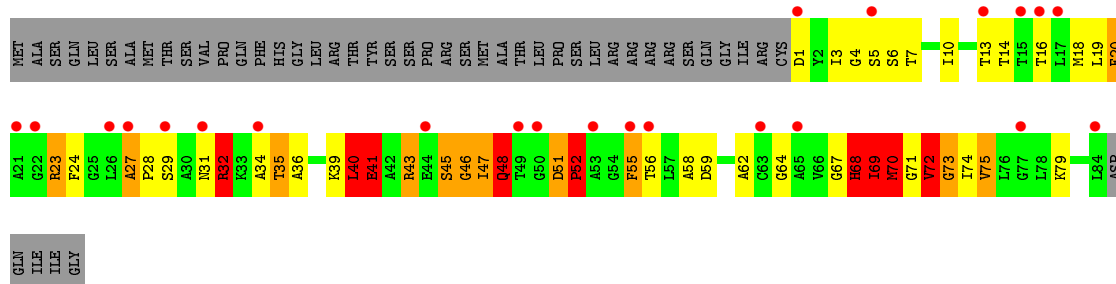
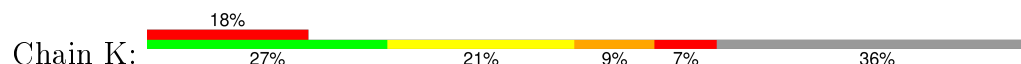
- Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



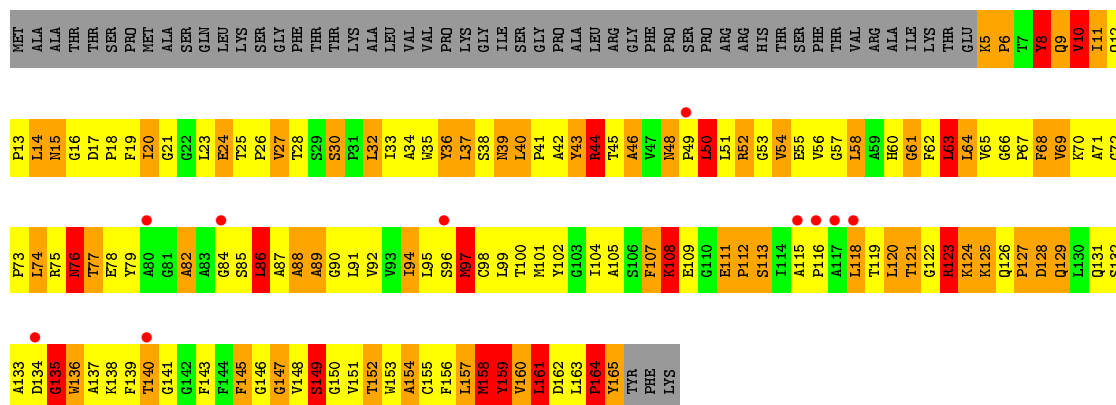
- Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX



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

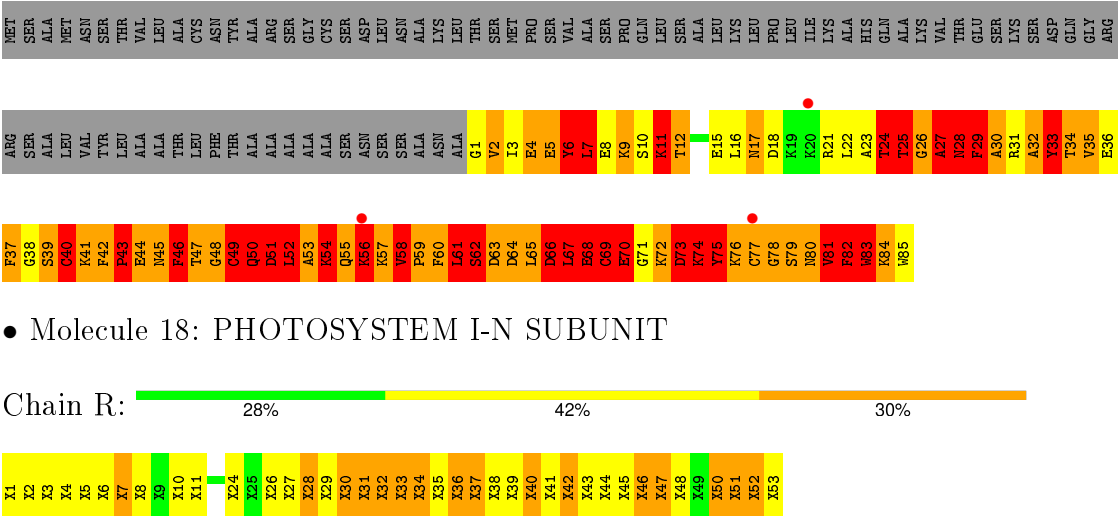


- Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

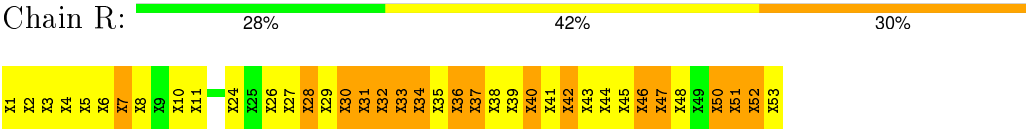


- Molecule 17: PHOTOSYSTEM I-N SUBUNIT





• 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, α , β , γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 49.14 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 98.5 (49.14-3.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.363 , 0.366 0.358 , 0.363	Depositor DCC
R_{free} test set	4345 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 81.2	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 93389 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	36379	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.48	0/1303	0.72	3/1774 (0.2%)
2	2	0.45	0/1420	0.71	0/1943
3	3	0.87	6/1292 (0.5%)	0.96	3/1743 (0.2%)
4	4	0.49	0/1359	0.75	2/1851 (0.1%)
5	A	0.95	3/5938 (0.1%)	1.04	11/8104 (0.1%)
6	B	0.95	2/6058 (0.0%)	1.02	14/8278 (0.2%)
7	C	1.43	7/632 (1.1%)	1.33	4/856 (0.5%)
8	D	1.10	0/1122	1.05	0/1514
9	E	1.15	0/530	1.17	2/718 (0.3%)
10	F	1.10	1/1250 (0.1%)	1.07	2/1687 (0.1%)
11	G	1.07	0/760	1.28	9/1031 (0.9%)
12	H	1.16	0/543	1.19	3/741 (0.4%)
13	I	1.00	0/235	0.97	0/320
14	J	1.02	0/349	1.09	1/475 (0.2%)
15	K	0.55	0/599	0.83	1/810 (0.1%)
16	L	1.08	0/1238	1.10	5/1691 (0.3%)
17	N	1.23	1/699 (0.1%)	1.33	7/936 (0.7%)
All	All	0.94	20/25327 (0.1%)	1.02	67/34472 (0.2%)

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	3
2	2	0	1
3	3	0	19
5	A	0	28
6	B	0	20
7	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	2
16	L	0	3
17	N	0	21
18	R	0	17
All	All	1	166

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.88	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
6	B	640	CYS	CB-SG	7.67	1.95	1.82
7	C	72	GLU	CD-OE1	-7.43	1.17	1.25
3	3	93	PHE	CD2-CE2	7.38	1.54	1.39
5	A	317	TYR	C-N	-7.34	1.17	1.34
7	C	58	CYS	CB-SG	6.76	1.93	1.82
3	3	93	PHE	CE2-CZ	6.63	1.50	1.37
7	C	72	GLU	CG-CD	-6.59	1.42	1.51
7	C	72	GLU	CD-OE2	-6.30	1.18	1.25
17	N	70	GLU	CB-CG	6.07	1.63	1.52
7	C	81	TYR	CE1-CZ	-5.97	1.30	1.38
10	F	47	GLU	CG-CD	5.72	1.60	1.51
7	C	54	CYS	CB-SG	-5.66	1.72	1.81
3	3	93	PHE	CD1-CE1	5.41	1.50	1.39
7	C	81	TYR	CD2-CE2	-5.39	1.31	1.39
6	B	401	GLU	CG-CD	5.25	1.59	1.51
3	3	92	TRP	CG-CD1	5.14	1.44	1.36
5	A	702	GLU	CG-CD	5.11	1.59	1.51
5	A	32	GLU	CG-CD	5.03	1.59	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	732	LYS	N-CA-C	-8.11	89.10	111.00
5	A	93	LEU	CA-CB-CG	8.06	133.84	115.30
5	A	530	LEU	CA-CB-CG	7.27	132.02	115.30
6	B	486	LEU	CA-CB-CG	7.27	132.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	315	LEU	CA-CB-CG	7.21	131.88	115.30
16	L	86	LEU	CA-CB-CG	7.18	131.82	115.30
17	N	33	TYR	N-CA-C	-7.15	91.70	111.00
5	A	540	LEU	CA-CB-CG	7.08	131.59	115.30
11	G	16	LEU	CA-CB-CG	7.00	131.40	115.30
5	A	554	LEU	CA-CB-CG	6.93	131.24	115.30
6	B	710	LEU	N-CA-C	-6.87	92.46	111.00
15	K	46	GLY	N-CA-C	-6.80	96.11	113.10
10	F	22	LEU	CB-CG-CD1	-6.55	99.87	111.00
4	4	147	LEU	CA-CB-CG	6.54	130.34	115.30
3	3	93	PHE	N-CA-CB	-6.42	99.05	110.60
5	A	271	THR	N-CA-C	-6.37	93.79	111.00
9	E	90	VAL	N-CA-C	-6.37	93.81	111.00
11	G	43	HIS	N-CA-C	-6.33	93.91	111.00
17	N	24	THR	N-CA-C	-6.29	94.03	111.00
7	C	79	LEU	CA-CB-CG	6.24	129.65	115.30
3	3	95	THR	N-CA-C	6.24	127.84	111.00
16	L	135	GLY	N-CA-C	-6.16	97.69	113.10
6	B	338	LEU	CA-CB-CG	6.15	129.45	115.30
1	1	183	ASP	C-N-CD	-6.14	107.10	120.60
6	B	494	LEU	CA-CB-CG	6.09	129.30	115.30
1	1	183	ASP	N-CA-C	6.08	127.42	111.00
17	N	27	ALA	N-CA-C	-6.06	94.63	111.00
11	G	91	ASN	N-CA-C	6.05	127.33	111.00
11	G	44	PHE	N-CA-C	-6.04	94.68	111.00
14	J	35	ASP	N-CA-C	6.04	127.30	111.00
7	C	69	LEU	CA-CB-CG	6.02	129.14	115.30
4	4	161	LEU	CA-CB-CG	5.93	128.93	115.30
6	B	194	LEU	CB-CG-CD1	-5.86	101.03	111.00
11	G	57	LEU	CA-CB-CG	5.79	128.62	115.30
11	G	51	ALA	N-CA-C	5.75	126.52	111.00
5	A	350	LEU	CA-CB-CG	-5.71	102.17	115.30
7	C	79	LEU	CB-CG-CD2	5.65	120.61	111.00
6	B	380	GLY	N-CA-C	-5.65	98.98	113.10
16	L	159	TYR	CA-CB-CG	5.63	124.10	113.40
12	H	27	ASP	N-CA-C	-5.63	95.81	111.00
17	N	62	SER	N-CA-C	-5.60	95.89	111.00
17	N	31	ARG	N-CA-C	-5.54	96.04	111.00
5	A	653	LEU	CA-CB-CG	5.50	127.94	115.30
6	B	104	PHE	N-CA-C	-5.47	96.23	111.00
7	C	75	ARG	CA-CB-CG	5.45	125.40	113.40
6	B	478	LEU	CA-CB-CG	5.44	127.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	60	LYS	N-CA-C	5.43	125.65	111.00
17	N	74	LYS	N-CA-C	5.41	125.61	111.00
5	A	626	GLY	N-CA-C	-5.35	99.72	113.10
17	N	6	TYR	N-CA-C	-5.34	96.58	111.00
6	B	289	LEU	CA-CB-CG	5.32	127.53	115.30
6	B	631	LEU	CA-CB-CG	5.28	127.44	115.30
12	H	52	LEU	N-CA-C	5.21	125.08	111.00
16	L	50	LEU	CA-CB-CG	5.19	127.23	115.30
12	H	57	LEU	CA-CB-CG	5.18	127.22	115.30
5	A	287	LEU	CA-CB-CG	5.18	127.20	115.30
5	A	385	LEU	CA-CB-CG	5.17	127.19	115.30
11	G	14	LEU	CA-CB-CG	-5.16	103.44	115.30
5	A	600	LEU	CA-CB-CG	5.12	127.07	115.30
16	L	158	MET	N-CA-C	-5.08	97.29	111.00
3	3	111	TYR	CA-CB-CG	5.07	123.04	113.40
6	B	72	GLY	N-CA-C	-5.07	100.44	113.10
10	F	59	TYR	CB-CA-C	-5.06	100.28	110.40
11	G	21	PHE	N-CA-C	5.05	124.64	111.00
6	B	596	TRP	N-CA-C	-5.04	97.38	111.00
11	G	16	LEU	N-CA-C	-5.04	97.40	111.00
1	1	85	LEU	CA-CB-CG	5.02	126.85	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

All (166) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	182	ALA	Peptide
1	1	183	ASP	Peptide
1	1	184	PRO	Peptide
2	2	120	ASN	Peptide
3	3	104	TYR	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

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Mol	Chain	Res	Type	Group
3	3	159	PRO	Peptide
3	3	169	PHE	Peptide
3	3	172	ASP	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
3	3	94	ARG	Peptide
3	3	95	THR	Peptide
5	A	103	PHE	Peptide
5	A	117	GLY	Peptide
5	A	123	VAL	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	240	LYS	Peptide
5	A	242	ILE	Peptide
5	A	25	ASP	Peptide
5	A	27	ILE	Peptide
5	A	29	THR	Peptide
5	A	315	HIS	Peptide
5	A	347	TYR	Peptide
5	A	37	PRO	Peptide
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	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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
15	K	45	SER	Peptide
15	K	46	GLY	Peptide
16	L	157	LEU	Mainchain
16	L	160	VAL	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

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Mol	Chain	Res	Type	Group
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	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
18	R	48	UNK	Peptide
18	R	50	UNK	Peptide
18	R	51	UNK	Peptide
18	R	52	UNK	Peptide
18	R	7	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	1264	0	1230	91	1
2	2	1374	0	1329	142	0
3	3	1254	0	1221	331	1
4	4	1319	0	1283	201	10
5	A	5745	0	5595	1659	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5848	0	5655	1447	1
7	C	619	0	608	236	0
8	D	1095	0	1112	226	0
9	E	520	0	528	150	0
10	F	1221	0	1246	289	0
11	G	740	0	709	296	7
12	H	529	0	514	120	0
13	I	229	0	252	58	0
14	J	338	0	340	80	0
15	K	593	0	619	65	1
16	L	1203	0	1213	326	10
17	N	685	0	671	447	7
18	R	265	0	67	77	0
19	1	644	0	429	113	1
19	2	658	0	480	160	0
19	3	548	0	326	115	0
19	4	699	0	454	157	0
19	A	2777	0	2599	1119	1
19	B	2372	0	2285	808	0
19	F	130	0	86	27	0
19	G	51	0	40	6	0
19	H	65	0	71	19	0
19	I	115	0	106	26	0
19	J	202	0	169	98	0
19	K	210	0	177	44	1
19	L	202	0	158	40	0
19	R	122	0	123	17	0
20	1	70	0	92	15	0
20	2	105	0	138	15	1
20	3	35	0	46	3	0
20	4	35	0	46	0	0
20	A	1153	0	1505	396	0
20	B	25	0	23	1	0
20	K	35	0	45	6	0
20	L	35	0	46	3	0
20	R	70	0	91	24	0
21	2	22	0	19	10	0
21	3	23	0	22	14	0
21	B	230	0	218	85	0
21	H	23	0	20	5	0
22	3	40	0	54	21	0
22	A	240	0	323	250	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	320	0	432	225	0
22	I	40	0	54	47	0
22	L	80	0	105	61	0
23	A	33	0	46	12	0
23	B	33	0	46	33	0
24	B	49	0	71	30	0
25	B	8	0	0	18	0
25	C	16	0	0	9	0
26	B	23	0	0	2	0
All	All	36379	0	35137	8375	21

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 117.

All (8375) 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)
4:4:160:MET:SD	19:4:1201:CLA:HBB1	1.28	1.66
19:A:1776:CLA:H92	22:A:1805:BCR:C37	1.17	1.58
6:B:25:ILE:HG21	22:L:1169:BCR:C29	1.11	1.58
5:A:51:THR:HG21	19:A:1795:CLA:CBB	1.24	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	1.33	1.56
16:L:163:LEU:CD2	16:L:164:PRO:HD2	1.34	1.56
23:B:1773:PQN:C19	22:B:1780:BCR:H10C	1.33	1.55
3:3:132:TRP:CZ3	3:3:155:GLU:HG2	1.37	1.55
19:1:1191:CLA:CAB	19:1:1197:CLA:HBC2	1.32	1.55
3:3:64:TYR:HB3	19:3:1218:CLA:C4	1.34	1.54
19:A:1772:CLA:CED	19:A:1772:CLA:H2A	1.33	1.54
23:B:1773:PQN:H162	22:B:1780:BCR:C33	1.29	1.53
19:A:1776:CLA:C9	22:A:1805:BCR:H373	1.33	1.53
19:A:1779:CLA:C4C	22:A:1805:BCR:H19C	1.32	1.52
19:3:3008:CLA:HBA2	19:3:3008:CLA:CB D	1.34	1.52
19:A:1816:CLA:C2	19:A:1816:CLA:HED1	1.29	1.52
18:R:32:UNK:CB	18:R:33:UNK:CB	1.85	1.51
20:A:7023:LMU:H91	20:A:7023:LMU:C2	1.41	1.50
11:G:45:GLU:CG	11:G:49:THR:HG23	1.38	1.50
19:2:1220:CLA:CGA	19:2:1220:CLA:HBD	1.35	1.50
17:N:45:ASN:ND2	17:N:54:LYS:HG2	1.24	1.50
17:N:62:SER:HB3	17:N:66:ASP:CB	1.41	1.49
5:A:328:LYS:CE	5:A:332:GLU:HG3	1.40	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:132:TRP:CZ3	3:3:155:GLU:CG	1.91	1.49
6:B:732:LYS:HG2	6:B:733:PHE:C	1.23	1.48
20:A:7016:LMU:C2	20:A:7016:LMU:H81	1.44	1.46
20:A:7042:LMU:C6'	20:A:7042:LMU:H32	1.41	1.46
6:B:25:ILE:CG2	22:L:1169:BCR:C29	1.95	1.45
19:A:1816:CLA:HAA1	19:A:1816:CLA:CGD	1.45	1.44
19:4:1198:CLA:HAA2	19:4:1198:CLA:CED	1.46	1.44
4:4:107:GLN:CA	19:4:1196:CLA:HMA3	1.47	1.44
7:C:14:CYS:HA	7:C:17:CYS:SG	1.56	1.43
19:2:1220:CLA:C4	3:3:140:LYS:HG2	1.45	1.43
21:B:8052:SUC:C5'	21:B:8052:SUC:H1	1.48	1.43
19:J:1043:CLA:HED3	19:J:1043:CLA:C1A	1.47	1.42
16:L:161:LEU:HD12	16:L:162:ASP:N	1.24	1.42
17:N:45:ASN:HD22	17:N:54:LYS:CG	1.28	1.41
11:G:48:ASP:CB	11:G:49:THR:HG22	1.47	1.41
19:2:1220:CLA:H41	3:3:140:LYS:CD	1.51	1.41
5:A:744:ALA:CB	22:A:1807:BCR:H391	1.51	1.40
3:3:74:ALA:HA	19:3:1215:CLA:C3D	1.51	1.40
11:G:93:TYR:HA	11:G:94:ASP:CB	1.43	1.40
17:N:48:GLY:HA2	17:N:49:CYS:SG	1.62	1.40
6:B:732:LYS:CG	6:B:733:PHE:C	1.83	1.40
19:A:1796:CLA:H141	22:A:1807:BCR:C2	1.51	1.39
19:B:1768:CLA:H152	22:B:1779:BCR:C31	1.52	1.39
19:A:1816:CLA:H2	19:A:1816:CLA:CED	1.51	1.39
19:A:1779:CLA:CHD	22:A:1805:BCR:H19C	1.52	1.39
5:A:21:LEU:CA	5:A:22:VAL:HB	1.47	1.39
17:N:61:LEU:HD11	17:N:63:ASP:C	1.40	1.39
19:K:1085:CLA:HMB2	19:K:1142:CLA:CED	1.49	1.39
19:J:1044:CLA:C7	19:J:1044:CLA:H41	1.49	1.38
17:N:58:VAL:HB	17:N:59:PRO:CD	1.47	1.38
6:B:732:LYS:HB3	6:B:733:PHE:CA	1.49	1.37
19:4:1201:CLA:HMA2	19:4:1201:CLA:CBA	1.54	1.37
5:A:368:LEU:HD21	19:A:1774:CLA:C9	1.55	1.36
3:3:205:GLY:N	5:A:252:ARG:HH22	1.16	1.36
17:N:62:SER:HB3	17:N:66:ASP:CG	1.46	1.36
17:N:72:LYS:HG3	17:N:74:LYS:CB	1.56	1.36
19:A:1783:CLA:H203	22:A:1808:BCR:C17	1.54	1.36
19:A:1770:CLA:C4B	22:A:1803:BCR:H19C	1.56	1.36
4:4:160:MET:CE	19:4:1201:CLA:CBB	2.02	1.35
19:A:1763:CLA:C3B	22:A:1808:BCR:H331	1.53	1.35
7:C:54:CYS:HB2	25:C:1082:SF4:S1	1.67	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:316:MET:HG2	5:A:317:TYR:CD1	1.62	1.35
17:N:72:LYS:HB3	17:N:73:ASP:CA	1.48	1.35
9:E:52:VAL:O	9:E:53:VAL:CG2	1.75	1.35
20:A:7037:LMU:C7	20:A:7037:LMU:H32	1.51	1.35
5:A:23:ASP:HB2	5:A:24:ARG:NE	1.42	1.34
20:A:7033:LMU:H3'	20:A:7033:LMU:C6B	1.55	1.34
4:4:160:MET:SD	19:4:1201:CLA:CBB	2.14	1.34
17:N:47:THR:HG21	17:N:54:LYS:NZ	1.37	1.34
17:N:61:LEU:HD11	17:N:63:ASP:CA	1.56	1.34
4:4:119:PRO:HG3	19:4:1206:CLA:C2D	1.56	1.33
5:A:567:ARG:NH1	8:D:35:GLY:HA2	1.43	1.33
19:B:1753:CLA:CBC	19:B:1753:CLA:HMC1	1.58	1.33
16:L:163:LEU:HD13	16:L:164:PRO:CB	1.57	1.33
5:A:453:LEU:CD2	19:A:1793:CLA:HBB2	1.57	1.33
19:B:1742:CLA:HAC2	19:B:1743:CLA:CBB	1.54	1.33
20:K:1086:LMU:H81	20:K:1086:LMU:C4	1.47	1.33
5:A:51:THR:CG2	19:A:1795:CLA:CBB	2.05	1.32
19:J:1044:CLA:H72	19:J:1044:CLA:C4	1.58	1.32
9:E:52:VAL:O	9:E:53:VAL:HG23	1.24	1.32
11:G:6:LEU:HB3	11:G:9:SER:CB	1.59	1.32
5:A:51:THR:CG2	19:A:1795:CLA:HBB2	1.60	1.32
5:A:269:PHE:CE1	15:K:14:THR:HG21	1.65	1.32
19:1:1187:CLA:HBC3	19:1:1187:CLA:CMC	1.46	1.32
20:A:7036:LMU:C7	20:A:7036:LMU:H31	1.45	1.31
19:4:1198:CLA:C20	19:4:1198:CLA:H151	1.59	1.31
4:4:107:GLN:CA	19:4:1196:CLA:CMA	2.09	1.31
4:4:107:GLN:HA	19:4:1196:CLA:CMA	1.61	1.31
10:F:24:LYS:CA	10:F:24:LYS:HE2	1.49	1.31
5:A:452:PHE:CE1	19:A:1793:CLA:HBB1	1.64	1.31
19:2:1220:CLA:C5	19:2:1220:CLA:H92	1.53	1.31
19:2:1220:CLA:C9	19:2:1220:CLA:H52	1.52	1.31
19:J:1045:CLA:CBC	19:J:1045:CLA:HHD	1.57	1.31
19:3:3008:CLA:CGD	19:3:3008:CLA:HBA2	1.61	1.31
20:A:7032:LMU:H31	20:A:7032:LMU:C2B	1.60	1.30
17:N:66:ASP:C	17:N:67:LEU:HD12	1.50	1.30
19:B:1768:CLA:CBB	19:B:1768:CLA:H93	1.61	1.29
20:A:7023:LMU:H82	20:A:7023:LMU:C3	1.61	1.29
19:A:1816:CLA:HHD	19:A:1816:CLA:CBC	1.62	1.29
19:A:1816:CLA:C1	19:A:1816:CLA:HED1	1.62	1.29
11:G:6:LEU:CB	11:G:9:SER:HB3	1.60	1.28
23:B:1773:PQN:C16	22:B:1780:BCR:C33	2.11	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7023:LMU:C9	20:A:7023:LMU:H21	1.60	1.28
19:2:1220:CLA:C4	3:3:140:LYS:CG	2.12	1.28
5:A:744:ALA:HB2	22:A:1807:BCR:C39	1.61	1.28
22:3:1220:BCR:H23C	22:3:1220:BCR:C39	1.55	1.28
22:A:1804:BCR:H23C	22:A:1804:BCR:C40	1.60	1.28
19:A:1763:CLA:C3B	22:A:1808:BCR:C33	2.10	1.28
19:4:4014:CLA:HED2	19:4:4014:CLA:C2A	1.62	1.28
19:A:1779:CLA:CBB	22:A:1805:BCR:C35	2.10	1.27
17:N:65:LEU:HD23	17:N:65:LEU:C	1.52	1.27
12:H:20:GLN:HB3	12:H:22:ASP:CB	1.63	1.27
6:B:732:LYS:CB	6:B:733:PHE:HA	1.63	1.27
19:A:1770:CLA:C3B	22:A:1803:BCR:H19C	1.63	1.27
3:3:132:TRP:CH2	3:3:155:GLU:CG	2.12	1.27
11:G:45:GLU:CG	11:G:49:THR:CG2	2.10	1.27
20:A:7037:LMU:H72	20:A:7037:LMU:C3	1.55	1.27
19:A:1781:CLA:HED1	19:A:1782:CLA:C2D	1.65	1.27
17:N:67:LEU:HB2	17:N:68:GLU:CG	1.65	1.27
20:A:7023:LMU:C9	20:A:7023:LMU:H41	1.64	1.26
17:N:41:LYS:HB2	17:N:42:PHE:CB	1.65	1.26
17:N:45:ASN:ND2	17:N:54:LYS:CB	1.99	1.26
11:G:93:TYR:CA	11:G:94:ASP:HB2	1.64	1.26
19:3:1219:CLA:C10	19:3:1219:CLA:H142	1.65	1.26
20:A:7020:LMU:H6E	20:A:7020:LMU:C5B	1.64	1.26
5:A:79:PHE:CE2	5:A:185:HIS:CD2	2.24	1.26
20:A:7036:LMU:H82	20:A:7036:LMU:C3	1.64	1.26
17:N:67:LEU:CB	17:N:68:GLU:HG2	1.66	1.26
19:4:4014:CLA:CED	19:4:4014:CLA:H2A	1.66	1.25
17:N:72:LYS:CG	17:N:74:LYS:HG3	1.66	1.25
7:C:17:CYS:HB2	7:C:58:CYS:SG	1.77	1.25
19:4:1201:CLA:CGD	19:4:1201:CLA:HAA2	1.67	1.25
7:C:62:PHE:CE2	9:E:42:GLU:OE1	1.90	1.25
19:2:1212:CLA:O1A	19:2:1212:CLA:H42	1.37	1.25
19:2:1220:CLA:H41	3:3:140:LYS:CG	1.67	1.25
12:H:25:GLY:CA	12:H:27:ASP:H	1.49	1.24
19:A:1776:CLA:CMD	19:A:1778:CLA:HBB2	1.67	1.24
6:B:25:ILE:CG2	22:L:1169:BCR:C28	2.14	1.24
20:A:7039:LMU:C6B	20:A:7039:LMU:H3'	1.66	1.24
22:B:1779:BCR:C8	22:B:1779:BCR:H321	1.55	1.24
12:H:20:GLN:CB	12:H:22:ASP:HB3	1.65	1.24
4:4:151:GLU:O	4:4:154:ILE:HG12	1.36	1.24
22:I:1032:BCR:HC8	22:I:1032:BCR:C31	1.62	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1187:CLA:CB	19:1:1187:CLA:HMC1	1.64	1.24
20:A:7042:LMU:C2	20:A:7042:LMU:H71	1.68	1.23
19:J:1045:CLA:CAD	19:J:1045:CLA:HED3	1.67	1.23
6:B:732:LYS:CB	6:B:733:PHE:CA	2.14	1.23
20:A:7042:LMU:C6	20:A:7042:LMU:H22	1.58	1.23
3:3:74:ALA:HA	19:3:1215:CLA:C4D	1.69	1.23
20:A:7016:LMU:C3	20:A:7016:LMU:H81	1.69	1.23
14:J:31:ARG:HH22	19:J:1043:CLA:C4B	1.50	1.23
4:4:106:TRP:CD1	19:4:1196:CLA:HED3	1.74	1.23
19:K:1085:CLA:O1A	19:K:1085:CLA:H3A	1.38	1.23
19:A:1783:CLA:C20	22:A:1808:BCR:H17C	1.68	1.23
13:I:11:LEU:CD1	22:I:1032:BCR:H10C	1.69	1.23
6:B:25:ILE:CG2	22:L:1169:BCR:H292	1.60	1.22
20:K:1086:LMU:H42	20:K:1086:LMU:C8	1.67	1.22
20:A:7032:LMU:C1B	20:A:7032:LMU:H31	1.67	1.22
5:A:81:ALA:CB	19:A:1760:CLA:HMA1	1.68	1.22
7:C:7:ILE:O	7:C:8:TYR:O	1.55	1.22
2:2:120:ASN:CB	14:J:5:LYS:HD2	1.68	1.22
19:A:1772:CLA:CB	19:A:1772:CLA:HMC1	1.70	1.22
6:B:732:LYS:HG2	6:B:734:GLY:N	0.90	1.22
19:A:1816:CLA:C2	19:A:1816:CLA:CED	2.13	1.22
19:4:1198:CLA:HED3	19:4:1198:CLA:CAA	1.70	1.22
6:B:517:PHE:O	6:B:517:PHE:CD2	1.93	1.22
5:A:328:LYS:CG	5:A:332:GLU:HB2	1.70	1.22
5:A:342:GLY:CA	5:A:430:ASP:HB2	1.70	1.22
19:B:1755:CLA:HBB1	19:B:1769:CLA:CMB	1.70	1.22
6:B:25:ILE:CG2	22:L:1169:BCR:H282	1.68	1.22
20:A:7020:LMU:C6'	20:A:7020:LMU:H5B	1.69	1.22
3:3:84:ILE:HB	19:A:1798:CLA:O1A	1.40	1.21
16:L:163:LEU:HD13	16:L:164:PRO:CD	1.69	1.21
20:A:7023:LMU:H2B	20:A:7023:LMU:C6B	1.65	1.21
20:A:7022:LMU:H2'	20:A:7022:LMU:C2	1.66	1.21
19:A:1779:CLA:CBB	22:A:1805:BCR:H351	1.70	1.21
19:2:1220:CLA:H61	3:3:140:LYS:CD	1.69	1.21
17:N:57:LYS:CG	17:N:58:VAL:H	1.52	1.21
9:E:86:GLU:HG3	9:E:87:VAL:N	1.49	1.21
19:A:1781:CLA:HED1	19:A:1782:CLA:C3D	1.70	1.21
5:A:331:LEU:HD11	5:A:346:LEU:CB	1.69	1.21
5:A:81:ALA:CB	19:A:1760:CLA:CMA	2.18	1.21
21:B:8056:SUC:H3'	21:B:8056:SUC:O2	1.39	1.21
16:L:161:LEU:C	16:L:161:LEU:HD12	1.51	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:1054:CLA:HED3	19:R:1054:CLA:C1A	1.69	1.21
16:L:164:PRO:HB3	16:L:165:TYR:CE2	1.75	1.20
17:N:45:ASN:ND2	17:N:54:LYS:HB2	1.53	1.20
19:A:1781:CLA:HED2	19:A:1782:CLA:CAD	1.71	1.20
20:A:7036:LMU:H22	20:A:7036:LMU:C8	1.71	1.20
3:3:48:PHE:CD2	3:3:49:ILE:HG22	1.74	1.20
20:A:7043:LMU:C6	20:A:7043:LMU:H102	1.69	1.20
19:4:1201:CLA:CMA	19:4:1201:CLA:HBA1	1.55	1.20
5:A:76:ARG:NH1	5:A:192:LYS:HG2	1.57	1.20
17:N:70:GLU:OE2	17:N:72:LYS:O	1.58	1.20
6:B:25:ILE:HG21	22:L:1169:BCR:C28	1.68	1.20
16:L:163:LEU:HD13	16:L:164:PRO:CG	1.72	1.20
3:3:205:GLY:H	5:A:252:ARG:NH2	1.39	1.20
11:G:46:ALA:N	11:G:48:ASP:HB3	1.56	1.19
20:A:7016:LMU:C9	20:A:7016:LMU:H32	1.72	1.19
4:4:33:ASP:HB3	4:4:34:PRO:HD2	1.23	1.19
6:B:403:ASN:O	6:B:406:ASN:CB	1.90	1.19
11:G:45:GLU:HG2	11:G:49:THR:HG23	1.19	1.19
5:A:541:VAL:HG11	5:A:615:HIS:CD2	1.77	1.19
16:L:164:PRO:HB3	16:L:165:TYR:CD2	1.78	1.19
17:N:61:LEU:HD12	17:N:62:SER:C	1.63	1.19
19:1:1198:CLA:H52	19:1:1198:CLA:C10	1.72	1.19
22:3:1220:BCR:C23	22:3:1220:BCR:H393	1.67	1.19
6:B:120:VAL:HA	6:B:123:TRP:CD1	1.76	1.19
6:B:293:THR:O	11:G:38:GLN:OE1	1.56	1.19
18:R:41:UNK:CB	18:R:42:UNK:HA	1.70	1.19
19:4:1196:CLA:HHD	19:4:1196:CLA:CBC	1.73	1.19
20:A:7021:LMU:C1'	20:A:7021:LMU:H31	1.67	1.19
19:B:1753:CLA:H43	19:B:1753:CLA:C1A	1.72	1.19
17:N:48:GLY:CA	17:N:49:CYS:SG	2.30	1.18
22:B:1779:BCR:C27	22:B:1779:BCR:H403	1.52	1.18
5:A:81:ALA:HB2	19:A:1760:CLA:CMA	1.71	1.18
5:A:702:GLU:OE2	6:B:550:LYS:NZ	1.76	1.18
18:R:52:UNK:HA	18:R:53:UNK:CB	1.68	1.18
19:B:1768:CLA:C15	22:B:1779:BCR:C31	2.20	1.18
19:1:1197:CLA:HED2	19:1:1197:CLA:CAD	1.67	1.18
17:N:79:SER:HA	17:N:80:ASN:O	1.39	1.18
20:A:7039:LMU:H6'2	20:A:7039:LMU:C3'	1.74	1.18
15:K:68:HIS:O	15:K:70:MET:HB2	1.41	1.18
5:A:331:LEU:HD23	5:A:331:LEU:O	1.42	1.18
17:N:57:LYS:HG3	17:N:58:VAL:N	1.44	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:8052:SUC:C4'	21:B:8052:SUC:H1	1.66	1.18
19:3:1219:CLA:HMC1	19:3:1219:CLA:HBC3	1.22	1.18
19:A:1801:CLA:HMA3	16:L:27:VAL:HA	1.24	1.18
5:A:51:THR:CB	19:A:1795:CLA:HBB2	1.70	1.18
5:A:342:GLY:HA3	5:A:430:ASP:CB	1.74	1.18
16:L:163:LEU:HD22	16:L:164:PRO:CD	1.72	1.18
3:3:132:TRP:CZ3	3:3:155:GLU:CD	2.06	1.18
22:A:1807:BCR:C31	19:A:1813:CLA:C14	2.21	1.17
5:A:27:ILE:O	5:A:28:LYS:HG3	1.41	1.17
4:4:107:GLN:C	19:4:1196:CLA:CMA	2.13	1.17
19:1:1198:CLA:CHD	19:1:1198:CLA:HBC3	1.74	1.17
19:J:1044:CLA:O1D	19:J:1045:CLA:H91	1.45	1.17
10:F:24:LYS:HE2	10:F:24:LYS:N	1.57	1.17
3:3:87:GLU:C	22:3:1220:BCR:C38	2.12	1.17
17:N:41:LYS:CB	17:N:42:PHE:HB3	1.75	1.17
5:A:316:MET:HB3	5:A:317:TYR:CB	1.73	1.17
19:B:1753:CLA:CMC	19:B:1753:CLA:HBC3	1.65	1.17
19:A:1779:CLA:C4C	22:A:1805:BCR:C19	2.23	1.17
19:B:1768:CLA:C9	19:B:1768:CLA:HBB2	1.75	1.17
19:3:3008:CLA:CBA	19:3:3008:CLA:HBD	1.75	1.17
5:A:79:PHE:CE2	5:A:185:HIS:NE2	2.13	1.16
5:A:590:CYS:SG	25:B:1784:SF4:S1	2.42	1.16
19:A:1781:CLA:HED1	19:A:1782:CLA:CMD	1.75	1.16
3:3:132:TRP:HH2	3:3:155:GLU:CD	1.21	1.16
19:A:1815:CLA:H61	19:A:1815:CLA:CMA	1.76	1.16
3:3:83:LEU:HA	19:A:1798:CLA:H43	1.25	1.16
7:C:1:MET:H2	7:C:3:HIS:N	1.42	1.16
3:3:132:TRP:HH2	3:3:155:GLU:OE2	0.82	1.16
3:3:64:TYR:CB	19:3:1218:CLA:C4	2.21	1.16
19:J:1044:CLA:CGD	19:J:1045:CLA:H92	1.75	1.16
20:A:7026:LMU:O3B	21:B:8062:SUC:H5'	1.37	1.16
19:A:1781:CLA:H72	19:A:1782:CLA:CED	1.74	1.16
5:A:25:ASP:OD1	5:A:26:PRO:HG3	1.44	1.16
6:B:87:ILE:HA	6:B:115:ASN:HA	1.25	1.16
25:B:1784:SF4:S2	25:B:1784:SF4:S4	2.44	1.16
19:2:1220:CLA:C9	3:3:137:SER:HB2	1.75	1.16
17:N:72:LYS:CB	17:N:73:ASP:HA	1.74	1.16
19:A:1797:CLA:C1	19:A:1797:CLA:HMA2	1.75	1.16
19:B:1768:CLA:H161	22:B:1779:BCR:H313	1.25	1.16
19:B:1753:CLA:H151	19:B:1753:CLA:C10	1.66	1.16
5:A:304:LEU:HD22	19:A:1772:CLA:HBB2	1.18	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:110:SER:C	3:3:111:TYR:HD2	1.48	1.15
19:B:1755:CLA:CBC	19:B:1755:CLA:HHD	1.76	1.15
20:A:7022:LMU:C2'	20:A:7022:LMU:H21	1.59	1.15
22:I:1032:BCR:HC31	19:I:1033:CLA:HAC2	1.28	1.15
17:N:63:ASP:H	17:N:64:ASP:CB	1.57	1.15
17:N:70:GLU:O	17:N:72:LYS:HD3	1.41	1.15
20:A:7016:LMU:H21	20:A:7016:LMU:C8	1.75	1.15
20:A:7043:LMU:C11	20:A:7043:LMU:H71	1.67	1.15
21:B:8062:SUC:H1'2	21:B:8062:SUC:C6'	1.70	1.15
19:L:1168:CLA:HBC3	19:L:1168:CLA:HHD	1.19	1.15
20:R:1057:LMU:H11	20:R:1057:LMU:H62	1.17	1.15
5:A:685:VAL:HG23	19:A:1796:CLA:HBB1	1.27	1.15
11:G:46:ALA:N	11:G:49:THR:HG21	1.59	1.15
19:1:1191:CLA:HMC1	19:1:1194:CLA:HHD	1.15	1.15
19:2:1220:CLA:HBD	19:2:1220:CLA:O1A	1.44	1.15
23:B:1773:PQN:C19	22:B:1780:BCR:C10	2.24	1.15
5:A:316:MET:CB	5:A:317:TYR:CD1	2.29	1.15
8:D:134:MET:SD	8:D:134:MET:N	2.20	1.15
7:C:1:MET:CB	7:C:4:SER:OG	1.94	1.14
22:A:1804:BCR:H23C	22:A:1804:BCR:H403	1.28	1.14
3:3:92:TRP:HA	3:3:93:PHE:CD1	1.80	1.14
5:A:316:MET:CG	5:A:317:TYR:CD1	2.29	1.14
6:B:22:TRP:NE1	19:B:1770:CLA:HBB1	1.60	1.14
3:3:74:ALA:HA	19:3:1215:CLA:C2D	1.77	1.14
17:N:72:LYS:HG3	17:N:74:LYS:CG	1.77	1.14
19:J:1045:CLA:CBA	19:J:1045:CLA:HBD	1.76	1.14
6:B:189:ALA:CB	19:B:1758:CLA:H203	1.76	1.14
11:G:33:LYS:CE	11:G:33:LYS:HA	1.68	1.14
17:N:61:LEU:C	17:N:61:LEU:HD12	1.65	1.14
19:3:1219:CLA:H101	19:3:1219:CLA:H142	1.23	1.14
20:A:7043:LMU:H62	20:A:7043:LMU:C10	1.76	1.14
3:3:194:ILE:CD1	19:3:1212:CLA:HMC2	1.75	1.14
20:1:7004:LMU:H12	20:1:7004:LMU:H3'	1.20	1.14
18:R:26:UNK:O	18:R:28:UNK:CB	1.96	1.14
5:A:304:LEU:HD22	19:A:1772:CLA:CBB	1.77	1.14
19:B:1786:CLA:C9	19:B:1787:CLA:H91	1.77	1.14
6:B:493:TRP:O	6:B:495:PRO:HD3	1.48	1.14
5:A:316:MET:HB3	5:A:317:TYR:CD1	1.81	1.14
21:B:8059:SUC:C1'	21:B:8059:SUC:H6'2	1.75	1.14
6:B:672:GLN:HA	6:B:672:GLN:HE21	1.09	1.14
19:A:1781:CLA:C4B	22:A:1806:BCR:H373	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:711:HIS:CD2	19:A:1795:CLA:HBC1	1.82	1.14
19:2:1220:CLA:H61	3:3:140:LYS:HD3	1.17	1.14
5:A:251:ASN:O	5:A:253:ASP:N	1.79	1.14
21:B:8059:SUC:H1'1	21:B:8059:SUC:H6'2	1.28	1.14
19:A:1797:CLA:HMA2	19:A:1797:CLA:H12	1.16	1.13
19:A:1788:CLA:H52	22:B:1780:BCR:H343	1.19	1.13
25:B:1784:SF4:S1	25:B:1784:SF4:S3	2.46	1.13
19:B:1751:CLA:HBC2	19:B:1751:CLA:HHD	1.14	1.13
21:3:1221:SUC:H6'2	21:3:1221:SUC:C1'	1.70	1.13
6:B:596:TRP:CH2	6:B:612:SER:O	2.02	1.13
19:A:1781:CLA:HBA2	19:A:1794:CLA:HED1	1.20	1.13
11:G:33:LYS:HE3	11:G:33:LYS:HA	1.26	1.13
22:I:1032:BCR:H313	22:I:1032:BCR:C8	1.75	1.13
4:4:104:ARG:HA	4:4:107:GLN:HB2	1.27	1.13
5:A:22:VAL:HG12	5:A:23:ASP:H	1.13	1.13
5:A:23:ASP:CA	5:A:24:ARG:HD2	1.78	1.13
19:B:1739:CLA:HBB2	19:B:1739:CLA:C9	1.78	1.13
17:N:61:LEU:HD12	17:N:62:SER:N	1.62	1.13
7:C:14:CYS:CA	7:C:17:CYS:SG	2.36	1.13
20:A:7009:LMU:H5B	20:A:7009:LMU:O3'	1.45	1.13
19:B:1742:CLA:CAC	19:B:1743:CLA:HBB2	1.78	1.13
5:A:160:SER:O	5:A:163:GLN:HG2	1.45	1.13
19:A:1779:CLA:CHD	22:A:1805:BCR:C19	2.26	1.13
6:B:403:ASN:O	6:B:406:ASN:HB3	0.97	1.13
19:1:1191:CLA:CAB	19:1:1197:CLA:CBC	2.25	1.13
19:1:1197:CLA:O1D	19:1:1197:CLA:HAA2	1.46	1.13
19:A:1816:CLA:HHD	19:A:1816:CLA:HBC3	1.18	1.13
3:3:110:SER:O	3:3:111:TYR:HD2	1.31	1.13
22:B:1779:BCR:HC8	22:B:1779:BCR:C32	1.66	1.13
12:H:69:SER:HB2	19:H:1079:CLA:H61	1.13	1.13
22:A:1807:BCR:H313	19:A:1813:CLA:C14	1.77	1.12
6:B:58:PHE:HB2	6:B:146:SER:HB3	1.27	1.12
19:B:1753:CLA:C15	19:B:1753:CLA:H102	1.77	1.12
13:I:7:LEU:CD1	22:I:1032:BCR:H333	1.79	1.12
16:L:164:PRO:CB	16:L:165:TYR:CD2	2.30	1.12
21:B:8060:SUC:O1'	21:B:8060:SUC:H5	1.49	1.12
5:A:451:ILE:HD12	19:A:1788:CLA:HED3	1.29	1.12
19:A:1772:CLA:H172	19:A:1772:CLA:H141	1.13	1.12
5:A:435:VAL:O	5:A:438:HIS:O	1.67	1.12
25:B:1784:SF4:S1	25:B:1784:SF4:S2	2.47	1.12
3:3:64:TYR:HB3	19:3:1218:CLA:H43	1.28	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:25:GLY:HA3	12:H:27:ASP:N	1.62	1.12
19:3:1217:CLA:CHA	19:3:3011:CLA:CBC	2.27	1.12
5:A:24:ARG:N	5:A:24:ARG:HD2	1.64	1.12
20:A:7036:LMU:C8	20:A:7036:LMU:H31	1.79	1.12
17:N:58:VAL:CB	17:N:59:PRO:HD2	1.77	1.12
3:3:158:TYR:HB3	3:3:159:PRO:HD2	1.31	1.12
5:A:423:ASP:HB3	5:A:424:PRO:HD3	1.20	1.12
16:L:163:LEU:CD1	16:L:164:PRO:HB2	1.78	1.12
17:N:75:TYR:O	17:N:76:LYS:O	1.68	1.12
20:A:7010:LMU:O2B	20:A:7010:LMU:H3'	1.49	1.12
19:A:1772:CLA:H141	19:A:1772:CLA:C17	1.78	1.11
19:4:1199:CLA:HAA1	19:F:1157:CLA:H42	1.31	1.11
19:A:1813:CLA:HMD3	6:B:578:LEU:HD23	1.13	1.11
19:4:1196:CLA:HHD	19:4:1196:CLA:HBC2	1.23	1.11
19:J:1045:CLA:HBA2	19:J:1045:CLA:CBD	1.79	1.11
11:G:12:THR:HG22	11:G:72:LEU:HG	1.19	1.11
3:3:84:ILE:HA	19:A:1798:CLA:H51	1.24	1.11
19:A:1791:CLA:HBC2	22:A:1806:BCR:HC31	1.32	1.11
6:B:131:THR:HB	6:B:134:ASP:HB2	1.16	1.11
6:B:608:GLN:HA	6:B:608:GLN:HE21	1.02	1.11
20:A:7033:LMU:C3'	20:A:7033:LMU:H6'2	1.78	1.11
10:F:25:LEU:CD2	10:F:46:MET:HB3	1.80	1.11
19:A:1781:CLA:CED	19:A:1782:CLA:HMD1	1.80	1.11
23:B:1773:PQN:H191	22:B:1780:BCR:C10	1.78	1.11
22:B:1780:BCR:H382	22:B:1780:BCR:H23C	1.21	1.11
25:B:1784:SF4:S1	25:B:1784:SF4:S4	2.47	1.11
5:A:472:ARG:HH12	16:L:74:LEU:HG	1.01	1.11
19:B:1735:CLA:HBB2	19:B:1735:CLA:H101	1.14	1.11
11:G:45:GLU:C	11:G:49:THR:HG21	1.70	1.11
19:1:1191:CLA:CMC	19:1:1194:CLA:HHD	1.77	1.11
17:N:61:LEU:CD1	17:N:63:ASP:HB2	1.80	1.11
10:F:22:LEU:CD1	10:F:22:LEU:H	1.64	1.11
15:K:69:ILE:HG22	15:K:70:MET:H	1.16	1.11
20:A:7030:LMU:C5	20:A:7030:LMU:H91	1.67	1.11
19:A:1817:CLA:HBC2	19:A:1817:CLA:HMC1	1.24	1.11
3:3:87:GLU:O	22:3:1220:BCR:H381	1.50	1.11
19:4:1199:CLA:HMC1	19:4:1199:CLA:HBC3	1.11	1.11
5:A:76:ARG:CZ	5:A:192:LYS:HG2	1.79	1.11
5:A:581:CYS:HB2	5:A:590:CYS:HA	1.23	1.11
19:B:1768:CLA:C16	22:B:1779:BCR:H313	1.79	1.11
5:A:588:GLY:CA	6:B:668:ARG:HD3	1.81	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1759:CLA:CBC	19:B:1759:CLA:HMC1	1.79	1.11
2:2:64:ILE:O	2:2:68:LEU:HB2	1.49	1.11
3:3:52:LYS:O	3:3:56:TYR:CD2	2.03	1.11
5:A:425:THR:HG21	8:D:59:GLU:OE2	1.48	1.11
19:B:1786:CLA:H93	19:B:1787:CLA:H91	1.16	1.11
7:C:66:ARG:HH21	7:C:66:ARG:HG2	1.16	1.11
20:A:7016:LMU:H22	20:A:7016:LMU:H61	1.26	1.11
5:A:316:MET:HB3	5:A:317:TYR:CG	1.85	1.11
2:2:127:ASN:ND2	14:J:2:ARG:HH12	1.47	1.10
5:A:685:VAL:HG23	19:A:1796:CLA:CBB	1.81	1.10
3:3:84:ILE:H	19:A:1798:CLA:C4	1.61	1.10
11:G:42:SER:HB2	11:G:45:GLU:CD	1.71	1.10
5:A:208:ALA:HA	5:A:310:PHE:O	1.50	1.10
17:N:67:LEU:C	17:N:68:GLU:HG3	1.72	1.10
22:A:1803:BCR:H23C	22:A:1803:BCR:H402	1.32	1.10
5:A:331:LEU:HD21	5:A:343:HIS:O	0.94	1.10
20:A:7036:LMU:C8	20:A:7036:LMU:C3	2.29	1.10
19:2:1220:CLA:CGA	19:2:1220:CLA:CBD	2.29	1.10
17:N:72:LYS:HG2	17:N:74:LYS:HG3	1.32	1.10
20:A:7026:LMU:O4'	21:B:8062:SUC:H3'	1.38	1.10
21:B:8062:SUC:H6'1	21:B:8062:SUC:H1'2	1.31	1.10
20:A:7030:LMU:C5	20:A:7030:LMU:C9	2.30	1.10
6:B:247:THR:CA	6:B:250:ALA:HB2	1.79	1.10
9:E:86:GLU:CG	9:E:87:VAL:H	1.65	1.10
8:D:113:HIS:NE2	8:D:118:VAL:HG11	1.63	1.10
19:1:1198:CLA:H71	19:1:1198:CLA:H41	1.11	1.10
20:A:7016:LMU:C8	20:A:7016:LMU:H32	1.81	1.10
19:A:1772:CLA:CED	19:A:1772:CLA:C2A	2.30	1.10
6:B:58:PHE:CB	6:B:146:SER:HB3	1.80	1.10
13:I:7:LEU:HD12	22:I:1032:BCR:C33	1.80	1.10
20:A:7023:LMU:H41	20:A:7023:LMU:H92	1.13	1.10
17:N:54:LYS:HB3	17:N:57:LYS:HE2	1.22	1.10
20:A:7016:LMU:C2	20:A:7016:LMU:C8	2.30	1.10
21:B:8052:SUC:H5'	21:B:8052:SUC:H1	1.20	1.10
19:K:1085:CLA:CMB	19:K:1142:CLA:CED	2.30	1.10
19:A:1760:CLA:H12	19:A:1767:CLA:H61	1.25	1.10
19:A:1770:CLA:HMB2	22:A:1803:BCR:H382	1.34	1.10
5:A:23:ASP:CB	5:A:24:ARG:HD2	1.82	1.10
19:3:3008:CLA:CGD	19:3:3008:CLA:CBA	2.30	1.10
18:R:38:UNK:O	18:R:42:UNK:HA	1.48	1.10
20:A:7023:LMU:C8	20:A:7023:LMU:C4	2.30	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7016:LMU:C3	20:A:7016:LMU:C8	2.29	1.10
19:1:1200:CLA:HMC1	19:1:1200:CLA:CBC	1.80	1.10
21:B:8052:SUC:C1	21:B:8052:SUC:C5'	2.29	1.10
20:A:7026:LMU:H41	20:A:7026:LMU:C8	1.80	1.10
5:A:328:LYS:HG2	5:A:332:GLU:HB2	1.31	1.09
5:A:331:LEU:HD11	5:A:346:LEU:HB3	1.23	1.09
19:A:1770:CLA:C4B	22:A:1803:BCR:C19	2.29	1.09
6:B:119:GLY:HA3	19:B:1758:CLA:HED1	1.14	1.09
22:I:1032:BCR:H322	22:I:1032:BCR:C4	1.61	1.09
16:L:163:LEU:CD1	16:L:164:PRO:CB	2.30	1.09
16:L:163:LEU:CD1	16:L:164:PRO:CG	2.29	1.09
10:F:22:LEU:N	10:F:22:LEU:HD12	1.52	1.09
19:A:1771:CLA:HBB1	22:A:1803:BCR:C35	1.81	1.09
5:A:23:ASP:CB	5:A:24:ARG:CD	2.30	1.09
6:B:103:ALA:O	6:B:104:PHE:HB2	1.48	1.09
22:I:1032:BCR:HC31	19:I:1033:CLA:CAC	1.80	1.09
20:A:7023:LMU:C9	20:A:7023:LMU:C4	2.30	1.09
17:N:72:LYS:HG3	17:N:74:LYS:CA	1.80	1.09
17:N:72:LYS:CG	17:N:74:LYS:CG	2.31	1.09
19:4:1198:CLA:CAA	19:4:1198:CLA:CED	2.29	1.09
19:J:1045:CLA:CAD	19:J:1045:CLA:CED	2.30	1.09
20:A:7037:LMU:C1	20:A:7037:LMU:C5	2.29	1.09
20:A:7033:LMU:C3'	20:A:7033:LMU:C6B	2.30	1.09
19:4:4014:CLA:HBC3	19:4:4014:CLA:HMC1	1.22	1.09
3:3:87:GLU:HB2	22:3:1220:BCR:H382	1.34	1.09
5:A:453:LEU:HD23	19:A:1793:CLA:HBB2	1.21	1.09
19:A:1791:CLA:CBC	22:A:1806:BCR:HC31	1.80	1.09
16:L:163:LEU:CD1	16:L:164:PRO:CD	2.29	1.09
19:A:1816:CLA:CGA	19:A:1816:CLA:CED	2.31	1.09
20:A:7023:LMU:C8	20:A:7023:LMU:C3	2.30	1.09
19:2:1220:CLA:CHA	19:2:1220:CLA:HBA2	1.63	1.09
17:N:72:LYS:CG	17:N:74:LYS:CB	2.31	1.09
19:K:1085:CLA:HMB2	19:K:1142:CLA:HED1	1.18	1.09
20:A:7039:LMU:C6B	20:A:7039:LMU:C3'	2.29	1.09
18:R:46:UNK:CB	18:R:47:UNK:CB	2.30	1.09
10:F:47:GLU:HG3	10:F:51:LYS:HE3	1.16	1.09
19:R:1055:CLA:HBA2	19:R:1055:CLA:HBD	1.28	1.09
19:A:1770:CLA:HHC	22:A:1803:BCR:H17C	1.32	1.09
8:D:117:GLY:O	8:D:118:VAL:HG23	1.52	1.09
18:R:34:UNK:CB	18:R:35:UNK:CB	2.30	1.09
5:A:316:MET:HG2	5:A:317:TYR:CE1	1.88	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7032:LMU:C3	20:A:7032:LMU:C1B	2.29	1.09
14:J:11:ALA:HB1	14:J:12:PRO:HD2	1.34	1.09
19:4:1201:CLA:CGA	19:4:1201:CLA:HMA2	1.82	1.09
19:A:1781:CLA:CED	19:A:1782:CLA:CMD	2.30	1.09
5:A:328:LYS:CE	5:A:332:GLU:CG	2.30	1.09
11:G:43:HIS:CA	11:G:44:PHE:HB3	1.81	1.09
16:L:164:PRO:CA	16:L:165:TYR:CE2	2.35	1.09
18:R:41:UNK:CB	18:R:42:UNK:CA	2.30	1.09
19:2:1220:CLA:H61	3:3:140:LYS:CE	1.83	1.09
17:N:62:SER:CB	17:N:66:ASP:CB	2.29	1.09
5:A:335:LYS:HG2	5:A:336:GLY:H	1.12	1.09
19:A:1776:CLA:HMD3	19:A:1778:CLA:HBB2	1.13	1.08
22:A:1805:BCR:H382	22:A:1805:BCR:H23C	1.21	1.08
22:B:1777:BCR:H382	22:B:1777:BCR:H23C	1.30	1.08
6:B:22:TRP:HE1	19:B:1770:CLA:CBB	1.65	1.08
19:B:1759:CLA:HBC2	19:B:1759:CLA:HMC1	1.29	1.08
16:L:164:PRO:CB	16:L:165:TYR:CE2	2.35	1.08
20:A:7043:LMU:H112	20:A:7043:LMU:H71	1.27	1.08
10:F:102:ARG:HG2	10:F:106:ILE:HD11	1.12	1.08
3:3:107:TRP:CD1	3:3:108:ALA:N	2.21	1.08
19:A:1788:CLA:H161	22:L:1169:BCR:H361	1.32	1.08
4:4:107:GLN:CB	19:4:1196:CLA:HMA3	1.84	1.08
20:A:7032:LMU:O5B	20:A:7032:LMU:H3'	1.35	1.08
11:G:48:ASP:CB	11:G:49:THR:CG2	2.30	1.08
19:A:1781:CLA:CED	19:A:1782:CLA:CAD	2.30	1.08
20:A:7042:LMU:C3	20:A:7042:LMU:H6D	1.82	1.08
16:L:163:LEU:HD13	16:L:164:PRO:N	1.67	1.08
19:1:1197:CLA:CAD	19:1:1197:CLA:CED	2.32	1.08
19:J:1044:CLA:C10	19:J:1044:CLA:H152	1.55	1.08
4:4:38:ARG:HH11	4:4:38:ARG:HG3	1.14	1.08
5:A:365:LEU:HD23	19:A:1761:CLA:HED3	1.29	1.08
5:A:402:ILE:HG13	19:A:1784:CLA:HBB2	1.32	1.08
19:A:1797:CLA:HHD	19:A:1797:CLA:HBC3	1.31	1.08
5:A:51:THR:HG21	19:A:1795:CLA:HBB1	1.17	1.08
20:A:7042:LMU:C3	20:A:7042:LMU:C6'	2.30	1.08
19:A:1816:CLA:CGD	19:A:1816:CLA:CAA	2.30	1.08
19:B:1755:CLA:HBB1	19:B:1769:CLA:HMB3	1.29	1.08
20:A:7036:LMU:C7	20:A:7036:LMU:C3	2.29	1.08
18:R:39:UNK:C	18:R:41:UNK:CB	2.30	1.08
17:N:51:ASP:C	17:N:52:LEU:HD23	1.74	1.08
19:K:1146:CLA:HBC2	19:K:1146:CLA:HMC1	1.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:23:LYS:HB2	10:F:24:LYS:HZ1	1.17	1.08
6:B:302:LYS:O	6:B:303:TYR:HB2	1.50	1.07
6:B:594:TRP:O	6:B:595:HIS:HB3	1.49	1.07
19:A:1780:CLA:OBD	19:A:1780:CLA:H92	1.51	1.07
19:2:1212:CLA:CBC	19:2:1212:CLA:HMC1	1.83	1.07
19:J:1043:CLA:HED3	19:J:1043:CLA:CHA	1.83	1.07
20:A:7032:LMU:H12	20:A:7032:LMU:O2'	1.45	1.07
3:3:198:PHE:HA	3:3:201:ALA:HB2	1.36	1.07
19:B:1755:CLA:HBC2	19:B:1755:CLA:HHD	1.15	1.07
9:E:52:VAL:HG12	9:E:53:VAL:H	1.18	1.07
11:G:46:ALA:HA	11:G:48:ASP:OD2	1.53	1.07
19:A:1797:CLA:H121	19:A:1797:CLA:H71	1.34	1.07
19:B:1753:CLA:O2D	19:B:1753:CLA:H2A	1.52	1.07
20:A:7036:LMU:C2	20:A:7036:LMU:C8	2.30	1.07
20:A:7023:LMU:C8	20:A:7023:LMU:H32	1.84	1.07
19:J:1044:CLA:O2D	19:J:1045:CLA:H92	1.50	1.07
19:J:1045:CLA:CHD	19:J:1045:CLA:CBC	2.30	1.07
5:A:316:MET:HB3	5:A:317:TYR:HB2	1.18	1.07
20:A:7043:LMU:C7	20:A:7043:LMU:C11	2.30	1.07
20:A:7021:LMU:H1'	20:A:7021:LMU:C3	1.81	1.07
20:R:1056:LMU:O6B	20:R:1056:LMU:H1B	1.50	1.07
16:L:164:PRO:HA	16:L:165:TYR:CE2	1.90	1.07
19:1:1198:CLA:C5	19:1:1198:CLA:H102	1.81	1.07
19:1:1198:CLA:CBC	19:1:1198:CLA:HHD	1.82	1.07
19:3:3008:CLA:CBA	19:3:3008:CLA:CBD	2.30	1.07
19:3:3008:CLA:HBC2	19:3:3008:CLA:HMC1	1.09	1.07
4:4:95:PHE:HZ	19:4:1208:CLA:C3C	1.67	1.07
10:F:42:ILE:HG13	10:F:43:LYS:H	1.15	1.07
19:A:1782:CLA:HMC1	19:A:1782:CLA:HBC2	1.33	1.07
6:B:58:PHE:HB2	6:B:146:SER:CB	1.83	1.07
16:L:164:PRO:C	16:L:165:TYR:CG	2.28	1.07
20:A:7023:LMU:O3B	20:A:7023:LMU:H6'1	1.46	1.07
17:N:45:ASN:HD22	17:N:54:LYS:CB	1.64	1.07
20:A:7016:LMU:H22	20:A:7016:LMU:C6	1.57	1.07
19:J:1044:CLA:CGD	19:J:1045:CLA:C9	2.32	1.07
19:B:1737:CLA:O1A	19:B:1737:CLA:H62	1.54	1.07
6:B:729:THR:O	6:B:729:THR:HG22	1.53	1.07
16:L:66:GLY:HA3	19:L:1168:CLA:CHC	1.85	1.07
20:A:7023:LMU:H32	20:A:7023:LMU:H82	1.13	1.07
19:2:1220:CLA:H42	3:3:140:LYS:HG2	1.35	1.07
3:3:93:PHE:N	3:3:93:PHE:CD2	2.22	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:1045:CLA:HBC2	19:J:1045:CLA:HHD	1.19	1.07
12:H:25:GLY:HA3	12:H:27:ASP:H	1.02	1.07
20:A:7039:LMU:H3'	20:A:7039:LMU:H6'2	1.08	1.07
19:R:1054:CLA:HED3	19:R:1054:CLA:CHA	1.85	1.07
5:A:21:LEU:HA	5:A:22:VAL:HB	1.14	1.06
6:B:202:SER:O	6:B:245:GLY:HA2	1.52	1.06
20:A:7042:LMU:H5'	20:A:7042:LMU:O2B	1.54	1.06
17:N:54:LYS:HB3	17:N:57:LYS:CE	1.85	1.06
6:B:25:ILE:HG23	22:L:1169:BCR:H282	1.37	1.06
19:A:1797:CLA:C7	19:A:1797:CLA:H121	1.85	1.06
5:A:249:ILE:HG12	5:A:250:LEU:N	1.67	1.06
19:J:1044:CLA:C8	19:J:1044:CLA:H41	1.84	1.06
20:A:7020:LMU:C6'	20:A:7020:LMU:C5B	2.29	1.06
20:A:7026:LMU:C5	20:A:7026:LMU:H12	1.82	1.06
12:H:58:ILE:HD11	16:L:97:MET:SD	1.94	1.06
3:3:87:GLU:C	22:3:1220:BCR:H381	1.75	1.06
22:A:1807:BCR:C31	19:A:1813:CLA:H142	1.84	1.06
11:G:28:ARG:HG2	11:G:28:ARG:HH21	1.20	1.06
22:I:1032:BCR:HC42	22:I:1032:BCR:H322	1.10	1.06
19:L:1168:CLA:HHD	19:L:1168:CLA:CBC	1.83	1.06
19:A:1779:CLA:CAB	22:A:1805:BCR:H351	1.85	1.06
19:A:1781:CLA:CBC	19:A:1781:CLA:HHD	1.86	1.06
19:A:1781:CLA:HBC2	19:A:1781:CLA:HHD	1.07	1.06
5:A:23:ASP:OD2	5:A:24:ARG:HD3	1.54	1.06
5:A:605:MET:HA	5:A:608:SER:OG	1.55	1.06
19:B:1768:CLA:H152	22:B:1779:BCR:H312	1.09	1.06
16:L:164:PRO:C	16:L:165:TYR:CD2	2.28	1.06
16:L:164:PRO:CA	16:L:165:TYR:CD2	2.37	1.06
5:A:197:GLN:HA	5:A:197:GLN:HE21	0.92	1.06
6:B:282:PHE:HZ	19:B:1746:CLA:C1	1.69	1.06
17:N:52:LEU:N	17:N:52:LEU:HD23	1.65	1.06
3:3:98:ILE:O	17:N:63:ASP:O	1.72	1.06
16:L:161:LEU:CD1	16:L:162:ASP:N	2.18	1.06
19:3:3011:CLA:H12	19:3:3011:CLA:HMA2	1.27	1.06
20:A:7030:LMU:H91	20:A:7030:LMU:H51	1.34	1.06
10:F:5:LEU:HG	10:F:6:THR:N	1.66	1.06
6:B:531:THR:HG22	19:B:1755:CLA:HMC2	1.11	1.06
19:B:1761:CLA:HHD	19:B:1761:CLA:HBC2	1.35	1.06
6:B:663:PHE:O	6:B:664:LEU:HB2	1.49	1.06
19:A:1770:CLA:CHC	22:A:1803:BCR:C19	2.34	1.06
5:A:21:LEU:N	5:A:22:VAL:HB	1.69	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1773:PQN:C16	22:B:1780:BCR:H333	1.80	1.06
6:B:310:PRO:HG3	19:B:1753:CLA:HMA1	1.09	1.06
4:4:107:GLN:HA	19:4:1196:CLA:HMA3	1.16	1.06
4:4:95:PHE:CZ	19:4:1208:CLA:C2C	2.38	1.06
9:E:87:VAL:O	9:E:87:VAL:HG12	1.56	1.05
11:G:42:SER:OG	11:G:45:GLU:HB2	1.56	1.05
11:G:45:GLU:HG3	11:G:49:THR:CG2	1.79	1.05
22:I:1032:BCR:HC22	19:I:1033:CLA:C4C	1.85	1.05
17:N:58:VAL:CB	17:N:59:PRO:CD	2.30	1.05
19:J:1044:CLA:C15	19:J:1044:CLA:C10	2.30	1.05
5:A:267:THR:O	5:A:269:PHE:HD2	1.39	1.05
11:G:46:ALA:H	11:G:48:ASP:CB	1.69	1.05
22:A:1803:BCR:HC8	22:A:1803:BCR:H311	1.07	1.05
19:B:1735:CLA:HMD3	22:B:1778:BCR:HC41	1.36	1.05
22:B:1780:BCR:H17C	19:B:1786:CLA:H101	1.39	1.05
6:B:560:ASP:OD1	6:B:561:GLY:N	1.90	1.05
19:3:3008:CLA:HMC1	19:3:3008:CLA:CBC	1.87	1.05
19:4:1198:CLA:H151	19:4:1198:CLA:H202	1.27	1.05
21:B:8052:SUC:C1	21:B:8052:SUC:H5'	1.84	1.05
11:G:68:ILE:CG2	11:G:72:LEU:HD13	1.86	1.05
19:4:1209:CLA:HBD	19:4:1209:CLA:HBA1	1.37	1.05
5:A:454:GLY:H	5:A:457:SER:HB3	1.15	1.05
19:B:1761:CLA:CBC	19:B:1761:CLA:HHD	1.86	1.05
19:A:1816:CLA:CHD	19:A:1816:CLA:CBC	2.33	1.05
17:N:48:GLY:HA3	17:N:49:CYS:O	1.55	1.05
17:N:46:PHE:O	17:N:47:THR:HG23	1.54	1.05
19:4:1198:CLA:H151	19:4:1198:CLA:H203	1.34	1.05
20:1:7004:LMU:H1B	20:1:7004:LMU:O6B	1.50	1.05
6:B:474:PHE:HE2	6:B:476:ILE:HG13	1.19	1.05
5:A:599:PHE:CE2	5:A:735:VAL:HG21	1.92	1.05
23:B:1773:PQN:H192	22:B:1780:BCR:H10C	1.35	1.05
17:N:65:LEU:HD23	17:N:65:LEU:O	1.54	1.05
19:4:1198:CLA:H2A	19:4:1198:CLA:O1D	1.56	1.05
19:J:1045:CLA:HBC3	19:J:1045:CLA:HHD	1.39	1.05
20:A:7037:LMU:C1	20:A:7037:LMU:H51	1.87	1.05
12:H:25:GLY:HA3	12:H:27:ASP:CB	1.86	1.05
20:A:7043:LMU:H62	20:A:7043:LMU:H102	1.06	1.05
11:G:12:THR:CG2	11:G:72:LEU:HG	1.85	1.05
22:A:1807:BCR:HC8	22:A:1807:BCR:C31	1.86	1.05
6:B:174:ARG:HB2	19:B:1743:CLA:HBC2	1.39	1.05
16:L:64:LEU:HB3	16:L:68:PHE:HE1	1.18	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1781:CLA:H72	19:A:1782:CLA:HED2	1.30	1.05
9:E:72:VAL:O	9:E:73:ASN:HB3	1.56	1.05
14:J:2:ARG:HH12	14:J:8:LEU:HD13	1.21	1.05
20:A:7036:LMU:H71	20:A:7036:LMU:C3	1.82	1.05
16:L:163:LEU:CD2	16:L:164:PRO:CD	2.30	1.05
20:A:7016:LMU:C2	20:A:7016:LMU:C6	2.30	1.05
19:A:1782:CLA:HMC1	19:A:1782:CLA:CBG	1.86	1.04
22:A:1804:BCR:H23C	22:A:1804:BCR:H402	1.38	1.04
5:A:402:ILE:CG1	19:A:1784:CLA:HBB2	1.87	1.04
11:G:43:HIS:O	11:G:45:GLU:HB2	1.56	1.04
19:1:1197:CLA:OBD	19:1:1197:CLA:HED2	1.56	1.04
16:L:161:LEU:HD11	16:L:162:ASP:O	1.57	1.04
10:F:151:ASP:O	10:F:154:PHE:HB3	1.56	1.04
6:B:560:ASP:HB2	7:C:66:ARG:NE	1.71	1.04
16:L:163:LEU:CG	16:L:164:PRO:HD2	1.85	1.04
17:N:45:ASN:HD22	17:N:57:LYS:NZ	1.53	1.04
5:A:316:MET:CB	5:A:317:TYR:HD1	1.64	1.04
19:B:1755:CLA:CED	19:B:1756:CLA:HMD1	1.88	1.04
8:D:78:ALA:HB3	8:D:82:GLN:HE22	1.16	1.04
9:E:85:ASP:O	9:E:86:GLU:HB3	1.52	1.04
20:A:7016:LMU:H6'	20:A:7016:LMU:H51	1.19	1.04
3:3:110:SER:O	3:3:111:TYR:CD2	2.10	1.04
5:A:81:ALA:HB1	19:A:1760:CLA:HMA1	1.38	1.04
19:A:1772:CLA:H172	19:A:1772:CLA:C14	1.86	1.04
5:A:21:LEU:CA	5:A:22:VAL:CB	2.35	1.04
7:C:1:MET:HG2	7:C:4:SER:HB3	1.37	1.04
22:I:1032:BCR:C3	19:I:1033:CLA:CAC	2.36	1.04
20:A:7042:LMU:C7	20:A:7042:LMU:C2	2.30	1.04
3:3:64:TYR:HB3	19:3:1218:CLA:H42	1.33	1.04
19:4:1198:CLA:C20	19:4:1198:CLA:C15	2.30	1.04
6:B:310:PRO:HG2	6:B:311:PRO:HD2	1.37	1.04
10:F:130:LEU:HG	10:F:131:PHE:H	1.16	1.04
19:B:1739:CLA:H92	19:B:1739:CLA:CBB	1.86	1.04
19:J:1045:CLA:HBA2	19:J:1045:CLA:HBD	1.04	1.04
10:F:24:LYS:CA	10:F:24:LYS:CE	2.36	1.04
10:F:23:LYS:O	10:F:26:GLN:HB2	1.57	1.04
21:3:1221:SUC:H6'2	21:3:1221:SUC:H1'1	1.07	1.04
5:A:370:ILE:HG22	5:A:400:MET:HA	1.40	1.03
19:A:1770:CLA:HMB2	22:A:1803:BCR:C38	1.87	1.03
22:B:1779:BCR:C40	22:B:1779:BCR:C27	2.30	1.03
11:G:45:GLU:HG3	11:G:49:THR:HG23	1.08	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:HD11	17:N:63:ASP:N	1.73	1.03
20:A:7032:LMU:H2B	20:A:7032:LMU:H31	1.34	1.03
6:B:708:VAL:O	6:B:712:HIS:HB2	1.56	1.03
19:A:1771:CLA:CBB	22:A:1803:BCR:H352	1.87	1.03
19:J:1045:CLA:O2A	19:J:1045:CLA:H2A	1.55	1.03
19:3:1219:CLA:C10	19:3:1219:CLA:C14	2.34	1.03
20:A:7021:LMU:H22	20:A:7021:LMU:H62	1.07	1.03
7:C:1:MET:HB3	7:C:4:SER:OG	1.54	1.03
6:B:419:ILE:O	6:B:420:SER:OG	1.77	1.03
7:C:54:CYS:CB	25:C:1082:SF4:S1	2.47	1.03
19:J:1044:CLA:C15	19:J:1044:CLA:H102	1.87	1.03
5:A:316:MET:CB	5:A:317:TYR:HB2	1.88	1.03
19:3:1219:CLA:H102	19:3:1219:CLA:C14	1.89	1.03
11:G:68:ILE:HG23	11:G:72:LEU:HD13	1.34	1.03
5:A:116:ILE:HG23	5:A:137:GLY:HA3	1.41	1.03
5:A:23:ASP:C	5:A:24:ARG:HD2	1.78	1.03
11:G:44:PHE:N	11:G:45:GLU:HB2	1.71	1.03
10:F:24:LYS:O	10:F:27:ALA:HB2	1.59	1.03
19:4:1199:CLA:CBC	19:4:1199:CLA:HMC1	1.88	1.03
19:A:1776:CLA:HMD3	19:A:1778:CLA:CBB	1.87	1.03
5:A:545:HIS:ND1	19:A:1792:CLA:HBB2	1.74	1.03
19:A:1796:CLA:C14	22:A:1807:BCR:C2	2.37	1.03
5:A:365:LEU:HD23	19:A:1761:CLA:CED	1.87	1.03
6:B:340:SER:HA	19:B:1756:CLA:H51	1.40	1.03
22:I:1032:BCR:C2	19:I:1033:CLA:C3C	2.36	1.03
19:1:1198:CLA:C7	19:1:1198:CLA:H41	1.78	1.03
12:H:20:GLN:HB3	12:H:22:ASP:HB3	1.03	1.03
15:K:71:GLY:O	15:K:72:VAL:O	1.76	1.03
6:B:65:LEU:HD22	6:B:124:TRP:HE3	1.21	1.02
19:B:1753:CLA:H43	19:B:1753:CLA:HAA1	1.41	1.02
5:A:707:ILE:HG22	5:A:711:HIS:NE2	1.74	1.02
23:B:1773:PQN:C16	22:B:1780:BCR:H331	1.87	1.02
19:2:1220:CLA:H41	3:3:140:LYS:HD3	1.40	1.02
9:E:51:SER:HB3	9:E:68:ARG:CZ	1.89	1.02
17:N:76:LYS:HG3	17:N:77:CYS:H	1.22	1.02
19:K:1085:CLA:CMB	19:K:1142:CLA:HED2	1.90	1.02
2:2:120:ASN:ND2	14:J:5:LYS:HE3	1.73	1.02
19:A:1791:CLA:CGA	19:A:1797:CLA:CBB	2.36	1.02
22:B:1779:BCR:H271	22:B:1779:BCR:H403	1.03	1.02
19:2:1213:CLA:HHD	19:2:1213:CLA:HBC2	1.41	1.02
19:J:1044:CLA:C15	19:J:1044:CLA:H91	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:24:LYS:HA	10:F:24:LYS:HE2	1.42	1.02
19:A:1762:CLA:H43	19:A:1785:CLA:H11	1.40	1.02
5:A:401:TRP:CD1	19:A:1783:CLA:HHC	1.95	1.02
22:A:1807:BCR:C31	19:A:1813:CLA:H143	1.87	1.02
6:B:558:PRO:HG2	6:B:703:VAL:HB	1.37	1.02
21:B:8052:SUC:O4'	21:B:8052:SUC:H1	1.59	1.02
14:J:31:ARG:NH2	19:J:1043:CLA:C4B	2.21	1.02
6:B:247:THR:HA	6:B:250:ALA:HB2	1.05	1.02
15:K:1:ASP:HA	15:K:5:SER:HB3	1.40	1.02
19:A:1772:CLA:CMC	19:A:1772:CLA:HBC3	1.82	1.02
16:L:88:ALA:C	16:L:90:GLY:H	1.56	1.02
10:F:23:LYS:C	10:F:24:LYS:HE2	1.79	1.02
4:4:160:MET:HE3	19:4:1201:CLA:CBB	1.87	1.01
19:B:1768:CLA:HBC1	10:F:83:PHE:CZ	1.95	1.01
9:E:45:TRP:CH2	9:E:78:SER:OG	2.12	1.01
11:G:48:ASP:HB3	11:G:49:THR:CG2	1.89	1.01
5:A:23:ASP:HB2	5:A:24:ARG:CZ	1.90	1.01
5:A:27:ILE:O	5:A:27:ILE:HG22	1.54	1.01
11:G:43:HIS:C	11:G:45:GLU:HB2	1.79	1.01
20:A:7042:LMU:H1B	20:A:7042:LMU:O3'	1.57	1.01
19:2:1212:CLA:CGA	19:2:1212:CLA:H42	1.89	1.01
19:3:1217:CLA:C2A	19:3:3011:CLA:HAC2	1.89	1.01
5:A:239:PRO:HA	5:A:242:ILE:CD1	1.90	1.01
5:A:511:THR:HG23	19:A:1773:CLA:O1A	1.58	1.01
6:B:382:ILE:HG22	6:B:383:MET:H	1.25	1.01
11:G:47:GLY:H	11:G:48:ASP:CB	1.73	1.01
5:A:355:HIS:ND1	5:A:416:ILE:HG21	1.76	1.01
17:N:61:LEU:CD1	17:N:63:ASP:CB	2.38	1.01
19:3:1217:CLA:CHA	19:3:3011:CLA:HBC2	1.90	1.01
19:B:1753:CLA:C4A	19:B:1753:CLA:H42	1.90	1.01
19:B:1767:CLA:HBC3	19:B:1767:CLA:HMC1	1.42	1.01
5:A:328:LYS:HE2	5:A:332:GLU:HG3	1.38	1.01
19:B:1735:CLA:HED3	19:B:1735:CLA:H2A	1.40	1.01
22:B:1780:BCR:H19C	19:B:1786:CLA:H151	1.41	1.01
19:3:3008:CLA:CGD	19:3:3008:CLA:CGA	2.38	1.01
5:A:249:ILE:HG12	5:A:250:LEU:H	0.89	1.01
20:1:7004:LMU:O2'	20:1:7004:LMU:H11	1.56	1.01
19:3:1217:CLA:CHA	19:3:3011:CLA:HBC1	1.87	1.01
12:H:44:ALA:CB	16:L:145:PHE:HD1	1.73	1.01
16:L:108:LYS:O	16:L:132:SER:HB2	1.59	1.01
19:A:1769:CLA:HBA1	19:A:1780:CLA:H41	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1755:CLA:HED1	19:B:1756:CLA:HMD1	1.42	1.01
16:L:122:GLY:C	16:L:124:LYS:H	1.61	1.01
19:A:1812:CLA:HMB3	19:B:1785:CLA:H18	1.43	1.01
20:A:7033:LMU:H3'	20:A:7033:LMU:H6'2	1.05	1.01
11:G:12:THR:HG22	11:G:72:LEU:CG	1.88	1.01
25:B:1784:SF4:S4	25:B:1784:SF4:S3	2.59	1.01
16:L:163:LEU:HD13	16:L:164:PRO:HB2	1.36	1.01
20:A:7023:LMU:H6'2	20:A:7023:LMU:C2B	1.87	1.01
2:2:169:LEU:HD22	19:2:1215:CLA:CAB	1.90	1.01
19:K:1085:CLA:NA	19:K:1142:CLA:HMD1	1.74	1.01
3:3:194:ILE:HD11	19:3:1212:CLA:HMC2	1.39	1.01
19:A:1781:CLA:C7	19:A:1782:CLA:CED	2.38	1.00
5:A:368:LEU:CD2	19:A:1774:CLA:C9	2.38	1.00
7:C:8:TYR:O	7:C:60:THR:HA	1.59	1.00
22:A:1807:BCR:HC8	22:A:1807:BCR:H311	1.01	1.00
22:A:1808:BCR:H393	22:A:1808:BCR:H23C	1.04	1.00
19:B:1768:CLA:H152	22:B:1779:BCR:H313	1.43	1.00
19:B:1735:CLA:HBB2	19:B:1735:CLA:C10	1.91	1.00
19:A:1788:CLA:H161	22:L:1169:BCR:C36	1.91	1.00
4:4:146:THR:OG1	19:4:1200:CLA:C5	2.09	1.00
19:A:1797:CLA:C12	19:A:1797:CLA:C7	2.35	1.00
5:A:390:ALA:HB2	5:A:754:ILE:HB	1.43	1.00
19:B:1740:CLA:H41	22:B:1781:BCR:C23	1.90	1.00
5:A:588:GLY:HA3	6:B:668:ARG:HD3	1.41	1.00
17:N:72:LYS:HB3	17:N:73:ASP:C	1.81	1.00
19:J:1044:CLA:C8	19:J:1044:CLA:H152	1.90	1.00
10:F:26:GLN:HA	10:F:26:GLN:OE1	1.61	1.00
3:3:48:PHE:HD2	3:3:49:ILE:HG22	0.85	1.00
20:A:7013:LMU:O6B	20:A:7013:LMU:H1B	1.57	1.00
19:A:1759:CLA:H42	19:A:1796:CLA:H61	1.03	1.00
19:A:1774:CLA:H121	19:A:1774:CLA:HBB2	1.42	1.00
19:B:1753:CLA:C4	19:B:1753:CLA:C4A	2.30	1.00
17:N:61:LEU:CD1	17:N:63:ASP:C	2.30	1.00
17:N:70:GLU:C	17:N:72:LYS:H	1.65	1.00
20:A:7026:LMU:H41	20:A:7026:LMU:H82	1.41	1.00
7:C:44:ARG:HH21	8:D:127:ARG:HB3	1.23	1.00
17:N:1:GLY:O	17:N:2:VAL:HG13	1.59	1.00
19:2:1220:CLA:C6	3:3:140:LYS:NZ	2.24	1.00
17:N:45:ASN:ND2	17:N:53:ALA:O	1.93	1.00
10:F:22:LEU:O	10:F:25:LEU:HB2	1.58	1.00
6:B:521:HIS:HE1	19:B:1768:CLA:NA	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:42:PHE:CD1	17:N:43:PRO:N	2.30	1.00
19:K:1085:CLA:HMB2	19:K:1142:CLA:HED2	1.40	1.00
9:E:39:LEU:H	9:E:40:ARG:NH1	1.58	1.00
11:G:43:HIS:HA	11:G:44:PHE:CB	1.91	1.00
17:N:54:LYS:CG	17:N:57:LYS:HZ3	1.74	1.00
10:F:23:LYS:C	10:F:24:LYS:CE	2.30	1.00
7:C:39:ILE:HG12	7:C:40:ALA:H	1.26	1.00
9:E:83:ALA:O	9:E:86:GLU:HG2	1.61	0.99
19:J:1043:CLA:CED	19:J:1043:CLA:CHA	2.39	0.99
19:A:1782:CLA:HBA1	19:A:1782:CLA:O1D	1.62	0.99
3:3:74:ALA:HB3	3:3:75:PRO:HD3	1.45	0.99
20:R:1057:LMU:C6	20:R:1057:LMU:H11	1.90	0.99
19:A:1801:CLA:CMA	16:L:27:VAL:HA	1.90	0.99
22:A:1807:BCR:H313	19:A:1813:CLA:H142	1.43	0.99
6:B:269:TRP:HB2	6:B:497:TRP:HH2	1.22	0.99
10:F:102:ARG:CG	10:F:106:ILE:HD11	1.92	0.99
17:N:18:ASP:CB	17:N:22:LEU:HG	1.92	0.99
19:2:1224:CLA:H152	19:2:1224:CLA:H192	1.43	0.99
19:A:1781:CLA:HBC2	19:A:1781:CLA:CHD	1.92	0.99
5:A:328:LYS:HE3	5:A:332:GLU:CG	1.90	0.99
11:G:48:ASP:HB3	11:G:49:THR:HG22	1.45	0.99
16:L:37:LEU:O	16:L:42:ALA:HB3	1.62	0.99
17:N:47:THR:OG1	17:N:54:LYS:HD3	1.61	0.99
17:N:62:SER:CB	17:N:66:ASP:CG	2.29	0.99
20:A:7021:LMU:H41	20:A:7021:LMU:C6'	1.91	0.99
6:B:361:ILE:HG23	6:B:368:GLN:OE1	1.63	0.99
3:3:205:GLY:N	5:A:252:ARG:NH2	1.99	0.99
18:R:52:UNK:CA	18:R:53:UNK:CB	2.36	0.99
16:L:82:ALA:CB	16:L:86:LEU:HD13	1.93	0.99
5:A:22:VAL:CG1	5:A:23:ASP:H	1.75	0.99
5:A:370:ILE:HG23	5:A:403:GLY:HA3	1.44	0.99
5:A:412:ALA:HB2	5:A:598:VAL:HG11	1.45	0.99
17:N:66:ASP:C	17:N:67:LEU:CD1	2.30	0.99
20:A:7037:LMU:O2B	20:A:7037:LMU:H5B	1.63	0.99
11:G:42:SER:CB	11:G:45:GLU:CD	2.30	0.99
19:2:1220:CLA:CBA	19:2:1220:CLA:HBD	1.92	0.99
20:A:7021:LMU:H31	20:A:7021:LMU:H1'	0.99	0.99
19:A:1763:CLA:C2B	22:A:1808:BCR:H331	1.92	0.99
22:A:1807:BCR:H311	22:A:1807:BCR:C8	1.85	0.99
5:A:453:LEU:HD21	19:A:1793:CLA:HBB2	1.41	0.99
5:A:672:LEU:O	5:A:674:ALA:N	1.95	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1786:CLA:H93	19:B:1787:CLA:C9	1.93	0.99
11:G:45:GLU:CA	11:G:49:THR:HG21	1.91	0.99
19:2:1215:CLA:O1A	19:2:1220:CLA:HBC2	1.61	0.99
17:N:32:ALA:HB1	17:N:35:VAL:HG22	1.45	0.99
8:D:44:GLU:HB2	8:D:46:TYR:HE2	1.26	0.98
11:G:42:SER:HB2	11:G:45:GLU:OE1	1.63	0.98
17:N:72:LYS:HB3	17:N:74:LYS:N	1.78	0.98
19:A:1770:CLA:CHC	22:A:1803:BCR:H19C	1.92	0.98
20:A:7021:LMU:C6	20:A:7021:LMU:H22	1.93	0.98
4:4:193:ILE:HG21	14:J:42:PHE:HD1	1.25	0.98
19:B:1787:CLA:HHB	19:B:1787:CLA:H43	1.45	0.98
17:N:63:ASP:CA	17:N:64:ASP:C	2.29	0.98
19:B:1768:CLA:H93	19:B:1768:CLA:HBB2	0.99	0.98
19:1:1200:CLA:HBC2	19:1:1200:CLA:HMC1	1.00	0.98
10:F:5:LEU:HG	10:F:6:THR:H	0.84	0.98
5:A:355:HIS:CE1	5:A:416:ILE:HG21	1.98	0.98
5:A:451:ILE:CD1	19:A:1788:CLA:CED	2.40	0.98
19:B:1737:CLA:O1A	19:B:1737:CLA:H2	1.19	0.98
20:A:7009:LMU:H3'	20:A:7009:LMU:O5B	1.61	0.98
4:4:169:GLN:NE2	19:4:1199:CLA:HHD	1.77	0.98
5:A:281:LEU:CG	19:A:1772:CLA:CED	2.40	0.98
19:B:1746:CLA:HHD	19:B:1746:CLA:HBC2	1.44	0.98
20:A:7042:LMU:H3'	20:A:7042:LMU:H2B	1.44	0.98
21:B:8054:SUC:H1'1	21:B:8054:SUC:C2	1.92	0.98
17:N:18:ASP:HB2	17:N:22:LEU:HG	1.42	0.98
5:A:170:GLY:O	5:A:173:VAL:HG22	1.63	0.98
5:A:204:ASN:O	5:A:205:HIS:HB2	1.63	0.98
5:A:302:HIS:O	5:A:306:ILE:HG12	1.64	0.98
19:B:1758:CLA:H142	22:B:1776:BCR:H10C	1.42	0.98
11:G:44:PHE:HD2	11:G:44:PHE:O	1.46	0.98
11:G:48:ASP:HB2	11:G:49:THR:CG2	1.91	0.98
22:I:1032:BCR:C8	22:I:1032:BCR:C31	2.29	0.98
10:F:22:LEU:HD12	10:F:22:LEU:H	0.83	0.98
15:K:64:GLY:O	15:K:68:HIS:ND1	1.96	0.98
19:A:1815:CLA:HMC1	19:A:1815:CLA:HBC3	1.43	0.98
5:A:210:LEU:CD1	19:A:1769:CLA:HMB2	1.94	0.98
11:G:46:ALA:H	11:G:49:THR:CG2	1.75	0.98
3:3:74:ALA:CA	19:3:1215:CLA:C3D	2.41	0.98
17:N:62:SER:HB3	17:N:66:ASP:HB3	1.41	0.98
9:E:68:ARG:C	9:E:68:ARG:HE	1.66	0.98
5:A:281:LEU:CD1	19:A:1772:CLA:O2D	2.11	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
19:B:1737:CLA:O1A	19:B:1737:CLA:C2	2.11	0.98
17:N:51:ASP:C	17:N:52:LEU:CD2	2.32	0.98
19:J:1045:CLA:HBC2	19:J:1045:CLA:CHD	1.92	0.98
2:2:103:GLY:N	19:2:1222:CLA:HBB2	1.79	0.98
19:A:1794:CLA:HMC1	19:A:1794:CLA:HBC3	1.43	0.98
19:A:1796:CLA:C14	22:A:1807:BCR:HC22	1.93	0.98
11:G:43:HIS:HA	11:G:44:PHE:HB3	0.99	0.98
4:4:107:GLN:C	19:4:1196:CLA:HMA2	1.82	0.98
3:3:173:GLU:HG2	3:3:174:LYS:H	1.29	0.98
22:A:1803:BCR:HC8	22:A:1803:BCR:C31	1.91	0.97
22:A:1804:BCR:C23	22:A:1804:BCR:C40	2.36	0.97
6:B:608:GLN:HA	6:B:608:GLN:NE2	1.79	0.97
10:F:5:LEU:CG	10:F:6:THR:H	1.74	0.97
5:A:365:LEU:CD2	19:A:1761:CLA:HED3	1.94	0.97
20:A:7023:LMU:H6 ²	20:A:7023:LMU:H2B	0.98	0.97
19:J:1043:CLA:CED	19:J:1043:CLA:C1A	2.42	0.97
16:L:160:VAL:O	16:L:160:VAL:HG22	1.64	0.97
19:4:1201:CLA:HAA2	19:4:1201:CLA:O1D	1.63	0.97
5:A:197:GLN:NE2	5:A:197:GLN:HA	1.72	0.97
6:B:269:TRP:HB2	6:B:497:TRP:CH2	2.00	0.97
6:B:11:GLY:HA3	7:C:71:HIS:HD2	1.26	0.97
17:N:61:LEU:CD1	17:N:63:ASP:CA	2.42	0.97
5:A:98:PHE:CZ	19:A:1763:CLA:HMD3	1.99	0.97
6:B:588:GLY:O	6:B:592:PHE:HB2	1.62	0.97
22:B:1780:BCR:C19	19:B:1786:CLA:H151	1.94	0.97
17:N:63:ASP:HA	17:N:64:ASP:O	1.64	0.97
17:N:65:LEU:C	17:N:65:LEU:CD2	2.30	0.97
6:B:247:THR:HA	6:B:250:ALA:CB	1.94	0.97
19:B:1768:CLA:C15	22:B:1779:BCR:H313	1.90	0.97
17:N:45:ASN:ND2	17:N:57:LYS:HZ1	1.61	0.97
19:J:1043:CLA:HHD	19:J:1043:CLA:HBC3	1.43	0.97
11:G:94:ASP:N	11:G:95:PRO:HD3	1.79	0.97
20:A:7037:LMU:H12	20:A:7037:LMU:H51	1.45	0.97
10:F:61:LEU:HD23	10:F:69:PRO:HB2	1.45	0.97
21:H:1080:SUC:H5	21:H:1080:SUC:O2	1.63	0.97
5:A:246:HIS:O	5:A:248:PHE:HD2	1.46	0.97
6:B:295:PHE:H	6:B:295:PHE:HD2	1.06	0.97
5:A:79:PHE:CZ	5:A:185:HIS:NE2	2.31	0.97
5:A:368:LEU:HD21	19:A:1774:CLA:H92	1.47	0.97
19:A:1800:CLA:HMD3	22:B:1780:BCR:HC31	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3008:CLA:O1A	19:3:3008:CLA:HED3	1.65	0.97
20:A:7023:LMU:H82	20:A:7023:LMU:C4	1.74	0.97
19:A:1771:CLA:HBB1	22:A:1803:BCR:H352	0.99	0.97
19:A:1781:CLA:CED	19:A:1782:CLA:C3D	2.43	0.97
19:A:1796:CLA:H141	22:A:1807:BCR:HC22	0.98	0.97
22:B:1777:BCR:C38	22:B:1777:BCR:H23C	1.92	0.97
6:B:461:GLN:O	6:B:464:GLN:HG2	1.65	0.97
17:N:70:GLU:O	17:N:72:LYS:CD	2.12	0.97
20:A:7032:LMU:C3	20:A:7032:LMU:C2B	2.42	0.97
4:4:160:MET:CE	19:4:1201:CLA:HBB1	1.80	0.97
19:A:1759:CLA:H42	19:A:1796:CLA:C6	1.93	0.97
19:A:1796:CLA:H141	22:A:1807:BCR:HC21	1.45	0.97
6:B:292:ARG:NE	6:B:292:ARG:HA	1.80	0.97
22:A:1808:BCR:C39	22:A:1808:BCR:H23C	1.91	0.96
6:B:586:THR:O	6:B:588:GLY:N	1.98	0.96
19:A:1812:CLA:H11	6:B:616:LEU:HG	1.47	0.96
13:I:11:LEU:HD12	22:I:1032:BCR:C10	1.94	0.96
16:L:163:LEU:HD22	16:L:164:PRO:HD2	1.00	0.96
19:K:1146:CLA:HMA2	19:K:1146:CLA:O1A	1.64	0.96
16:L:82:ALA:HB2	16:L:86:LEU:CD1	1.94	0.96
24:B:1783:LMG:O3	7:C:70:TRP:CZ2	2.16	0.96
6:B:22:TRP:HE1	19:B:1770:CLA:HBB1	0.80	0.96
6:B:530:THR:HG21	19:B:1755:CLA:HAC1	1.42	0.96
13:I:26:LEU:HA	13:I:29:GLU:O	1.64	0.96
19:1:1187:CLA:HMA2	19:1:1187:CLA:HBA1	1.46	0.96
19:A:1797:CLA:C12	19:A:1797:CLA:H72	1.94	0.96
6:B:122:GLN:O	6:B:126:THR:OG1	1.83	0.96
17:N:72:LYS:HB3	17:N:73:ASP:HA	0.97	0.96
5:A:40:PHE:HE1	5:A:53:TRP:CD1	1.83	0.96
25:B:1784:SF4:S2	25:B:1784:SF4:S3	2.63	0.96
11:G:44:PHE:N	11:G:45:GLU:CB	2.29	0.96
17:N:61:LEU:CD1	17:N:62:SER:C	2.34	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
5:A:361:ASN:HD21	19:A:1761:CLA:CED	1.76	0.96
17:N:79:SER:HA	17:N:80:ASN:C	1.84	0.96
19:1:1187:CLA:CBC	19:1:1187:CLA:CMC	2.30	0.96
5:A:368:LEU:HD21	19:A:1774:CLA:H93	1.44	0.96
5:A:451:ILE:CD1	19:A:1788:CLA:HED3	1.95	0.96
5:A:545:HIS:HB3	19:A:1792:CLA:HBB1	1.46	0.96
19:B:1735:CLA:H191	10:F:104:TYR:HB3	1.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1780:BCR:H19C	19:B:1786:CLA:H112	1.44	0.96
6:B:732:LYS:CG	6:B:734:GLY:CA	2.43	0.96
11:G:28:ARG:HG2	11:G:29:GLU:N	1.80	0.96
17:N:67:LEU:N	17:N:67:LEU:HD12	1.79	0.96
2:2:120:ASN:HB3	14:J:5:LYS:HD2	1.45	0.96
12:H:44:ALA:HB2	16:L:145:PHE:CD1	1.99	0.96
1:1:37:GLU:HA	1:1:40:LYS:HB2	1.45	0.96
19:A:1783:CLA:C20	22:A:1808:BCR:C17	2.35	0.96
5:A:79:PHE:HE2	5:A:185:HIS:CD2	1.81	0.96
6:B:87:ILE:CA	6:B:115:ASN:HA	1.94	0.96
10:F:24:LYS:CE	10:F:24:LYS:N	2.27	0.96
3:3:84:ILE:H	19:A:1798:CLA:C3	1.78	0.96
7:C:62:PHE:HE2	9:E:42:GLU:OE1	1.49	0.96
20:A:7016:LMU:C2	20:A:7016:LMU:H61	1.92	0.96
12:H:20:GLN:CB	12:H:22:ASP:CB	2.34	0.96
5:A:714:LEU:HD13	22:B:1779:BCR:C39	1.96	0.96
17:N:57:LYS:N	17:N:60:PHE:O	1.88	0.96
3:3:83:LEU:CA	19:A:1798:CLA:H43	1.96	0.96
5:A:368:LEU:CD2	19:A:1774:CLA:H92	1.93	0.96
19:B:1768:CLA:C16	22:B:1779:BCR:C31	2.41	0.96
2:2:127:ASN:ND2	14:J:2:ARG:NH1	2.14	0.96
11:G:94:ASP:N	11:G:95:PRO:CD	2.29	0.96
19:4:1209:CLA:HBC3	19:4:1209:CLA:HHD	1.46	0.96
5:A:331:LEU:HD21	5:A:343:HIS:C	1.85	0.95
19:A:1816:CLA:HBC3	19:A:1816:CLA:CHD	1.92	0.95
20:A:7027:LMU:O2'	20:A:7027:LMU:H12	1.64	0.95
6:B:421:HIS:NE2	19:B:1761:CLA:ND	2.13	0.95
17:N:62:SER:HB3	17:N:66:ASP:CA	1.96	0.95
5:A:335:LYS:HG2	5:A:336:GLY:N	1.82	0.95
9:E:68:ARG:HH21	9:E:69:PHE:HA	1.30	0.95
19:A:1764:CLA:CHC	19:A:1765:CLA:HMD2	1.96	0.95
19:A:1797:CLA:CMA	19:A:1797:CLA:H12	1.94	0.95
5:A:328:LYS:HE3	5:A:332:GLU:HG3	0.98	0.95
5:A:382:TYR:OH	19:A:1784:CLA:H42	1.64	0.95
5:A:547:PHE:O	5:A:551:VAL:HG13	1.64	0.95
6:B:608:GLN:CA	6:B:608:GLN:HE21	1.80	0.95
17:N:56:LYS:O	17:N:60:PHE:HD1	1.49	0.95
19:1:1200:CLA:HBC2	19:1:1200:CLA:CMC	1.91	0.95
5:A:246:HIS:O	5:A:248:PHE:N	1.99	0.95
7:C:63:LEU:HG	7:C:64:SER:N	1.78	0.95
19:2:1220:CLA:C6	3:3:140:LYS:CE	2.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1783:CLA:H43	19:A:1783:CLA:HBA1	1.48	0.95
5:A:394:SER:HB2	19:A:1783:CLA:HMA1	1.44	0.95
5:A:328:LYS:HE2	5:A:332:GLU:CG	1.94	0.95
5:A:87:SER:HB2	5:A:178:MET:O	1.65	0.95
19:B:1743:CLA:H151	19:B:1758:CLA:HMD2	1.47	0.95
9:E:52:VAL:O	9:E:53:VAL:HG22	1.64	0.95
19:F:1157:CLA:OBD	19:F:1157:CLA:HED2	1.66	0.95
5:A:472:ARG:NH1	16:L:74:LEU:HG	1.81	0.95
20:A:7009:LMU:C3'	20:A:7009:LMU:H5B	1.96	0.95
19:B:1786:CLA:HBB2	19:B:1787:CLA:C1B	1.97	0.95
11:G:13:GLY:HA2	11:G:16:LEU:HG	1.47	0.95
1:1:89:VAL:HB	1:1:90:PRO:HD3	1.46	0.95
19:A:1781:CLA:HED3	19:A:1782:CLA:HMD1	1.45	0.95
5:A:23:ASP:CG	5:A:24:ARG:CD	2.35	0.95
5:A:51:THR:HG21	19:A:1795:CLA:HBB2	1.11	0.95
5:A:545:HIS:CG	19:A:1792:CLA:CBB	2.49	0.95
7:C:52:LYS:HG3	7:C:52:LYS:O	1.66	0.95
6:B:167:TRP:HB2	11:G:41:MET:HE2	1.47	0.95
16:L:161:LEU:CD1	16:L:161:LEU:C	2.30	0.95
3:3:110:SER:C	3:3:111:TYR:CD2	2.40	0.95
5:A:442:ILE:HG23	19:A:1786:CLA:HMC3	1.47	0.95
5:A:21:LEU:N	5:A:22:VAL:CB	2.30	0.95
5:A:599:PHE:CE2	5:A:731:ARG:HB3	2.02	0.95
6:B:648:TRP:CZ3	22:B:1780:BCR:H392	2.01	0.95
7:C:1:MET:HG2	7:C:4:SER:CB	1.96	0.95
7:C:1:MET:HB3	7:C:4:SER:HG	1.29	0.95
11:G:46:ALA:H	11:G:48:ASP:HB3	1.16	0.95
11:G:60:SER:HA	11:G:63:PRO:HD2	1.49	0.95
3:3:87:GLU:CB	22:3:1220:BCR:H382	1.95	0.95
19:A:1759:CLA:C4	19:A:1796:CLA:H61	1.96	0.95
19:1:1198:CLA:C4	19:1:1198:CLA:H71	1.93	0.95
19:J:1043:CLA:O1A	19:J:1043:CLA:H143	1.67	0.95
20:A:7032:LMU:C3	20:A:7032:LMU:H2B	1.96	0.95
9:E:56:ASP:HB2	9:E:64:PRO:HB3	1.46	0.95
5:A:23:ASP:OD1	5:A:33:GLN:OE1	1.83	0.95
19:B:1771:CLA:HMC1	19:B:1771:CLA:HBC2	1.47	0.95
5:A:567:ARG:HH11	8:D:35:GLY:HA2	1.31	0.95
18:R:40:UNK:N	18:R:41:UNK:CB	2.30	0.95
10:F:23:LYS:CB	10:F:24:LYS:NZ	2.30	0.95
4:4:95:PHE:CZ	19:4:1208:CLA:C3C	2.50	0.95
20:A:7042:LMU:H32	20:A:7042:LMU:H6D	0.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:34:UNK:N	18:R:36:UNK:CB	2.30	0.94
19:4:1198:CLA:C15	19:4:1198:CLA:H203	1.95	0.94
20:A:7026:LMU:O4'	21:B:8062:SUC:C3'	1.98	0.94
20:R:1056:LMU:O6'	20:R:1056:LMU:H1'	1.65	0.94
1:1:161:PHE:H	19:1:1189:CLA:CBB	1.79	0.94
4:4:52:MET:HG3	4:4:160:MET:HG3	1.47	0.94
5:A:21:LEU:N	5:A:22:VAL:CG2	2.30	0.94
11:G:47:GLY:N	11:G:48:ASP:CB	2.30	0.94
19:2:1220:CLA:H42	3:3:140:LYS:CG	1.92	0.94
17:N:54:LYS:CG	17:N:57:LYS:NZ	2.30	0.94
19:A:1781:CLA:CHC	22:A:1806:BCR:H373	1.97	0.94
19:B:1755:CLA:CBB	19:B:1769:CLA:HMB3	1.96	0.94
6:B:266:GLN:O	6:B:267:SER:HB3	1.66	0.94
7:C:73:THR:OG1	7:C:76:SER:HB3	1.67	0.94
22:I:1032:BCR:C3	19:I:1033:CLA:HAC1	1.98	0.94
5:A:340:GLY:O	5:A:343:HIS:HB2	1.68	0.94
6:B:422:LEU:HD13	6:B:535:VAL:HG11	1.46	0.94
10:F:100:VAL:HA	10:F:103:SER:OG	1.66	0.94
17:N:52:LEU:N	17:N:52:LEU:CD2	2.30	0.94
17:N:61:LEU:CD1	17:N:62:SER:N	2.29	0.94
5:A:22:VAL:CG1	5:A:23:ASP:N	2.30	0.94
13:I:12:VAL:O	13:I:17:PRO:HD3	1.65	0.94
3:3:74:ALA:CA	19:3:1215:CLA:C2D	2.45	0.94
5:A:114:THR:HG22	5:A:115:HIS:ND1	1.82	0.94
5:A:246:HIS:HE1	19:A:1798:CLA:HMA3	1.31	0.94
13:I:11:LEU:HD12	22:I:1032:BCR:H10C	0.97	0.94
19:2:1212:CLA:HMC1	19:2:1212:CLA:HBC3	1.49	0.94
17:N:54:LYS:CB	17:N:57:LYS:NZ	2.30	0.94
17:N:67:LEU:C	17:N:68:GLU:CG	2.33	0.94
5:A:316:MET:CG	5:A:317:TYR:HD1	1.70	0.94
19:4:1201:CLA:HBA1	19:4:1201:CLA:HMA2	0.95	0.94
11:G:46:ALA:CA	11:G:48:ASP:CG	2.36	0.94
19:2:1220:CLA:H93	3:3:137:SER:HB2	1.45	0.94
17:N:66:ASP:O	17:N:67:LEU:HG	1.68	0.94
21:B:8062:SUC:O2	21:B:8062:SUC:H5	1.66	0.94
16:L:82:ALA:HB2	16:L:86:LEU:HD13	0.98	0.94
12:H:72:ALA:HA	21:H:1080:SUC:C6'	1.96	0.94
5:A:23:ASP:HB2	5:A:24:ARG:CD	1.93	0.94
19:B:1751:CLA:CHD	19:B:1751:CLA:HBC2	1.96	0.94
19:B:1755:CLA:CHD	19:B:1755:CLA:HBC2	1.96	0.94
8:D:39:LYS:HD2	8:D:42:VAL:CG1	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:81:ALA:HB2	19:A:1760:CLA:HMA2	1.50	0.94
5:A:381:PRO:HB2	19:A:1774:CLA:HAA2	1.48	0.94
19:B:1747:CLA:H52	19:B:1756:CLA:HMB1	1.47	0.94
11:G:46:ALA:N	11:G:48:ASP:CB	2.30	0.94
19:A:1816:CLA:HAA1	19:A:1816:CLA:O2D	1.66	0.94
20:A:7023:LMU:C9	20:A:7023:LMU:C2	2.30	0.94
20:A:7021:LMU:H41	20:A:7021:LMU:O6'	1.67	0.94
21:B:8059:SUC:O6	21:B:8059:SUC:H1	1.68	0.94
6:B:493:TRP:CH2	19:B:1765:CLA:HMA2	2.02	0.94
17:N:62:SER:CB	17:N:66:ASP:HB3	1.96	0.94
17:N:72:LYS:NZ	17:N:74:LYS:HG2	1.82	0.94
19:3:1219:CLA:CBC	19:3:1219:CLA:HMC1	1.96	0.94
19:A:1764:CLA:H142	22:A:1808:BCR:C14	1.98	0.94
22:I:1032:BCR:C32	22:I:1032:BCR:C4	2.39	0.94
3:3:64:TYR:HB3	19:3:1218:CLA:H41	1.49	0.94
17:N:51:ASP:O	17:N:52:LEU:HD22	1.67	0.94
19:J:1044:CLA:H72	19:J:1044:CLA:H41	0.95	0.94
5:A:328:LYS:HG2	5:A:332:GLU:CB	1.98	0.93
5:A:331:LEU:CD1	5:A:346:LEU:HB3	1.96	0.93
6:B:127:ILE:HD13	6:B:198:ALA:HB2	1.51	0.93
6:B:50:HIS:HD2	19:B:1737:CLA:HAA2	1.31	0.93
19:B:1755:CLA:HED1	19:B:1756:CLA:CMD	1.97	0.93
7:C:1:MET:H1	7:C:4:SER:N	1.66	0.93
17:N:63:ASP:H	17:N:64:ASP:HB3	1.32	0.93
19:J:1044:CLA:OBD	19:J:1044:CLA:HED3	1.66	0.93
17:N:72:LYS:CB	17:N:73:ASP:CA	2.31	0.93
6:B:390:GLY:O	22:B:1777:BCR:HC42	1.69	0.93
6:B:715:VAL:HG23	6:B:719:PHE:CD2	2.03	0.93
6:B:732:LYS:HG2	6:B:734:GLY:H	1.23	0.93
19:A:1816:CLA:HHD	19:A:1816:CLA:HBC2	1.47	0.93
17:N:61:LEU:CD1	17:N:63:ASP:N	2.30	0.93
19:K:1085:CLA:NA	19:K:1142:CLA:CMD	2.30	0.93
5:A:162:LEU:O	5:A:165:TYR:HB3	1.66	0.93
19:B:1743:CLA:H42	22:B:1775:BCR:H10C	1.50	0.93
22:B:1779:BCR:C8	22:B:1779:BCR:C32	2.29	0.93
17:N:47:THR:HG21	17:N:54:LYS:HZ3	0.88	0.93
2:2:99:LEU:CD2	19:2:1222:CLA:HMC3	1.99	0.93
22:A:1804:BCR:C23	22:A:1804:BCR:H402	1.96	0.93
6:B:517:PHE:O	6:B:517:PHE:HD2	1.36	0.93
20:2:7006:LMU:O2'	20:2:7006:LMU:H22	1.69	0.93
19:A:1776:CLA:C9	22:A:1805:BCR:C37	2.12	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1813:CLA:HMD3	6:B:578:LEU:CD2	1.99	0.93
5:A:358:LEU:HD11	5:A:413:HIS:CG	2.03	0.93
7:C:5:VAL:C	7:C:65:VAL:HG22	1.88	0.93
17:N:72:LYS:CB	17:N:74:LYS:N	2.31	0.93
20:A:7032:LMU:O1'	20:A:7032:LMU:H1B	1.68	0.93
19:4:4014:CLA:CBC	19:4:4014:CLA:HMC1	1.98	0.93
19:3:3011:CLA:H122	19:3:3011:CLA:H172	1.51	0.93
19:A:1783:CLA:C7	22:A:1807:BCR:C37	2.47	0.93
5:A:23:ASP:CB	5:A:24:ARG:NE	2.30	0.93
20:A:7041:LMU:O2'	20:A:7041:LMU:H5'	1.66	0.93
11:G:68:ILE:O	11:G:72:LEU:HB3	1.68	0.93
6:B:124:TRP:NE1	6:B:129:LEU:HD22	1.84	0.93
6:B:556:SER:C	6:B:558:PRO:HD2	1.88	0.93
15:K:69:ILE:CG2	15:K:70:MET:N	2.29	0.93
4:4:160:MET:HE3	19:4:1201:CLA:HBB2	1.51	0.93
22:A:1805:BCR:C38	22:A:1805:BCR:H23C	1.99	0.93
22:B:1778:BCR:H371	10:F:93:ILE:HG21	1.51	0.93
20:A:7016:LMU:H51	20:A:7016:LMU:O6'	1.67	0.93
1:1:160:GLY:HA3	19:1:1189:CLA:HBB2	1.48	0.93
5:A:81:ALA:HB1	19:A:1760:CLA:CMA	1.91	0.93
19:A:1770:CLA:HHC	22:A:1803:BCR:C17	1.98	0.93
22:A:1803:BCR:C23	22:A:1803:BCR:H402	1.94	0.93
5:A:239:PRO:HA	5:A:242:ILE:HD11	1.49	0.93
5:A:73:GLU:O	5:A:76:ARG:N	2.02	0.93
11:G:45:GLU:HG2	11:G:49:THR:CG2	1.87	0.93
20:A:7033:LMU:C5B	20:A:7033:LMU:H3'	1.99	0.93
5:A:103:PHE:HE1	19:A:1763:CLA:O1D	1.51	0.92
5:A:462:ILE:HD11	19:B:1786:CLA:H51	1.47	0.92
2:2:90:ASP:HB3	2:2:94:LEU:HB2	1.49	0.92
19:A:1781:CLA:O1A	19:A:1781:CLA:H2	1.67	0.92
19:A:1781:CLA:H2	19:A:1782:CLA:HED3	1.52	0.92
22:A:1808:BCR:C23	22:A:1808:BCR:H393	1.94	0.92
5:A:626:GLY:HA3	5:A:636:HIS:HA	1.51	0.92
19:3:3008:CLA:HBA2	19:3:3008:CLA:HBD	0.93	0.92
11:G:93:TYR:CA	11:G:94:ASP:CB	2.30	0.92
7:C:79:LEU:HD22	7:C:81:TYR:O	1.70	0.92
9:E:61:THR:HG22	9:E:62:ARG:H	1.34	0.92
16:L:118:LEU:HD12	16:L:119:THR:H	1.31	0.92
5:A:331:LEU:HD11	5:A:346:LEU:HB2	1.50	0.92
22:B:1779:BCR:C40	22:B:1779:BCR:H271	1.95	0.92
11:G:7:VAL:CG2	11:G:8:ILE:H	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:67:GLY:O	15:K:70:MET:HB2	1.69	0.92
21:B:8059:SUC:C6'	21:B:8059:SUC:H1'1	2.00	0.92
5:A:100:GLY:HA3	5:A:153:TRP:CH2	2.05	0.92
5:A:715:LYS:HD2	10:F:153:ASN:OD1	1.70	0.92
4:4:107:GLN:CA	19:4:1196:CLA:HMA2	1.99	0.92
4:4:124:TYR:HB2	4:4:143:PHE:CD1	2.05	0.92
21:3:1221:SUC:C6'	21:3:1221:SUC:C1'	2.39	0.92
1:1:25:ASP:H	6:B:314:ARG:HH22	1.17	0.92
8:D:111:TYR:HD2	8:D:114:PRO:HB3	1.33	0.92
3:3:64:TYR:CB	19:3:1218:CLA:H42	1.91	0.92
10:F:40:LEU:HA	10:F:42:ILE:HG12	1.50	0.92
19:A:1788:CLA:C16	22:L:1169:BCR:C36	2.47	0.92
19:A:1788:CLA:H52	22:B:1780:BCR:C34	1.99	0.92
22:B:1780:BCR:C38	22:B:1780:BCR:H23C	1.99	0.92
19:2:1220:CLA:CBA	19:2:1220:CLA:CHA	2.44	0.92
4:4:122:LYS:HG2	4:4:150:LYS:HD2	1.48	0.92
20:A:7009:LMU:C5B	20:A:7009:LMU:C3'	2.47	0.92
5:A:259:TYR:HB3	5:A:260:PRO:HD2	1.51	0.92
22:A:1807:BCR:H313	19:A:1813:CLA:H143	1.48	0.92
5:A:195:TRP:CZ2	19:A:1766:CLA:HMA1	2.05	0.92
6:B:612:SER:HA	6:B:615:TYR:HE1	1.32	0.92
7:C:1:MET:CG	7:C:4:SER:OG	2.17	0.92
6:B:697:PRO:O	7:C:79:LEU:CD1	2.17	0.92
11:G:47:GLY:H	11:G:48:ASP:CA	1.82	0.92
11:G:46:ALA:N	11:G:49:THR:CG2	2.31	0.92
17:N:47:THR:CG2	17:N:54:LYS:HZ3	1.81	0.92
17:N:72:LYS:NZ	17:N:74:LYS:CG	2.32	0.92
20:A:7016:LMU:H21	20:A:7016:LMU:H81	0.94	0.92
19:K:1085:CLA:CGA	19:K:1085:CLA:H3A	2.00	0.92
4:4:169:GLN:CG	19:4:1199:CLA:HAC2	1.99	0.91
5:A:103:PHE:CE1	19:A:1763:CLA:O1D	2.23	0.91
5:A:648:THR:HG23	5:A:651:GLY:H	1.33	0.91
17:N:72:LYS:CG	17:N:74:LYS:HB2	1.99	0.91
5:A:478:SER:HB3	5:A:644:GLN:OE1	1.70	0.91
19:A:1779:CLA:C1D	22:A:1805:BCR:H19C	2.00	0.91
19:A:1763:CLA:C3B	22:A:1808:BCR:H333	1.99	0.91
7:C:5:VAL:HB	7:C:65:VAL:HA	1.52	0.91
16:L:30:SER:OG	16:L:32:LEU:HB2	1.67	0.91
19:A:1816:CLA:HAA1	19:A:1816:CLA:O1D	1.71	0.91
12:H:25:GLY:HA2	12:H:27:ASP:OD2	1.68	0.91
5:A:304:LEU:CD2	19:A:1772:CLA:HBB2	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1779:CLA:NC	22:A:1805:BCR:H19C	1.84	0.91
19:A:1783:CLA:H203	22:A:1808:BCR:H17C	0.92	0.91
23:B:1773:PQN:H191	22:B:1780:BCR:H10C	0.92	0.91
6:B:492:ILE:H	6:B:492:ILE:HD13	1.36	0.91
3:3:93:PHE:H	3:3:95:THR:H	1.10	0.91
4:4:154:ILE:HG13	4:4:155:ALA:H	1.36	0.91
5:A:25:ASP:CG	5:A:26:PRO:HG3	1.89	0.91
6:B:596:TRP:HH2	6:B:612:SER:O	1.48	0.91
6:B:602:TRP:O	6:B:604:GLY:N	2.02	0.91
11:G:46:ALA:C	11:G:48:ASP:CG	2.29	0.91
17:N:61:LEU:HD11	17:N:63:ASP:CB	1.98	0.91
11:G:93:TYR:HA	11:G:94:ASP:CG	1.90	0.91
20:A:7022:LMU:C2'	20:A:7022:LMU:C2	2.32	0.91
6:B:189:ALA:HB2	19:B:1758:CLA:H203	1.49	0.91
20:A:7036:LMU:H71	20:A:7036:LMU:H31	0.93	0.91
19:B:1786:CLA:C9	19:B:1787:CLA:C9	2.48	0.91
20:A:7020:LMU:H6E	20:A:7020:LMU:H5B	1.29	0.91
2:2:120:ASN:ND2	14:J:5:LYS:CE	2.33	0.91
20:A:7009:LMU:H3'	20:A:7009:LMU:C5B	2.00	0.91
10:F:42:ILE:HG13	10:F:43:LYS:N	1.82	0.91
6:B:525:LEU:HD22	6:B:525:LEU:O	1.70	0.91
11:G:45:GLU:CB	11:G:49:THR:HG21	1.99	0.91
11:G:48:ASP:HB2	11:G:49:THR:HG22	0.94	0.91
5:A:453:LEU:HB3	5:A:547:PHE:HB2	1.52	0.91
6:B:661:PHE:HB2	19:B:1787:CLA:CMC	2.00	0.91
19:4:1196:CLA:CBC	19:4:1196:CLA:CHD	2.44	0.91
8:D:124:ASN:HB3	8:D:125:PRO:HD3	1.52	0.91
19:A:1811:CLA:HAA1	19:B:1785:CLA:HBB2	1.51	0.91
5:A:217:SER:HA	22:A:1803:BCR:H351	1.51	0.91
6:B:353:TYR:CG	6:B:594:TRP:HZ3	1.88	0.91
11:G:40:GLY:O	11:G:41:MET:SD	2.29	0.91
19:2:1220:CLA:H71	3:3:140:LYS:HZ2	1.33	0.91
21:B:8054:SUC:H1'1	21:B:8054:SUC:O2	1.71	0.91
6:B:5:ILE:HB	6:B:6:PRO:HD2	1.51	0.91
4:4:169:GLN:CD	19:4:1199:CLA:HHD	1.91	0.91
11:G:42:SER:HB2	11:G:45:GLU:OE2	1.70	0.91
20:A:7042:LMU:H22	20:A:7042:LMU:H71	0.92	0.91
8:D:102:ARG:NH1	8:D:104:PHE:CE1	2.39	0.90
13:I:11:LEU:HG	22:I:1032:BCR:C7	2.00	0.90
16:L:123:ARG:HA	16:L:123:ARG:CZ	2.00	0.90
22:3:1220:BCR:H311	22:3:1220:BCR:C8	1.99	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:248:PHE:H	5:A:248:PHE:HD2	1.11	0.90
5:A:328:LYS:HG3	5:A:332:GLU:HB2	1.50	0.90
19:B:1740:CLA:HBB2	19:B:1786:CLA:H13	1.53	0.90
19:A:1813:CLA:CMD	6:B:578:LEU:HD23	2.00	0.90
19:H:1079:CLA:O2A	19:H:1079:CLA:HMA2	1.71	0.90
19:L:1168:CLA:HAA1	19:L:1168:CLA:CGD	1.99	0.90
16:L:95:LEU:HD13	22:L:1169:BCR:C31	2.01	0.90
18:R:33:UNK:C	18:R:36:UNK:CB	2.50	0.90
17:N:47:THR:CG2	17:N:54:LYS:NZ	2.32	0.90
19:3:1219:CLA:O1A	19:3:1219:CLA:HMA2	1.71	0.90
20:A:7021:LMU:C2	20:A:7021:LMU:H62	1.98	0.90
6:B:369:ALA:O	6:B:725:LEU:HD11	1.71	0.90
7:C:78:GLY:O	7:C:81:TYR:HE1	1.54	0.90
2:2:120:ASN:HD22	14:J:5:LYS:HE3	1.35	0.90
6:B:120:VAL:HA	6:B:123:TRP:NE1	1.85	0.90
10:F:23:LYS:C	10:F:24:LYS:HZ3	1.74	0.90
7:C:44:ARG:NH2	8:D:127:ARG:HB3	1.85	0.90
1:1:160:GLY:CA	19:1:1189:CLA:HBB2	2.01	0.90
19:A:1791:CLA:O1A	19:A:1797:CLA:HBB1	1.72	0.90
6:B:382:ILE:CG2	6:B:383:MET:H	1.85	0.90
16:L:161:LEU:CD1	16:L:162:ASP:O	2.19	0.90
19:R:1054:CLA:CHA	19:R:1054:CLA:CED	2.49	0.90
11:G:46:ALA:H	11:G:49:THR:HG21	1.33	0.90
17:N:54:LYS:CB	17:N:57:LYS:HZ1	1.84	0.90
17:N:63:ASP:HA	17:N:64:ASP:C	1.91	0.90
6:B:504:ASN:HD22	6:B:504:ASN:H	1.14	0.90
19:1:1192:CLA:HHD	19:1:1192:CLA:CBC	2.01	0.90
19:A:1780:CLA:HMD2	19:A:1780:CLA:H142	1.51	0.90
19:B:1786:CLA:HBB2	19:B:1787:CLA:CHB	2.00	0.90
6:B:382:ILE:O	6:B:384:THR:N	2.05	0.90
6:B:732:LYS:CB	6:B:733:PHE:C	2.39	0.90
8:D:48:ILE:HB	8:D:100:PHE:HB3	1.52	0.90
19:2:1220:CLA:H91	3:3:137:SER:HB2	1.52	0.90
19:A:1781:CLA:C6	19:A:1782:CLA:CED	2.50	0.90
19:A:1781:CLA:C6	19:A:1782:CLA:HED1	2.02	0.90
5:A:361:ASN:HD21	19:A:1761:CLA:HED3	1.37	0.90
5:A:472:ARG:HE	5:A:474:GLN:HG3	1.33	0.90
6:B:65:LEU:HD22	6:B:124:TRP:CE3	2.06	0.90
19:3:1218:CLA:H2A	19:3:1218:CLA:O1D	1.70	0.90
6:B:5:ILE:HB	6:B:6:PRO:CD	2.01	0.90
6:B:666:SER:HB3	6:B:671:TRP:HE1	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:672:GLN:HE21	6:B:672:GLN:CA	1.85	0.90
19:4:1196:CLA:HBC2	19:4:1196:CLA:CHD	2.01	0.90
6:B:370:ALA:O	19:B:1757:CLA:HMA1	1.71	0.90
17:N:45:ASN:HB2	17:N:57:LYS:HZ2	1.35	0.90
21:3:1221:SUC:H5	21:3:1221:SUC:O2'	1.72	0.90
5:A:452:PHE:HE1	19:A:1793:CLA:HBB1	1.07	0.89
6:B:172:GLU:O	6:B:176:ASN:HB2	1.72	0.89
17:N:40:CYS:SG	17:N:40:CYS:O	2.30	0.89
2:2:76:THR:HG23	17:N:7:LEU:HB2	1.54	0.89
5:A:210:LEU:HD13	19:A:1769:CLA:HMB2	1.53	0.89
5:A:368:LEU:HD11	19:A:1782:CLA:H61	1.52	0.89
5:A:452:PHE:HE1	19:A:1793:CLA:CBB	1.84	0.89
5:A:659:ALA:O	5:A:662:SER:OG	1.88	0.89
19:B:1752:CLA:HBC2	19:B:1753:CLA:HBA1	1.54	0.89
19:1:1188:CLA:HMC1	19:1:1188:CLA:HBC3	1.54	0.89
19:A:1772:CLA:HMC1	19:A:1772:CLA:HBC3	0.91	0.89
22:A:1807:BCR:H23C	22:A:1807:BCR:H393	1.52	0.89
6:B:11:GLY:HA3	7:C:71:HIS:CD2	2.07	0.89
20:A:7038:LMU:H101	20:A:7038:LMU:C6	2.00	0.89
5:A:131:ILE:O	5:A:671:SER:HA	1.72	0.89
6:B:351:HIS:HB3	19:B:1747:CLA:HED1	1.52	0.89
19:2:1212:CLA:C4	19:2:1212:CLA:CGA	2.50	0.89
20:A:7026:LMU:H4O1	21:B:8062:SUC:H3'	1.32	0.89
19:A:1781:CLA:C7	19:A:1782:CLA:HED1	2.02	0.89
19:B:1755:CLA:HBB1	19:B:1769:CLA:HMB2	1.54	0.89
4:4:158:ARG:HB2	19:4:1202:CLA:C3A	2.02	0.89
12:H:44:ALA:CB	16:L:145:PHE:CD1	2.56	0.89
19:B:1755:CLA:CBC	19:B:1755:CLA:CHD	2.46	0.89
19:B:1768:CLA:H161	22:B:1779:BCR:C31	2.03	0.89
20:A:7040:LMU:O3'	20:A:7040:LMU:H1B	1.65	0.89
3:3:84:ILE:N	19:A:1798:CLA:C4	2.34	0.89
19:A:1779:CLA:C1D	22:A:1805:BCR:C19	2.49	0.89
19:A:1779:CLA:CBB	22:A:1805:BCR:H353	2.02	0.89
5:A:402:ILE:CD1	19:A:1784:CLA:HBB2	2.02	0.89
19:B:1753:CLA:C2	19:B:1753:CLA:H71	2.00	0.89
6:B:292:ARG:O	6:B:293:THR:OG1	1.91	0.89
6:B:362:ALA:HB2	6:B:368:GLN:HG2	1.55	0.89
6:B:635:ILE:O	6:B:636:THR:O	1.91	0.89
7:C:62:PHE:CZ	9:E:42:GLU:OE1	2.26	0.89
19:2:1220:CLA:H41	3:3:140:LYS:CE	2.02	0.89
19:4:1204:CLA:H41	19:4:1204:CLA:C10	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1781:CLA:C7	19:A:1782:CLA:HED2	2.01	0.89
6:B:174:ARG:HB2	19:B:1743:CLA:CBC	2.02	0.89
8:D:102:ARG:HE	8:D:110:GLN:HB2	1.38	0.89
16:L:64:LEU:HB3	16:L:68:PHE:CE1	2.08	0.89
20:A:7039:LMU:O6B	20:A:7039:LMU:H4'	1.73	0.89
21:B:8059:SUC:H3	21:B:8059:SUC:O2'	1.72	0.89
6:B:393:PHE:HD2	6:B:397:ASP:OD1	1.55	0.89
6:B:442:VAL:HG21	19:B:1763:CLA:HAC2	1.55	0.89
19:1:1198:CLA:HBC3	19:1:1198:CLA:HHD	0.91	0.89
17:N:72:LYS:CG	17:N:74:LYS:N	2.35	0.89
5:A:269:PHE:HE1	15:K:14:THR:HG21	1.06	0.89
19:3:1219:CLA:H142	19:3:1219:CLA:H102	1.50	0.89
5:A:24:ARG:N	5:A:24:ARG:CD	2.34	0.89
6:B:282:PHE:CZ	19:B:1746:CLA:C1	2.55	0.89
6:B:574:ASP:HA	6:B:577:TYR:HB3	1.52	0.89
10:F:93:ILE:O	10:F:96:TRP:HD1	1.56	0.89
19:4:1198:CLA:C2A	19:4:1198:CLA:CGD	2.50	0.89
4:4:147:LEU:HD22	4:4:148:GLU:H	1.38	0.89
4:4:154:ILE:HG13	4:4:155:ALA:N	1.88	0.89
19:A:1779:CLA:CAB	22:A:1805:BCR:C35	2.48	0.88
19:A:1796:CLA:C14	22:A:1807:BCR:HC21	2.00	0.88
22:B:1777:BCR:H321	22:B:1777:BCR:HC8	1.55	0.88
19:3:1218:CLA:HBC2	19:3:1218:CLA:HHD	1.54	0.88
21:B:8059:SUC:O2	21:B:8059:SUC:H1'2	1.71	0.88
20:A:7030:LMU:C9	20:A:7030:LMU:H52	2.01	0.88
19:B:1738:CLA:H2A	19:B:1738:CLA:O1D	1.73	0.88
6:B:621:ARG:O	6:B:625:TRP:HB3	1.72	0.88
6:B:91:ILE:HD12	6:B:104:PHE:HE2	1.38	0.88
19:1:1198:CLA:H52	19:1:1198:CLA:H102	0.92	0.88
20:A:7032:LMU:C5B	20:A:7032:LMU:H3'	2.03	0.88
19:A:1795:CLA:C1C	19:B:1735:CLA:HBC2	2.03	0.88
6:B:87:ILE:HA	6:B:115:ASN:CA	2.04	0.88
19:B:1746:CLA:HHD	19:B:1746:CLA:CBC	2.02	0.88
25:B:1784:SF4:FE3	25:B:1784:SF4:S1	1.65	0.88
20:A:7036:LMU:H22	20:A:7036:LMU:H82	0.90	0.88
18:R:39:UNK:HA	18:R:42:UNK:CB	2.04	0.88
19:A:1765:CLA:CBB	19:B:1763:CLA:HMD2	2.03	0.88
5:A:470:LEU:CD1	6:B:95:HIS:HB3	2.03	0.88
5:A:578:ARG:CZ	5:A:578:ARG:HB2	2.02	0.88
6:B:137:THR:HA	6:B:140:ILE:HG13	1.54	0.88
6:B:167:TRP:HB2	11:G:41:MET:CE	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1784:SF4:FE1	25:B:1784:SF4:S2	1.64	0.88
19:J:1044:CLA:HED2	19:J:1045:CLA:HMA3	1.53	0.88
19:J:1044:CLA:HED2	19:J:1045:CLA:CMA	2.03	0.88
2:2:81:THR:HG23	2:2:82:ALA:H	1.36	0.88
19:A:1771:CLA:HMC1	19:A:1771:CLA:HBC3	1.55	0.88
5:A:355:HIS:ND1	5:A:416:ILE:CG2	2.36	0.88
24:B:1783:LMG:O3	7:C:70:TRP:CE2	2.24	0.88
19:2:1218:CLA:HMD2	19:2:1220:CLA:HMD3	1.55	0.88
19:K:1085:CLA:CMB	19:K:1142:CLA:HED1	1.96	0.88
19:B:1735:CLA:CBB	19:B:1735:CLA:H101	2.03	0.88
3:3:205:GLY:CA	5:A:252:ARG:HH22	1.85	0.88
4:4:193:ILE:HG21	14:J:42:PHE:CD1	2.07	0.88
5:A:309:LEU:HD21	19:A:1776:CLA:CMC	2.03	0.88
6:B:732:LYS:HG2	6:B:734:GLY:CA	2.04	0.88
5:A:267:THR:O	5:A:269:PHE:CD2	2.26	0.88
15:K:74:ILE:HG22	15:K:75:VAL:HG22	1.56	0.88
6:B:50:HIS:CD2	19:B:1737:CLA:HAA2	2.09	0.88
19:B:1739:CLA:H92	19:B:1739:CLA:HBB2	0.90	0.88
6:B:119:GLY:CA	19:B:1758:CLA:HED1	2.01	0.88
7:C:14:CYS:HA	7:C:17:CYS:HG	1.01	0.88
16:L:115:ALA:H	16:L:116:PRO:HD2	1.36	0.88
3:3:112:THR:OG1	3:3:113:LEU:N	2.04	0.87
19:A:1781:CLA:C5	19:A:1782:CLA:HED1	2.03	0.87
5:A:246:HIS:CE1	19:A:1798:CLA:HMA3	2.08	0.87
5:A:358:LEU:HD11	5:A:413:HIS:CB	2.03	0.87
5:A:356:ALA:HB2	5:A:417:PHE:HD2	1.39	0.87
5:A:581:CYS:CB	5:A:590:CYS:HA	2.04	0.87
6:B:275:HIS:O	6:B:279:ALA:N	2.05	0.87
6:B:531:THR:O	6:B:535:VAL:HG12	1.74	0.87
6:B:561:GLY:HA3	7:C:52:LYS:HG2	1.55	0.87
8:D:30:ALA:O	16:L:18:PRO:HB2	1.74	0.87
17:N:67:LEU:HB2	17:N:68:GLU:HG2	0.90	0.87
4:4:160:MET:HE1	19:4:1201:CLA:CBB	2.02	0.87
5:A:22:VAL:HG12	5:A:23:ASP:N	1.82	0.87
5:A:151:GLN:NE2	5:A:384:TYR:O	2.06	0.87
6:B:91:ILE:HG21	19:B:1740:CLA:HMD1	1.57	0.87
16:L:163:LEU:HD13	16:L:164:PRO:CA	2.04	0.87
19:2:1220:CLA:C6	3:3:140:LYS:HD3	2.03	0.87
5:A:249:ILE:CG1	5:A:250:LEU:H	1.83	0.87
17:N:48:GLY:HA2	17:N:49:CYS:HG	1.05	0.87
9:E:42:GLU:HG2	9:E:43:SER:N	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:56:VAL:HA	19:L:1167:CLA:HED2	1.55	0.87
20:A:7023:LMU:C9	20:A:7023:LMU:C3	2.50	0.87
10:F:23:LYS:HB2	10:F:24:LYS:NZ	1.88	0.87
5:A:425:THR:HG1	5:A:428:TYR:HE1	0.93	0.87
19:A:1760:CLA:HBB2	19:A:1762:CLA:C3D	2.04	0.87
6:B:310:PRO:CG	6:B:311:PRO:HD2	2.04	0.87
8:D:113:HIS:H	8:D:114:PRO:HD2	1.39	0.87
20:A:7032:LMU:H31	20:A:7032:LMU:O5B	1.73	0.87
5:A:349:ILE:HG23	5:A:352:THR:O	1.72	0.87
19:A:1761:CLA:H42	22:A:1804:BCR:H313	1.56	0.87
6:B:279:ALA:O	19:B:1746:CLA:HMB3	1.73	0.87
8:D:113:HIS:NE2	8:D:118:VAL:CG1	2.37	0.87
5:A:567:ARG:HH12	8:D:35:GLY:HA2	1.34	0.87
17:N:32:ALA:CB	17:N:35:VAL:HG22	2.05	0.87
19:A:1781:CLA:HMB3	22:A:1806:BCR:C18	2.04	0.87
6:B:427:LEU:HD23	6:B:431:PHE:CZ	2.09	0.87
9:E:68:ARG:NE	9:E:68:ARG:O	2.06	0.87
3:3:84:ILE:CA	19:A:1798:CLA:H51	2.04	0.87
19:B:1765:CLA:HMB1	22:B:1777:BCR:H292	1.56	0.87
6:B:230:TRP:HB3	19:B:1746:CLA:HED3	1.55	0.87
6:B:661:PHE:HB2	19:B:1787:CLA:HMC3	1.56	0.87
6:B:70:TRP:CD1	6:B:71:GLN:OE1	2.27	0.87
6:B:732:LYS:CG	6:B:733:PHE:CA	2.49	0.87
20:A:7043:LMU:H111	20:A:7043:LMU:H71	1.57	0.87
5:A:661:ALA:O	5:A:664:VAL:HG22	1.75	0.87
6:B:469:LYS:HG2	6:B:471:THR:OG1	1.75	0.87
19:2:1220:CLA:C4	3:3:140:LYS:CD	2.42	0.87
19:4:1198:CLA:C15	19:4:1198:CLA:H202	2.00	0.87
5:A:194:ALA:O	5:A:198:ASP:N	2.07	0.87
13:I:24:LEU:C	13:I:26:LEU:H	1.77	0.87
20:A:7041:LMU:O6'	20:A:7041:LMU:H1B	1.75	0.87
17:N:48:GLY:CA	17:N:49:CYS:CB	2.50	0.87
12:H:21:TRP:H	12:H:22:ASP:HA	1.38	0.87
11:G:68:ILE:O	11:G:72:LEU:CB	2.22	0.87
6:B:317:ARG:NH1	6:B:405:ASP:O	2.08	0.87
19:A:1792:CLA:HBA2	19:A:1792:CLA:O1D	1.74	0.86
6:B:203:ARG:HG2	6:B:204:GLY:N	1.88	0.86
6:B:732:LYS:HG2	6:B:733:PHE:CA	2.04	0.86
16:L:95:LEU:HD13	22:L:1169:BCR:H312	1.57	0.86
6:B:110:LEU:HD12	6:B:111:GLY:H	1.40	0.86
19:A:1795:CLA:CGA	19:A:1795:CLA:H42	2.03	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:393:LEU:HG	5:A:394:SER:H	1.40	0.86
19:B:1755:CLA:H52	19:B:1769:CLA:CAD	2.05	0.86
6:B:474:PHE:CE2	6:B:476:ILE:HG13	2.10	0.86
19:A:1790:CLA:OBD	19:A:1791:CLA:HAC1	1.75	0.86
5:A:370:ILE:HD11	19:A:1781:CLA:C3D	2.05	0.86
19:B:1753:CLA:C2	19:B:1753:CLA:C7	2.51	0.86
19:B:1755:CLA:CBB	19:B:1769:CLA:HHB	2.05	0.86
23:B:1773:PQN:H162	22:B:1780:BCR:H333	0.88	0.86
19:1:1198:CLA:CHD	19:1:1198:CLA:CBC	2.45	0.86
19:3:1218:CLA:H91	19:3:1218:CLA:H121	1.54	0.86
4:4:104:ARG:HH11	4:4:105:ARG:HB2	1.38	0.86
19:J:1043:CLA:H2	19:J:1043:CLA:C16	2.05	0.86
19:1:1193:CLA:HBC3	19:1:1193:CLA:HMC1	1.54	0.86
6:B:25:ILE:CG2	22:L:1169:BCR:H291	2.04	0.86
6:B:86:PRO:O	6:B:87:ILE:HG13	1.74	0.86
21:B:8052:SUC:C1	21:B:8052:SUC:C4'	2.52	0.86
15:K:69:ILE:HG22	15:K:70:MET:N	1.84	0.86
4:4:75:TRP:HA	19:4:1204:CLA:HMD3	1.58	0.86
5:A:411:ALA:HB2	22:A:1806:BCR:H392	1.57	0.86
5:A:356:ALA:HB2	5:A:417:PHE:CD2	2.09	0.86
19:A:1816:CLA:H2	19:A:1816:CLA:HED3	1.58	0.86
19:J:1044:CLA:C16	19:J:1044:CLA:H91	2.05	0.86
10:F:20:GLN:C	10:F:20:GLN:NE2	2.29	0.86
17:N:32:ALA:HB1	17:N:35:VAL:CG2	2.06	0.86
19:A:1783:CLA:H171	22:A:1808:BCR:H15C	1.55	0.86
22:A:1806:BCR:C33	22:A:1806:BCR:HC8	2.06	0.86
19:B:1735:CLA:C19	10:F:104:TYR:HB3	2.05	0.86
19:A:1788:CLA:C16	22:L:1169:BCR:H361	2.06	0.86
19:2:1220:CLA:H91	3:3:137:SER:CB	2.06	0.86
1:1:57:ILE:HG23	1:1:58:LEU:H	1.41	0.86
19:A:1790:CLA:CBC	19:A:1790:CLA:HMC1	2.06	0.86
19:A:1761:CLA:H151	22:A:1803:BCR:H393	1.57	0.86
5:A:281:LEU:HD12	19:A:1772:CLA:O2D	1.73	0.86
19:A:1788:CLA:C5	22:B:1780:BCR:H343	2.05	0.86
6:B:693:TRP:HD1	19:B:1770:CLA:C2D	1.89	0.86
10:F:153:ASN:HD22	10:F:153:ASN:C	1.78	0.86
16:L:161:LEU:HD12	16:L:162:ASP:CA	2.04	0.86
5:A:370:ILE:CG2	5:A:400:MET:HA	2.06	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	1.87	0.86
7:C:1:MET:CG	7:C:4:SER:CB	2.54	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
17:N:61:LEU:HD11	17:N:63:ASP:O	1.76	0.86
7:C:14:CYS:SG	7:C:18:VAL:O	2.32	0.86
19:A:1800:CLA:CMD	22:B:1780:BCR:HC31	2.05	0.86
5:A:606:TYR:O	5:A:610:SER:HB2	1.76	0.86
6:B:310:PRO:CG	19:B:1753:CLA:HMA1	2.02	0.86
6:B:142:LEU:CD2	22:B:1776:BCR:H333	2.06	0.86
6:B:527:LEU:HD12	19:B:1755:CLA:C1D	2.05	0.86
20:A:7042:LMU:C2	20:A:7042:LMU:H61	2.01	0.86
19:2:1212:CLA:HBC2	19:2:1212:CLA:HMC1	1.55	0.86
10:F:24:LYS:CA	10:F:26:GLN:H	1.89	0.86
3:3:63:ARG:HH22	3:3:189:LEU:HD23	1.40	0.86
6:B:216:LEU:HD21	6:B:221:GLY:HA2	1.57	0.86
19:A:1763:CLA:CBA	19:A:1765:CLA:H12	2.06	0.86
5:A:581:CYS:SG	25:B:1784:SF4:S2	2.73	0.86
7:C:1:MET:N	7:C:3:HIS:C	2.29	0.86
6:B:551:LYS:NZ	8:D:140:ASN:O	2.09	0.86
16:L:164:PRO:O	16:L:165:TYR:CD1	2.29	0.86
17:N:58:VAL:HG23	17:N:60:PHE:CE1	2.11	0.86
2:2:120:ASN:CG	14:J:5:LYS:HD2	1.95	0.86
5:A:21:LEU:HD12	5:A:21:LEU:O	1.75	0.85
5:A:331:LEU:HD23	5:A:331:LEU:C	1.95	0.85
19:B:1761:CLA:HMA2	19:B:1761:CLA:H12	1.56	0.85
6:B:432:HIS:HE1	19:B:1762:CLA:NB	1.74	0.85
7:C:74:THR:OG1	7:C:80:ALA:HB2	1.75	0.85
16:L:56:VAL:HA	19:L:1167:CLA:CED	2.04	0.85
17:N:63:ASP:H	17:N:64:ASP:CA	1.89	0.85
19:A:1815:CLA:HMA1	19:A:1815:CLA:H61	1.56	0.85
19:4:1201:CLA:CGD	19:4:1201:CLA:CAA	2.52	0.85
22:A:1807:BCR:C8	22:A:1807:BCR:C31	2.47	0.85
19:B:1743:CLA:H141	19:B:1748:CLA:H2	1.59	0.85
6:B:310:PRO:HG3	19:B:1753:CLA:CMA	2.03	0.85
6:B:374:HIS:HB2	19:B:1757:CLA:C1B	2.06	0.85
12:H:69:SER:CB	19:H:1079:CLA:H61	2.04	0.85
17:N:72:LYS:HG3	17:N:74:LYS:N	1.89	0.85
10:F:23:LYS:CB	10:F:24:LYS:HZ1	1.89	0.85
12:H:25:GLY:HA3	12:H:27:ASP:CA	2.04	0.85
2:2:70:LYS:HG3	2:2:73:ILE:HG13	1.56	0.85
12:H:45:ALA:O	12:H:48:THR:N	2.08	0.85
13:I:1:MET:O	13:I:2:ILE:HG22	1.75	0.85
19:A:1783:CLA:H72	22:A:1807:BCR:H371	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:66:GLY:HA3	19:L:1168:CLA:HHC	1.57	0.85
16:L:164:PRO:O	16:L:165:TYR:CG	2.30	0.85
17:N:70:GLU:HB3	17:N:72:LYS:N	1.89	0.85
12:H:21:TRP:H	12:H:22:ASP:CA	1.88	0.85
19:A:1776:CLA:H92	22:A:1805:BCR:H371	1.51	0.85
5:A:453:LEU:CD2	19:A:1793:CLA:CBB	2.50	0.85
6:B:142:LEU:HD22	22:B:1776:BCR:H333	1.58	0.85
6:B:594:TRP:O	6:B:595:HIS:CB	2.24	0.85
19:L:1168:CLA:HBC3	19:L:1168:CLA:CHD	2.04	0.85
3:3:132:TRP:CH2	3:3:155:GLU:HG3	2.08	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:H	1.78	0.85
17:N:5:GLU:OE1	17:N:6:TYR:CD2	2.30	0.85
17:N:5:GLU:OE1	17:N:6:TYR:CG	2.30	0.85
19:A:1767:CLA:HMC1	19:A:1767:CLA:HBC3	1.58	0.85
19:A:1796:CLA:NC	19:A:1796:CLA:C4	2.40	0.85
5:A:197:GLN:HE21	5:A:197:GLN:CA	1.84	0.85
6:B:388:ALA:C	6:B:391:PRO:HD2	1.95	0.85
6:B:571:SER:OG	6:B:574:ASP:OD1	1.95	0.85
9:E:39:LEU:N	9:E:40:ARG:NH1	2.24	0.85
17:N:63:ASP:N	17:N:64:ASP:CB	2.38	0.85
5:A:349:ILE:HG22	5:A:349:ILE:O	1.74	0.85
1:1:185:TRP:O	1:1:186:HIS:HB2	1.75	0.85
9:E:35:LYS:NZ	9:E:89:GLU:OE2	2.09	0.85
19:1:1191:CLA:HMC1	19:1:1194:CLA:CHD	2.03	0.85
17:N:61:LEU:HD21	17:N:63:ASP:O	1.74	0.85
12:H:25:GLY:HA3	12:H:27:ASP:HB2	1.56	0.85
6:B:374:HIS:HB2	19:B:1757:CLA:NB	1.91	0.85
19:B:1768:CLA:H121	22:B:1779:BCR:H312	1.58	0.85
2:2:169:LEU:HD22	19:2:1215:CLA:CBB	2.05	0.85
3:3:98:ILE:C	17:N:63:ASP:O	2.15	0.85
20:A:7020:LMU:H5B	20:A:7020:LMU:O6'	1.76	0.85
17:N:4:GLU:O	17:N:4:GLU:HG3	1.74	0.85
19:A:1781:CLA:H52	19:A:1782:CLA:HED1	1.57	0.85
5:A:62:HIS:HB2	19:A:1785:CLA:HBA1	1.58	0.85
19:B:1753:CLA:CMC	19:B:1753:CLA:CBC	2.31	0.85
19:B:1757:CLA:O1D	19:B:1758:CLA:HMA1	1.77	0.85
6:B:304:ILE:HD11	19:B:1749:CLA:CED	2.07	0.85
6:B:656:VAL:HG22	19:B:1771:CLA:HMB3	1.59	0.85
19:A:1816:CLA:CGA	19:A:1816:CLA:HED1	2.00	0.85
20:A:7023:LMU:O6'	20:A:7023:LMU:H1'	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:80:LYS:HD3	3:3:105:ASN:HB2	1.59	0.85
19:4:1199:CLA:HAA1	19:F:1157:CLA:C4	2.05	0.85
19:A:1797:CLA:CHD	19:A:1797:CLA:HBC3	2.05	0.85
16:L:163:LEU:HD11	16:L:164:PRO:HG2	1.57	0.85
7:C:59:PRO:O	25:C:1083:SF4:S3	2.35	0.85
10:F:20:GLN:CD	10:F:21:ALA:N	2.29	0.85
5:A:207:LEU:HA	5:A:211:LEU:HG	1.57	0.85
5:A:58:HIS:HE1	19:A:1759:CLA:ND	1.73	0.85
19:B:1753:CLA:HMD2	19:B:1754:CLA:CBB	2.06	0.85
10:F:96:TRP:HZ3	10:F:134:PHE:HB2	1.42	0.85
19:A:1817:CLA:HBA2	19:A:1817:CLA:O1D	1.76	0.85
5:A:685:VAL:CG2	19:A:1796:CLA:CBB	2.55	0.84
22:B:1774:BCR:H343	11:G:21:PHE:CD1	2.11	0.84
19:A:1776:CLA:C3C	19:A:1782:CLA:H172	2.06	0.84
22:A:1803:BCR:C8	22:A:1803:BCR:H311	1.98	0.84
5:A:370:ILE:CD1	19:A:1781:CLA:CAD	2.54	0.84
6:B:230:TRP:CH2	11:G:11:SER:HB2	2.12	0.84
9:E:58:ASP:OD2	9:E:60:LYS:HG2	1.76	0.84
19:1:1197:CLA:CGD	19:1:1197:CLA:HAA2	2.05	0.84
3:3:158:TYR:HB3	3:3:159:PRO:CD	2.06	0.84
2:2:99:LEU:HD22	19:2:1222:CLA:HMC3	1.58	0.84
16:L:48:ASN:HB3	16:L:49:PRO:HD2	1.56	0.84
24:B:1783:LMG:HC61	7:C:70:TRP:CH2	2.12	0.84
6:B:464:GLN:CD	6:B:469:LYS:HD3	1.96	0.84
19:H:1079:CLA:HBB2	13:I:13:GLY:O	1.77	0.84
17:N:45:ASN:ND2	17:N:57:LYS:NZ	2.22	0.84
4:4:58:MET:SD	4:4:59:LEU:N	2.50	0.84
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.57	0.84
6:B:174:ARG:CB	19:B:1743:CLA:HBC2	2.06	0.84
20:A:7037:LMU:H6E	20:A:7037:LMU:O3'	1.76	0.84
20:A:7033:LMU:H6'2	20:A:7033:LMU:O2'	1.77	0.84
19:A:1763:CLA:HAA2	19:A:1765:CLA:CED	2.07	0.84
6:B:391:PRO:HB3	6:B:538:ALA:HA	1.58	0.84
20:K:1086:LMU:H42	20:K:1086:LMU:H81	0.85	0.84
10:F:24:LYS:C	10:F:26:GLN:N	2.30	0.84
10:F:23:LYS:C	10:F:24:LYS:NZ	2.29	0.84
12:H:20:GLN:CA	12:H:22:ASP:HB3	2.07	0.84
20:1:7004:LMU:C1	20:1:7004:LMU:H3'	2.06	0.84
5:A:581:CYS:HB2	5:A:590:CYS:CA	2.05	0.84
25:B:1784:SF4:S1	25:B:1784:SF4:FE2	1.69	0.84
6:B:427:LEU:HD23	6:B:431:PHE:HZ	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:63:LEU:HG	7:C:64:SER:H	1.39	0.84
12:H:28:ALA:N	12:H:29:PRO:HD3	1.89	0.84
3:3:88:THR:N	22:3:1220:BCR:H383	1.93	0.84
19:A:1797:CLA:H122	19:A:1797:CLA:H72	1.59	0.84
11:G:44:PHE:CD2	11:G:44:PHE:O	2.30	0.84
19:J:1044:CLA:C7	19:J:1044:CLA:C4	2.30	0.84
17:N:5:GLU:OE1	17:N:6:TYR:CD1	2.31	0.84
3:3:199:VAL:HG22	19:3:1214:CLA:C3C	2.07	0.84
20:A:7042:LMU:C6	20:A:7042:LMU:C2	2.30	0.84
19:2:1220:CLA:CBA	19:2:1220:CLA:CBD	2.55	0.84
19:A:1783:CLA:H71	22:A:1807:BCR:H372	1.58	0.84
19:B:1739:CLA:H141	19:B:1757:CLA:H91	1.60	0.84
16:L:14:LEU:HA	16:L:24:GLU:HG3	1.59	0.84
20:A:7038:LMU:H101	20:A:7038:LMU:H61	1.59	0.84
5:A:53:TRP:HA	5:A:56:ASN:HB2	1.60	0.83
19:B:1739:CLA:H142	19:B:1739:CLA:H102	1.60	0.83
19:B:1768:CLA:C20	22:B:1779:BCR:HC41	2.07	0.83
6:B:202:SER:HB3	6:B:270:LEU:HD11	1.60	0.83
12:H:65:LEU:HD23	19:H:1079:CLA:H52	1.60	0.83
4:4:106:TRP:CD1	19:4:1196:CLA:CED	2.60	0.83
5:A:269:PHE:CD1	15:K:14:THR:HG21	2.12	0.83
10:F:61:LEU:HD23	10:F:69:PRO:CB	2.06	0.83
25:B:1784:SF4:S2	25:B:1784:SF4:FE4	1.68	0.83
6:B:560:ASP:HB2	7:C:66:ARG:HE	1.39	0.83
22:L:1169:BCR:H271	22:L:1169:BCR:H403	1.60	0.83
3:3:74:ALA:N	19:3:1215:CLA:C2D	2.41	0.83
17:N:61:LEU:CG	17:N:62:SER:N	2.35	0.83
20:A:7037:LMU:C5	20:A:7037:LMU:H11	2.05	0.83
17:N:5:GLU:OE2	17:N:5:GLU:HA	1.75	0.83
5:A:133:ASN:ND2	5:A:142:GLY:HA2	1.92	0.83
5:A:393:LEU:HG	5:A:394:SER:N	1.92	0.83
22:B:1776:BCR:H331	22:B:1776:BCR:C8	2.06	0.83
6:B:516:ASP:O	6:B:520:HIS:HB2	1.78	0.83
2:2:181:HIS:CD2	19:2:1214:CLA:C1D	2.62	0.83
5:A:110:LEU:HD11	5:A:239:PRO:HG2	1.58	0.83
22:A:1807:BCR:H23C	22:A:1807:BCR:C39	2.09	0.83
5:A:207:LEU:CB	19:A:1776:CLA:HBB2	2.07	0.83
6:B:294:ASN:HB3	11:G:36:PRO:HD2	1.58	0.83
11:G:26:PHE:HB2	11:G:27:GLN:HE21	1.41	0.83
19:A:1800:CLA:C20	16:L:64:LEU:HD21	2.08	0.83
3:3:132:TRP:HZ3	3:3:155:GLU:CG	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1198:CLA:C5	19:1:1198:CLA:C10	2.41	0.83
3:3:74:ALA:HA	19:3:1215:CLA:C1D	2.09	0.83
15:K:69:ILE:HA	15:K:72:VAL:HG12	1.60	0.83
19:A:1800:CLA:H201	16:L:64:LEU:HD21	1.61	0.83
19:B:1753:CLA:C1A	19:B:1753:CLA:C4	2.41	0.83
9:E:60:LYS:HG3	9:E:61:THR:H	1.41	0.83
20:A:7038:LMU:C10	20:A:7038:LMU:C6	2.49	0.83
3:3:80:LYS:HD3	3:3:105:ASN:CB	2.07	0.83
5:A:711:HIS:NE2	19:A:1795:CLA:HAC1	1.94	0.83
6:B:353:TYR:CG	6:B:594:TRP:CZ3	2.66	0.83
6:B:711:VAL:HG12	6:B:711:VAL:O	1.76	0.83
8:D:78:ALA:HB3	8:D:82:GLN:NE2	1.92	0.83
19:A:1788:CLA:O1A	19:A:1800:CLA:H11	1.78	0.83
5:A:207:LEU:HD12	5:A:310:PHE:HD1	1.42	0.83
5:A:28:LYS:O	5:A:29:THR:HG22	1.78	0.83
5:A:567:ARG:NH1	8:D:35:GLY:CA	2.35	0.83
22:I:1032:BCR:HC22	19:I:1033:CLA:C3C	2.03	0.83
19:L:1168:CLA:CBC	19:L:1168:CLA:CHD	2.55	0.83
16:L:124:LYS:NZ	16:L:124:LYS:HB2	1.93	0.83
20:A:7042:LMU:H32	20:A:7042:LMU:C5'	2.09	0.83
19:3:1218:CLA:HBC2	19:3:1218:CLA:CHD	2.09	0.83
21:B:8054:SUC:H1'1	21:B:8054:SUC:H2	1.61	0.83
5:A:269:PHE:HE1	15:K:14:THR:CG2	1.88	0.83
5:A:451:ILE:CD1	19:A:1788:CLA:HED1	2.07	0.83
5:A:497:ALA:HB2	5:A:515:TRP:HB2	1.59	0.83
19:B:1735:CLA:CMD	22:B:1778:BCR:HC41	2.08	0.83
6:B:732:LYS:HG3	6:B:733:PHE:C	1.98	0.83
10:F:62:LEU:HG	10:F:72:ILE:HD13	1.59	0.83
19:2:1220:CLA:C7	3:3:140:LYS:NZ	2.41	0.83
12:H:25:GLY:C	12:H:27:ASP:H	1.74	0.83
5:A:397:THR:HB	5:A:613:ILE:CG1	2.09	0.83
19:B:1768:CLA:C15	22:B:1779:BCR:H312	1.94	0.83
5:A:586:ARG:HG3	7:C:49:VAL:HG21	1.61	0.83
17:N:56:LYS:O	17:N:60:PHE:CD1	2.30	0.83
17:N:67:LEU:O	17:N:68:GLU:HG3	1.78	0.83
20:A:7037:LMU:H51	20:A:7037:LMU:H11	1.57	0.83
3:3:83:LEU:HD12	19:A:1798:CLA:HED2	1.61	0.83
5:A:207:LEU:HD21	5:A:314:GLY:HA2	1.61	0.83
6:B:131:THR:HB	6:B:134:ASP:CB	2.06	0.83
7:C:2:SER:O	7:C:69:LEU:HB2	1.79	0.83
8:D:39:LYS:HD2	8:D:42:VAL:HG13	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:63:LEU:HD22	16:L:64:LEU:H	1.41	0.83
17:N:59:PRO:HB3	17:N:75:TYR:HE1	1.43	0.83
17:N:58:VAL:HB	17:N:59:PRO:HD2	0.83	0.83
17:N:63:ASP:N	17:N:64:ASP:C	2.33	0.83
19:1:1200:CLA:HBC2	19:4:1198:CLA:HMB3	1.60	0.83
3:3:89:ALA:HB1	3:3:90:LEU:HG	1.61	0.83
19:A:1760:CLA:H2A	19:A:1760:CLA:O2D	1.79	0.82
22:B:1778:BCR:C37	10:F:93:ILE:HG21	2.08	0.82
18:R:41:UNK:CB	18:R:42:UNK:CB	2.56	0.82
17:N:48:GLY:HA3	17:N:49:CYS:CB	2.08	0.82
3:3:87:GLU:C	22:3:1220:BCR:H383	1.96	0.82
19:B:1744:CLA:HMB2	22:B:1776:BCR:C8	2.09	0.82
19:B:1755:CLA:HMB3	22:B:1777:BCR:C35	2.10	0.82
5:A:668:TYR:OH	6:B:441:ASP:OD1	1.96	0.82
20:A:7020:LMU:H6E	20:A:7020:LMU:O6B	1.78	0.82
11:G:16:LEU:HD23	11:G:68:ILE:CG2	2.09	0.82
1:1:24:PHE:HB3	6:B:314:ARG:HH21	1.43	0.82
5:A:373:ALA:HB1	5:A:396:PHE:HD1	1.44	0.82
22:B:1780:BCR:H19C	19:B:1786:CLA:C11	2.09	0.82
25:B:1784:SF4:S1	25:B:1784:SF4:FE4	1.69	0.82
19:B:1787:CLA:H3A	19:B:1787:CLA:O2A	1.79	0.82
6:B:664:LEU:C	6:B:667:TRP:HZ3	1.81	0.82
22:I:1032:BCR:HC21	19:I:1033:CLA:C3C	2.08	0.82
19:B:1771:CLA:H102	13:I:21:MET:SD	2.19	0.82
3:3:157:ALA:C	3:3:158:TYR:HD2	1.83	0.82
20:R:1056:LMU:H6D	20:R:1056:LMU:O5B	1.80	0.82
14:J:9:SER:O	14:J:10:VAL:HB	1.79	0.82
5:A:100:GLY:HA3	5:A:153:TRP:HH2	1.42	0.82
19:B:1768:CLA:H121	22:B:1779:BCR:C31	2.09	0.82
10:F:130:LEU:HG	10:F:131:PHE:N	1.94	0.82
11:G:47:GLY:N	11:G:48:ASP:CA	2.41	0.82
20:A:7041:LMU:O6B	20:A:7041:LMU:H1B	1.77	0.82
19:A:1817:CLA:HBC2	19:A:1817:CLA:CMC	2.09	0.82
2:2:120:ASN:CA	14:J:5:LYS:HD2	2.10	0.82
19:R:1055:CLA:HBA2	19:R:1055:CLA:CBD	2.08	0.82
20:2:7006:LMU:O5B	20:2:7006:LMU:H5'	1.74	0.82
5:A:349:ILE:CG2	5:A:349:ILE:O	2.27	0.82
15:K:6:SER:O	15:K:10:ILE:HD13	1.80	0.82
19:1:1190:CLA:HBC3	19:1:1190:CLA:HMC1	1.61	0.82
5:A:711:HIS:NE2	19:A:1795:CLA:CAC	2.43	0.82
5:A:693:LEU:HD21	5:A:735:VAL:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7016:LMU:H91	20:A:7016:LMU:H32	1.60	0.82
5:A:239:PRO:HA	5:A:242:ILE:HD13	1.62	0.82
5:A:90:PHE:CE1	19:A:1761:CLA:H91	2.15	0.82
6:B:53:GLN:C	6:B:55:ALA:H	1.83	0.82
19:A:1812:CLA:C3B	6:B:589:TRP:HH2	1.93	0.82
22:A:1807:BCR:H312	19:A:1813:CLA:H143	1.61	0.82
5:A:286:GLY:C	5:A:287:LEU:HD22	2.00	0.82
23:B:1773:PQN:H161	22:B:1780:BCR:H331	1.61	0.82
6:B:414:HIS:CD2	19:B:1760:CLA:HMA3	2.15	0.82
7:C:7:ILE:HG22	7:C:65:VAL:CG2	2.09	0.82
7:C:74:THR:C	7:C:76:SER:N	2.30	0.82
1:1:97:ILE:HG22	19:1:1197:CLA:HBB2	1.59	0.82
19:1:1187:CLA:HMA2	19:1:1187:CLA:CBA	2.08	0.82
5:A:141:ARG:HH21	5:A:141:ARG:HG3	1.42	0.82
2:2:102:ILE:C	19:2:1222:CLA:HBB2	1.97	0.82
5:A:368:LEU:CD1	19:A:1782:CLA:H61	2.09	0.82
19:A:1770:CLA:HMC2	22:A:1803:BCR:C16	2.10	0.82
5:A:393:LEU:CD1	5:A:750:PHE:CE1	2.62	0.82
16:L:88:ALA:C	16:L:90:GLY:N	2.31	0.82
16:L:163:LEU:CD1	16:L:164:PRO:HD2	2.00	0.82
20:A:7026:LMU:H41	20:A:7026:LMU:H81	1.62	0.82
10:F:81:GLY:O	14:J:38:THR:HG23	1.79	0.82
19:A:1770:CLA:C3B	22:A:1803:BCR:C19	2.54	0.82
5:A:555:ILE:HG21	19:B:1787:CLA:HMD1	1.62	0.82
19:B:1742:CLA:HAC2	19:B:1743:CLA:HBB2	0.86	0.82
6:B:323:TYR:CE1	19:B:1754:CLA:HBC1	2.15	0.82
9:E:45:TRP:HH2	9:E:78:SER:OG	1.63	0.82
17:N:61:LEU:C	17:N:61:LEU:CD1	2.37	0.82
20:A:7022:LMU:H21	20:A:7022:LMU:H2'	0.83	0.82
19:2:1223:CLA:HMC1	19:2:1223:CLA:HBC3	1.62	0.82
5:A:470:LEU:HD11	6:B:95:HIS:HB3	1.61	0.81
19:2:1220:CLA:C9	3:3:137:SER:CB	2.58	0.81
17:N:45:ASN:HD22	17:N:57:LYS:HZ1	1.17	0.81
4:4:154:ILE:HD12	19:4:1202:CLA:CHA	2.10	0.81
19:A:1787:CLA:H52	19:A:1801:CLA:HHB	1.61	0.81
19:B:1753:CLA:H12	19:B:1753:CLA:HAA1	1.60	0.81
17:N:72:LYS:HZ3	17:N:74:LYS:HG2	1.43	0.81
20:A:7017:LMU:H1B	20:A:7017:LMU:O3'	1.78	0.81
5:A:187:HIS:CD2	19:A:1767:CLA:NC	2.29	0.81
5:A:621:GLN:HG2	5:A:637:ILE:HD12	1.60	0.81
6:B:464:GLN:OE1	6:B:469:LYS:HD3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:1199:CLA:CAA	19:F:1157:CLA:H42	2.09	0.81
19:A:1781:CLA:CHC	22:A:1806:BCR:C37	2.57	0.81
19:B:1751:CLA:HHD	19:B:1751:CLA:CBC	2.00	0.81
16:L:122:GLY:C	16:L:124:LYS:N	2.31	0.81
21:B:8062:SUC:O6'	21:B:8062:SUC:H1'2	1.80	0.81
21:B:8059:SUC:C3	21:B:8059:SUC:O2'	2.28	0.81
12:H:53:LEU:HG	12:H:54:LEU:H	1.44	0.81
5:A:373:ALA:HB1	5:A:396:PHE:CD1	2.16	0.81
5:A:599:PHE:HD1	5:A:600:LEU:HD23	1.43	0.81
6:B:697:PRO:O	7:C:79:LEU:HD13	1.78	0.81
8:D:44:GLU:HB2	8:D:46:TYR:CE2	2.15	0.81
10:F:26:GLN:O	10:F:27:ALA:HB3	1.80	0.81
8:D:124:ASN:CB	8:D:125:PRO:HD3	2.10	0.81
21:H:1080:SUC:C5	21:H:1080:SUC:O2	2.29	0.81
2:2:189:ILE:HD13	2:2:189:ILE:H	1.45	0.81
19:A:1781:CLA:HBA2	19:A:1794:CLA:CED	2.05	0.81
5:A:746:THR:HA	5:A:749:PHE:HB3	1.62	0.81
19:B:1740:CLA:H41	22:B:1781:BCR:H23C	1.62	0.81
7:C:74:THR:OG1	7:C:80:ALA:CB	2.29	0.81
17:N:47:THR:HB	17:N:52:LEU:O	1.79	0.81
17:N:72:LYS:N	17:N:72:LYS:CD	2.42	0.81
20:A:7032:LMU:C1	20:A:7032:LMU:O5B	2.29	0.81
2:2:181:HIS:NE2	19:2:1214:CLA:C4D	2.44	0.81
19:A:1774:CLA:H202	19:A:1782:CLA:H3A	1.62	0.81
11:G:8:ILE:O	11:G:8:ILE:HG13	1.79	0.81
20:A:7039:LMU:C6B	20:A:7039:LMU:C4'	2.58	0.81
17:N:34:THR:OG1	17:N:36:GLU:HB3	1.79	0.81
16:L:118:LEU:CD1	16:L:119:THR:H	1.93	0.81
8:D:94:TYR:O	8:D:95:LYS:HG2	1.78	0.81
19:A:1812:CLA:CAD	19:A:1812:CLA:HED2	2.09	0.81
5:A:23:ASP:CG	5:A:24:ARG:HD2	2.00	0.81
5:A:362:LEU:HB3	5:A:410:ALA:HB2	1.62	0.81
9:E:88:GLU:O	9:E:90:VAL:CB	2.29	0.81
17:N:47:THR:HG21	17:N:54:LYS:HZ2	1.41	0.81
5:A:711:HIS:CE1	19:A:1795:CLA:HAC1	2.15	0.81
6:B:131:THR:O	6:B:135:LEU:N	2.14	0.81
5:A:466:THR:HG21	19:B:1740:CLA:CBB	2.11	0.81
19:A:1800:CLA:HBB2	19:B:1770:CLA:HMD1	1.63	0.81
6:B:293:THR:O	6:B:294:ASN:ND2	2.14	0.81
8:D:104:PHE:HB3	8:D:106:SER:H	1.46	0.81
19:2:1220:CLA:C7	3:3:140:LYS:HZ2	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7016:LMU:O6'	20:A:7016:LMU:C1	2.29	0.81
5:A:108:ALA:HB1	5:A:138:GLY:HA3	1.61	0.81
5:A:244:LEU:HD22	5:A:247:GLU:OE2	1.81	0.81
6:B:128:GLY:HA2	6:B:130:ARG:HE	1.44	0.81
6:B:212:PHE:HE1	19:B:1744:CLA:HHD	1.44	0.81
25:B:1784:SF4:S4	25:B:1784:SF4:FE2	1.72	0.81
19:B:1787:CLA:H3A	19:B:1787:CLA:CGA	2.11	0.81
6:B:334:LEU:HG	6:B:334:LEU:O	1.79	0.81
8:D:102:ARG:NH1	8:D:104:PHE:CD1	2.47	0.81
10:F:20:GLN:NE2	10:F:21:ALA:N	2.29	0.81
15:K:67:GLY:O	15:K:70:MET:CB	2.29	0.81
17:N:18:ASP:HB2	17:N:22:LEU:CG	2.11	0.81
19:A:1783:CLA:C7	22:A:1807:BCR:H371	2.10	0.81
19:A:1816:CLA:C1	19:A:1816:CLA:CED	2.54	0.81
16:L:160:VAL:O	16:L:160:VAL:CG2	2.29	0.81
11:G:17:PHE:O	11:G:20:ARG:HB2	1.81	0.81
20:A:7013:LMU:O6B	20:A:7013:LMU:C1B	2.29	0.81
20:A:7038:LMU:H1B	20:A:7038:LMU:O6'	1.81	0.81
19:A:1791:CLA:H3A	19:A:1797:CLA:CBB	2.11	0.80
6:B:189:ALA:HB1	19:B:1758:CLA:H203	1.61	0.80
6:B:586:THR:C	6:B:588:GLY:H	1.84	0.80
17:N:50:GLN:CA	17:N:51:ASP:O	2.28	0.80
20:A:7016:LMU:C3	20:A:7016:LMU:O6'	2.30	0.80
20:A:7032:LMU:O1'	20:A:7032:LMU:C1B	2.29	0.80
11:G:16:LEU:HD12	11:G:17:PHE:CE2	2.15	0.80
8:D:93:LYS:HB3	8:D:93:LYS:NZ	1.95	0.80
3:3:86:GLN:HB2	3:3:88:THR:HB	1.60	0.80
5:A:21:LEU:CD1	5:A:21:LEU:O	2.30	0.80
5:A:588:GLY:N	6:B:668:ARG:HD3	1.96	0.80
5:A:596:ASP:HA	5:A:599:PHE:HB3	1.62	0.80
6:B:373:THR:HA	6:B:376:GLN:HB2	1.62	0.80
18:R:33:UNK:O	18:R:36:UNK:CB	2.30	0.80
20:A:7020:LMU:C1B	20:A:7020:LMU:O6'	2.30	0.80
21:B:8060:SUC:O1'	21:B:8060:SUC:C5	2.29	0.80
1:1:45:ILE:HD12	19:1:1195:CLA:HMD2	1.63	0.80
20:A:7038:LMU:C1B	20:A:7038:LMU:O6'	2.29	0.80
5:A:284:ARG:HA	5:A:284:ARG:CZ	2.09	0.80
6:B:85:ARG:O	6:B:86:PRO:O	1.98	0.80
6:B:542:ARG:NH2	8:D:143:PRO:HG3	1.96	0.80
9:E:43:SER:HB2	9:E:82:TYR:HE1	1.45	0.80
11:G:46:ALA:CA	11:G:48:ASP:OD2	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:23:ALA:O	14:J:26:LEU:HB3	1.82	0.80
17:N:48:GLY:CA	17:N:49:CYS:O	2.30	0.80
19:J:1044:CLA:OBD	19:J:1044:CLA:CED	2.30	0.80
19:J:1045:CLA:C1	19:J:1045:CLA:O1D	2.30	0.80
20:A:7037:LMU:O3'	20:A:7037:LMU:C6'	2.29	0.80
20:A:7033:LMU:C6B	20:A:7033:LMU:O2'	2.30	0.80
5:A:269:PHE:CE1	15:K:14:THR:CG2	2.57	0.80
3:3:104:TYR:HB2	3:3:106:TYR:N	1.96	0.80
5:A:21:LEU:HA	5:A:22:VAL:CB	2.05	0.80
5:A:27:ILE:O	5:A:27:ILE:CG2	2.28	0.80
5:A:545:HIS:O	5:A:549:ILE:HG13	1.81	0.80
6:B:395:ILE:HD12	6:B:396:ARG:HG2	1.63	0.80
6:B:404:ALA:C	6:B:406:ASN:H	1.84	0.80
7:C:7:ILE:O	7:C:8:TYR:C	2.18	0.80
9:E:85:ASP:O	9:E:86:GLU:CB	2.30	0.80
19:3:3008:CLA:CED	19:3:3008:CLA:O1A	2.30	0.80
19:3:3008:CLA:HBC2	19:3:3008:CLA:CMC	2.00	0.80
12:H:25:GLY:CA	12:H:27:ASP:OD2	2.30	0.80
5:A:423:ASP:CB	5:A:424:PRO:HD3	2.09	0.80
21:B:8055:SUC:C1'	21:B:8055:SUC:O2	2.30	0.80
5:A:545:HIS:CG	19:A:1792:CLA:HBB2	2.14	0.80
5:A:393:LEU:O	5:A:397:THR:HG23	1.82	0.80
5:A:684:PHE:C	5:A:684:PHE:CD2	2.55	0.80
7:C:73:THR:OG1	7:C:76:SER:CB	2.30	0.80
9:E:88:GLU:O	9:E:90:VAL:CA	2.29	0.80
11:G:43:HIS:C	11:G:45:GLU:N	2.30	0.80
21:B:8054:SUC:O2	21:B:8054:SUC:C1'	2.30	0.80
20:A:7021:LMU:C2	20:A:7021:LMU:O6'	2.30	0.80
20:A:7026:LMU:H2B	20:A:7026:LMU:O3'	1.80	0.80
22:3:1220:BCR:HC8	22:3:1220:BCR:H311	1.62	0.80
19:A:1800:CLA:C9	22:L:1169:BCR:H321	2.12	0.80
13:I:12:VAL:HG21	19:I:1031:CLA:O1A	1.81	0.80
17:N:72:LYS:HZ2	17:N:74:LYS:CG	1.91	0.80
19:4:1198:CLA:O1D	19:4:1198:CLA:C2A	2.29	0.80
19:J:1044:CLA:C9	19:J:1044:CLA:C15	2.59	0.80
10:F:22:LEU:O	10:F:25:LEU:CB	2.30	0.80
10:F:26:GLN:CA	10:F:26:GLN:OE1	2.29	0.80
20:A:7043:LMU:H62	20:A:7043:LMU:C11	2.12	0.80
21:3:1221:SUC:C6'	21:3:1221:SUC:O1'	2.29	0.80
11:G:16:LEU:HD23	11:G:68:ILE:HG23	1.64	0.80
20:A:7028:LMU:O6'	20:A:7028:LMU:C1'	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:107:GLU:OE1	5:A:161:GLU:HG3	1.82	0.80
19:A:1789:CLA:H41	16:L:64:LEU:HD23	1.62	0.80
5:A:21:LEU:N	5:A:22:VAL:HG23	1.95	0.80
19:B:1756:CLA:C8	22:B:1777:BCR:H14C	2.11	0.80
6:B:557:PHE:N	6:B:558:PRO:CD	2.44	0.80
16:L:165:TYR:N	16:L:165:TYR:CD2	2.50	0.80
17:N:45:ASN:HD21	17:N:54:LYS:CB	1.93	0.80
17:N:67:LEU:HB2	17:N:68:GLU:CB	2.11	0.80
17:N:72:LYS:HG2	17:N:74:LYS:CG	2.04	0.80
10:F:24:LYS:O	10:F:27:ALA:CB	2.30	0.80
20:A:7032:LMU:C3	20:A:7032:LMU:H1B	2.08	0.80
12:H:20:GLN:HB3	12:H:22:ASP:HB2	1.60	0.80
11:G:60:SER:OG	11:G:63:PRO:HB2	1.81	0.80
5:A:615:HIS:CE1	19:A:1792:CLA:HBC3	2.16	0.80
5:A:207:LEU:O	5:A:310:PHE:HB3	1.80	0.80
8:D:46:TYR:HE1	8:D:80:LYS:HE2	1.44	0.80
11:G:7:VAL:HG22	11:G:8:ILE:H	1.46	0.80
16:L:56:VAL:HG13	19:L:1167:CLA:CED	2.12	0.80
19:A:1816:CLA:CGA	19:A:1816:CLA:O2D	2.30	0.80
18:R:34:UNK:O	18:R:38:UNK:CB	2.30	0.80
20:A:7032:LMU:C3	20:A:7032:LMU:O5B	2.29	0.80
20:A:7020:LMU:H3B	20:A:7020:LMU:O6'	1.81	0.80
20:A:7039:LMU:C3'	20:A:7039:LMU:O6B	2.30	0.80
20:A:7021:LMU:O6'	20:A:7021:LMU:H1'	1.82	0.80
20:A:7028:LMU:O2'	20:A:7028:LMU:C1	2.30	0.80
11:G:73:ALA:O	11:G:75:GLY:N	2.15	0.80
19:A:1781:CLA:CHB	22:A:1806:BCR:H363	2.11	0.80
5:A:496:HIS:HB3	5:A:515:TRP:CE3	2.17	0.80
16:L:8:TYR:HE1	16:L:11:ILE:HG23	1.47	0.80
18:R:35:UNK:O	18:R:38:UNK:CB	2.29	0.80
17:N:63:ASP:N	17:N:65:LEU:N	2.29	0.80
17:N:66:ASP:O	17:N:67:LEU:CD1	2.29	0.80
20:A:7016:LMU:C7	20:A:7016:LMU:H112	2.12	0.80
19:J:1045:CLA:CGA	19:J:1045:CLA:O1D	2.29	0.80
19:K:1146:CLA:O1A	19:K:1146:CLA:C2A	2.30	0.80
20:A:7020:LMU:O5B	20:A:7020:LMU:C6'	2.30	0.80
21:3:1221:SUC:C5	21:3:1221:SUC:O2'	2.29	0.80
17:N:5:GLU:OE2	17:N:6:TYR:CB	2.29	0.80
6:B:317:ARG:NE	6:B:317:ARG:HA	1.95	0.80
12:H:50:ARG:HH12	12:H:53:LEU:C	1.86	0.80
5:A:726:SER:O	5:A:728:VAL:N	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:680:LEU:HB3	19:A:1812:CLA:O2A	1.81	0.80
5:A:248:PHE:CD2	5:A:248:PHE:N	2.49	0.80
19:B:1759:CLA:H62	24:B:1783:LMG:H182	1.64	0.80
22:B:1778:BCR:C37	10:F:93:ILE:CG2	2.60	0.80
11:G:47:GLY:H	11:G:48:ASP:HB3	1.45	0.80
22:I:1032:BCR:H313	22:I:1032:BCR:HC8	0.84	0.80
20:A:7042:LMU:O2B	20:A:7042:LMU:C5'	2.30	0.80
19:2:1215:CLA:H43	19:2:1220:CLA:HBC3	1.61	0.80
17:N:65:LEU:CD2	17:N:65:LEU:O	2.30	0.80
20:A:7016:LMU:C1'	20:A:7016:LMU:O6'	2.30	0.80
4:4:107:GLN:HA	19:4:1196:CLA:HMA2	1.57	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:8062:SUC:O6'	21:B:8062:SUC:C1'	2.30	0.80
19:1:1192:CLA:HAA1	20:1:1202:LMU:O3'	1.82	0.80
19:A:1781:CLA:CMA	19:A:1782:CLA:O1A	2.30	0.79
5:A:308:ILE:O	5:A:312:ILE:N	2.15	0.79
19:B:1753:CLA:HBD	19:B:1753:CLA:HAA2	1.64	0.79
6:B:655:LEU:HD21	19:B:1771:CLA:CBB	2.11	0.79
9:E:60:LYS:HG3	9:E:61:THR:N	1.97	0.79
10:F:103:SER:C	10:F:105:LEU:H	1.86	0.79
11:G:19:GLY:C	11:G:21:PHE:N	2.30	0.79
19:A:1787:CLA:H42	16:L:33:ILE:HG12	1.64	0.79
20:A:7036:LMU:O5B	20:A:7036:LMU:C6'	2.30	0.79
19:3:3008:CLA:CGA	19:3:3008:CLA:O1D	2.30	0.79
18:R:36:UNK:O	18:R:38:UNK:CB	2.30	0.79
17:N:61:LEU:CD1	17:N:63:ASP:O	2.30	0.79
19:K:1146:CLA:C3A	19:K:1146:CLA:O1A	2.30	0.79
12:H:21:TRP:N	12:H:22:ASP:HB3	1.96	0.79
20:A:7039:LMU:H6'2	20:A:7039:LMU:C4'	2.11	0.79
20:A:7039:LMU:C4'	20:A:7039:LMU:O6B	2.29	0.79
21:B:8059:SUC:O2	21:B:8059:SUC:C2'	2.30	0.79
10:F:102:ARG:HG2	10:F:106:ILE:CD1	2.05	0.79
21:2:1226:SUC:O2	21:2:1226:SUC:C5'	2.29	0.79
19:4:1201:CLA:CAA	19:4:1201:CLA:O1D	2.30	0.79
3:3:107:TRP:CG	3:3:108:ALA:N	2.38	0.79
19:A:1791:CLA:CGA	19:A:1797:CLA:HBB2	2.12	0.79
19:B:1742:CLA:CAC	19:B:1743:CLA:CBB	2.48	0.79
19:B:1737:CLA:H43	22:B:1775:BCR:H313	1.63	0.79
6:B:398:TYR:HD1	6:B:542:ARG:HH21	1.28	0.79
20:A:7041:LMU:O6'	20:A:7041:LMU:C1B	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7042:LMU:O6'	20:A:7042:LMU:C4	2.29	0.79
18:R:38:UNK:O	18:R:42:UNK:CA	2.29	0.79
17:N:48:GLY:C	17:N:49:CYS:SG	2.58	0.79
17:N:66:ASP:O	17:N:67:LEU:CG	2.30	0.79
19:J:1043:CLA:C14	19:J:1043:CLA:O1A	2.30	0.79
19:K:1146:CLA:CMA	19:K:1146:CLA:O1A	2.29	0.79
20:A:7020:LMU:C3B	20:A:7020:LMU:O6'	2.29	0.79
20:A:7020:LMU:C5B	20:A:7020:LMU:O6'	2.30	0.79
21:B:8059:SUC:C1	21:B:8059:SUC:O6	2.30	0.79
2:2:181:HIS:NE2	19:2:1214:CLA:C3D	2.46	0.79
19:A:1783:CLA:H71	22:A:1807:BCR:C37	2.10	0.79
5:A:78:VAL:O	5:A:82:HIS:HB2	1.82	0.79
6:B:119:GLY:HA3	19:B:1758:CLA:CED	2.04	0.79
19:B:1755:CLA:CED	19:B:1756:CLA:OBD	2.30	0.79
6:B:546:LEU:HD11	6:B:567:THR:HG22	1.62	0.79
11:G:45:GLU:CG	11:G:49:THR:HG21	2.12	0.79
11:G:45:GLU:CB	11:G:49:THR:CG2	2.59	0.79
19:L:1167:CLA:HBC3	19:L:1167:CLA:HMC1	1.63	0.79
20:A:7042:LMU:O6'	20:A:7042:LMU:C3	2.30	0.79
19:2:1220:CLA:H71	3:3:140:LYS:NZ	1.95	0.79
17:N:45:ASN:CB	17:N:57:LYS:NZ	2.45	0.79
10:F:22:LEU:O	10:F:25:LEU:CD1	2.29	0.79
17:N:4:GLU:O	17:N:4:GLU:CG	2.29	0.79
20:A:7040:LMU:O3'	20:A:7040:LMU:C1B	2.29	0.79
2:2:196:HIS:CE1	21:2:1226:SUC:O3	2.34	0.79
16:L:152:THR:O	16:L:156:PHE:N	2.11	0.79
5:A:401:TRP:CD1	19:A:1783:CLA:CHC	2.65	0.79
6:B:331:HIS:CE1	6:B:392:ILE:HG21	2.17	0.79
11:G:30:ASN:O	11:G:33:LYS:NZ	2.16	0.79
2:2:68:LEU:HD11	19:2:1217:CLA:H192	1.64	0.79
17:N:51:ASP:O	17:N:52:LEU:CD2	2.30	0.79
17:N:60:PHE:CA	17:N:61:LEU:O	2.30	0.79
12:H:23:VAL:O	12:H:23:VAL:CG1	2.30	0.79
2:2:124:ILE:HB	2:2:129:LYS:HB3	1.63	0.79
22:B:1779:BCR:H321	22:B:1779:BCR:HC8	0.83	0.79
6:B:672:GLN:HA	6:B:672:GLN:NE2	1.94	0.79
17:N:61:LEU:CD2	17:N:63:ASP:O	2.29	0.79
19:4:1198:CLA:CAA	19:4:1198:CLA:O2D	2.30	0.79
20:A:7020:LMU:C2B	20:A:7020:LMU:O6'	2.30	0.79
1:1:185:TRP:O	1:1:186:HIS:CB	2.30	0.79
5:A:281:LEU:HD12	19:A:1772:CLA:CED	1.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:278:LEU:HD12	19:B:1746:CLA:CMA	2.12	0.79
19:B:1753:CLA:O2D	19:B:1753:CLA:C2A	2.31	0.79
19:B:1762:CLA:HBB2	22:B:1778:BCR:H272	1.65	0.79
25:B:1784:SF4:FE1	25:B:1784:SF4:S3	1.73	0.79
6:B:531:THR:HG22	19:B:1755:CLA:CMC	2.05	0.79
6:B:415:LYS:HE3	6:B:539:LEU:O	1.82	0.79
9:E:90:VAL:CG1	9:E:90:VAL:O	2.30	0.79
19:F:1157:CLA:CED	19:F:1157:CLA:OBD	2.31	0.79
11:G:28:ARG:NH2	11:G:28:ARG:HG2	1.94	0.79
11:G:46:ALA:HA	11:G:48:ASP:CG	2.01	0.79
16:L:148:VAL:O	16:L:149:SER:HB3	1.80	0.79
16:L:163:LEU:HD11	16:L:164:PRO:CG	2.11	0.79
17:N:45:ASN:HB2	17:N:57:LYS:NZ	1.98	0.79
19:J:1043:CLA:CHD	19:J:1043:CLA:HBC3	2.13	0.79
10:F:30:LYS:O	10:F:31:LEU:HB2	1.80	0.79
20:A:7026:LMU:H51	20:A:7026:LMU:H12	1.64	0.79
3:3:158:TYR:O	3:3:160:GLY:N	2.16	0.79
25:B:1784:SF4:FE3	25:B:1784:SF4:S2	1.70	0.79
19:F:1156:CLA:HBC2	19:F:1156:CLA:HHD	1.64	0.79
11:G:42:SER:OG	11:G:45:GLU:CB	2.30	0.79
20:A:7023:LMU:O3B	20:A:7023:LMU:C6B	2.30	0.79
17:N:62:SER:CB	17:N:66:ASP:OD1	2.30	0.79
20:A:7026:LMU:H3O1	21:B:8062:SUC:H5'	1.48	0.79
20:A:7010:LMU:C3'	20:A:7010:LMU:O2B	2.30	0.79
11:G:67:ASN:HA	11:G:70:ASP:OD2	1.83	0.79
7:C:39:ILE:CG1	7:C:40:ALA:H	1.92	0.79
1:1:160:GLY:HA3	19:1:1189:CLA:CBB	2.11	0.79
19:A:1770:CLA:HMC2	22:A:1803:BCR:C17	2.13	0.79
22:B:1781:BCR:H392	19:I:1031:CLA:H142	1.63	0.79
6:B:255:LEU:HD13	6:B:275:HIS:HB2	1.64	0.79
11:G:43:HIS:O	11:G:45:GLU:CB	2.29	0.79
20:A:7016:LMU:C4	20:A:7016:LMU:O6'	2.30	0.79
20:A:7032:LMU:O5B	20:A:7032:LMU:C2	2.29	0.79
22:A:1803:BCR:C40	22:A:1803:BCR:C23	2.61	0.79
6:B:120:VAL:HA	6:B:123:TRP:HD1	1.46	0.79
19:B:1756:CLA:H122	22:B:1777:BCR:C14	2.13	0.79
19:B:1744:CLA:HMA1	22:B:1776:BCR:H313	1.64	0.79
19:B:1759:CLA:H72	24:B:1783:LMG:H311	1.64	0.79
7:C:1:MET:N	7:C:4:SER:N	2.31	0.79
19:F:1157:CLA:CAD	19:F:1157:CLA:HED2	2.12	0.79
10:F:147:GLY:CA	10:F:150:VAL:HB	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:92:TRP:HA	3:3:93:PHE:CG	2.18	0.79
20:A:7016:LMU:C2	20:A:7016:LMU:O6'	2.30	0.79
19:4:1196:CLA:HHD	19:4:1196:CLA:HBC3	1.62	0.79
21:B:8059:SUC:O2	21:B:8059:SUC:C1'	2.30	0.79
14:J:11:ALA:CB	14:J:12:PRO:HD2	2.13	0.79
17:N:1:GLY:O	17:N:2:VAL:CG1	2.30	0.79
17:N:29:PHE:CD1	17:N:32:ALA:HB3	2.18	0.79
1:1:39:TYR:CB	19:1:1196:CLA:OBD	2.31	0.79
5:A:58:HIS:CE1	19:A:1759:CLA:ND	2.50	0.79
19:A:1772:CLA:C17	19:A:1772:CLA:C14	2.45	0.79
19:A:1781:CLA:O1A	19:A:1782:CLA:HED3	1.83	0.79
6:B:438:VAL:HG22	19:B:1763:CLA:CMC	2.12	0.79
5:A:555:ILE:HG22	6:B:670:TYR:CE2	2.18	0.79
6:B:558:PRO:CG	6:B:703:VAL:HB	2.13	0.79
7:C:63:LEU:CG	7:C:64:SER:H	1.96	0.79
12:H:65:LEU:HD23	19:H:1079:CLA:C5	2.12	0.79
20:A:7023:LMU:O6'	20:A:7023:LMU:C1'	2.29	0.79
20:A:7016:LMU:C5	20:A:7016:LMU:O6'	2.30	0.79
21:B:8052:SUC:O4'	21:B:8052:SUC:C1	2.30	0.79
20:A:7030:LMU:H92	20:A:7030:LMU:H52	1.64	0.79
7:C:26:LEU:H	7:C:43:PRO:HG3	1.48	0.79
25:B:1784:SF4:FE4	25:B:1784:SF4:S3	1.74	0.78
22:B:1778:BCR:H371	10:F:93:ILE:CG2	2.13	0.78
22:I:1032:BCR:HC32	19:I:1033:CLA:HAC1	1.65	0.78
17:N:61:LEU:HD13	17:N:63:ASP:HB2	1.64	0.78
20:A:7021:LMU:O6'	20:A:7021:LMU:C4	2.30	0.78
20:A:7021:LMU:H41	20:A:7021:LMU:H6D	1.65	0.78
21:B:8062:SUC:C6'	21:B:8062:SUC:C1'	2.48	0.78
20:1:7004:LMU:O2'	20:1:7004:LMU:C1	2.30	0.78
21:B:8060:SUC:H5	21:B:8060:SUC:HO1'	1.46	0.78
9:E:51:SER:HB3	9:E:68:ARG:NH1	1.97	0.78
1:1:25:ASP:H	6:B:314:ARG:NH2	1.81	0.78
5:A:157:GLY:HA2	5:A:229:ILE:HG21	1.66	0.78
5:A:242:ILE:HG12	5:A:243:PRO:HD3	1.64	0.78
5:A:27:ILE:O	5:A:28:LYS:CG	2.29	0.78
5:A:669:GLY:H	6:B:445:ALA:HA	1.47	0.78
19:3:1218:CLA:C2A	19:3:1218:CLA:O1D	2.31	0.78
17:N:45:ASN:HD22	17:N:54:LYS:HG2	0.79	0.78
4:4:119:PRO:CG	19:4:1206:CLA:C2D	2.51	0.78
2:2:70:LYS:HG3	2:2:73:ILE:CG1	2.13	0.78
19:4:1201:CLA:CMA	19:4:1201:CLA:CBA	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1760:CLA:HMC3	19:A:1762:CLA:O2D	1.82	0.78
19:A:1776:CLA:C1C	19:A:1782:CLA:H171	2.13	0.78
5:A:700:TRP:O	5:A:704:ILE:HB	1.83	0.78
17:N:54:LYS:CB	17:N:57:LYS:CE	2.61	0.78
7:C:17:CYS:CB	7:C:58:CYS:SG	2.68	0.78
17:N:5:GLU:OE2	17:N:5:GLU:CA	2.30	0.78
5:A:217:SER:CA	22:A:1803:BCR:H351	2.12	0.78
5:A:308:ILE:HG22	5:A:309:LEU:N	1.99	0.78
5:A:197:GLN:HE22	5:A:351:THR:HB	1.49	0.78
6:B:172:GLU:O	6:B:176:ASN:CB	2.32	0.78
19:B:1739:CLA:HMC2	22:B:1780:BCR:H281	1.64	0.78
6:B:353:TYR:O	6:B:354:SER:OG	2.01	0.78
16:L:124:LYS:C	16:L:126:GLN:H	1.86	0.78
20:A:7041:LMU:C5'	20:A:7041:LMU:O2'	2.29	0.78
17:N:62:SER:O	17:N:63:ASP:CB	2.30	0.78
11:G:88:THR:OG1	11:G:92:GLY:HA3	1.83	0.78
19:A:1776:CLA:C2C	19:A:1782:CLA:C17	2.61	0.78
6:B:120:VAL:CA	6:B:123:TRP:CD1	2.64	0.78
19:B:1749:CLA:OBD	19:B:1752:CLA:HBC3	1.83	0.78
11:G:21:PHE:O	11:G:23:PHE:HB2	1.82	0.78
16:L:123:ARG:HA	16:L:123:ARG:NE	1.97	0.78
16:L:99:LEU:CD1	22:L:1169:BCR:HC7	2.13	0.78
17:N:45:ASN:CB	17:N:57:LYS:HZ2	1.96	0.78
20:A:7033:LMU:C3'	20:A:7033:LMU:O5B	2.29	0.78
12:H:25:GLY:CA	12:H:27:ASP:N	2.29	0.78
19:A:1794:CLA:HBA2	19:A:1794:CLA:CHA	2.12	0.78
19:A:1813:CLA:H11	6:B:431:PHE:CE1	2.18	0.78
6:B:382:ILE:HG22	6:B:383:MET:N	1.98	0.78
7:C:79:LEU:CD2	7:C:81:TYR:O	2.29	0.78
19:A:1816:CLA:O2D	19:A:1816:CLA:CBA	2.31	0.78
17:N:62:SER:O	17:N:63:ASP:HB2	1.80	0.78
15:K:68:HIS:O	15:K:70:MET:CB	2.29	0.78
15:K:69:ILE:CG2	15:K:70:MET:H	1.90	0.78
2:2:54:TRP:CG	19:2:1222:CLA:O1D	2.37	0.78
5:A:146:THR:O	19:A:1783:CLA:HMA2	1.83	0.78
5:A:23:ASP:OD2	5:A:24:ARG:CD	2.29	0.78
6:B:348:VAL:HA	19:B:1748:CLA:H42	1.66	0.78
6:B:280:ILE:HA	6:B:283:LEU:HD12	1.64	0.78
6:B:438:VAL:CG2	19:B:1763:CLA:HMC1	2.12	0.78
13:I:8:PHE:HB2	19:I:1031:CLA:OBD	1.84	0.78
2:2:59:ALA:O	2:2:62:ILE:HG22	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:1220:CLA:H43	3:3:140:LYS:HG2	1.62	0.78
20:A:7037:LMU:H61	20:A:7037:LMU:H11	1.65	0.78
20:A:7026:LMU:H52	20:A:7026:LMU:H12	1.63	0.78
20:A:7009:LMU:C5B	20:A:7009:LMU:O3'	2.30	0.78
19:A:1816:CLA:O1A	19:A:1816:CLA:CED	2.31	0.78
10:F:12:LYS:HG2	10:F:13:GLN:N	1.99	0.78
6:B:58:PHE:HB3	6:B:146:SER:HB3	1.65	0.78
6:B:521:HIS:CE1	19:B:1768:CLA:NA	2.49	0.78
7:C:1:MET:H2	7:C:3:HIS:CA	1.96	0.78
11:G:47:GLY:N	11:G:48:ASP:CG	2.37	0.78
17:N:70:GLU:HB3	17:N:72:LYS:H	1.47	0.78
4:4:149:ALA:HB1	4:4:150:LYS:HE3	1.66	0.78
19:J:1044:CLA:H151	19:J:1044:CLA:H102	1.65	0.78
3:3:112:THR:O	3:3:114:PHE:N	2.17	0.78
19:A:1781:CLA:O2A	19:A:1794:CLA:O2D	2.02	0.78
5:A:545:HIS:CB	19:A:1792:CLA:HBB1	2.14	0.78
5:A:443:ILE:HG21	5:A:558:LYS:HB2	1.66	0.78
19:B:1761:CLA:CBC	19:B:1761:CLA:CHD	2.62	0.78
6:B:188:LEU:O	6:B:191:ALA:N	2.17	0.78
8:D:48:ILE:HG22	8:D:83:CYS:HB2	1.65	0.78
11:G:42:SER:CB	11:G:45:GLU:OE1	2.29	0.78
19:A:1800:CLA:H92	22:L:1169:BCR:H321	1.64	0.78
22:L:1170:BCR:H383	22:L:1170:BCR:H23C	1.64	0.78
16:L:163:LEU:HD21	16:L:164:PRO:HD2	1.57	0.78
3:3:205:GLY:H	5:A:252:ARG:HH22	0.78	0.78
21:B:8060:SUC:C1'	21:B:8060:SUC:O5	2.30	0.78
20:A:7013:LMU:H1B	20:A:7013:LMU:H6B	1.49	0.78
20:A:7025:LMU:O2'	20:A:7025:LMU:H21	1.84	0.78
15:K:27:ALA:CB	15:K:28:PRO:HD3	2.14	0.78
19:A:1787:CLA:HBB1	19:A:1793:CLA:H192	1.64	0.77
19:A:1791:CLA:HBC1	22:A:1806:BCR:HC31	1.66	0.77
19:A:1764:CLA:H111	22:A:1808:BCR:C11	2.13	0.77
11:G:42:SER:CB	11:G:45:GLU:OE2	2.30	0.77
17:N:54:LYS:HB2	17:N:57:LYS:HZ1	1.48	0.77
19:J:1045:CLA:HBC3	19:J:1045:CLA:CHD	2.05	0.77
20:A:7037:LMU:C5B	20:A:7037:LMU:O2B	2.31	0.77
20:A:7033:LMU:C2'	20:A:7033:LMU:H6'2	2.13	0.77
4:4:33:ASP:HB3	4:4:34:PRO:CD	2.10	0.77
17:N:5:GLU:OE1	17:N:6:TYR:CE1	2.37	0.77
15:K:51:ASP:HB3	15:K:52:PRO:CD	2.13	0.77
6:B:160:LYS:HG3	6:B:161:TRP:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:197:LEU:HD21	5:A:162:LEU:HD21	1.66	0.77
5:A:454:GLY:H	5:A:457:SER:CB	1.96	0.77
5:A:723:ARG:HH11	5:A:723:ARG:HG2	1.50	0.77
6:B:137:THR:HA	6:B:140:ILE:CG1	2.14	0.77
6:B:527:LEU:HD12	19:B:1755:CLA:CHD	2.13	0.77
6:B:190:TRP:HA	19:B:1744:CLA:HBB2	1.66	0.77
19:2:1220:CLA:CBD	19:2:1220:CLA:O1A	2.30	0.77
17:N:46:PHE:O	17:N:47:THR:CG2	2.29	0.77
11:G:93:TYR:HA	11:G:94:ASP:HB2	0.78	0.77
2:2:128:ASN:ND2	14:J:4:PHE:H	1.83	0.77
5:A:168:ALA:O	5:A:171:ALA:HB3	1.82	0.77
19:A:1781:CLA:CBC	19:A:1781:CLA:CHD	2.53	0.77
5:A:375:HIS:CE1	19:A:1782:CLA:NC	2.53	0.77
22:A:1807:BCR:C23	22:A:1807:BCR:H393	2.12	0.77
5:A:80:SER:O	5:A:83:PHE:HB2	1.84	0.77
19:B:1746:CLA:CBA	19:B:1746:CLA:HED2	2.13	0.77
6:B:655:LEU:CD2	19:B:1771:CLA:CBB	2.61	0.77
6:B:76:ALA:O	6:B:78:VAL:N	2.18	0.77
19:A:1816:CLA:CAA	19:A:1816:CLA:O2D	2.31	0.77
19:A:1816:CLA:C2	19:A:1816:CLA:O1A	2.32	0.77
17:N:79:SER:CA	17:N:80:ASN:O	2.29	0.77
20:A:7037:LMU:H72	20:A:7037:LMU:H32	0.78	0.77
20:A:7022:LMU:H5'	20:A:7022:LMU:O2'	1.83	0.77
19:R:1054:CLA:CED	19:R:1054:CLA:C1A	2.58	0.77
20:1:7004:LMU:C1B	20:1:7004:LMU:O6B	2.30	0.77
18:R:27:UNK:O	18:R:29:UNK:O	2.03	0.77
1:1:28:GLY:HA2	19:1:1199:CLA:C3C	2.15	0.77
19:A:1787:CLA:O2A	16:L:27:VAL:O	2.02	0.77
5:A:214:GLY:HA3	22:A:1804:BCR:H15C	1.66	0.77
5:A:331:LEU:CD2	5:A:331:LEU:C	2.53	0.77
6:B:124:TRP:O	6:B:129:LEU:HB3	1.85	0.77
19:B:1764:CLA:HMD2	19:B:1765:CLA:C2C	2.14	0.77
6:B:664:LEU:O	6:B:667:TRP:CZ3	2.37	0.77
9:E:52:VAL:HG12	9:E:53:VAL:N	1.99	0.77
10:F:62:LEU:HG	10:F:72:ILE:CD1	2.13	0.77
19:1:1197:CLA:O1D	19:1:1197:CLA:CAA	2.31	0.77
19:J:1045:CLA:CBA	19:J:1045:CLA:CBD	2.51	0.77
6:B:409:ALA:O	6:B:411:MET:N	2.17	0.77
19:A:1783:CLA:C10	22:A:1807:BCR:H372	2.14	0.77
5:A:28:LYS:C	5:A:29:THR:HG22	2.04	0.77
5:A:737:HIS:HA	5:A:740:LEU:CD2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:11:LEU:CD1	22:I:1032:BCR:C10	2.56	0.77
20:A:7021:LMU:O3B	20:A:7021:LMU:C6B	2.29	0.77
18:R:3:UNK:O	18:R:4:UNK:CB	2.33	0.77
19:A:1776:CLA:HAA2	19:A:1780:CLA:HBB2	1.67	0.77
19:A:1781:CLA:CBA	19:A:1794:CLA:HED1	2.10	0.77
5:A:40:PHE:HE1	5:A:53:TRP:HD1	1.29	0.77
6:B:278:LEU:HD12	19:B:1746:CLA:HMA2	1.66	0.77
8:D:78:ALA:CB	8:D:82:GLN:HE22	1.97	0.77
20:A:7042:LMU:C1B	20:A:7042:LMU:O3'	2.29	0.77
17:N:5:GLU:OE1	17:N:6:TYR:CE2	2.37	0.77
5:A:422:TYR:N	5:A:422:TYR:CD1	2.51	0.77
5:A:392:GLN:HA	5:A:395:LEU:HD23	1.67	0.77
5:A:624:VAL:O	5:A:636:HIS:CD2	2.38	0.77
6:B:75:GLU:HB2	6:B:132:ASN:HB3	1.67	0.77
19:B:1755:CLA:HMB3	22:B:1777:BCR:H352	1.67	0.77
17:N:45:ASN:HD21	17:N:54:LYS:CG	1.93	0.77
10:F:23:LYS:CB	10:F:24:LYS:HZ3	1.98	0.77
6:B:317:ARG:HE	6:B:317:ARG:HA	1.48	0.77
19:B:1739:CLA:HBA1	19:B:1757:CLA:OBD	1.85	0.77
6:B:353:TYR:CD2	6:B:594:TRP:CZ3	2.72	0.77
9:E:44:TYR:CE1	9:E:73:ASN:HA	2.20	0.77
17:N:57:LYS:O	17:N:60:PHE:CD1	2.37	0.77
7:C:14:CYS:C	7:C:17:CYS:SG	2.62	0.77
21:B:8052:SUC:O3	21:B:8052:SUC:H62	1.85	0.77
5:A:423:ASP:HB3	5:A:424:PRO:CD	2.07	0.77
6:B:507:SER:O	6:B:508:LEU:HB2	1.82	0.77
5:A:107:GLU:CD	5:A:161:GLU:HG3	2.05	0.77
19:B:1760:CLA:HED2	19:B:1760:CLA:HAA1	1.67	0.77
19:B:1760:CLA:HED2	19:B:1760:CLA:CAA	2.15	0.77
19:B:1768:CLA:HBC1	10:F:83:PHE:HZ	1.44	0.77
6:B:437:TYR:HB3	6:B:616:LEU:CD2	2.14	0.77
6:B:732:LYS:HB3	6:B:733:PHE:HA	0.79	0.77
17:N:65:LEU:CD2	17:N:66:ASP:O	2.33	0.77
19:K:1085:CLA:HMC1	19:K:1085:CLA:HBC2	1.67	0.77
10:F:25:LEU:HD22	10:F:46:MET:HB3	1.65	0.77
19:4:1209:CLA:HBC3	19:4:1209:CLA:CHD	2.14	0.77
21:B:8055:SUC:O2	21:B:8055:SUC:C2'	2.33	0.77
5:A:132:LEU:HD11	5:A:674:ALA:HB2	1.65	0.77
6:B:354:SER:O	6:B:355:LEU:HD13	1.85	0.77
11:G:44:PHE:H	11:G:45:GLU:HB2	1.49	0.77
19:A:1815:CLA:HMC1	19:A:1815:CLA:CBC	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:121:GLN:NE2	19:A:1765:CLA:HMD1	2.00	0.76
6:B:189:ALA:HB2	19:B:1758:CLA:C20	2.14	0.76
7:C:1:MET:N	7:C:4:SER:OG	2.18	0.76
13:I:23:SER:O	13:I:26:LEU:HD23	1.85	0.76
20:A:7023:LMU:H91	20:A:7023:LMU:C3	2.08	0.76
19:2:1212:CLA:O1A	19:2:1212:CLA:C1A	2.33	0.76
19:2:1220:CLA:CBD	19:2:1220:CLA:HBA2	2.15	0.76
3:3:48:PHE:HD2	3:3:49:ILE:CG2	1.82	0.76
19:4:1199:CLA:H2A	19:4:1199:CLA:O2A	1.85	0.76
5:A:491:TRP:CD1	5:A:492:ILE:HG23	2.20	0.76
5:A:711:HIS:HB3	5:A:717:ALA:HB2	1.66	0.76
19:B:1759:CLA:HMC1	19:B:1759:CLA:HBC3	1.67	0.76
6:B:475:ASP:HA	6:B:480:SER:O	1.85	0.76
2:2:103:GLY:CA	19:2:1222:CLA:HBB2	2.16	0.76
1:1:161:PHE:H	19:1:1189:CLA:HBB2	1.51	0.76
19:1:1192:CLA:HHD	19:1:1192:CLA:HBC2	1.66	0.76
10:F:33:ALA:HA	10:F:36:SER:HB2	1.65	0.76
5:A:747:TRP:CD2	22:A:1807:BCR:C40	2.67	0.76
5:A:28:LYS:O	5:A:29:THR:CB	2.30	0.76
19:B:1755:CLA:CMB	22:B:1777:BCR:H352	2.15	0.76
6:B:127:ILE:CD1	6:B:198:ALA:HB2	2.14	0.76
3:3:74:ALA:CA	19:3:1215:CLA:C4D	2.59	0.76
4:4:33:ASP:CB	4:4:34:PRO:HD2	2.11	0.76
21:3:1221:SUC:O1'	21:3:1221:SUC:C4'	2.30	0.76
1:1:161:PHE:N	19:1:1189:CLA:HBB2	2.00	0.76
19:A:1791:CLA:CGA	19:A:1797:CLA:HBB1	2.14	0.76
6:B:374:HIS:O	6:B:374:HIS:CG	2.38	0.76
11:G:45:GLU:O	11:G:46:ALA:HB3	1.84	0.76
19:2:1220:CLA:H61	3:3:140:LYS:NZ	1.94	0.76
19:J:1044:CLA:C9	19:J:1044:CLA:H41	2.14	0.76
4:4:154:ILE:HB	19:4:1202:CLA:CHA	2.16	0.76
19:A:1760:CLA:C1	19:A:1767:CLA:H61	2.12	0.76
19:A:1793:CLA:C1A	19:A:1793:CLA:CGA	2.63	0.76
9:E:90:VAL:HG12	9:E:90:VAL:O	1.85	0.76
18:R:34:UNK:H	18:R:36:UNK:CB	1.99	0.76
17:N:70:GLU:CD	17:N:72:LYS:O	2.24	0.76
20:A:7032:LMU:C1	20:A:7032:LMU:O2'	2.30	0.76
6:B:454:LEU:HD11	10:F:69:PRO:O	1.84	0.76
5:A:259:TYR:CB	5:A:260:PRO:HD2	2.14	0.76
17:N:5:GLU:OE2	17:N:6:TYR:CG	2.38	0.76
20:A:7038:LMU:H4'	20:A:7038:LMU:O2B	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:233:LEU:O	5:A:235:ALA:N	2.19	0.76
6:B:323:TYR:CD1	19:B:1754:CLA:HBC1	2.21	0.76
18:R:37:UNK:O	18:R:42:UNK:C	2.34	0.76
4:4:106:TRP:CG	19:4:1196:CLA:CED	2.69	0.76
19:J:1043:CLA:O1A	19:J:1043:CLA:C16	2.34	0.76
9:E:48:ASN:ND2	9:E:71:LYS:NZ	2.34	0.76
5:A:464:ASN:HD22	5:A:464:ASN:N	1.82	0.76
5:A:714:LEU:HD13	22:B:1779:BCR:H392	1.66	0.76
6:B:325:THR:O	6:B:329:SER:HB2	1.86	0.76
6:B:596:TRP:CD1	6:B:623:TYR:HB2	2.19	0.76
17:N:42:PHE:H	17:N:43:PRO:HD3	1.50	0.76
3:3:173:GLU:CG	3:3:174:LYS:H	1.98	0.76
7:C:20:ALA:O	7:C:21:CYS:HB2	1.84	0.76
19:A:1783:CLA:C17	22:A:1808:BCR:H15C	2.14	0.76
19:A:1783:CLA:C7	22:A:1807:BCR:H372	2.15	0.76
6:B:414:HIS:HD2	19:B:1760:CLA:HMA3	1.48	0.76
6:B:693:TRP:CD1	19:B:1770:CLA:C2D	2.69	0.76
11:G:41:MET:O	11:G:42:SER:O	2.04	0.76
20:A:7037:LMU:C6	20:A:7037:LMU:H11	2.16	0.76
20:R:1057:LMU:H62	20:R:1057:LMU:C1	2.08	0.76
19:R:1055:CLA:H92	20:R:1056:LMU:O4'	1.85	0.76
6:B:195:VAL:HA	6:B:199:ILE:HG13	1.66	0.76
7:C:70:TRP:O	7:C:72:GLU:HB2	1.85	0.76
11:G:44:PHE:H	11:G:45:GLU:CB	1.96	0.76
2:2:68:LEU:CG	19:2:1217:CLA:H192	2.15	0.76
5:A:259:TYR:CE2	5:A:280:PHE:HA	2.21	0.76
6:B:503:GLU:HB3	6:B:507:SER:CB	2.16	0.76
5:A:23:ASP:CG	5:A:24:ARG:HD3	2.02	0.76
5:A:353:SER:O	5:A:354:TRP:HB2	1.85	0.76
17:N:59:PRO:HB3	17:N:75:TYR:CE1	2.20	0.76
7:C:29:ILE:HG23	8:D:126:GLY:HA2	1.68	0.76
19:2:1223:CLA:HMC1	19:2:1223:CLA:CBC	2.15	0.76
21:2:1226:SUC:O2'	21:2:1226:SUC:C2	2.32	0.76
3:3:87:GLU:CB	22:3:1220:BCR:C38	2.64	0.75
19:A:1781:CLA:HMA2	19:A:1782:CLA:O1A	1.86	0.75
6:B:295:PHE:N	6:B:295:PHE:CD2	2.54	0.75
10:F:96:TRP:CZ3	10:F:134:PHE:HB2	2.20	0.75
16:L:164:PRO:HA	16:L:165:TYR:CZ	2.21	0.75
19:J:1043:CLA:O1A	19:J:1043:CLA:C15	2.33	0.75
15:K:24:PHE:HB3	15:K:52:PRO:HG2	1.68	0.75
17:N:11:LYS:HG2	17:N:12:THR:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:94:ALA:HA	10:F:97:ILE:HG12	1.68	0.75
19:A:1769:CLA:HMA2	19:A:1769:CLA:C2	2.16	0.75
5:A:402:ILE:HG13	19:A:1784:CLA:CBB	2.14	0.75
5:A:626:GLY:CA	5:A:636:HIS:HA	2.17	0.75
6:B:130:ARG:O	6:B:135:LEU:HD23	1.85	0.75
6:B:493:TRP:HE1	19:B:1746:CLA:HAC2	1.51	0.75
6:B:337:ALA:HA	19:B:1754:CLA:HAA1	1.68	0.75
9:E:44:TYR:CD1	9:E:73:ASN:HB2	2.20	0.75
10:F:83:PHE:O	10:F:87:GLY:HA3	1.87	0.75
8:D:32:SER:O	16:L:21:GLY:HA2	1.85	0.75
16:L:164:PRO:HB3	16:L:165:TYR:HD2	1.48	0.75
20:R:1056:LMU:O6B	20:R:1056:LMU:C1B	2.31	0.75
19:A:1782:CLA:CGD	19:A:1782:CLA:HBA1	2.17	0.75
5:A:735:VAL:O	5:A:739:LEU:HG	1.86	0.75
19:B:1756:CLA:HED1	19:B:1764:CLA:CBB	2.15	0.75
11:G:7:VAL:CG2	11:G:8:ILE:N	2.48	0.75
16:L:64:LEU:HA	16:L:67:PRO:CG	2.16	0.75
17:N:50:GLN:HA	17:N:51:ASP:O	1.86	0.75
17:N:65:LEU:HD23	17:N:66:ASP:C	2.07	0.75
4:4:106:TRP:CG	19:4:1196:CLA:HED3	2.20	0.75
7:C:12:ILE:HD12	7:C:12:ILE:N	2.01	0.75
5:A:661:ALA:HA	5:A:664:VAL:HG13	1.68	0.75
19:B:1758:CLA:OBD	19:B:1758:CLA:O1D	1.93	0.75
6:B:596:TRP:NE1	6:B:623:TYR:HB2	2.01	0.75
6:B:630:GLN:HE21	6:B:731:GLY:HA3	1.50	0.75
5:A:558:LYS:NZ	6:B:674:LEU:HB3	2.01	0.75
7:C:7:ILE:HG22	7:C:65:VAL:HG23	1.69	0.75
20:A:7020:LMU:H6E	20:A:7020:LMU:C6B	2.16	0.75
21:B:8060:SUC:H1'2	21:B:8060:SUC:O5	1.86	0.75
19:A:1796:CLA:H62	19:A:1813:CLA:H193	1.68	0.75
5:A:56:ASN:O	5:A:57:LEU:HB3	1.86	0.75
19:B:1739:CLA:H42	19:B:1739:CLA:C4C	2.17	0.75
6:B:123:TRP:CZ3	19:B:1743:CLA:H191	2.22	0.75
19:A:1788:CLA:C16	22:L:1169:BCR:H362	2.15	0.75
22:I:1032:BCR:H391	22:L:1169:BCR:H401	1.66	0.75
16:L:164:PRO:HB3	16:L:165:TYR:HE2	1.44	0.75
10:F:20:GLN:O	10:F:21:ALA:CB	2.31	0.75
20:A:7022:LMU:O3B	20:A:7022:LMU:C6B	2.30	0.75
16:L:115:ALA:N	16:L:116:PRO:HD2	2.01	0.75
8:D:93:LYS:HB3	8:D:93:LYS:HZ3	1.49	0.75
6:B:315:LEU:HD13	6:B:315:LEU:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:370:ILE:HD11	19:A:1781:CLA:CAD	2.14	0.75
19:A:1783:CLA:H43	19:A:1783:CLA:CBA	2.16	0.75
5:A:281:LEU:CD1	19:A:1772:CLA:H2A	2.13	0.75
5:A:342:GLY:HA3	5:A:430:ASP:HB2	0.82	0.75
5:A:648:THR:CG2	5:A:651:GLY:H	2.00	0.75
19:B:1753:CLA:H151	19:B:1753:CLA:H102	0.81	0.75
6:B:292:ARG:NH1	6:B:296:GLY:H	1.85	0.75
8:D:28:ILE:HG12	8:D:67:ILE:HG13	1.69	0.75
14:J:26:LEU:C	14:J:26:LEU:HD23	2.07	0.75
4:4:193:ILE:CG2	14:J:42:PHE:HD1	1.99	0.75
5:A:361:ASN:ND2	19:A:1761:CLA:CED	2.50	0.75
19:A:1777:CLA:CAD	19:A:1778:CLA:HMA1	2.17	0.75
5:A:246:HIS:O	5:A:248:PHE:CD2	2.37	0.75
5:A:591:GLN:HA	5:A:591:GLN:HE21	1.50	0.75
5:A:636:HIS:C	5:A:638:THR:N	2.39	0.75
16:L:124:LYS:HZ2	16:L:124:LYS:HB2	1.48	0.75
2:2:68:LEU:HD21	19:2:1217:CLA:H172	1.68	0.75
19:A:1817:CLA:CBC	19:A:1817:CLA:HMC1	2.10	0.75
15:K:27:ALA:HB3	15:K:28:PRO:HD3	1.67	0.75
19:A:1789:CLA:C4	16:L:64:LEU:HD23	2.16	0.75
5:A:284:ARG:HA	5:A:284:ARG:NH1	2.01	0.75
6:B:196:HIS:CE1	19:B:1745:CLA:HED2	2.21	0.75
22:B:1777:BCR:C23	22:B:1777:BCR:H382	2.09	0.75
7:C:52:LYS:O	7:C:52:LYS:CG	2.35	0.75
5:A:567:ARG:HH11	8:D:35:GLY:CA	1.97	0.75
1:1:97:ILE:HG22	19:1:1197:CLA:CBB	2.16	0.75
19:2:1220:CLA:H42	3:3:140:LYS:CB	2.16	0.75
20:A:7032:LMU:H6'2	20:A:7032:LMU:H22	1.66	0.75
20:A:7043:LMU:C6	20:A:7043:LMU:C11	2.63	0.75
11:G:13:GLY:CA	11:G:16:LEU:HG	2.17	0.75
4:4:38:ARG:HG3	4:4:39:TRP:H	1.52	0.75
3:3:112:THR:OG1	3:3:113:LEU:HG	1.87	0.75
19:B:1739:CLA:HMC2	22:B:1780:BCR:C28	2.17	0.75
6:B:347:LEU:HD22	6:B:351:HIS:CE1	2.22	0.75
8:D:78:ALA:O	8:D:79:ARG:HD3	1.85	0.75
19:2:1215:CLA:O1A	19:2:1220:CLA:CBC	2.34	0.75
19:J:1045:CLA:CGA	19:J:1045:CLA:HBD	2.16	0.75
7:C:31:TRP:O	7:C:33:GLY:N	2.19	0.75
17:N:4:GLU:OE2	17:N:5:GLU:HB2	1.87	0.75
21:B:8055:SUC:H1'1	21:B:8055:SUC:O2	1.87	0.75
19:A:1761:CLA:C4	22:A:1804:BCR:H313	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:747:TRP:CE3	22:A:1807:BCR:H401	2.22	0.74
5:A:29:THR:O	5:A:29:THR:HG23	1.85	0.74
5:A:491:TRP:HE1	19:A:1792:CLA:H12	1.51	0.74
5:A:54:ILE:O	5:A:58:HIS:CD2	2.40	0.74
5:A:690:LEU:HD23	5:A:693:LEU:HD12	1.69	0.74
5:A:91:LEU:O	19:A:1763:CLA:HMC3	1.87	0.74
19:B:1764:CLA:HBB2	22:B:1777:BCR:H381	1.67	0.74
6:B:180:SER:HB2	6:B:288:GLY:HA3	1.68	0.74
7:C:54:CYS:SG	25:C:1082:SF4:S1	2.85	0.74
8:D:111:TYR:CD2	8:D:114:PRO:HB3	2.21	0.74
11:G:28:ARG:HA	19:G:1099:CLA:HMA3	1.68	0.74
19:2:1212:CLA:O2A	19:2:1212:CLA:C4	2.30	0.74
2:2:169:LEU:CD2	19:2:1215:CLA:CBB	2.65	0.74
17:N:54:LYS:HG2	17:N:57:LYS:HZ3	1.50	0.74
5:A:488:PHE:CE2	5:A:533:PRO:HB3	2.22	0.74
5:A:684:PHE:HD2	5:A:685:VAL:N	1.85	0.74
5:A:462:ILE:CD1	19:B:1786:CLA:H72	2.17	0.74
6:B:709:GLY:O	6:B:710:LEU:HB2	1.86	0.74
9:E:58:ASP:OD2	9:E:60:LYS:NZ	2.18	0.74
14:J:31:ARG:NH2	19:J:1043:CLA:C3B	2.50	0.74
19:A:1815:CLA:H2	19:A:1815:CLA:HMA2	1.69	0.74
5:A:32:GLU:OE2	19:A:1767:CLA:HMA2	1.87	0.74
5:A:711:HIS:CD2	19:A:1795:CLA:CBC	2.68	0.74
6:B:122:GLN:HG3	6:B:361:ILE:HG12	1.69	0.74
6:B:58:PHE:HB2	6:B:146:SER:HB2	1.69	0.74
11:G:40:GLY:C	11:G:41:MET:SD	2.65	0.74
11:G:94:ASP:H	11:G:95:PRO:CD	1.99	0.74
18:R:44:UNK:O	18:R:45:UNK:C	2.35	0.74
3:3:87:GLU:CA	22:3:1220:BCR:C38	2.65	0.74
19:4:1199:CLA:HBC3	19:4:1199:CLA:CMC	2.03	0.74
19:A:1776:CLA:C2C	19:A:1782:CLA:H171	2.18	0.74
19:A:1787:CLA:H3A	6:B:685:THR:OG1	1.87	0.74
3:3:84:ILE:CB	19:A:1798:CLA:O1A	2.29	0.74
5:A:411:ALA:HB2	22:A:1806:BCR:C39	2.17	0.74
5:A:214:GLY:O	5:A:215:SER:HB3	1.86	0.74
19:B:1746:CLA:HED2	19:B:1746:CLA:HBA2	1.67	0.74
6:B:269:TRP:CB	6:B:497:TRP:HH2	2.00	0.74
5:A:472:ARG:HH22	16:L:74:LEU:HD21	1.52	0.74
12:H:23:VAL:HG12	12:H:23:VAL:O	1.87	0.74
18:R:24:UNK:O	18:R:27:UNK:CB	2.35	0.74
14:J:11:ALA:HB1	14:J:12:PRO:CD	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:99:LEU:HD21	19:2:1222:CLA:HMC3	1.70	0.74
1:1:39:TYR:HB3	19:1:1196:CLA:OBD	1.87	0.74
2:2:36:SER:O	2:2:37:ASP:HB2	1.87	0.74
19:A:1772:CLA:CMC	19:A:1772:CLA:CBC	2.46	0.74
6:B:471:THR:HG23	6:B:502:ASN:ND2	2.02	0.74
16:L:36:TYR:CG	16:L:36:TYR:O	2.40	0.74
17:N:45:ASN:HD22	17:N:57:LYS:HZ3	1.33	0.74
17:N:61:LEU:CG	17:N:62:SER:H	1.98	0.74
19:J:1043:CLA:HED3	19:J:1043:CLA:C2A	2.17	0.74
19:2:1224:CLA:H8	19:2:1224:CLA:H151	1.69	0.74
5:A:103:PHE:N	5:A:103:PHE:CD2	2.55	0.74
5:A:692:PHE:CZ	19:A:1796:CLA:HBC3	2.22	0.74
5:A:588:GLY:H	6:B:668:ARG:NH1	1.85	0.74
12:H:44:ALA:HB3	16:L:145:PHE:HD1	1.51	0.74
7:C:12:ILE:HB	7:C:39:ILE:HA	1.68	0.74
10:F:7:PRO:HA	10:F:61:LEU:O	1.88	0.74
18:R:7:UNK:O	18:R:11:UNK:N	2.20	0.74
5:A:187:HIS:CE1	19:A:1767:CLA:C4D	2.67	0.74
5:A:224:HIS:O	5:A:225:VAL:HG22	1.88	0.74
5:A:475:ASP:OD2	16:L:74:LEU:HA	1.87	0.74
5:A:78:VAL:HG11	19:A:1761:CLA:HBC3	1.69	0.74
19:B:1753:CLA:H43	19:B:1753:CLA:CAA	2.16	0.74
6:B:292:ARG:CZ	6:B:292:ARG:HA	2.16	0.74
6:B:347:LEU:CD2	6:B:351:HIS:CE1	2.71	0.74
11:G:46:ALA:H	11:G:49:THR:HG22	1.53	0.74
11:G:47:GLY:H	11:G:48:ASP:HA	1.52	0.74
19:1:1190:CLA:CBC	19:1:1190:CLA:HMC1	2.16	0.74
19:A:1792:CLA:HBA2	19:A:1792:CLA:CGD	2.17	0.74
19:A:1788:CLA:CBC	19:A:1793:CLA:HBC2	2.17	0.74
19:A:1801:CLA:HED1	16:L:32:LEU:HD13	1.69	0.74
5:A:270:PHE:CE1	19:A:1797:CLA:H2	2.22	0.74
5:A:76:ARG:NH1	5:A:192:LYS:CG	2.45	0.74
19:B:1755:CLA:H72	19:B:1769:CLA:C2D	2.18	0.74
6:B:292:ARG:C	6:B:293:THR:HG1	1.91	0.74
4:4:126:LEU:N	4:4:127:PRO:HD3	2.03	0.74
20:1:7004:LMU:C1	20:1:7004:LMU:C3'	2.66	0.74
14:J:10:VAL:HG13	14:J:14:LEU:HG	1.69	0.74
5:A:216:LEU:HD12	22:A:1803:BCR:H353	1.70	0.74
5:A:457:SER:O	5:A:544:ILE:HD13	1.87	0.74
9:E:88:GLU:O	9:E:90:VAL:HB	1.88	0.74
19:B:1748:CLA:H3A	19:B:1748:CLA:CGA	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:233:TYR:CD2	19:B:1746:CLA:HED1	2.23	0.74
20:1:7004:LMU:C3'	20:1:7004:LMU:H12	2.01	0.74
3:3:80:LYS:HB2	19:3:1214:CLA:C3D	2.17	0.74
19:A:1760:CLA:H2A	19:A:1760:CLA:CED	2.18	0.73
19:A:1787:CLA:H52	19:A:1801:CLA:CHB	2.18	0.73
19:A:1779:CLA:HBB2	22:A:1805:BCR:H351	1.70	0.73
5:A:459:GLY:O	5:A:462:ILE:HG22	1.88	0.73
5:A:553:VAL:H	5:A:556:LEU:HD12	1.53	0.73
6:B:732:LYS:HG3	6:B:734:GLY:CA	2.18	0.73
9:E:55:VAL:HG23	9:E:65:VAL:HB	1.70	0.73
16:L:8:TYR:CE1	16:L:11:ILE:HG23	2.23	0.73
3:3:194:ILE:CG1	19:3:1212:CLA:HMC2	2.18	0.73
20:A:7010:LMU:O3'	20:A:7010:LMU:H1B	1.88	0.73
19:A:1796:CLA:H43	19:A:1796:CLA:NC	2.03	0.73
5:A:452:PHE:CE1	19:A:1793:CLA:CBB	2.57	0.73
6:B:700:LEU:N	6:B:700:LEU:HD23	2.02	0.73
18:R:35:UNK:O	18:R:36:UNK:C	2.35	0.73
19:2:1215:CLA:C3	19:2:1220:CLA:CBC	2.66	0.73
17:N:63:ASP:H	17:N:64:ASP:C	1.90	0.73
16:L:49:PRO:HB2	16:L:139:PHE:HB2	1.70	0.73
6:B:98:GLN:C	6:B:100:ALA:H	1.92	0.73
19:4:1199:CLA:H2	19:4:1199:CLA:HED1	1.69	0.73
19:A:1763:CLA:CMB	22:A:1808:BCR:HC7	2.17	0.73
19:A:1790:CLA:HMC1	19:A:1790:CLA:HBC2	1.70	0.73
5:A:227:LEU:HD23	5:A:231:GLN:HE22	1.53	0.73
6:B:664:LEU:O	6:B:667:TRP:HZ3	1.71	0.73
6:B:91:ILE:HD12	6:B:104:PHE:CE2	2.23	0.73
19:L:1168:CLA:HAA1	19:L:1168:CLA:O1D	1.87	0.73
16:L:63:LEU:HD22	16:L:64:LEU:N	2.02	0.73
2:2:68:LEU:CD1	19:2:1217:CLA:H192	2.18	0.73
17:N:72:LYS:HZ2	17:N:74:LYS:HG3	1.53	0.73
1:1:45:ILE:HA	1:1:48:ARG:HB2	1.68	0.73
5:A:364:MET:O	5:A:368:LEU:N	2.20	0.73
2:2:127:ASN:CG	14:J:2:ARG:NH1	2.41	0.73
18:R:38:UNK:O	18:R:41:UNK:CB	2.36	0.73
19:3:1217:CLA:C2A	19:3:3011:CLA:CAC	2.64	0.73
17:N:5:GLU:OE1	17:N:6:TYR:CZ	2.41	0.73
22:A:1807:BCR:H312	19:A:1813:CLA:C14	2.17	0.73
5:A:28:LYS:O	5:A:29:THR:CG2	2.36	0.73
5:A:684:PHE:C	5:A:684:PHE:HD2	1.91	0.73
6:B:489:GLY:O	6:B:490:ARG:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:64:ILE:O	2:2:68:LEU:CB	2.35	0.73
3:3:98:ILE:HB	17:N:61:LEU:HB2	1.70	0.73
20:A:7020:LMU:O5B	20:A:7020:LMU:H6E	1.86	0.73
19:A:1776:CLA:C8	22:A:1805:BCR:H373	2.18	0.73
19:A:1783:CLA:H172	22:A:1808:BCR:H17C	1.70	0.73
5:A:328:LYS:HE2	5:A:332:GLU:CD	2.09	0.73
6:B:124:TRP:CG	6:B:129:LEU:HD13	2.23	0.73
17:N:60:PHE:HA	17:N:61:LEU:O	1.87	0.73
10:F:30:LYS:O	10:F:31:LEU:CB	2.37	0.73
22:A:1806:BCR:HC8	22:A:1806:BCR:H331	1.70	0.73
5:A:542:HIS:HA	5:A:545:HIS:HD2	1.54	0.73
19:B:1771:CLA:C19	13:I:21:MET:HB3	2.18	0.73
6:B:8:PHE:O	6:B:35:ASP:HB2	1.87	0.73
6:B:394:PHE:O	6:B:542:ARG:NE	2.18	0.73
5:A:447:ASN:ND2	6:B:678:LEU:HD21	2.04	0.73
9:E:39:LEU:O	9:E:40:ARG:HD3	1.88	0.73
9:E:86:GLU:HG3	9:E:87:VAL:H	0.71	0.73
17:N:67:LEU:CB	17:N:68:GLU:CG	2.45	0.73
19:K:1085:CLA:C1A	19:K:1142:CLA:CMD	2.67	0.73
3:3:50:GLU:N	3:3:51:PRO:CD	2.52	0.73
19:4:1209:CLA:CBD	19:4:1209:CLA:HBA1	2.17	0.73
19:1:1190:CLA:HMC3	19:1:1196:CLA:CAC	2.18	0.73
5:A:387:THR:CG2	5:A:523:VAL:HG11	2.18	0.73
5:A:628:ILE:HG13	5:A:632:GLY:HA2	1.69	0.73
5:A:692:PHE:CE2	19:A:1796:CLA:HBC3	2.24	0.73
19:A:1800:CLA:HMB2	19:L:1167:CLA:HBC1	1.69	0.73
19:A:1779:CLA:CHD	22:A:1805:BCR:C20	2.66	0.73
5:A:309:LEU:HD21	19:A:1776:CLA:HMC3	1.71	0.73
5:A:472:ARG:HH12	16:L:74:LEU:CG	1.91	0.73
6:B:329:SER:O	6:B:330:ILE:HG22	1.88	0.73
6:B:438:VAL:HG23	19:B:1763:CLA:HAC1	1.71	0.73
9:E:39:LEU:C	9:E:40:ARG:HD3	2.08	0.73
17:N:67:LEU:CA	17:N:68:GLU:HG2	2.18	0.73
5:A:316:MET:CB	5:A:317:TYR:CB	2.56	0.73
19:4:1201:CLA:C2	19:4:1201:CLA:O1A	2.29	0.73
19:A:1783:CLA:H102	22:A:1807:BCR:H372	1.70	0.73
19:A:1787:CLA:HAC2	19:A:1801:CLA:HMC3	1.71	0.73
5:A:393:LEU:HD11	5:A:750:PHE:CE1	2.23	0.73
6:B:533:ILE:HD11	6:B:575:ASP:O	1.88	0.73
7:C:1:MET:H1	7:C:4:SER:CB	2.00	0.73
17:N:72:LYS:CG	17:N:74:LYS:H	1.98	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7016:LMU:C7	20:A:7016:LMU:C11	2.67	0.73
20:A:7032:LMU:H32	20:A:7032:LMU:H1B	1.70	0.73
3:3:194:ILE:HG13	19:3:1212:CLA:CMC	2.19	0.73
20:R:1056:LMU:O5B	20:R:1056:LMU:C5'	2.33	0.73
4:4:38:ARG:NH1	4:4:38:ARG:HG3	1.94	0.73
5:A:270:PHE:CZ	19:A:1797:CLA:H2	2.24	0.73
5:A:442:ILE:CG2	19:A:1786:CLA:HMC3	2.18	0.73
5:A:54:ILE:O	5:A:58:HIS:HD2	1.71	0.73
6:B:304:ILE:HG22	19:B:1752:CLA:CGD	2.19	0.73
10:F:125:LEU:O	10:F:126:ALA:CB	2.36	0.73
19:A:1816:CLA:HBC2	19:A:1816:CLA:CHD	2.10	0.73
11:G:13:GLY:O	11:G:16:LEU:HG	1.89	0.73
12:H:42:THR:HG22	12:H:45:ALA:HB2	1.70	0.73
3:3:208:PRO:HB3	3:3:210:GLN:OE1	1.89	0.73
5:A:289:PRO:O	5:A:290:LEU:HB2	1.89	0.73
19:A:1781:CLA:H61	19:A:1782:CLA:CED	2.19	0.72
19:A:1770:CLA:CHC	22:A:1803:BCR:C17	2.66	0.72
22:A:1807:BCR:C32	22:A:1808:BCR:H391	2.19	0.72
19:B:1756:CLA:H122	22:B:1777:BCR:C13	2.18	0.72
16:L:36:TYR:O	16:L:36:TYR:CD1	2.41	0.72
17:N:75:TYR:C	17:N:76:LYS:O	2.26	0.72
19:4:1198:CLA:O1A	19:4:1198:CLA:C2	2.29	0.72
19:J:1045:CLA:CGA	19:J:1045:CLA:CBD	2.67	0.72
20:A:7021:LMU:O6'	20:A:7021:LMU:C1	2.37	0.72
20:A:1810:LMU:O6B	20:A:1810:LMU:O1'	2.06	0.72
5:A:220:ARG:O	5:A:221:HIS:HB2	1.88	0.72
4:4:169:GLN:HG2	19:4:1199:CLA:HAC2	1.71	0.72
19:A:1763:CLA:HBA2	19:A:1765:CLA:H12	1.71	0.72
19:A:1769:CLA:HBA1	19:A:1780:CLA:C4	2.18	0.72
19:A:1781:CLA:HED3	19:A:1782:CLA:CMD	2.09	0.72
5:A:281:LEU:HD11	19:A:1772:CLA:CED	0.95	0.72
5:A:707:ILE:O	5:A:711:HIS:CD2	2.42	0.72
19:B:1738:CLA:H91	19:B:1738:CLA:H193	1.71	0.72
19:B:1753:CLA:HBC3	19:B:1753:CLA:HMC1	0.78	0.72
19:B:1755:CLA:HMB2	19:B:1769:CLA:O1A	1.89	0.72
6:B:378:ILE:O	6:B:380:GLY:N	2.21	0.72
7:C:6:LYS:HB3	7:C:63:LEU:HD21	1.71	0.72
13:I:12:VAL:O	13:I:17:PRO:CD	2.36	0.72
17:N:72:LYS:CB	17:N:74:LYS:HB2	2.19	0.72
2:2:99:LEU:HB3	19:2:1222:CLA:HBB1	1.71	0.72
20:2:7006:LMU:C2'	20:2:7006:LMU:H22	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:131:ILE:HD13	6:B:446:PHE:C	2.10	0.72
5:A:210:LEU:HD12	19:A:1769:CLA:HMB2	1.72	0.72
17:N:41:LYS:HB2	17:N:42:PHE:HB3	0.80	0.72
11:G:68:ILE:HG23	11:G:72:LEU:CD1	2.14	0.72
19:A:1776:CLA:HMD2	19:A:1778:CLA:HBB2	1.67	0.72
5:A:51:THR:CB	19:A:1795:CLA:CBB	2.53	0.72
5:A:98:PHE:HZ	19:A:1763:CLA:HMD3	1.54	0.72
6:B:38:THR:OG1	6:B:41:ARG:HB2	1.89	0.72
5:A:755:ILE:O	5:A:756:ALA:HB3	1.87	0.72
5:A:685:VAL:CG2	19:A:1796:CLA:HBB1	2.12	0.72
5:A:514:THR:O	5:A:531:PRO:O	2.07	0.72
17:N:47:THR:CB	17:N:52:LEU:O	2.37	0.72
17:N:61:LEU:HD12	17:N:62:SER:CA	2.19	0.72
17:N:62:SER:CB	17:N:66:ASP:CA	2.65	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
5:A:426:THR:HA	5:A:428:TYR:CE2	2.25	0.72
12:H:49:LYS:O	12:H:51:GLY:N	2.22	0.72
19:4:1201:CLA:CMA	19:4:1201:CLA:CGA	2.66	0.72
3:3:106:TYR:CD2	3:3:107:TRP:CD1	2.78	0.72
5:A:23:ASP:OD1	5:A:33:GLN:CD	2.26	0.72
19:2:1212:CLA:O2A	19:2:1212:CLA:H43	1.89	0.72
21:B:8054:SUC:C2	21:B:8054:SUC:C1'	2.64	0.72
17:N:48:GLY:HA3	17:N:49:CYS:HB2	1.71	0.72
20:A:7016:LMU:H81	20:A:7016:LMU:H32	1.46	0.72
19:A:1800:CLA:HMD3	22:B:1780:BCR:C3	2.20	0.72
5:A:76:ARG:O	5:A:186:TYR:HD2	1.71	0.72
5:A:187:HIS:CD2	19:A:1767:CLA:C4C	2.73	0.72
5:A:218:TRP:O	5:A:222:GLN:HB2	1.89	0.72
5:A:79:PHE:HE2	5:A:185:HIS:CE1	2.06	0.72
5:A:85:GLN:O	5:A:89:ILE:HG13	1.90	0.72
19:B:1768:CLA:H61	22:B:1779:BCR:H323	1.70	0.72
6:B:707:LEU:CD1	6:B:711:VAL:HG21	2.20	0.72
22:I:1032:BCR:H402	22:I:1032:BCR:H382	1.71	0.72
21:B:8052:SUC:O3	21:B:8052:SUC:C6	2.30	0.72
19:A:1815:CLA:CMA	19:A:1815:CLA:C6	2.64	0.72
16:L:48:ASN:HD22	16:L:115:ALA:HB2	1.54	0.72
8:D:69:ARG:O	8:D:70:GLU:HB2	1.90	0.72
5:A:479:ASP:HA	5:A:536:THR:HG23	1.72	0.72
5:A:340:GLY:O	5:A:343:HIS:N	2.22	0.72
22:L:1169:BCR:C27	22:L:1169:BCR:H403	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:28:SER:O	10:F:29:LEU:C	2.27	0.72
3:3:52:LYS:O	3:3:56:TYR:HD2	1.63	0.72
19:A:1815:CLA:H2	19:A:1815:CLA:CMA	2.20	0.72
10:F:53:PHE:C	10:F:55:ASN:H	1.93	0.72
6:B:492:ILE:CD1	6:B:492:ILE:H	2.01	0.72
16:L:124:LYS:O	16:L:126:GLN:N	2.23	0.72
16:L:40:LEU:HB3	16:L:41:PRO:HD3	1.71	0.72
11:G:92:GLY:C	11:G:94:ASP:OD1	2.28	0.72
19:K:1085:CLA:C1A	19:K:1142:CLA:HMD1	2.20	0.72
21:B:8059:SUC:HO2	21:B:8059:SUC:H1'2	1.53	0.72
16:L:107:PHE:HB2	16:L:109:GLU:OE1	1.89	0.72
5:A:103:PHE:N	5:A:103:PHE:HD2	1.87	0.72
5:A:174:PHE:CE2	19:A:1761:CLA:H152	2.24	0.72
19:A:1765:CLA:CBB	19:B:1763:CLA:CMD	2.66	0.72
16:L:66:GLY:N	16:L:67:PRO:HD2	2.05	0.72
2:2:120:ASN:HA	14:J:5:LYS:HB2	1.71	0.72
11:G:13:GLY:O	11:G:16:LEU:CG	2.38	0.72
8:D:60:MET:SD	8:D:61:PRO:HD2	2.30	0.72
7:C:11:CYS:SG	7:C:12:ILE:N	2.63	0.72
19:2:1224:CLA:ND	19:2:1224:CLA:H18	2.04	0.72
20:A:7027:LMU:C6B	20:A:7027:LMU:H2B	2.18	0.72
17:N:5:GLU:CD	17:N:6:TYR:CG	2.63	0.72
12:H:37:SER:HB3	16:L:51:LEU:HG	1.72	0.72
19:A:1763:CLA:HAA2	19:A:1765:CLA:HED1	1.72	0.71
19:A:1789:CLA:HBC3	19:A:1789:CLA:HMC1	1.71	0.71
22:A:1803:BCR:H341	22:A:1803:BCR:C12	2.17	0.71
22:A:1807:BCR:HC31	22:B:1778:BCR:H17C	1.72	0.71
5:A:41:SER:O	5:A:44:ILE:HA	1.89	0.71
5:A:747:TRP:CD2	22:A:1807:BCR:H401	2.25	0.71
6:B:427:LEU:HD13	19:B:1735:CLA:OBD	1.90	0.71
6:B:615:TYR:HD1	6:B:615:TYR:H	1.38	0.71
5:A:668:TYR:CE2	6:B:617:MET:SD	2.83	0.71
7:C:1:MET:N	7:C:3:HIS:N	2.30	0.71
11:G:21:PHE:O	11:G:23:PHE:CB	2.37	0.71
11:G:42:SER:OG	11:G:45:GLU:CD	2.29	0.71
19:L:1167:CLA:HHC	22:L:1170:BCR:HC8	1.71	0.71
16:L:95:LEU:HA	16:L:98:CYS:HB2	1.71	0.71
17:N:50:GLN:HA	17:N:51:ASP:C	2.10	0.71
12:H:21:TRP:H	12:H:22:ASP:HB3	1.55	0.71
4:4:39:TRP:CG	4:4:40:PHE:N	2.58	0.71
6:B:504:ASN:ND2	6:B:504:ASN:H	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7028:LMU:H1'	20:A:7028:LMU:O6'	1.86	0.71
21:2:1226:SUC:O2	21:2:1226:SUC:H5'	1.87	0.71
5:A:475:ASP:HB3	19:A:1789:CLA:HED3	1.72	0.71
6:B:188:LEU:HD11	19:B:1745:CLA:CBB	2.19	0.71
19:B:1752:CLA:CBB	19:B:1752:CLA:H72	2.19	0.71
10:F:93:ILE:O	10:F:96:TRP:CD1	2.40	0.71
3:3:93:PHE:HD2	3:3:93:PHE:H	1.38	0.71
3:3:92:TRP:CZ2	5:A:250:LEU:HD12	2.25	0.71
19:1:1187:CLA:CBA	19:1:1187:CLA:CMA	2.59	0.71
19:4:4014:CLA:HED3	19:4:4014:CLA:O1A	1.90	0.71
5:A:119:SER:HB2	5:A:136:VAL:HG21	1.71	0.71
5:A:747:TRP:CE3	22:A:1807:BCR:C40	2.73	0.71
5:A:79:PHE:CE2	5:A:185:HIS:CE1	2.79	0.71
5:A:381:PRO:CB	19:A:1774:CLA:HAA2	2.18	0.71
5:A:708:VAL:HA	5:A:711:HIS:HD2	1.54	0.71
6:B:145:LEU:HA	6:B:148:ILE:HD12	1.71	0.71
19:B:1745:CLA:OBD	19:B:1745:CLA:O2D	2.06	0.71
23:B:1773:PQN:H291	24:B:1783:LMG:H201	1.71	0.71
6:B:437:TYR:HB3	6:B:616:LEU:HD23	1.72	0.71
8:D:113:HIS:N	8:D:114:PRO:HD2	2.05	0.71
10:F:80:TRP:HE3	19:F:1157:CLA:HMC2	1.54	0.71
16:L:10:VAL:O	16:L:10:VAL:HG22	1.89	0.71
17:N:49:CYS:O	17:N:50:GLN:C	2.29	0.71
10:F:42:ILE:CG1	10:F:43:LYS:H	1.99	0.71
20:A:7027:LMU:H6'1	20:A:7027:LMU:H2B	1.72	0.71
8:D:94:TYR:O	8:D:95:LYS:CG	2.38	0.71
10:F:17:ARG:HE	10:F:17:ARG:HA	1.54	0.71
19:A:1759:CLA:C4	19:A:1796:CLA:H8	2.20	0.71
22:A:1806:BCR:H331	22:A:1806:BCR:C8	2.20	0.71
5:A:397:THR:HB	5:A:613:ILE:HD11	1.73	0.71
6:B:91:ILE:CD1	6:B:104:PHE:HE2	2.04	0.71
6:B:444:LEU:O	6:B:445:ALA:HB3	1.90	0.71
7:C:74:THR:CB	7:C:80:ALA:HB2	2.20	0.71
20:A:7042:LMU:H1B	20:A:7042:LMU:H3O2	1.53	0.71
17:N:45:ASN:CG	17:N:45:ASN:O	2.29	0.71
19:J:1044:CLA:H151	19:J:1044:CLA:H91	1.71	0.71
16:L:118:LEU:HD12	16:L:119:THR:N	2.04	0.71
19:A:1796:CLA:H161	22:A:1807:BCR:HC22	1.70	0.71
5:A:370:ILE:HG22	5:A:400:MET:CA	2.19	0.71
5:A:443:ILE:HD11	5:A:557:LEU:HG	1.73	0.71
6:B:299:HIS:CE1	19:B:1752:CLA:HMD1	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:654:HIS:CE1	19:B:1785:CLA:NB	2.58	0.71
9:E:53:VAL:HG12	9:E:54:ALA:H	1.55	0.71
17:N:54:LYS:O	17:N:56:LYS:N	2.22	0.71
14:J:31:ARG:HA	14:J:34:PRO:HA	1.72	0.71
19:3:1219:CLA:H102	19:3:1219:CLA:H143	1.70	0.71
17:N:35:VAL:HG12	17:N:37:PHE:CZ	2.26	0.71
15:K:51:ASP:HB3	15:K:52:PRO:HD3	1.70	0.71
19:A:1788:CLA:H152	22:L:1169:BCR:C36	2.20	0.71
19:A:1796:CLA:H102	19:A:1813:CLA:H152	1.73	0.71
5:A:550:HIS:O	5:A:552:THR:O	2.07	0.71
6:B:545:LYS:HG2	6:B:546:LEU:N	2.03	0.71
5:A:555:ILE:HG22	6:B:670:TYR:HE2	1.53	0.71
9:E:39:LEU:H	9:E:40:ARG:HH11	1.37	0.71
9:E:44:TYR:CG	9:E:73:ASN:HB2	2.25	0.71
16:L:99:LEU:HD11	22:L:1169:BCR:HC7	1.72	0.71
2:2:98:GLU:HG2	2:2:99:LEU:HG	1.71	0.71
5:A:387:THR:HG23	5:A:523:VAL:HG11	1.71	0.71
6:B:44:GLN:OE1	6:B:163:PRO:HB2	1.90	0.71
6:B:496:GLY:O	6:B:499:ASN:HB2	1.91	0.71
5:A:281:LEU:HA	5:A:297:THR:O	1.91	0.71
6:B:144:PHE:CD2	6:B:144:PHE:O	2.42	0.71
22:B:1775:BCR:HC8	22:B:1775:BCR:C33	2.20	0.71
6:B:334:LEU:HB2	19:B:1737:CLA:HMD3	1.72	0.71
6:B:362:ALA:O	6:B:363:GLN:HG3	1.90	0.71
6:B:46:ILE:HD11	19:B:1737:CLA:H192	1.72	0.71
6:B:25:ILE:HG22	22:L:1169:BCR:C29	2.14	0.71
17:N:74:LYS:O	17:N:76:LYS:N	2.24	0.71
3:3:52:LYS:O	3:3:56:TYR:N	2.21	0.71
9:E:68:ARG:NH2	9:E:69:PHE:HA	2.05	0.71
7:C:26:LEU:N	7:C:43:PRO:HG3	2.05	0.71
19:A:1781:CLA:H2	19:A:1782:CLA:CED	2.20	0.71
19:B:1749:CLA:C3	19:B:1754:CLA:H92	2.20	0.71
19:B:1753:CLA:HAA2	19:B:1753:CLA:CBD	2.20	0.71
19:B:1756:CLA:H8	22:B:1777:BCR:H12C	1.71	0.71
23:B:1773:PQN:H192	22:B:1780:BCR:C8	2.21	0.71
6:B:375:HIS:HE1	19:B:1758:CLA:NC	1.89	0.71
19:1:1200:CLA:HMC1	19:4:1198:CLA:HMB3	1.73	0.71
15:K:47:ILE:HG23	15:K:48:GLN:H	1.54	0.71
1:1:163:VAL:HA	1:1:166:SER:HB3	1.71	0.71
19:A:1782:CLA:C4	19:A:1782:CLA:O2A	2.39	0.71
11:G:28:ARG:CG	11:G:29:GLU:N	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:1220:CLA:C6	3:3:140:LYS:HZ2	2.04	0.71
5:A:249:ILE:O	5:A:251:ASN:N	2.23	0.71
17:N:61:LEU:HG	17:N:62:SER:H	1.55	0.71
17:N:65:LEU:O	17:N:66:ASP:C	2.29	0.71
10:F:24:LYS:C	10:F:26:GLN:H	1.93	0.71
20:A:7009:LMU:O2'	20:A:7009:LMU:H12	1.90	0.71
6:B:454:LEU:CD1	10:F:69:PRO:O	2.38	0.71
6:B:152:ALA:O	6:B:153:GLY:C	2.28	0.71
5:A:166:CYS:HB3	19:A:1798:CLA:HBB1	1.73	0.71
19:A:1783:CLA:H111	22:A:1808:BCR:H353	1.73	0.71
5:A:223:VAL:HG23	5:A:227:LEU:HD13	1.73	0.71
6:B:25:ILE:HG21	22:L:1169:BCR:H292	0.72	0.71
11:G:46:ALA:C	11:G:48:ASP:OD1	2.28	0.71
16:L:126:GLN:N	16:L:127:PRO:HD2	2.05	0.71
16:L:52:ARG:O	16:L:56:VAL:HG23	1.90	0.71
17:N:11:LYS:HD2	17:N:12:THR:O	1.91	0.71
5:A:479:ASP:OD2	5:A:536:THR:HG23	1.90	0.71
19:4:1199:CLA:CBC	19:4:1199:CLA:CMC	2.65	0.70
19:A:1776:CLA:C4C	19:A:1782:CLA:H172	2.20	0.70
19:A:1774:CLA:O1A	19:A:1784:CLA:H71	1.91	0.70
19:A:1800:CLA:H112	19:A:1800:CLA:C6	2.18	0.70
5:A:211:LEU:O	5:A:214:GLY:O	2.09	0.70
6:B:295:PHE:N	6:B:295:PHE:HD2	1.85	0.70
6:B:400:PRO:HD2	8:D:143:PRO:HD3	1.74	0.70
17:N:42:PHE:O	17:N:43:PRO:C	2.30	0.70
3:3:106:TYR:O	3:3:108:ALA:HB2	1.91	0.70
5:A:331:LEU:CD2	5:A:331:LEU:O	2.30	0.70
5:A:445:HIS:O	5:A:446:LEU:CB	2.39	0.70
5:A:454:GLY:N	5:A:457:SER:HB3	1.99	0.70
6:B:130:ARG:HG2	6:B:130:ARG:HH11	1.56	0.70
6:B:463:ILE:O	6:B:464:GLN:HB3	1.91	0.70
8:D:28:ILE:HG12	8:D:67:ILE:CG1	2.21	0.70
17:N:42:PHE:HD1	17:N:43:PRO:N	1.84	0.70
19:3:3011:CLA:C1	19:3:3011:CLA:HMA2	2.14	0.70
5:A:645:SER:HB3	6:B:637:PRO:HG3	1.72	0.70
19:B:1755:CLA:HED2	19:B:1756:CLA:OBD	1.91	0.70
6:B:199:ILE:HG23	6:B:270:LEU:HD22	1.71	0.70
24:B:1783:LMG:O3	7:C:70:TRP:NE1	2.24	0.70
9:E:42:GLU:HG2	9:E:43:SER:H	1.54	0.70
3:3:74:ALA:CA	19:3:1215:CLA:C1D	2.69	0.70
18:R:37:UNK:O	18:R:43:UNK:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:79:SER:CA	17:N:80:ASN:C	2.57	0.70
4:4:126:LEU:HG	4:4:126:LEU:O	1.89	0.70
19:J:1044:CLA:H72	19:J:1044:CLA:H42	1.71	0.70
11:G:68:ILE:HG22	11:G:72:LEU:HD13	1.70	0.70
19:A:1763:CLA:C4B	22:A:1808:BCR:C33	2.67	0.70
5:A:51:THR:OG1	19:A:1795:CLA:CBB	2.40	0.70
19:A:1795:CLA:H42	19:A:1795:CLA:O1A	1.91	0.70
5:A:497:ALA:HB2	5:A:515:TRP:CB	2.20	0.70
6:B:172:GLU:HG3	6:B:301:ILE:HG13	1.72	0.70
13:I:20:ALA:O	13:I:24:LEU:HB3	1.91	0.70
19:2:1218:CLA:O1D	19:2:1218:CLA:H2A	1.91	0.70
17:N:54:LYS:HG2	17:N:57:LYS:NZ	2.06	0.70
20:A:7016:LMU:H12	20:A:7016:LMU:O6'	1.89	0.70
19:4:1198:CLA:CAA	19:4:1198:CLA:CGD	2.69	0.70
7:C:17:CYS:C	7:C:58:CYS:HB2	2.11	0.70
19:J:1043:CLA:H152	19:J:1044:CLA:HMB1	1.73	0.70
2:2:120:ASN:CG	14:J:5:LYS:CD	2.59	0.70
3:3:157:ALA:C	3:3:158:TYR:CD2	2.64	0.70
1:1:24:PHE:HB3	6:B:314:ARG:NH2	2.06	0.70
17:N:4:GLU:C	17:N:4:GLU:OE2	2.30	0.70
10:F:116:GLN:C	10:F:118:GLU:H	1.93	0.70
5:A:485:GLN:O	5:A:487:VAL:N	2.24	0.70
6:B:438:VAL:HG22	19:B:1763:CLA:HMC3	1.72	0.70
7:C:5:VAL:HB	7:C:65:VAL:CA	2.13	0.70
9:E:52:VAL:C	9:E:53:VAL:HG23	2.10	0.70
19:2:1213:CLA:H93	19:2:1213:CLA:H51	1.71	0.70
17:N:70:GLU:C	17:N:72:LYS:N	2.34	0.70
19:4:4014:CLA:O1A	19:4:4014:CLA:CED	2.39	0.70
4:4:159:LEU:O	4:4:163:PHE:HB2	1.91	0.70
19:A:1782:CLA:H42	19:A:1782:CLA:O2A	1.91	0.70
5:A:242:ILE:HG12	5:A:243:PRO:CD	2.20	0.70
5:A:467:MET:HA	5:A:470:LEU:HB2	1.72	0.70
5:A:690:LEU:HD21	5:A:738:TYR:HE1	1.56	0.70
23:B:1773:PQN:H2M1	23:B:1773:PQN:H142	1.74	0.70
6:B:730:SER:C	6:B:731:GLY:O	2.29	0.70
7:C:1:MET:H2	7:C:3:HIS:C	1.91	0.70
10:F:83:PHE:O	10:F:87:GLY:CA	2.39	0.70
22:L:1170:BCR:C33	22:L:1170:BCR:HC8	2.22	0.70
2:2:169:LEU:CD2	19:2:1215:CLA:HBB2	2.21	0.70
17:N:63:ASP:H	17:N:65:LEU:N	1.88	0.70
12:H:21:TRP:H	12:H:22:ASP:CB	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:K:3009:CLA:O2D	19:K:3009:CLA:HBA1	1.92	0.70
19:A:1781:CLA:HBB2	19:A:1794:CLA:H3A	1.73	0.70
5:A:438:HIS:CE1	5:A:442:ILE:HD11	2.26	0.70
5:A:458:PHE:CD2	19:B:1786:CLA:HMB2	2.26	0.70
5:A:723:ARG:NH1	5:A:723:ARG:HG2	2.06	0.70
6:B:293:THR:HG22	6:B:294:ASN:ND2	2.07	0.70
8:D:28:ILE:HG21	8:D:67:ILE:HG13	1.74	0.70
6:B:294:ASN:OD1	11:G:38:GLN:N	2.20	0.70
2:2:120:ASN:HA	14:J:5:LYS:CB	2.21	0.70
10:F:63:CYS:HA	10:F:69:PRO:HA	1.74	0.70
12:H:45:ALA:HB3	12:H:46:PRO:CD	2.21	0.70
3:3:163:PHE:O	3:3:164:PHE:HB2	1.91	0.70
5:A:545:HIS:CE1	5:A:612:VAL:HG22	2.27	0.70
5:A:680:LEU:HD21	6:B:617:MET:CE	2.22	0.70
5:A:685:VAL:HG12	5:A:741:GLY:HA2	1.74	0.70
6:B:174:ARG:NH1	19:B:1754:CLA:CMD	2.54	0.70
6:B:174:ARG:NH1	19:B:1754:CLA:HMD1	2.07	0.70
19:B:1787:CLA:HMC1	19:B:1787:CLA:CBC	2.21	0.70
6:B:29:HIS:CG	19:B:1737:CLA:HBB2	2.27	0.70
6:B:91:ILE:CD1	6:B:104:PHE:CE2	2.75	0.70
7:C:1:MET:CA	7:C:4:SER:OG	2.40	0.70
6:B:561:GLY:HA3	7:C:52:LYS:CG	2.22	0.70
7:C:5:VAL:CB	7:C:65:VAL:HG22	2.22	0.70
6:B:293:THR:O	11:G:38:GLN:CD	2.29	0.70
19:2:1215:CLA:C5	19:2:1220:CLA:HBC1	2.21	0.70
5:A:396:PHE:CE2	5:A:616:PHE:CG	2.80	0.70
22:B:1780:BCR:H17C	19:B:1786:CLA:C10	2.18	0.70
13:I:9:VAL:HG12	13:I:10:PRO:HD3	1.73	0.70
20:A:7042:LMU:H32	20:A:7042:LMU:O5'	1.91	0.70
19:2:1220:CLA:C4	3:3:140:LYS:HD3	2.18	0.70
17:N:76:LYS:HG3	17:N:77:CYS:N	2.00	0.70
20:A:7022:LMU:C5'	20:A:7022:LMU:O2'	2.30	0.70
16:L:5:LYS:HA	16:L:5:LYS:HE2	1.73	0.70
6:B:230:TRP:HH2	11:G:11:SER:HB2	1.54	0.70
8:D:47:VAL:HB	8:D:76:LYS:HA	1.74	0.70
4:4:95:PHE:CE2	19:4:1208:CLA:C2C	2.75	0.70
12:H:45:ALA:O	12:H:47:PHE:N	2.25	0.70
6:B:141:PHE:O	6:B:143:LEU:N	2.25	0.69
6:B:421:HIS:NE2	19:B:1761:CLA:C4D	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:697:ARG:NH2	6:B:566:GLY:O	2.18	0.69
5:A:558:LYS:HZ2	6:B:674:LEU:HB3	1.56	0.69
11:G:37:GLU:OE2	11:G:42:SER:HA	1.92	0.69
17:N:74:LYS:O	17:N:75:TYR:C	2.30	0.69
7:C:44:ARG:HH22	8:D:127:ARG:NE	1.90	0.69
5:A:691:MET:HE2	23:A:1802:PQN:H2M2	1.75	0.69
5:A:207:LEU:HD12	5:A:310:PHE:CD1	2.26	0.69
5:A:453:LEU:HD13	5:A:547:PHE:HA	1.74	0.69
6:B:594:TRP:C	6:B:594:TRP:CD1	2.66	0.69
6:B:696:LYS:HG2	7:C:80:ALA:HA	1.72	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
19:J:1045:CLA:H12	19:J:1045:CLA:O1D	1.91	0.69
4:4:38:ARG:CG	4:4:39:TRP:H	2.04	0.69
12:H:53:LEU:CG	12:H:54:LEU:H	2.03	0.69
6:B:15:ASP:O	6:B:20:ARG:HG2	1.90	0.69
19:L:1166:CLA:HED2	19:L:1166:CLA:HAA2	1.74	0.69
19:A:1764:CLA:HMB1	19:A:1765:CLA:H11	1.74	0.69
19:A:1782:CLA:CBC	19:A:1782:CLA:CMC	2.65	0.69
5:A:25:ASP:OD1	5:A:26:PRO:CG	2.32	0.69
6:B:269:TRP:HE3	6:B:270:LEU:H	1.38	0.69
8:D:111:TYR:HD2	8:D:114:PRO:CB	2.05	0.69
11:G:62:ASP:HB2	11:G:63:PRO:HD3	1.73	0.69
10:F:47:GLU:CG	10:F:51:LYS:HE3	2.09	0.69
7:C:44:ARG:HH21	8:D:127:ARG:CB	2.04	0.69
19:A:1790:CLA:CAD	19:A:1791:CLA:HAC1	2.21	0.69
19:B:1747:CLA:H52	19:B:1756:CLA:CMB	2.22	0.69
19:B:1764:CLA:HMD2	19:B:1765:CLA:C1C	2.22	0.69
23:B:1773:PQN:H192	22:B:1780:BCR:C10	2.09	0.69
6:B:188:LEU:HD11	19:B:1745:CLA:HBB2	1.74	0.69
6:B:645:VAL:HG11	19:B:1739:CLA:HAC1	1.74	0.69
16:L:64:LEU:HA	16:L:67:PRO:HG2	1.73	0.69
20:R:1056:LMU:O5B	20:R:1056:LMU:C6'	2.39	0.69
6:B:242:HIS:O	6:B:243:LEU:HG	1.92	0.69
5:A:390:ALA:HA	5:A:393:LEU:HD23	1.74	0.69
5:A:472:ARG:O	5:A:474:GLN:HG3	1.92	0.69
6:B:655:LEU:HD21	19:B:1771:CLA:HBB1	1.74	0.69
17:N:54:LYS:HG3	17:N:57:LYS:HZ3	1.55	0.69
18:R:51:UNK:O	18:R:52:UNK:CB	2.41	0.69
11:G:13:GLY:HA2	11:G:16:LEU:CG	2.22	0.69
7:C:31:TRP:HB2	7:C:39:ILE:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:43:TYR:O	16:L:44:ARG:HB2	1.90	0.69
19:B:1771:CLA:H192	13:I:21:MET:HB3	1.73	0.69
7:C:75:ARG:HH22	8:D:110:GLN:CD	1.95	0.69
9:E:72:VAL:O	9:E:73:ASN:CB	2.39	0.69
16:L:96:SER:OG	16:L:143:PHE:HD2	1.76	0.69
19:J:1045:CLA:CGD	19:J:1045:CLA:CGA	2.69	0.69
10:F:22:LEU:C	10:F:24:LYS:H	1.93	0.69
10:F:47:GLU:HG3	10:F:51:LYS:CE	2.10	0.69
17:N:18:ASP:HB3	17:N:22:LEU:HG	1.74	0.69
6:B:369:ALA:O	6:B:725:LEU:CD1	2.39	0.69
16:L:158:MET:CG	16:L:159:TYR:H	2.04	0.69
22:3:1220:BCR:H23C	22:3:1220:BCR:H393	0.77	0.69
4:4:165:GLY:O	4:4:169:GLN:HG2	1.93	0.69
19:A:1764:CLA:C4	22:A:1807:BCR:H383	2.23	0.69
5:A:402:ILE:HD11	19:A:1784:CLA:HBB2	1.74	0.69
6:B:124:TRP:HD1	6:B:124:TRP:O	1.76	0.69
6:B:693:TRP:HD1	19:B:1770:CLA:C1D	2.06	0.69
22:I:1032:BCR:HC21	19:I:1033:CLA:C2C	2.23	0.69
19:2:1215:CLA:C4	19:2:1220:CLA:CBC	2.71	0.69
19:K:1085:CLA:C4A	19:K:1142:CLA:HMD1	2.22	0.69
20:A:7037:LMU:C1	20:A:7037:LMU:C6	2.71	0.69
5:A:259:TYR:CD2	5:A:280:PHE:HA	2.28	0.69
6:B:409:ALA:C	6:B:411:MET:H	1.96	0.69
5:A:157:GLY:HA2	5:A:229:ILE:CG2	2.23	0.69
19:A:1774:CLA:OBD	19:A:1784:CLA:H43	1.92	0.69
19:A:1800:CLA:HMC2	19:B:1770:CLA:H11	1.75	0.69
22:A:1807:BCR:H311	19:A:1813:CLA:H142	1.73	0.69
5:A:225:VAL:O	5:A:229:ILE:HB	1.91	0.69
19:B:1755:CLA:H72	19:B:1769:CLA:C3D	2.23	0.69
19:B:1768:CLA:H202	22:B:1779:BCR:HC41	1.75	0.69
5:A:281:LEU:HD13	19:A:1772:CLA:H2A	1.71	0.69
19:B:1750:CLA:NB	19:B:1750:CLA:H2	2.07	0.69
19:B:1756:CLA:H72	19:B:1756:CLA:H41	1.73	0.69
6:B:595:HIS:HD2	6:B:623:TYR:OH	1.75	0.69
19:J:1045:CLA:O2A	19:J:1045:CLA:C2A	2.30	0.69
21:B:8056:SUC:C3'	21:B:8056:SUC:O2	2.30	0.69
6:B:503:GLU:HB3	6:B:507:SER:HB2	1.73	0.69
3:3:83:LEU:HA	19:A:1798:CLA:C4	2.15	0.69
5:A:453:LEU:HD21	19:A:1793:CLA:CBB	2.17	0.69
5:A:396:PHE:HE2	5:A:616:PHE:CB	2.06	0.69
5:A:618:TRP:CZ2	5:A:655:ASP:HB2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1759:CLA:HBC2	19:B:1759:CLA:CMC	2.11	0.69
23:A:1802:PQN:C13	22:B:1778:BCR:H322	2.23	0.69
6:B:347:LEU:HD13	6:B:351:HIS:HD1	1.58	0.69
6:B:404:ALA:C	6:B:406:ASN:N	2.45	0.69
9:E:52:VAL:CG1	9:E:53:VAL:H	1.95	0.69
16:L:99:LEU:HD11	22:L:1169:BCR:H313	1.74	0.69
18:R:34:UNK:C	18:R:38:UNK:CB	2.71	0.69
20:A:7016:LMU:C7	20:A:7016:LMU:C2	2.71	0.69
10:F:21:ALA:O	10:F:22:LEU:C	2.29	0.69
12:H:44:ALA:HB2	16:L:145:PHE:CE1	2.27	0.69
16:L:77:THR:HG21	16:L:82:ALA:HB1	1.74	0.69
19:A:1782:CLA:H101	19:A:1782:CLA:H143	1.73	0.69
5:A:466:THR:O	5:A:470:LEU:HG	1.92	0.69
6:B:124:TRP:CD1	6:B:129:LEU:HD13	2.27	0.69
6:B:124:TRP:HE1	6:B:129:LEU:HD22	1.58	0.69
19:B:1747:CLA:CAD	19:B:1756:CLA:CBB	2.71	0.69
19:B:1762:CLA:H51	22:B:1779:BCR:H401	1.75	0.69
6:B:693:TRP:CD1	19:B:1770:CLA:C1D	2.76	0.69
8:D:102:ARG:NE	8:D:110:GLN:HB2	2.07	0.69
13:I:8:PHE:CB	19:I:1031:CLA:OBD	2.40	0.69
16:L:163:LEU:CG	16:L:164:PRO:CD	2.60	0.69
3:3:97:PHE:CD2	3:3:97:PHE:N	2.59	0.69
20:A:7026:LMU:H3'	20:A:7026:LMU:H11	1.72	0.69
20:A:7027:LMU:O2'	20:A:7027:LMU:C1	2.39	0.69
19:3:3007:CLA:HAC2	19:K:3009:CLA:H91	1.75	0.69
19:A:1760:CLA:H12	19:A:1767:CLA:C6	2.16	0.68
5:A:545:HIS:CE1	19:A:1792:CLA:HBB2	2.26	0.68
5:A:193:LEU:HA	5:A:196:PHE:CE2	2.28	0.68
5:A:385:LEU:O	5:A:386:ALA:CB	2.39	0.68
5:A:620:MET:HG3	5:A:625:TRP:CE2	2.28	0.68
6:B:46:ILE:HG21	19:B:1737:CLA:HBC3	1.73	0.68
7:C:65:VAL:HG12	7:C:66:ARG:H	1.57	0.68
12:H:14:ILE:HG13	12:H:17:THR:OG1	1.93	0.68
5:A:207:LEU:HB2	19:A:1776:CLA:HBB2	1.73	0.68
5:A:582:ASP:OD1	5:A:586:ARG:NH1	2.18	0.68
6:B:697:PRO:HB3	19:B:1770:CLA:HBC3	1.75	0.68
7:C:78:GLY:O	7:C:81:TYR:CE1	2.42	0.68
2:2:81:THR:HG23	2:2:82:ALA:N	2.06	0.68
19:A:1811:CLA:HBC3	19:A:1811:CLA:HHD	1.75	0.68
5:A:28:LYS:O	5:A:29:THR:HB	1.93	0.68
5:A:59:ALA:O	5:A:61:ALA:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1749:CLA:HBB2	19:B:1754:CLA:H41	1.76	0.68
6:B:438:VAL:CG2	19:B:1763:CLA:CMC	2.69	0.68
6:B:711:VAL:O	6:B:711:VAL:CG1	2.42	0.68
8:D:48:ILE:CG2	8:D:83:CYS:HB2	2.22	0.68
22:B:1779:BCR:HC32	19:F:1156:CLA:CMA	2.23	0.68
19:1:1198:CLA:C9	19:1:1198:CLA:C12	2.72	0.68
3:3:74:ALA:HA	19:3:1215:CLA:ND	2.09	0.68
19:4:1198:CLA:HED3	19:4:1198:CLA:HAA2	0.73	0.68
19:J:1045:CLA:C2	19:J:1045:CLA:H2A	2.24	0.68
3:3:52:LYS:C	3:3:56:TYR:CD2	2.65	0.68
19:A:1763:CLA:HMB3	19:A:1764:CLA:HHB	1.74	0.68
19:A:1782:CLA:HBD	19:A:1782:CLA:HBA1	1.74	0.68
5:A:51:THR:OG1	19:A:1795:CLA:HBB2	1.93	0.68
5:A:370:ILE:HG23	5:A:403:GLY:CA	2.22	0.68
6:B:438:VAL:HG21	19:B:1763:CLA:HMC1	1.75	0.68
13:I:14:LEU:C	13:I:17:PRO:HD2	2.14	0.68
16:L:161:LEU:CD1	16:L:162:ASP:C	2.60	0.68
15:K:16:THR:O	15:K:20:PHE:HB3	1.94	0.68
4:4:169:GLN:NE2	19:4:1199:CLA:CHD	2.55	0.68
5:A:309:LEU:O	5:A:310:PHE:HB2	1.93	0.68
19:B:1744:CLA:HMB3	22:B:1776:BCR:H311	1.73	0.68
6:B:576:PHE:CE2	19:B:1759:CLA:HAC1	2.28	0.68
7:C:1:MET:SD	7:C:4:SER:CB	2.82	0.68
10:F:95:GLY:O	10:F:99:TRP:HB2	1.93	0.68
19:3:3008:CLA:CBC	19:3:3008:CLA:CMC	2.63	0.68
20:R:1056:LMU:O6'	20:R:1056:LMU:C1'	2.41	0.68
5:A:464:ASN:HD22	5:A:464:ASN:H	1.40	0.68
19:A:1776:CLA:H162	19:A:1776:CLA:H111	1.76	0.68
5:A:431:LEU:O	5:A:435:VAL:HG12	1.93	0.68
6:B:290:MET:HA	19:B:1751:CLA:HAC2	1.74	0.68
19:B:1758:CLA:H101	22:B:1776:BCR:H343	1.75	0.68
6:B:388:ALA:C	6:B:391:PRO:CD	2.61	0.68
6:B:568:CYS:O	6:B:570:ILE:N	2.26	0.68
9:E:34:SER:O	9:E:35:LYS:HB3	1.92	0.68
16:L:163:LEU:O	16:L:164:PRO:C	2.29	0.68
1:1:97:ILE:CG2	19:1:1197:CLA:CBB	2.71	0.68
3:3:63:ARG:CZ	3:3:185:LYS:HG2	2.24	0.68
6:B:468:GLY:O	6:B:470:THR:N	2.26	0.68
7:C:20:ALA:O	7:C:21:CYS:CB	2.42	0.68
19:A:1771:CLA:HAA1	19:A:1771:CLA:CED	2.23	0.68
5:A:370:ILE:HD13	19:A:1781:CLA:CAD	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:625:TRP:CB	5:A:637:ILE:HD11	2.23	0.68
6:B:140:ILE:H	6:B:140:ILE:HD13	1.59	0.68
22:B:1780:BCR:C20	19:B:1786:CLA:H151	2.23	0.68
6:B:711:VAL:HG22	24:B:1783:LMG:H391	1.75	0.68
9:E:53:VAL:O	9:E:55:VAL:N	2.25	0.68
9:E:44:TYR:CZ	9:E:73:ASN:HA	2.29	0.68
19:A:1816:CLA:H2	19:A:1816:CLA:H72	1.75	0.68
19:J:1045:CLA:HBA2	19:J:1045:CLA:CHA	2.24	0.68
10:F:25:LEU:HD23	10:F:46:MET:HB3	1.72	0.68
11:G:12:THR:HG22	11:G:72:LEU:CD1	2.24	0.68
4:4:39:TRP:HE1	4:4:41:VAL:HG23	1.59	0.68
4:4:171:ASN:O	4:4:172:VAL:HB	1.92	0.68
5:A:585:GLY:O	5:A:589:THR:OG1	2.12	0.68
19:B:1753:CLA:C4	19:B:1753:CLA:HAA1	2.20	0.68
19:B:1755:CLA:HHD	19:B:1755:CLA:HBC3	1.76	0.68
6:B:438:VAL:O	6:B:441:ASP:N	2.27	0.68
8:D:49:THR:HG22	8:D:99:GLN:HB3	1.76	0.68
11:G:28:ARG:HD2	11:G:33:LYS:HE2	1.76	0.68
16:L:69:VAL:HG11	16:L:84:GLY:H	1.58	0.68
3:3:93:PHE:H	3:3:95:THR:N	1.89	0.68
15:K:67:GLY:O	15:K:68:HIS:O	2.12	0.68
19:A:1779:CLA:HBB2	22:A:1805:BCR:C35	2.19	0.68
19:A:1781:CLA:H172	22:A:1805:BCR:H332	1.75	0.68
5:A:618:TRP:O	5:A:622:SER:HB3	1.94	0.68
5:A:663:GLN:HB3	5:A:752:ALA:O	1.93	0.68
14:J:22:LEU:O	14:J:25:LEU:N	2.27	0.68
3:3:92:TRP:CA	3:3:93:PHE:CG	2.74	0.68
17:N:65:LEU:HD23	17:N:66:ASP:O	1.94	0.68
14:J:31:ARG:NH2	19:J:1043:CLA:CHC	2.56	0.68
19:3:1219:CLA:O2D	19:3:1219:CLA:H2A	1.94	0.68
1:1:161:PHE:N	19:1:1189:CLA:CBB	2.54	0.68
3:3:84:ILE:HA	19:A:1798:CLA:C5	2.15	0.68
22:B:1781:BCR:C4	19:B:1787:CLA:H142	2.24	0.68
20:A:7016:LMU:H71	20:A:7016:LMU:C11	2.24	0.68
19:J:1044:CLA:C9	19:J:1044:CLA:H152	2.24	0.68
3:3:50:GLU:O	3:3:53:TRP:N	2.27	0.68
5:A:141:ARG:HD3	10:F:39:ALA:HA	1.75	0.68
19:1:1188:CLA:HED2	19:1:1188:CLA:OBD	1.93	0.68
6:B:450:GLU:O	6:B:452:GLN:N	2.25	0.68
19:A:1785:CLA:H101	19:A:1785:CLA:H152	1.76	0.67
5:A:203:LEU:H	5:A:203:LEU:HD12	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:204:ASN:O	5:A:205:HIS:CB	2.36	0.67
5:A:396:PHE:HE2	5:A:616:PHE:CG	2.11	0.67
5:A:400:MET:O	5:A:609:ILE:HD12	1.94	0.67
5:A:470:LEU:HD13	6:B:95:HIS:HB3	1.74	0.67
6:B:174:ARG:O	6:B:175:LEU:HB3	1.95	0.67
19:B:1753:CLA:CHB	19:B:1753:CLA:H42	2.23	0.67
6:B:30:ASP:OD2	6:B:396:ARG:NH1	2.25	0.67
3:3:93:PHE:N	3:3:95:THR:H	1.89	0.67
19:A:1759:CLA:H42	19:A:1796:CLA:H8	1.75	0.67
5:A:390:ALA:HA	5:A:393:LEU:CD2	2.24	0.67
6:B:141:PHE:HD2	6:B:144:PHE:CE1	2.12	0.67
19:B:1762:CLA:HBB2	22:B:1778:BCR:C27	2.25	0.67
19:B:1755:CLA:CAD	19:B:1767:CLA:HBB1	2.24	0.67
22:B:1780:BCR:HC8	22:B:1780:BCR:C33	2.24	0.67
6:B:269:TRP:CD1	6:B:497:TRP:CH2	2.82	0.67
6:B:646:TRP:CH2	6:B:726:ILE:HD13	2.28	0.67
7:C:55:GLU:C	7:C:57:ALA:H	1.98	0.67
20:A:7041:LMU:O6B	20:A:7041:LMU:C1B	2.42	0.67
17:N:67:LEU:CA	17:N:68:GLU:CG	2.71	0.67
19:J:1044:CLA:H93	19:J:1044:CLA:H41	1.76	0.67
19:K:1085:CLA:O2A	19:K:1085:CLA:H43	1.93	0.67
18:R:26:UNK:O	18:R:27:UNK:C	2.42	0.67
14:J:10:VAL:CG1	14:J:11:ALA:N	2.57	0.67
15:K:4:GLY:HA2	15:K:7:THR:HB	1.75	0.67
6:B:160:LYS:HZ3	6:B:160:LYS:HB2	1.58	0.67
6:B:160:LYS:HE3	6:B:161:TRP:CD2	2.29	0.67
19:B:1735:CLA:H191	10:F:104:TYR:CB	2.20	0.67
6:B:290:MET:HA	19:B:1751:CLA:CAC	2.23	0.67
7:C:66:ARG:NH2	7:C:66:ARG:HG2	1.95	0.67
8:D:91:ARG:HH12	8:D:119:TYR:HE1	1.39	0.67
20:A:7020:LMU:O2'	20:A:7020:LMU:H5'	1.92	0.67
10:F:52:ARG:NH1	10:F:55:ASN:OD1	2.28	0.67
16:L:113:SER:O	16:L:116:PRO:HD2	1.93	0.67
10:F:15:ALA:O	10:F:18:GLU:HB2	1.94	0.67
5:A:263:ALA:O	5:A:264:GLU:HG3	1.95	0.67
5:A:382:TYR:CE2	19:A:1784:CLA:HED3	2.29	0.67
5:A:603:PHE:HZ	5:A:693:LEU:HD21	1.60	0.67
5:A:88:ILE:HG22	5:A:89:ILE:N	2.09	0.67
19:B:1787:CLA:HHB	19:B:1787:CLA:C4	2.23	0.67
6:B:178:HIS:O	6:B:180:SER:N	2.27	0.67
8:D:39:LYS:CD	8:D:42:VAL:CG1	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:HD12	17:N:63:ASP:HB2	1.74	0.67
15:K:69:ILE:HA	15:K:72:VAL:CG1	2.23	0.67
7:C:12:ILE:HB	7:C:38:GLN:O	1.95	0.67
5:A:720:THR:HG22	5:A:720:THR:O	1.94	0.67
12:H:67:TYR:O	12:H:70:ALA:O	2.13	0.67
2:2:126:PRO:CD	2:2:129:LYS:HB2	2.25	0.67
19:A:1790:CLA:C3D	19:A:1791:CLA:HAC1	2.24	0.67
5:A:408:VAL:HG11	5:A:602:LEU:HD23	1.76	0.67
5:A:436:LEU:O	5:A:439:ARG:HB3	1.95	0.67
6:B:127:ILE:CD1	6:B:193:HIS:CE1	2.78	0.67
19:B:1764:CLA:HMB3	19:B:1767:CLA:HED3	1.77	0.67
22:B:1779:BCR:H333	19:F:1156:CLA:HHB	1.76	0.67
19:B:1786:CLA:H91	19:B:1787:CLA:C9	2.24	0.67
6:B:273:VAL:O	6:B:277:HIS:HD2	1.76	0.67
11:G:28:ARG:NH2	11:G:29:GLU:O	2.28	0.67
22:L:1170:BCR:C38	22:L:1170:BCR:H23C	2.25	0.67
19:A:1815:CLA:HAA2	19:A:1815:CLA:O1D	1.94	0.67
18:R:26:UNK:O	18:R:28:UNK:N	2.27	0.67
6:B:426:SER:O	6:B:430:GLY:N	2.26	0.67
5:A:107:GLU:OE1	5:A:161:GLU:CG	2.43	0.67
19:A:1790:CLA:O1A	19:A:1791:CLA:HBC3	1.94	0.67
19:A:1812:CLA:CED	19:A:1812:CLA:CAD	2.72	0.67
6:B:347:LEU:HD21	6:B:351:HIS:HE1	1.60	0.67
6:B:612:SER:HA	6:B:615:TYR:CE1	2.23	0.67
19:F:1157:CLA:CED	19:F:1157:CLA:CAD	2.73	0.67
19:A:1817:CLA:O1D	19:A:1817:CLA:CBA	2.43	0.67
4:4:38:ARG:HH11	4:4:38:ARG:CG	2.01	0.67
4:4:192:THR:HG22	4:4:193:ILE:H	1.58	0.67
6:B:98:GLN:O	6:B:100:ALA:N	2.28	0.67
12:H:10:ASP:HB3	12:H:13:ASP:HB2	1.75	0.67
3:3:107:TRP:CD1	3:3:108:ALA:CA	2.77	0.67
5:A:170:GLY:O	5:A:173:VAL:CG2	2.40	0.67
5:A:491:TRP:NE1	19:A:1792:CLA:H12	2.10	0.67
19:A:1800:CLA:H152	22:L:1170:BCR:H352	1.76	0.67
6:B:469:LYS:HE2	6:B:471:THR:OG1	1.94	0.67
6:B:633:ASN:ND2	6:B:636:THR:HB	2.09	0.67
7:C:2:SER:O	7:C:3:HIS:ND1	2.28	0.67
15:K:31:ASN:H	15:K:32:ARG:HH11	1.39	0.67
19:2:1220:CLA:C6	3:3:140:LYS:HZ3	2.07	0.67
17:N:62:SER:HB2	17:N:66:ASP:OD1	1.95	0.67
19:1:1192:CLA:H61	19:1:1192:CLA:H122	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:694:ARG:HE	16:L:105:ALA:HA	1.60	0.67
19:A:1776:CLA:H61	22:A:1806:BCR:H19C	1.76	0.67
19:A:1781:CLA:O1A	19:A:1781:CLA:C2	2.41	0.67
19:A:1812:CLA:C1	6:B:616:LEU:HG	2.22	0.67
5:A:397:THR:HB	5:A:613:ILE:CD1	2.25	0.67
6:B:178:HIS:C	6:B:180:SER:H	1.96	0.67
6:B:598:HIS:HB3	6:B:602:TRP:CZ3	2.30	0.67
6:B:689:ASN:O	6:B:691:ILE:N	2.27	0.67
8:D:28:ILE:CG2	8:D:67:ILE:HG13	2.25	0.67
22:I:1032:BCR:C2	19:I:1033:CLA:CAC	2.72	0.67
16:L:25:THR:O	16:L:28:THR:HB	1.94	0.67
19:K:1085:CLA:O2A	19:K:1085:CLA:C4	2.42	0.67
6:B:154:TRP:HD1	6:B:158:GLN:HG2	1.58	0.67
2:2:114:LEU:O	2:2:116:PRO:HD3	1.94	0.67
12:H:74:GLN:OE1	12:H:74:GLN:O	2.13	0.67
5:A:164:LEU:HA	5:A:167:THR:HG23	1.75	0.67
19:A:1788:CLA:O1A	19:A:1800:CLA:C1	2.43	0.67
19:A:1764:CLA:H43	22:A:1807:BCR:H383	1.77	0.67
19:B:1755:CLA:HED2	19:B:1756:CLA:HMD1	1.76	0.67
6:B:390:GLY:HA3	22:B:1777:BCR:HC22	1.76	0.67
16:L:13:PRO:O	16:L:14:LEU:HB2	1.95	0.67
8:D:31:GLY:HA3	16:L:23:LEU:HD21	1.77	0.67
17:N:40:CYS:N	17:N:41:LYS:HA	2.10	0.67
17:N:80:ASN:OD1	17:N:82:PHE:HA	1.95	0.67
3:3:47:GLY:O	3:3:49:ILE:N	2.27	0.67
19:A:1787:CLA:C4	16:L:33:ILE:HG12	2.24	0.67
19:A:1812:CLA:H92	19:A:1812:CLA:H122	1.77	0.67
5:A:368:LEU:HD21	19:A:1774:CLA:H91	1.69	0.67
6:B:576:PHE:HE2	19:B:1759:CLA:HAC1	1.59	0.67
6:B:81:PRO:HG2	6:B:360:PHE:CD1	2.30	0.67
7:C:66:ARG:HH21	7:C:66:ARG:CG	2.03	0.67
19:2:1220:CLA:H62	3:3:140:LYS:CE	2.24	0.67
3:3:63:ARG:NH1	3:3:185:LYS:O	2.28	0.67
20:A:7043:LMU:H62	20:A:7043:LMU:H111	1.76	0.67
3:3:173:GLU:CG	3:3:174:LYS:N	2.57	0.67
4:4:52:MET:HG3	4:4:160:MET:CG	2.22	0.66
5:A:708:VAL:HA	5:A:711:HIS:CD2	2.30	0.66
6:B:418:ILE:O	6:B:422:LEU:HD12	1.94	0.66
10:F:140:ALA:O	10:F:144:LEU:HB3	1.96	0.66
16:L:65:VAL:C	16:L:67:PRO:HD2	2.14	0.66
3:3:97:PHE:O	3:3:98:ILE:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:108:ARG:NH2	19:2:1224:CLA:O1D	2.28	0.66
3:3:106:TYR:CG	3:3:107:TRP:CD1	2.84	0.66
5:A:114:THR:CG2	5:A:115:HIS:CE1	2.75	0.66
19:B:1739:CLA:CMC	22:B:1780:BCR:H282	2.25	0.66
19:B:1740:CLA:H12	19:B:1740:CLA:HAA1	1.76	0.66
6:B:190:TRP:HE3	19:B:1744:CLA:CBB	2.08	0.66
5:A:555:ILE:HG23	19:B:1787:CLA:OBD	1.95	0.66
6:B:267:SER:HA	6:B:356:PRO:O	1.95	0.66
7:C:70:TRP:O	7:C:72:GLU:CB	2.43	0.66
2:2:49:LEU:HB3	19:2:1215:CLA:HAC2	1.76	0.66
4:4:108:ASP:N	19:4:1196:CLA:HMA2	2.08	0.66
5:A:425:THR:O	5:A:427:ARG:NE	2.28	0.66
6:B:692:ARG:HH22	6:B:694:ARG:HG2	1.60	0.66
5:A:129:GLN:O	5:A:130:GLU:HB2	1.95	0.66
19:A:1785:CLA:C10	19:A:1785:CLA:H152	2.26	0.66
5:A:216:LEU:HD12	22:A:1803:BCR:C35	2.25	0.66
19:A:1811:CLA:CHD	19:A:1811:CLA:HBC3	2.25	0.66
5:A:370:ILE:HD12	19:A:1781:CLA:O1D	1.94	0.66
5:A:660:GLN:O	5:A:661:ALA:CB	2.42	0.66
6:B:127:ILE:CD1	6:B:193:HIS:HE1	2.08	0.66
19:B:1746:CLA:CHD	19:B:1746:CLA:CBC	2.74	0.66
19:B:1748:CLA:CGA	19:B:1748:CLA:C3A	2.73	0.66
17:N:40:CYS:H	17:N:41:LYS:HA	1.59	0.66
21:B:8052:SUC:O4'	21:B:8052:SUC:H2	1.96	0.66
19:A:1815:CLA:HMA1	19:A:1815:CLA:C6	2.24	0.66
20:A:7026:LMU:C4	20:A:7026:LMU:C8	2.65	0.66
17:N:33:TYR:O	17:N:34:THR:HG22	1.96	0.66
5:A:629:ASN:HD21	5:A:633:VAL:HG23	1.59	0.66
5:A:539:PHE:HD2	5:A:539:PHE:O	1.78	0.66
5:A:173:VAL:HG23	5:A:174:PHE:HD1	1.61	0.66
5:A:578:ARG:O	5:A:579:PHE:CD1	2.49	0.66
19:B:1736:CLA:HBC3	19:B:1759:CLA:H51	1.77	0.66
6:B:349:ALA:HB2	6:B:375:HIS:HB3	1.78	0.66
7:C:55:GLU:O	7:C:57:ALA:N	2.21	0.66
19:1:1192:CLA:HHD	19:1:1192:CLA:HBC3	1.76	0.66
20:A:1810:LMU:H5'	20:A:1810:LMU:O5B	1.94	0.66
12:H:63:SER:O	12:H:67:TYR:HB2	1.95	0.66
3:3:114:PHE:CD1	19:3:1216:CLA:CHA	2.79	0.66
3:3:84:ILE:N	19:A:1798:CLA:H43	2.10	0.66
5:A:154:ARG:HH21	5:A:233:LEU:HD13	1.60	0.66
5:A:229:ILE:CG1	5:A:243:PRO:HB3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1780:BCR:H19C	19:B:1786:CLA:C15	2.23	0.66
6:B:187:SER:O	6:B:189:ALA:N	2.28	0.66
6:B:203:ARG:H	6:B:270:LEU:HD11	1.60	0.66
6:B:292:ARG:NH2	6:B:297:ILE:HG13	2.10	0.66
6:B:649:MET:O	6:B:653:GLY:N	2.27	0.66
7:C:73:THR:N	7:C:76:SER:OG	2.29	0.66
9:E:87:VAL:O	9:E:89:GLU:N	2.27	0.66
19:H:1079:CLA:HBB2	13:I:13:GLY:C	2.15	0.66
17:N:45:ASN:HD21	17:N:54:LYS:HB2	1.51	0.66
17:N:70:GLU:HB3	17:N:72:LYS:CA	2.25	0.66
4:4:118:ASP:O	4:4:122:LYS:HA	1.96	0.66
16:L:161:LEU:HD11	16:L:162:ASP:C	2.15	0.66
15:K:71:GLY:O	15:K:72:VAL:C	2.31	0.66
5:A:255:LEU:CD1	5:A:280:PHE:HZ	2.09	0.66
5:A:636:HIS:O	5:A:638:THR:N	2.29	0.66
6:B:141:PHE:HA	6:B:144:PHE:CD1	2.31	0.66
7:C:74:THR:O	7:C:76:SER:N	2.28	0.66
8:D:39:LYS:NZ	8:D:43:GLU:OE2	2.28	0.66
19:A:1788:CLA:C15	22:L:1169:BCR:C36	2.74	0.66
16:L:69:VAL:HG11	16:L:84:GLY:N	2.10	0.66
19:R:1054:CLA:H2A	19:R:1054:CLA:O1A	1.94	0.66
20:A:7026:LMU:H52	20:A:7026:LMU:C1	2.22	0.66
17:N:18:ASP:HB2	17:N:22:LEU:CD1	2.24	0.66
5:A:68:THR:C	5:A:70:ASP:H	1.99	0.66
5:A:123:VAL:HG22	5:A:133:ASN:OD1	1.94	0.66
19:A:1812:CLA:HMB3	19:B:1785:CLA:C18	2.24	0.66
6:B:292:ARG:NH2	6:B:297:ILE:H	1.94	0.66
7:C:1:MET:CB	7:C:4:SER:HG	1.92	0.66
10:F:147:GLY:HA2	10:F:150:VAL:HB	1.78	0.66
16:L:10:VAL:O	16:L:10:VAL:CG2	2.44	0.66
17:N:61:LEU:O	17:N:62:SER:HB2	1.93	0.66
20:A:7016:LMU:H112	20:A:7016:LMU:H71	1.78	0.66
19:K:1085:CLA:C3A	19:K:1085:CLA:O1A	2.32	0.66
6:B:247:THR:CG2	6:B:250:ALA:HB3	2.25	0.66
8:D:126:GLY:C	8:D:127:ARG:HG2	2.15	0.66
5:A:160:SER:HB2	5:A:163:GLN:OE1	1.96	0.66
5:A:302:HIS:HB2	19:A:1773:CLA:C1B	2.25	0.66
19:A:1777:CLA:H2A	19:A:1777:CLA:O1D	1.95	0.66
19:A:1781:CLA:C3B	22:A:1806:BCR:H373	2.26	0.66
5:A:206:HIS:C	5:A:211:LEU:HD23	2.16	0.66
5:A:624:VAL:O	5:A:636:HIS:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:55:ALA:HB1	6:B:150:LEU:CD1	2.26	0.66
6:B:595:HIS:CD2	6:B:623:TYR:OH	2.49	0.66
11:G:49:THR:OG1	11:G:50:ARG:N	2.29	0.66
19:A:1816:CLA:HED3	19:A:1816:CLA:O1A	1.96	0.66
17:N:62:SER:HB3	17:N:66:ASP:OD1	1.89	0.66
19:K:1146:CLA:O1A	19:K:1146:CLA:H2A	1.95	0.66
10:F:22:LEU:O	10:F:24:LYS:N	2.28	0.66
19:3:1219:CLA:O1A	19:3:1219:CLA:CMA	2.43	0.66
21:B:8059:SUC:C1'	21:B:8059:SUC:HO2	2.07	0.66
4:4:91:PHE:CD1	19:4:1205:CLA:C3C	2.79	0.66
5:A:118:PRO:HB3	5:A:150:PHE:CE2	2.31	0.66
5:A:691:MET:CE	23:A:1802:PQN:H2M2	2.26	0.66
5:A:207:LEU:HA	5:A:211:LEU:CG	2.25	0.66
5:A:244:LEU:HB2	5:A:247:GLU:HB2	1.77	0.66
6:B:124:TRP:CD1	6:B:124:TRP:O	2.48	0.66
9:E:65:VAL:HG13	9:E:82:TYR:O	1.95	0.66
11:G:24:PHE:CE1	11:G:27:GLN:O	2.49	0.66
3:3:93:PHE:HD2	3:3:95:THR:H	1.41	0.66
17:N:44:GLU:O	17:N:46:PHE:N	2.29	0.66
17:N:49:CYS:C	17:N:51:ASP:O	2.34	0.66
17:N:65:LEU:O	17:N:67:LEU:N	2.29	0.66
19:K:1085:CLA:C3A	19:K:1085:CLA:CGA	2.73	0.66
6:B:247:THR:C	6:B:250:ALA:HB2	2.15	0.66
20:A:7038:LMU:H1B	20:A:7038:LMU:C6'	2.26	0.66
5:A:631:GLN:HG3	5:A:631:GLN:O	1.96	0.66
26:B:8057:UNL:C6	26:B:8057:UNL:C2	2.65	0.66
19:A:1764:CLA:HMC3	19:A:1765:CLA:HHD	1.76	0.66
19:A:1776:CLA:H8	22:A:1806:BCR:H19C	1.76	0.66
5:A:615:HIS:ND1	19:A:1792:CLA:HBC3	2.10	0.66
5:A:206:HIS:O	5:A:211:LEU:HD23	1.96	0.66
5:A:374:GLN:O	5:A:377:TYR:HD2	1.79	0.66
7:C:79:LEU:CD2	7:C:81:TYR:C	2.64	0.66
8:D:101:TYR:CD1	8:D:114:PRO:HD3	2.30	0.66
8:D:44:GLU:CB	8:D:46:TYR:HE2	2.05	0.66
9:E:89:GLU:HG2	9:E:92:ALA:H	1.61	0.66
22:I:1032:BCR:C27	22:I:1032:BCR:H403	2.19	0.66
16:L:36:TYR:O	16:L:37:LEU:HB3	1.95	0.66
20:A:7042:LMU:O6'	20:A:7042:LMU:H32	1.92	0.66
19:2:1215:CLA:C4	19:2:1220:CLA:HBC3	2.24	0.66
17:N:69:CYS:O	17:N:72:LYS:CE	2.44	0.66
21:B:8052:SUC:O4'	21:B:8052:SUC:C2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7037:LMU:C1	20:A:7037:LMU:H61	2.25	0.66
2:2:131:THR:HG23	2:2:132:GLY:H	1.60	0.66
5:A:606:TYR:O	5:A:610:SER:CB	2.43	0.65
6:B:336:LEU:HD13	19:B:1754:CLA:HBB1	1.78	0.65
17:N:58:VAL:O	17:N:60:PHE:N	2.29	0.65
10:F:21:ALA:O	10:F:23:LYS:N	2.29	0.65
20:A:7022:LMU:H1B	20:A:7022:LMU:O2'	1.96	0.65
11:G:13:GLY:O	11:G:16:LEU:CB	2.44	0.65
10:F:151:ASP:C	10:F:154:PHE:HB3	2.15	0.65
20:A:7031:LMU:H4'	20:A:7031:LMU:O2B	1.94	0.65
19:A:1777:CLA:HBC3	19:A:1779:CLA:HED1	1.77	0.65
19:A:1781:CLA:C4B	22:A:1806:BCR:C37	2.67	0.65
19:A:1781:CLA:C6	19:A:1782:CLA:HED2	2.24	0.65
5:A:328:LYS:O	5:A:330:ILE:N	2.30	0.65
6:B:388:ALA:O	6:B:391:PRO:HD2	1.94	0.65
6:B:366:THR:HG23	6:B:729:THR:HG22	1.78	0.65
11:G:23:PHE:CD2	11:G:24:PHE:HB2	2.31	0.65
11:G:28:ARG:HG2	11:G:29:GLU:H	1.57	0.65
11:G:33:LYS:CA	11:G:33:LYS:HE3	2.16	0.65
22:I:1032:BCR:H311	22:I:1032:BCR:C8	2.24	0.65
16:L:128:ASP:OD2	16:L:129:GLN:N	2.27	0.65
16:L:60:HIS:HD2	19:L:1167:CLA:HED1	1.61	0.65
16:L:64:LEU:HD22	16:L:91:LEU:HD22	1.79	0.65
19:2:1213:CLA:HBC2	19:2:1213:CLA:CHD	2.21	0.65
17:N:80:ASN:OD1	17:N:82:PHE:N	2.30	0.65
17:N:82:PHE:O	17:N:84:LYS:N	2.30	0.65
5:A:95:GLY:H	19:A:1763:CLA:HMC3	1.60	0.65
19:A:1792:CLA:H2	19:A:1792:CLA:O1A	1.96	0.65
5:A:42:ARG:C	5:A:44:ILE:H	1.99	0.65
6:B:119:GLY:O	6:B:121:TYR:N	2.29	0.65
1:1:97:ILE:CG2	19:1:1197:CLA:HBB2	2.27	0.65
19:2:1215:CLA:C3	19:2:1220:CLA:HBC1	2.25	0.65
19:J:1044:CLA:C4A	19:J:1044:CLA:HBA2	2.25	0.65
3:3:52:LYS:O	3:3:56:TYR:CG	2.49	0.65
1:1:45:ILE:HD12	19:1:1195:CLA:CMD	2.25	0.65
3:3:107:TRP:CD1	3:3:108:ALA:HA	2.32	0.65
19:A:1776:CLA:CBC	19:A:1776:CLA:HMC1	2.25	0.65
19:A:1782:CLA:CBD	19:A:1782:CLA:HBA1	2.26	0.65
19:A:1782:CLA:HBC2	19:A:1782:CLA:CMC	2.18	0.65
5:A:679:PHE:CE2	5:A:683:HIS:HD2	2.14	0.65
19:B:1762:CLA:HBB2	22:B:1778:BCR:C26	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1756:CLA:HED1	19:B:1764:CLA:HBB1	1.77	0.65
6:B:293:THR:C	6:B:294:ASN:ND2	2.50	0.65
7:C:1:MET:N	7:C:4:SER:CB	2.60	0.65
7:C:74:THR:O	7:C:75:ARG:C	2.30	0.65
7:C:7:ILE:C	7:C:8:TYR:O	2.34	0.65
11:G:47:GLY:N	11:G:48:ASP:OD1	2.30	0.65
8:D:32:SER:H	16:L:23:LEU:HG	1.59	0.65
4:4:103:ILE:HG13	19:4:1197:CLA:HMD1	1.78	0.65
14:J:4:PHE:O	14:J:5:LYS:HB2	1.95	0.65
6:B:247:THR:HG23	6:B:250:ALA:HB3	1.77	0.65
6:B:20:ARG:HB3	6:B:20:ARG:HH11	1.60	0.65
11:G:83:TYR:O	11:G:83:TYR:CG	2.48	0.65
19:A:1783:CLA:H202	22:A:1808:BCR:C15	2.26	0.65
19:A:1791:CLA:O1A	19:A:1797:CLA:CBB	2.38	0.65
5:A:23:ASP:OD2	5:A:24:ARG:NH1	2.29	0.65
5:A:432:LEU:HA	5:A:435:VAL:HG13	1.78	0.65
6:B:174:ARG:HH11	19:B:1754:CLA:HMD1	1.60	0.65
6:B:349:ALA:CB	6:B:375:HIS:HB3	2.26	0.65
6:B:663:PHE:O	6:B:664:LEU:CB	2.33	0.65
6:B:646:TRP:CH2	6:B:726:ILE:HG21	2.32	0.65
12:H:69:SER:OG	19:H:1079:CLA:H2	1.96	0.65
14:J:2:ARG:NH1	14:J:8:LEU:HD13	2.04	0.65
19:2:1220:CLA:H91	3:3:137:SER:OG	1.97	0.65
17:N:61:LEU:HD21	17:N:63:ASP:C	2.16	0.65
17:N:65:LEU:HD23	17:N:66:ASP:N	2.10	0.65
19:J:1044:CLA:CED	19:J:1045:CLA:HMA3	2.24	0.65
19:J:1045:CLA:H2A	19:J:1045:CLA:H2	1.77	0.65
10:F:22:LEU:O	10:F:25:LEU:N	2.30	0.65
15:K:68:HIS:O	15:K:70:MET:N	2.29	0.65
12:H:50:ARG:HG2	16:L:137:ALA:HB1	1.77	0.65
15:K:27:ALA:HB3	15:K:28:PRO:CD	2.25	0.65
3:3:163:PHE:C	3:3:163:PHE:HD1	1.99	0.65
6:B:324:ASP:O	6:B:328:ASN:HB2	1.96	0.65
6:B:62:SER:OG	6:B:63:GLY:N	2.29	0.65
19:A:1776:CLA:HMD1	19:A:1777:CLA:HHD	1.79	0.65
5:A:81:ALA:CB	19:A:1760:CLA:HMA3	2.22	0.65
6:B:398:TYR:HD1	6:B:542:ARG:NH2	1.94	0.65
19:A:1812:CLA:H11	6:B:616:LEU:CG	2.23	0.65
7:C:60:THR:CG2	7:C:63:LEU:O	2.44	0.65
8:D:31:GLY:HA2	16:L:13:PRO:HB3	1.79	0.65
10:F:62:LEU:CG	10:F:72:ILE:HD13	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:10:PRO:HA	13:I:14:LEU:HB2	1.78	0.65
13:I:14:LEU:O	13:I:17:PRO:HD2	1.97	0.65
17:N:54:LYS:O	17:N:57:LYS:N	2.29	0.65
17:N:81:VAL:O	17:N:83:TRP:N	2.30	0.65
20:A:7033:LMU:C3'	20:A:7033:LMU:O6B	2.44	0.65
12:H:30:SER:O	12:H:31:PRO:O	2.13	0.65
20:2:7006:LMU:O5B	20:2:7006:LMU:C5'	2.42	0.65
19:A:1786:CLA:HMB2	19:A:1787:CLA:C1D	2.26	0.65
5:A:197:GLN:NE2	5:A:351:THR:HB	2.11	0.65
5:A:362:LEU:CB	5:A:410:ALA:HB2	2.26	0.65
19:B:1740:CLA:H91	22:B:1781:BCR:H361	1.77	0.65
22:B:1778:BCR:C39	10:F:90:PHE:HA	2.27	0.65
6:B:414:HIS:O	6:B:414:HIS:CG	2.50	0.65
6:B:551:LYS:CE	8:D:143:PRO:HA	2.26	0.65
18:R:36:UNK:O	18:R:38:UNK:N	2.30	0.65
7:C:14:CYS:O	7:C:14:CYS:SG	2.54	0.65
11:G:16:LEU:HA	11:G:68:ILE:HG13	1.77	0.65
23:A:1802:PQN:H142	22:B:1778:BCR:HC22	1.78	0.65
5:A:217:SER:CB	22:A:1803:BCR:H351	2.26	0.65
5:A:353:SER:HB2	5:A:356:ALA:HB3	1.79	0.65
6:B:131:THR:CB	6:B:134:ASP:HB2	2.11	0.65
19:B:1747:CLA:HBD	19:B:1756:CLA:HBB2	1.77	0.65
6:B:392:ILE:HD13	19:B:1759:CLA:CED	2.27	0.65
6:B:175:LEU:O	6:B:179:LEU:HG	1.96	0.65
8:D:102:ARG:HE	8:D:110:GLN:CB	2.08	0.65
10:F:123:VAL:HB	10:F:126:ALA:C	2.17	0.65
16:L:13:PRO:HG2	16:L:18:PRO:HB3	1.77	0.65
20:A:7021:LMU:O6'	20:A:7021:LMU:H12	1.96	0.65
10:F:42:ILE:C	10:F:43:LYS:HE3	2.17	0.65
12:H:54:LEU:HD13	12:H:55:LYS:HG3	1.78	0.65
8:D:93:LYS:CB	8:D:93:LYS:NZ	2.60	0.65
6:B:607:SER:HA	6:B:610:ASN:ND2	2.12	0.65
5:A:368:LEU:HD22	19:A:1774:CLA:H92	1.79	0.65
5:A:618:TRP:CZ2	5:A:655:ASP:CB	2.79	0.65
10:F:104:TYR:O	10:F:104:TYR:CD2	2.49	0.65
10:F:130:LEU:HD12	10:F:131:PHE:CD1	2.32	0.65
14:J:2:ARG:HH12	14:J:8:LEU:CD1	2.04	0.65
19:2:1220:CLA:H41	3:3:140:LYS:HE2	1.77	0.65
17:N:61:LEU:HD12	17:N:62:SER:O	1.95	0.65
17:N:2:VAL:O	17:N:2:VAL:HG23	1.97	0.65
3:3:84:ILE:H	19:A:1798:CLA:H43	1.56	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:158:ILE:HG22	19:A:1770:CLA:HED3	1.79	0.65
5:A:361:ASN:HD22	5:A:362:LEU:N	1.95	0.65
5:A:455:PHE:HD1	19:A:1788:CLA:CMA	2.10	0.65
5:A:705:GLU:HA	5:A:708:VAL:HB	1.79	0.65
5:A:98:PHE:O	5:A:99:HIS:HB2	1.96	0.65
19:B:1759:CLA:CBC	19:B:1759:CLA:CMC	2.57	0.65
6:B:493:TRP:HB3	19:B:1765:CLA:HED2	1.78	0.65
6:B:387:PHE:O	6:B:391:PRO:HD3	1.97	0.65
6:B:538:ALA:O	6:B:540:ASP:N	2.30	0.65
6:B:558:PRO:HG2	6:B:703:VAL:CB	2.21	0.65
7:C:7:ILE:HG22	7:C:65:VAL:HG21	1.76	0.65
9:E:40:ARG:HB2	9:E:42:GLU:OE2	1.97	0.65
19:1:1198:CLA:H91	19:1:1198:CLA:C12	2.26	0.65
21:B:8061:SUC:H1'2	21:B:8061:SUC:O5	1.96	0.65
6:B:224:PRO:HA	6:B:227:THR:OG1	1.97	0.65
19:A:1796:CLA:H192	14:J:19:PHE:CD2	2.32	0.64
5:A:281:LEU:O	5:A:283:PHE:N	2.29	0.64
5:A:334:HIS:HB3	19:A:1777:CLA:CMA	2.26	0.64
19:B:1742:CLA:H11	19:B:1742:CLA:H61	1.79	0.64
6:B:661:PHE:CB	19:B:1787:CLA:CMC	2.75	0.64
6:B:666:SER:O	6:B:667:TRP:HB2	1.96	0.64
6:B:551:LYS:HE2	8:D:143:PRO:HA	1.79	0.64
10:F:130:LEU:HD12	10:F:131:PHE:HD1	1.62	0.64
11:G:28:ARG:HH21	11:G:29:GLU:H	1.46	0.64
11:G:48:ASP:N	11:G:48:ASP:OD1	2.29	0.64
20:A:7042:LMU:H3'	20:A:7042:LMU:C2B	2.11	0.64
19:4:1198:CLA:O2D	19:4:1198:CLA:HAA1	1.96	0.64
19:K:1085:CLA:CHB	19:K:1142:CLA:OBD	2.46	0.64
2:2:128:ASN:HD21	14:J:4:PHE:H	1.44	0.64
2:2:120:ASN:HA	14:J:5:LYS:CG	2.27	0.64
8:D:60:MET:HG3	8:D:61:PRO:O	1.97	0.64
19:A:1763:CLA:HMB2	22:A:1808:BCR:HC7	1.79	0.64
19:A:1812:CLA:H91	19:A:1812:CLA:H152	1.78	0.64
5:A:544:ILE:O	5:A:548:THR:OG1	2.09	0.64
6:B:527:LEU:HD13	6:B:586:THR:HG21	1.78	0.64
6:B:625:TRP:HE3	6:B:626:LEU:N	1.95	0.64
6:B:708:VAL:O	6:B:710:LEU:O	2.16	0.64
8:D:118:VAL:CG1	8:D:119:TYR:N	2.59	0.64
8:D:113:HIS:CD2	8:D:118:VAL:HG21	2.32	0.64
16:L:40:LEU:HB3	16:L:41:PRO:CD	2.28	0.64
16:L:163:LEU:HD12	16:L:164:PRO:HB2	1.72	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:41:LYS:HB2	17:N:42:PHE:CA	2.25	0.64
4:4:126:LEU:H	4:4:127:PRO:HD3	1.61	0.64
11:G:93:TYR:N	11:G:94:ASP:OD1	2.29	0.64
20:A:7033:LMU:H3'	20:A:7033:LMU:O5B	1.78	0.64
21:3:1221:SUC:H4'	21:3:1221:SUC:O1'	1.96	0.64
10:F:151:ASP:O	10:F:154:PHE:CB	2.40	0.64
5:A:390:ALA:HB1	5:A:754:ILE:HD13	1.80	0.64
6:B:527:LEU:HB3	19:B:1755:CLA:C4C	2.27	0.64
22:B:1780:BCR:C35	19:B:1787:CLA:H111	2.27	0.64
6:B:424:TRP:CZ2	19:B:1761:CLA:HAC1	2.33	0.64
6:B:661:PHE:CB	19:B:1787:CLA:HMC1	2.27	0.64
20:A:7036:LMU:O5B	20:A:7036:LMU:H6E	1.95	0.64
20:A:7042:LMU:C1	20:A:7042:LMU:H71	2.26	0.64
18:R:38:UNK:C	18:R:39:UNK:O	2.45	0.64
19:2:1212:CLA:NA	19:2:1212:CLA:O1A	2.30	0.64
19:1:1200:CLA:CMC	19:1:1200:CLA:CBC	2.57	0.64
4:4:118:ASP:C	4:4:122:LYS:HA	2.18	0.64
16:L:48:ASN:HB3	16:L:49:PRO:CD	2.27	0.64
19:A:1759:CLA:O1D	19:A:1759:CLA:HBA2	1.96	0.64
5:A:453:LEU:HD23	19:A:1793:CLA:CBB	2.13	0.64
19:B:1735:CLA:CBC	22:B:1778:BCR:H332	2.28	0.64
19:B:1751:CLA:CHD	19:B:1751:CLA:CBC	2.65	0.64
9:E:36:VAL:C	9:E:49:VAL:HG13	2.18	0.64
9:E:35:LYS:CE	9:E:89:GLU:OE2	2.46	0.64
16:L:30:SER:HG	16:L:32:LEU:HB2	1.62	0.64
19:1:1197:CLA:HMD1	19:1:1197:CLA:OBD	1.96	0.64
2:2:68:LEU:HG	19:2:1217:CLA:H192	1.80	0.64
17:N:39:SER:OG	17:N:40:CYS:N	2.29	0.64
17:N:83:TRP:O	17:N:83:TRP:HE3	1.79	0.64
19:3:1217:CLA:C2A	19:3:3011:CLA:CBC	2.76	0.64
8:D:90:LEU:HD13	8:D:90:LEU:O	1.97	0.64
16:L:158:MET:SD	16:L:159:TYR:N	2.67	0.64
12:H:75:ASP:CG	12:H:77:LEU:HG	2.18	0.64
19:A:1770:CLA:CHC	22:A:1803:BCR:C18	2.75	0.64
5:A:401:TRP:O	5:A:405:PHE:HB2	1.97	0.64
6:B:171:ALA:O	6:B:172:GLU:HB2	1.98	0.64
19:B:1755:CLA:HMB3	22:B:1777:BCR:H351	1.79	0.64
19:B:1787:CLA:HED3	19:B:1787:CLA:CBA	2.28	0.64
6:B:334:LEU:CG	6:B:334:LEU:O	2.46	0.64
6:B:17:THR:HA	6:B:696:LYS:H	1.62	0.64
9:E:89:GLU:O	9:E:90:VAL:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:73:ILE:C	19:3:1215:CLA:C2D	2.65	0.64
3:3:205:GLY:CA	5:A:252:ARG:HH12	2.09	0.64
17:N:63:ASP:CA	17:N:64:ASP:O	2.40	0.64
15:K:69:ILE:O	15:K:70:MET:C	2.35	0.64
14:J:10:VAL:HG13	14:J:11:ALA:H	1.61	0.64
3:3:198:PHE:HA	3:3:201:ALA:CB	2.18	0.64
6:B:37:ILE:HD12	6:B:37:ILE:O	1.97	0.64
19:A:1760:CLA:HBC3	19:A:1760:CLA:HHD	1.78	0.64
19:A:1770:CLA:H2A	19:A:1770:CLA:HED2	1.80	0.64
19:A:1790:CLA:HMC1	19:A:1790:CLA:HBC3	1.79	0.64
5:A:302:HIS:HE1	19:A:1774:CLA:CHB	2.11	0.64
5:A:207:LEU:CD2	5:A:314:GLY:HA2	2.28	0.64
5:A:340:GLY:O	5:A:343:HIS:CB	2.43	0.64
19:B:1768:CLA:HHB	19:B:1769:CLA:OBD	1.97	0.64
19:B:1786:CLA:CBB	19:B:1787:CLA:CHB	2.73	0.64
19:J:1043:CLA:O2A	19:J:1043:CLA:C16	2.45	0.64
19:A:1817:CLA:O1D	19:A:1817:CLA:CAA	2.46	0.64
5:A:187:HIS:CE1	19:A:1767:CLA:C1A	2.67	0.64
19:A:1788:CLA:C14	19:A:1788:CLA:H101	2.28	0.64
19:A:1793:CLA:H11	19:A:1793:CLA:ND	2.12	0.64
6:B:545:LYS:HD3	6:B:546:LEU:H	1.61	0.64
19:I:1197:CLA:H41	19:I:1198:CLA:O1D	1.96	0.64
3:3:64:TYR:CB	19:3:1218:CLA:H41	2.15	0.64
4:4:75:TRP:HA	19:4:1204:CLA:CMD	2.27	0.64
12:H:45:ALA:HB3	12:H:46:PRO:HD3	1.78	0.64
1:1:185:TRP:O	1:1:186:HIS:ND1	2.30	0.64
19:3:3007:CLA:HAC2	19:K:3009:CLA:C9	2.28	0.64
12:H:63:SER:O	12:H:67:TYR:CB	2.46	0.64
3:3:87:GLU:CA	22:3:1220:BCR:H382	2.27	0.64
19:A:1784:CLA:CHD	22:A:1804:BCR:H333	2.28	0.64
19:A:1795:CLA:O1A	19:A:1795:CLA:C3	2.46	0.64
5:A:434:ARG:O	5:A:437:ARG:HB2	1.98	0.64
19:B:1771:CLA:HED1	24:B:1783:LMG:C21	2.28	0.64
5:A:668:TYR:CD1	6:B:445:ALA:HB2	2.33	0.64
6:B:577:TYR:HE2	6:B:578:LEU:HD12	1.63	0.64
22:B:1779:BCR:H333	19:F:1156:CLA:HMA1	1.79	0.64
10:F:153:ASN:C	10:F:153:ASN:ND2	2.48	0.64
11:G:28:ARG:NH2	11:G:29:GLU:H	1.95	0.64
11:G:7:VAL:HG23	11:G:8:ILE:N	2.12	0.64
19:3:3008:CLA:O2A	19:3:3008:CLA:H2A	1.96	0.64
17:N:77:CYS:O	17:N:79:SER:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:69:ILE:HG23	15:K:70:MET:N	2.13	0.64
4:4:91:PHE:CG	19:4:1205:CLA:C3C	2.81	0.64
5:A:631:GLN:O	20:A:1809:LMU:H6E	1.98	0.64
5:A:132:LEU:HD11	5:A:674:ALA:CB	2.27	0.64
5:A:40:PHE:CE1	5:A:53:TRP:CD1	2.76	0.64
6:B:366:THR:HG23	6:B:729:THR:CG2	2.28	0.64
6:B:535:VAL:HG13	6:B:536:LYS:N	2.13	0.64
6:B:556:SER:C	6:B:558:PRO:CD	2.62	0.64
10:F:125:LEU:O	10:F:126:ALA:HB2	1.98	0.64
17:N:59:PRO:C	17:N:66:ASP:OD1	2.37	0.64
19:4:4014:CLA:CB	19:4:4014:CLA:CMC	2.74	0.64
18:R:27:UNK:O	18:R:29:UNK:N	2.31	0.64
11:G:68:ILE:O	11:G:72:LEU:HB2	1.96	0.64
17:N:11:LYS:HG2	17:N:12:THR:N	2.13	0.64
17:N:24:THR:O	17:N:26:GLY:N	2.31	0.64
4:4:169:GLN:CD	19:4:1199:CLA:HAC2	2.19	0.64
5:A:101:ALA:O	5:A:104:SER:HA	1.98	0.64
19:A:1760:CLA:HBB2	19:A:1762:CLA:C4D	2.27	0.64
19:A:1779:CLA:NC	22:A:1805:BCR:H17C	2.12	0.64
19:A:1796:CLA:H142	19:A:1813:CLA:H143	1.80	0.64
19:A:1812:CLA:HED1	19:B:1785:CLA:H61	1.80	0.64
5:A:202:MET:HG3	19:A:1769:CLA:HBC2	1.79	0.64
5:A:207:LEU:O	5:A:310:PHE:CB	2.46	0.64
5:A:362:LEU:HD11	19:A:1785:CLA:HBB2	1.78	0.64
5:A:492:ILE:HA	5:A:495:THR:HG23	1.78	0.64
6:B:103:ALA:O	6:B:104:PHE:CB	2.34	0.64
5:A:131:ILE:HD13	6:B:447:GLY:N	2.13	0.64
6:B:73:ASN:HB3	6:B:76:ALA:HB3	1.78	0.64
11:G:28:ARG:HG3	11:G:29:GLU:CG	2.28	0.64
16:L:99:LEU:O	16:L:102:TYR:N	2.29	0.64
20:A:7016:LMU:C7	20:A:7016:LMU:C3	2.76	0.64
21:B:8060:SUC:C5	21:B:8060:SUC:C1'	2.75	0.64
11:G:16:LEU:HD23	11:G:68:ILE:HG21	1.81	0.64
14:J:10:VAL:HG13	14:J:11:ALA:N	2.13	0.64
5:A:126:ILE:HG12	19:A:1765:CLA:HMA3	1.80	0.63
19:A:1796:CLA:C6	19:A:1813:CLA:H193	2.27	0.63
5:A:360:ILE:HD13	22:A:1805:BCR:H371	1.79	0.63
5:A:700:TRP:CZ2	23:A:1802:PQN:H2M3	2.33	0.63
19:B:1756:CLA:H8	22:B:1777:BCR:H14C	1.79	0.63
6:B:292:ARG:HH22	6:B:297:ILE:HG13	1.62	0.63
7:C:55:GLU:C	7:C:57:ALA:N	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:46:TYR:HE1	8:D:80:LYS:CE	2.11	0.63
11:G:42:SER:OG	11:G:43:HIS:C	2.37	0.63
19:A:1815:CLA:HMA2	19:A:1815:CLA:H61	1.74	0.63
7:C:28:MET:HG2	7:C:38:GLN:HE21	1.63	0.63
6:B:216:LEU:O	6:B:218:TYR:N	2.31	0.63
3:3:163:PHE:C	3:3:163:PHE:CD1	2.72	0.63
5:A:418:MET:O	5:A:564:ARG:HD2	1.98	0.63
10:F:11:SER:OG	10:F:14:PHE:HB3	1.98	0.63
3:3:106:TYR:HB3	3:3:107:TRP:CD1	2.32	0.63
19:A:1763:CLA:CGA	19:A:1765:CLA:H12	2.28	0.63
5:A:281:LEU:HD13	19:A:1772:CLA:CED	1.04	0.63
5:A:360:ILE:O	5:A:361:ASN:CB	2.45	0.63
5:A:53:TRP:HA	5:A:56:ASN:CB	2.28	0.63
5:A:625:TRP:HB2	5:A:637:ILE:HD11	1.79	0.63
19:B:1742:CLA:CMC	22:B:1775:BCR:H373	2.27	0.63
19:B:1756:CLA:H71	22:B:1777:BCR:H14C	1.79	0.63
22:B:1780:BCR:C17	19:B:1786:CLA:H101	2.22	0.63
6:B:67:HIS:O	6:B:68:VAL:HG23	1.98	0.63
10:F:100:VAL:CA	10:F:103:SER:OG	2.45	0.63
10:F:123:VAL:HB	10:F:126:ALA:O	1.99	0.63
10:F:147:GLY:C	10:F:150:VAL:HB	2.19	0.63
10:F:62:LEU:CD2	10:F:72:ILE:HD13	2.28	0.63
16:L:128:ASP:CG	16:L:129:GLN:H	2.01	0.63
16:L:63:LEU:CD2	16:L:64:LEU:H	2.10	0.63
20:A:7042:LMU:C3	20:A:7042:LMU:O5'	2.46	0.63
17:N:41:LYS:CB	17:N:42:PHE:CB	2.55	0.63
19:J:1043:CLA:O1A	19:J:1043:CLA:H152	1.98	0.63
10:F:12:LYS:HG2	10:F:13:GLN:H	1.60	0.63
5:A:114:THR:CG2	5:A:115:HIS:ND1	2.59	0.63
5:A:205:HIS:CE1	19:A:1769:CLA:HMC2	2.33	0.63
5:A:229:ILE:HG12	5:A:243:PRO:HB3	1.80	0.63
6:B:203:ARG:HG2	6:B:204:GLY:H	1.63	0.63
6:B:79:GLN:O	6:B:80:ASP:HB3	1.96	0.63
8:D:36:LEU:HD12	8:D:78:ALA:H	1.63	0.63
9:E:44:TYR:HB3	9:E:45:TRP:CE3	2.33	0.63
19:J:1043:CLA:CGA	19:J:1043:CLA:C16	2.77	0.63
4:4:91:PHE:O	4:4:95:PHE:HD1	1.82	0.63
17:N:29:PHE:CE1	17:N:32:ALA:HB3	2.33	0.63
6:B:317:ARG:NE	6:B:317:ARG:CA	2.56	0.63
19:A:1783:CLA:H102	22:A:1807:BCR:C37	2.29	0.63
19:A:1793:CLA:O1A	19:A:1793:CLA:CHA	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:24:ARG:HG2	5:A:29:THR:HG21	1.81	0.63
5:A:308:ILE:CG2	5:A:309:LEU:N	2.61	0.63
19:B:1758:CLA:H142	22:B:1776:BCR:C10	2.24	0.63
5:A:547:PHE:HE2	19:B:1787:CLA:O1A	1.82	0.63
6:B:282:PHE:O	6:B:286:ILE:HG13	1.98	0.63
6:B:510:LEU:HD21	19:B:1767:CLA:HHD	1.80	0.63
5:A:558:LYS:NZ	6:B:674:LEU:HD23	2.14	0.63
8:D:79:ARG:O	8:D:82:GLN:HB2	1.98	0.63
5:A:249:ILE:C	5:A:251:ASN:H	2.00	0.63
3:3:180:LYS:O	3:3:182:LYS:N	2.31	0.63
20:A:7043:LMU:O3B	20:A:7043:LMU:C6B	2.45	0.63
5:A:520:LEU:O	5:A:522:ALA:N	2.27	0.63
5:A:455:PHE:HD1	19:A:1788:CLA:HMA2	1.63	0.63
5:A:284:ARG:HH12	5:A:507:ALA:HB1	1.63	0.63
5:A:530:LEU:HB2	5:A:531:PRO:HD2	1.81	0.63
5:A:612:VAL:O	5:A:615:HIS:HB3	1.98	0.63
5:A:618:TRP:CH2	5:A:655:ASP:HB2	2.34	0.63
6:B:193:HIS:HB2	19:B:1744:CLA:CHC	2.28	0.63
16:L:36:TYR:OH	19:L:1167:CLA:HBA2	1.97	0.63
16:L:99:LEU:HD11	22:L:1169:BCR:C31	2.28	0.63
17:N:72:LYS:N	17:N:72:LYS:HD2	2.07	0.63
10:F:20:GLN:CD	10:F:20:GLN:C	2.54	0.63
10:F:22:LEU:O	10:F:25:LEU:HD12	1.97	0.63
20:A:7010:LMU:O3'	20:A:7010:LMU:C1B	2.47	0.63
11:G:60:SER:CA	11:G:63:PRO:HD2	2.27	0.63
5:A:426:THR:HA	5:A:428:TYR:CZ	2.33	0.63
20:2:7006:LMU:C2	20:2:7006:LMU:C2'	2.77	0.63
18:R:7:UNK:O	18:R:10:UNK:CB	2.47	0.63
5:A:370:ILE:CD1	19:A:1781:CLA:C3D	2.75	0.63
6:B:178:HIS:HE1	19:B:1743:CLA:NC	1.97	0.63
19:B:1760:CLA:HMB2	19:B:1761:CLA:CHB	2.28	0.63
3:3:205:GLY:HA3	5:A:252:ARG:HH12	1.62	0.63
17:N:66:ASP:N	17:N:66:ASP:OD2	2.29	0.63
19:R:1054:CLA:NA	19:R:1054:CLA:HED3	2.11	0.63
6:B:224:PRO:CB	6:B:227:THR:HB	2.28	0.63
19:A:1774:CLA:H193	19:A:1774:CLA:H93	1.78	0.63
5:A:398:HIS:CD2	19:A:1783:CLA:ND	2.67	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	2.13	0.63
16:L:122:GLY:O	16:L:124:LYS:N	2.32	0.63
11:G:93:TYR:CA	11:G:94:ASP:CG	2.59	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:14:ILE:O	12:H:16:ASN:N	2.31	0.63
7:C:12:ILE:CB	7:C:39:ILE:HA	2.28	0.63
19:A:1765:CLA:HBD	19:A:1765:CLA:HBA2	1.80	0.63
19:A:1781:CLA:HMA3	19:A:1782:CLA:O1A	1.98	0.63
5:A:451:ILE:HD11	19:A:1788:CLA:HED1	1.79	0.63
5:A:281:LEU:O	5:A:282:THR:C	2.36	0.63
5:A:701:GLN:O	5:A:704:ILE:N	2.32	0.63
6:B:429:LEU:HB3	6:B:525:LEU:HB2	1.80	0.63
6:B:670:TYR:C	6:B:670:TYR:CD1	2.72	0.63
7:C:77:MET:O	7:C:79:LEU:N	2.29	0.63
19:2:1220:CLA:HBC3	19:2:1220:CLA:HHD	1.80	0.63
17:N:57:LYS:HG3	17:N:58:VAL:H	0.61	0.63
4:4:107:GLN:HB3	19:4:1196:CLA:HMA3	1.75	0.63
11:G:92:GLY:O	11:G:93:TYR:C	2.36	0.63
3:3:50:GLU:N	3:3:51:PRO:HD3	2.13	0.63
2:2:196:HIS:NE2	21:2:1226:SUC:O3	2.28	0.63
5:A:520:LEU:HD22	20:A:1809:LMU:O2'	1.98	0.63
19:A:1764:CLA:H142	22:A:1808:BCR:H14C	1.79	0.63
5:A:330:ILE:O	5:A:330:ILE:HG22	1.99	0.63
5:A:346:LEU:HD11	19:A:1779:CLA:CHD	2.29	0.63
6:B:438:VAL:CG2	19:B:1763:CLA:HAC1	2.29	0.63
6:B:458:ILE:HG23	19:B:1768:CLA:CMD	2.29	0.63
6:B:545:LYS:CG	6:B:546:LEU:N	2.61	0.63
6:B:704:GLN:O	6:B:708:VAL:HG23	1.99	0.63
6:B:25:ILE:CB	22:L:1169:BCR:H292	2.28	0.63
19:L:1167:CLA:CHC	22:L:1170:BCR:HC8	2.28	0.63
19:A:1816:CLA:O2A	19:A:1816:CLA:HED1	1.99	0.63
18:R:31:UNK:C	18:R:32:UNK:O	2.47	0.63
17:N:80:ASN:C	17:N:82:PHE:H	2.02	0.63
17:N:80:ASN:O	17:N:82:PHE:N	2.29	0.63
4:4:124:TYR:CB	4:4:143:PHE:CD1	2.80	0.63
2:2:54:TRP:CD1	19:2:1222:CLA:O1D	2.52	0.63
6:B:92:TRP:O	6:B:92:TRP:CD1	2.52	0.63
5:A:665:ILE:C	5:A:665:ILE:HD12	2.19	0.62
19:B:1747:CLA:CBD	19:B:1756:CLA:CBB	2.77	0.62
6:B:378:ILE:HG22	6:B:379:ALA:H	1.63	0.62
6:B:687:LEU:HD12	22:L:1170:BCR:HC31	1.81	0.62
7:C:62:PHE:CE1	9:E:42:GLU:HB2	2.34	0.62
19:B:1771:CLA:C19	13:I:21:MET:CB	2.76	0.62
19:4:1198:CLA:H2A	19:4:1198:CLA:CGD	2.18	0.62
1:1:160:GLY:O	1:1:162:CYS:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:7:THR:HA	15:K:10:ILE:HB	1.81	0.62
6:B:49:SER:O	6:B:52:GLY:N	2.33	0.62
5:A:195:TRP:CZ2	19:A:1766:CLA:CMA	2.80	0.62
5:A:24:ARG:C	5:A:25:ASP:O	2.33	0.62
5:A:599:PHE:CD2	5:A:735:VAL:HG21	2.35	0.62
5:A:664:VAL:CG2	5:A:665:ILE:HG23	2.29	0.62
23:B:1773:PQN:H162	22:B:1780:BCR:H332	1.64	0.62
19:B:1742:CLA:HMC1	22:B:1775:BCR:H373	1.80	0.62
6:B:269:TRP:HD1	6:B:497:TRP:CH2	2.17	0.62
6:B:371:LEU:HD21	19:B:1758:CLA:HED3	1.80	0.62
1:1:57:ILE:O	1:1:59:VAL:N	2.32	0.62
5:A:109:TRP:HA	5:A:116:ILE:HG13	1.81	0.62
5:A:174:PHE:O	5:A:175:ALA:HB2	1.98	0.62
19:A:1796:CLA:H62	19:A:1813:CLA:H171	1.80	0.62
19:A:1812:CLA:HED1	19:B:1785:CLA:H2	1.80	0.62
5:A:79:PHE:HE2	5:A:185:HIS:CG	2.17	0.62
6:B:77:TRP:CZ2	6:B:122:GLN:NE2	2.68	0.62
19:B:1771:CLA:CBC	19:B:1771:CLA:HMC1	2.27	0.62
6:B:661:PHE:HB3	19:B:1787:CLA:HBC3	1.81	0.62
19:F:1156:CLA:CHD	19:F:1156:CLA:HBC2	2.27	0.62
11:G:28:ARG:HA	19:G:1099:CLA:CMA	2.28	0.62
11:G:37:GLU:OE2	11:G:42:SER:N	2.32	0.62
13:I:24:LEU:C	13:I:26:LEU:N	2.51	0.62
16:L:64:LEU:HA	16:L:67:PRO:HG3	1.80	0.62
4:4:147:LEU:CD2	4:4:148:GLU:H	2.12	0.62
4:4:70:ILE:O	4:4:73:PRO:HD3	1.99	0.62
2:2:174:VAL:O	2:2:178:TRP:HD1	1.82	0.62
5:A:302:HIS:HB2	19:A:1773:CLA:CHB	2.28	0.62
19:A:1781:CLA:C3B	22:A:1806:BCR:C22	2.78	0.62
5:A:201:SER:O	5:A:204:ASN:HB2	1.99	0.62
5:A:23:ASP:CA	5:A:24:ARG:CD	2.63	0.62
5:A:393:LEU:HD11	5:A:750:PHE:CD1	2.33	0.62
22:B:1776:BCR:H331	22:B:1776:BCR:HC8	1.80	0.62
19:B:1768:CLA:C12	22:B:1779:BCR:C31	2.76	0.62
6:B:284:PHE:O	6:B:288:GLY:N	2.27	0.62
5:A:254:LEU:C	5:A:256:ALA:H	2.03	0.62
7:C:59:PRO:HB3	7:C:61:ASP:OD1	2.00	0.62
12:H:21:TRP:N	12:H:22:ASP:CB	2.61	0.62
3:3:59:ILE:O	3:3:63:ARG:HG3	1.99	0.62
7:C:28:MET:HB3	8:D:122:LYS:O	1.98	0.62
6:B:221:GLY:C	6:B:223:GLY:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:94:TYR:O	8:D:95:LYS:CB	2.48	0.62
19:A:1791:CLA:HAA2	19:A:1797:CLA:HBB2	1.81	0.62
19:A:1797:CLA:CHD	19:A:1797:CLA:CBC	2.77	0.62
19:A:1783:CLA:C18	22:A:1808:BCR:H17C	2.28	0.62
19:A:1812:CLA:C3B	6:B:589:TRP:CH2	2.78	0.62
5:A:377:TYR:CD1	5:A:616:PHE:HE1	2.18	0.62
19:B:1756:CLA:H41	19:B:1756:CLA:C7	2.29	0.62
19:B:1738:CLA:HBB2	19:B:1758:CLA:HHC	1.79	0.62
6:B:530:THR:HG22	19:B:1755:CLA:HMC1	1.80	0.62
6:B:53:GLN:C	6:B:55:ALA:N	2.53	0.62
7:C:73:THR:C	7:C:76:SER:OG	2.37	0.62
11:G:33:LYS:NZ	11:G:33:LYS:HA	2.14	0.62
22:L:1170:BCR:C23	22:L:1170:BCR:C38	2.76	0.62
3:3:104:TYR:HB2	3:3:106:TYR:H	1.64	0.62
19:A:1787:CLA:CBB	19:A:1793:CLA:H192	2.30	0.62
5:A:281:LEU:HG	5:A:282:THR:H	1.63	0.62
5:A:514:THR:HB	5:A:532:ILE:HG23	1.82	0.62
5:A:604:TRP:O	5:A:607:ASN:N	2.28	0.62
5:A:466:THR:HG22	19:B:1740:CLA:HHC	1.80	0.62
19:B:1743:CLA:C4	22:B:1775:BCR:H10C	2.27	0.62
22:B:1780:BCR:H382	22:B:1780:BCR:C23	2.11	0.62
6:B:374:HIS:HB2	19:B:1757:CLA:C4B	2.29	0.62
8:D:118:VAL:HG12	8:D:119:TYR:N	2.14	0.62
9:E:61:THR:HG22	9:E:62:ARG:N	2.11	0.62
13:I:22:ALA:O	13:I:23:SER:C	2.36	0.62
17:N:62:SER:CA	17:N:66:ASP:H	2.13	0.62
17:N:72:LYS:HZ3	17:N:74:LYS:CG	2.01	0.62
19:1:1187:CLA:HBC3	19:1:1187:CLA:HMC1	0.70	0.62
20:A:7032:LMU:C1B	20:A:7032:LMU:H32	2.25	0.62
12:H:25:GLY:CA	12:H:27:ASP:HB2	2.28	0.62
20:A:7010:LMU:C2B	20:A:7010:LMU:C3'	2.77	0.62
17:N:34:THR:C	17:N:36:GLU:H	2.02	0.62
15:K:27:ALA:CB	15:K:28:PRO:CD	2.78	0.62
6:B:42:LEU:O	6:B:43:TYR:C	2.36	0.62
1:1:61:GLU:HG2	1:1:61:GLU:O	1.98	0.62
19:A:1788:CLA:HAA1	22:L:1170:BCR:C13	2.29	0.62
19:A:1783:CLA:H72	22:A:1807:BCR:C37	2.20	0.62
5:A:308:ILE:HG22	5:A:309:LEU:H	1.64	0.62
5:A:553:VAL:O	5:A:557:LEU:N	2.29	0.62
5:A:705:GLU:CB	6:B:545:LYS:HZ2	2.12	0.62
10:F:103:SER:C	10:F:105:LEU:N	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1816:CLA:HAA1	19:A:1816:CLA:CED	2.28	0.62
20:A:7016:LMU:H1'	20:A:7016:LMU:H31	1.81	0.62
4:4:106:TRP:CE3	19:4:1207:CLA:HMA2	2.35	0.62
20:A:7043:LMU:C6	20:A:7043:LMU:H111	2.28	0.62
6:B:247:THR:HG23	6:B:250:ALA:CB	2.29	0.62
6:B:456:GLU:HG2	10:F:70:HIS:HB3	1.80	0.62
17:N:5:GLU:OE2	17:N:6:TYR:HB2	1.99	0.62
5:A:210:LEU:CD1	19:A:1769:CLA:CMB	2.75	0.62
5:A:445:HIS:O	5:A:446:LEU:HB2	1.99	0.62
5:A:555:ILE:CG2	19:B:1787:CLA:OBD	2.47	0.62
5:A:578:ARG:HA	5:A:595:TRP:HB2	1.80	0.62
5:A:690:LEU:CD2	6:B:661:PHE:HE1	2.13	0.62
5:A:707:ILE:C	5:A:711:HIS:CD2	2.73	0.62
6:B:334:LEU:CA	19:B:1737:CLA:HMD3	2.30	0.62
6:B:664:LEU:C	6:B:667:TRP:CZ3	2.69	0.62
6:B:697:PRO:CB	19:B:1770:CLA:HBC3	2.30	0.62
9:E:45:TRP:CZ3	9:E:78:SER:OG	2.53	0.62
17:N:81:VAL:O	17:N:82:PHE:C	2.38	0.62
10:F:40:LEU:HA	10:F:42:ILE:CG1	2.26	0.62
19:1:1193:CLA:H43	19:1:1193:CLA:CGA	2.29	0.62
5:A:66:SER:O	5:A:67:HIS:HB2	2.00	0.62
2:2:41:LEU:O	2:2:43:TRP:N	2.30	0.62
19:B:1746:CLA:HED2	19:B:1746:CLA:HBA1	1.81	0.62
5:A:709:TRP:CH2	6:B:417:ALA:HB2	2.35	0.62
7:C:62:PHE:CE2	8:D:137:ILE:HB	2.34	0.62
16:L:163:LEU:CD1	16:L:164:PRO:N	2.51	0.62
12:H:26:SER:C	12:H:27:ASP:O	2.33	0.62
4:4:151:GLU:HA	4:4:154:ILE:HG23	1.81	0.62
5:A:425:THR:OG1	5:A:428:TYR:HE1	1.74	0.62
19:A:1774:CLA:C20	19:A:1782:CLA:H3A	2.30	0.62
5:A:207:LEU:HB3	19:A:1776:CLA:HBB2	1.82	0.62
5:A:448:TRP:CD1	19:A:1788:CLA:HED2	2.35	0.62
5:A:270:PHE:CZ	19:A:1797:CLA:C2	2.83	0.62
10:F:84:ILE:O	10:F:87:GLY:N	2.26	0.62
16:L:30:SER:C	16:L:32:LEU:H	2.03	0.62
19:2:1213:CLA:H42	19:2:1213:CLA:C4C	2.29	0.62
12:H:16:ASN:HD22	12:H:19:GLY:HA2	1.65	0.62
10:F:151:ASP:HA	10:F:154:PHE:HB3	1.80	0.62
6:B:456:GLU:OE1	10:F:70:HIS:ND1	2.32	0.62
4:4:169:GLN:HE22	19:4:1199:CLA:HHD	1.62	0.61
22:A:1807:BCR:H353	19:A:1812:CLA:H41	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:633:ASN:ND2	6:B:636:THR:CB	2.62	0.61
6:B:658:ALA:O	6:B:661:PHE:HD2	1.83	0.61
8:D:48:ILE:CB	8:D:100:PHE:HB3	2.29	0.61
3:3:62:GLY:HA2	3:3:65:ALA:HB3	1.82	0.61
19:A:1765:CLA:H51	22:A:1808:BCR:H10C	1.83	0.61
5:A:401:TRP:HD1	19:A:1783:CLA:CHC	2.13	0.61
5:A:449:VAL:HG22	19:A:1794:CLA:HMC3	1.82	0.61
5:A:472:ARG:O	5:A:474:GLN:CG	2.47	0.61
5:A:697:ARG:HD3	6:B:566:GLY:O	2.00	0.61
6:B:555:TYR:CD2	6:B:573:TRP:HB2	2.34	0.61
6:B:732:LYS:CD	6:B:734:GLY:N	2.61	0.61
10:F:130:LEU:CD1	10:F:131:PHE:HD1	2.13	0.61
19:L:1167:CLA:CMC	19:L:1167:CLA:HBC3	2.30	0.61
16:L:30:SER:O	16:L:32:LEU:N	2.33	0.61
19:1:1191:CLA:HMC3	19:1:1194:CLA:HHD	1.77	0.61
19:1:1198:CLA:C9	19:1:1198:CLA:H121	2.30	0.61
2:2:52:SER:OG	2:2:169:LEU:HG	1.99	0.61
20:A:7020:LMU:H92	20:A:7020:LMU:C5	2.19	0.61
6:B:475:ASP:HA	6:B:480:SER:HA	1.80	0.61
6:B:31:PHE:HB2	6:B:42:LEU:CD1	2.29	0.61
5:A:58:HIS:HB3	19:A:1760:CLA:HBC1	1.80	0.61
5:A:25:ASP:CB	5:A:26:PRO:HG3	2.30	0.61
5:A:307:ALA:O	5:A:308:ILE:C	2.39	0.61
19:B:1747:CLA:HBD	19:B:1756:CLA:CBB	2.30	0.61
19:B:1753:CLA:CMC	19:B:1753:CLA:HBC2	2.30	0.61
19:B:1771:CLA:HMC3	19:B:1787:CLA:HMB3	1.83	0.61
6:B:447:GLY:O	6:B:449:PRO:HD3	2.00	0.61
6:B:622:ASP:HA	6:B:626:LEU:HB3	1.82	0.61
6:B:732:LYS:CG	6:B:733:PHE:O	2.43	0.61
14:J:20:GLY:O	14:J:21:SER:HB2	2.01	0.61
4:4:118:ASP:HB3	19:4:1200:CLA:HMB3	1.83	0.61
4:4:106:TRP:HE3	19:4:1207:CLA:CMA	2.13	0.61
20:A:7030:LMU:C2'	20:A:7030:LMU:C6'	2.64	0.61
7:C:29:ILE:CG2	8:D:126:GLY:HA2	2.29	0.61
5:A:224:HIS:CE1	19:A:1771:CLA:C4C	2.84	0.61
5:A:514:THR:HB	5:A:532:ILE:CG2	2.31	0.61
5:A:87:SER:OG	5:A:179:LEU:HB2	1.99	0.61
19:B:1753:CLA:HAA1	19:B:1753:CLA:C1	2.30	0.61
19:B:1756:CLA:C10	22:B:1777:BCR:H14C	2.31	0.61
19:B:1761:CLA:CHD	19:B:1761:CLA:HBC2	2.20	0.61
6:B:592:PHE:HA	6:B:721:TYR:OH	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:608:GLN:O	6:B:612:SER:HB3	1.99	0.61
6:B:689:ASN:OD1	6:B:689:ASN:N	2.32	0.61
9:E:32:ARG:HH22	9:E:53:VAL:HA	1.65	0.61
16:L:46:ALA:HB2	16:L:52:ARG:NH2	2.16	0.61
20:A:7036:LMU:H92	20:A:7036:LMU:H11	1.81	0.61
17:N:57:LYS:O	17:N:60:PHE:N	2.33	0.61
1:1:140:LEU:HG	1:1:142:GLU:H	1.65	0.61
3:3:52:LYS:CA	3:3:55:ALA:HB3	2.30	0.61
6:B:213:LEU:HD12	6:B:214:ASP:N	2.15	0.61
5:A:113:PRO:C	5:A:115:HIS:H	2.03	0.61
19:A:1768:CLA:C3D	19:A:1769:CLA:HMC3	2.31	0.61
19:A:1787:CLA:H92	19:A:1801:CLA:H2	1.81	0.61
19:A:1783:CLA:C17	22:A:1808:BCR:H17C	2.30	0.61
6:B:124:TRP:C	6:B:124:TRP:CD1	2.73	0.61
6:B:275:HIS:HD1	19:B:1747:CLA:HMB1	1.64	0.61
6:B:382:ILE:CG2	6:B:383:MET:N	2.53	0.61
6:B:433:THR:O	6:B:436:LEU:O	2.17	0.61
6:B:451:LYS:HD2	19:B:1763:CLA:O2D	2.00	0.61
9:E:73:ASN:ND2	9:E:75:ALA:H	1.99	0.61
5:A:249:ILE:CG1	5:A:250:LEU:N	2.48	0.61
17:N:65:LEU:HD21	17:N:66:ASP:O	2.00	0.61
4:4:124:TYR:HD2	4:4:144:ALA:H	1.49	0.61
19:J:1045:CLA:CGD	19:J:1045:CLA:O1A	2.48	0.61
12:H:14:ILE:O	12:H:14:ILE:HD13	2.00	0.61
6:B:475:ASP:CA	6:B:480:SER:HA	2.29	0.61
6:B:98:GLN:C	6:B:100:ALA:N	2.53	0.61
19:A:1779:CLA:C1B	22:A:1805:BCR:C15	2.79	0.61
6:B:560:ASP:CG	6:B:561:GLY:N	2.54	0.61
8:D:84:LEU:HD12	8:D:100:PHE:HZ	1.64	0.61
19:B:1768:CLA:CBC	10:F:83:PHE:HZ	2.13	0.61
19:G:1099:CLA:H3A	19:G:1099:CLA:O2A	2.00	0.61
17:N:58:VAL:C	17:N:60:PHE:H	2.04	0.61
17:N:73:ASP:N	17:N:73:ASP:OD1	2.32	0.61
5:A:210:LEU:HD13	19:A:1769:CLA:HHB	1.83	0.61
19:A:1781:CLA:H61	19:A:1782:CLA:HED2	1.82	0.61
5:A:508:THR:O	5:A:509:ALA:CB	2.49	0.61
6:B:130:ARG:CG	6:B:130:ARG:HH11	2.13	0.61
19:B:1755:CLA:H52	19:B:1769:CLA:CBD	2.30	0.61
7:C:74:THR:C	7:C:76:SER:H	2.01	0.61
6:B:697:PRO:O	7:C:79:LEU:HD11	2.00	0.61
8:D:78:ALA:O	8:D:79:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:158:TYR:OH	19:3:1213:CLA:C3B	2.49	0.61
4:4:193:ILE:HG22	4:4:194:VAL:H	1.66	0.61
6:B:216:LEU:HD21	6:B:221:GLY:CA	2.31	0.61
12:H:41:GLU:OE2	12:H:42:THR:OG1	2.16	0.61
6:B:211:ASN:HB2	6:B:214:ASP:HB3	1.82	0.61
19:A:1791:CLA:C3A	19:A:1797:CLA:CBB	2.79	0.61
5:A:360:ILE:O	5:A:361:ASN:HB3	2.01	0.61
6:B:462:TRP:HZ3	19:B:1764:CLA:CBC	2.13	0.61
19:B:1768:CLA:CGA	19:B:1768:CLA:C1A	2.79	0.61
19:B:1758:CLA:C14	22:B:1776:BCR:H10C	2.25	0.61
6:B:91:ILE:HD11	6:B:104:PHE:CD2	2.35	0.61
8:D:117:GLY:O	8:D:118:VAL:CG2	2.39	0.61
9:E:73:ASN:C	9:E:73:ASN:HD22	2.04	0.61
19:2:1215:CLA:H2	19:2:1218:CLA:HMD3	1.82	0.61
17:N:66:ASP:C	17:N:67:LEU:CG	2.69	0.61
17:N:5:GLU:CD	17:N:6:TYR:CD2	2.74	0.61
3:3:106:TYR:CD1	3:3:107:TRP:N	2.68	0.61
19:A:1781:CLA:CAA	19:A:1781:CLA:HED2	2.30	0.61
19:A:1796:CLA:C10	19:A:1813:CLA:H152	2.31	0.61
5:A:399:HIS:O	5:A:400:MET:HB2	1.98	0.61
5:A:39:HIS:O	5:A:40:PHE:HB3	2.01	0.61
5:A:581:CYS:CB	5:A:590:CYS:O	2.49	0.61
6:B:493:TRP:HH2	19:B:1765:CLA:HMA2	1.65	0.61
5:A:458:PHE:CD2	19:B:1786:CLA:CMB	2.83	0.61
5:A:462:ILE:HD11	19:B:1786:CLA:H72	1.80	0.61
6:B:715:VAL:HG23	6:B:719:PHE:HD2	1.64	0.61
7:C:60:THR:HG23	7:C:63:LEU:O	2.01	0.61
6:B:552:ASP:HA	8:D:144:ILE:HG22	1.81	0.61
9:E:41:ARG:HG3	9:E:46:PHE:CZ	2.36	0.61
5:A:105:ASN:HB2	5:A:140:PHE:HZ	1.66	0.61
19:A:1781:CLA:HAA2	19:A:1782:CLA:CAD	2.31	0.61
19:A:1782:CLA:HMC1	19:A:1782:CLA:HBC3	1.77	0.61
5:A:368:LEU:CD1	19:A:1782:CLA:C6	2.79	0.61
5:A:389:TYR:HE1	5:A:625:TRP:CD1	2.19	0.61
6:B:120:VAL:CA	6:B:123:TRP:HD1	2.09	0.61
6:B:143:LEU:C	6:B:145:LEU:H	2.03	0.61
19:B:1755:CLA:H11	19:B:1769:CLA:CBD	2.31	0.61
19:B:1755:CLA:CMB	22:B:1777:BCR:C35	2.77	0.61
5:A:604:TRP:HE1	19:B:1787:CLA:C1D	2.13	0.61
6:B:348:VAL:HG12	6:B:349:ALA:N	2.16	0.61
6:B:347:LEU:CD2	6:B:351:HIS:HE1	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:559:CYS:HB2	6:B:702:ILE:HD12	1.82	0.61
6:B:655:LEU:HD22	19:B:1771:CLA:CBB	2.29	0.61
6:B:707:LEU:HD12	6:B:711:VAL:HG21	1.80	0.61
8:D:102:ARG:NH2	8:D:109:VAL:O	2.34	0.61
17:N:72:LYS:CB	17:N:73:ASP:C	2.59	0.61
19:J:1045:CLA:C1	19:J:1045:CLA:H2A	2.30	0.61
20:A:7038:LMU:H62	20:A:7038:LMU:C10	2.30	0.61
12:H:39:PHE:O	12:H:40:PHE:CD1	2.53	0.61
2:2:196:HIS:CE1	21:2:1226:SUC:HO3	2.17	0.61
5:A:123:VAL:O	5:A:124:TRP:HB2	2.01	0.60
19:A:1783:CLA:H172	22:A:1808:BCR:C17	2.30	0.60
19:A:1787:CLA:H93	16:L:36:TYR:CE1	2.35	0.60
19:A:1795:CLA:H42	19:A:1795:CLA:O2A	2.00	0.60
5:A:446:LEU:CD1	5:A:554:LEU:HA	2.30	0.60
5:A:662:SER:HA	5:A:665:ILE:HD11	1.82	0.60
19:B:1756:CLA:C7	22:B:1777:BCR:H14C	2.31	0.60
6:B:467:HIS:NE2	19:B:1764:CLA:C1A	2.64	0.60
6:B:494:LEU:HD12	19:B:1765:CLA:HED1	1.83	0.60
19:B:1739:CLA:HMC1	22:B:1780:BCR:H282	1.82	0.60
18:R:41:UNK:CA	18:R:42:UNK:CB	2.77	0.60
19:2:1220:CLA:H62	3:3:140:LYS:NZ	2.16	0.60
19:J:1043:CLA:C2	19:J:1043:CLA:C16	2.76	0.60
3:3:173:GLU:HG2	3:3:174:LYS:N	2.08	0.60
1:1:44:LEU:HD22	1:1:154:ALA:HB3	1.82	0.60
10:F:17:ARG:HA	10:F:17:ARG:NE	2.15	0.60
2:2:148:TRP:O	2:2:150:SER:N	2.34	0.60
19:A:1800:CLA:H141	16:L:95:LEU:HD22	1.83	0.60
5:A:84:GLY:O	5:A:87:SER:O	2.19	0.60
6:B:51:PHE:CD1	19:B:1743:CLA:HED1	2.36	0.60
8:D:37:LEU:O	8:D:39:LYS:N	2.34	0.60
13:I:26:LEU:HD13	13:I:30:LYS:HB3	1.82	0.60
18:R:35:UNK:C	18:R:38:UNK:CB	2.79	0.60
4:4:150:LYS:HE3	4:4:150:LYS:H	1.66	0.60
19:J:1044:CLA:O1D	19:J:1045:CLA:H93	1.95	0.60
19:K:1146:CLA:CBC	19:K:1146:CLA:HMC1	2.20	0.60
20:A:7040:LMU:C1B	20:A:7040:LMU:H3O2	2.14	0.60
20:A:7028:LMU:H11	20:A:7028:LMU:O2'	2.00	0.60
6:B:500:ALA:HB2	6:B:508:LEU:HD22	1.83	0.60
5:A:158:ILE:CG2	19:A:1770:CLA:HED3	2.32	0.60
5:A:406:LEU:HD11	19:A:1762:CLA:HMB3	1.83	0.60
19:A:1779:CLA:HBC1	22:A:1805:BCR:C39	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1811:CLA:CAA	19:B:1785:CLA:HBB2	2.29	0.60
6:B:127:ILE:HG12	6:B:193:HIS:HE1	1.66	0.60
6:B:560:ASP:OD1	7:C:66:ARG:HB3	2.00	0.60
7:C:1:MET:H2	7:C:3:HIS:H	1.43	0.60
22:I:1032:BCR:C39	22:L:1169:BCR:H401	2.30	0.60
22:L:1170:BCR:C8	22:L:1170:BCR:C33	2.73	0.60
16:L:164:PRO:CB	16:L:165:TYR:HD2	2.01	0.60
17:N:54:LYS:CB	17:N:57:LYS:HE2	2.14	0.60
20:A:7016:LMU:H92	20:A:7016:LMU:H32	1.77	0.60
4:4:38:ARG:O	4:4:39:TRP:HD1	1.85	0.60
4:4:133:TYR:CD1	4:4:134:PRO:HD2	2.36	0.60
22:3:1220:BCR:C23	22:3:1220:BCR:C39	2.37	0.60
5:A:91:LEU:O	19:A:1763:CLA:CMC	2.49	0.60
5:A:346:LEU:O	5:A:347:TYR:HB2	2.01	0.60
5:A:389:TYR:CE1	5:A:625:TRP:CD1	2.89	0.60
19:B:1762:CLA:H71	22:B:1779:BCR:H402	1.84	0.60
6:B:646:TRP:O	6:B:649:MET:HB2	2.00	0.60
16:L:9:GLN:C	16:L:11:ILE:H	2.03	0.60
20:A:7023:LMU:H21	20:A:7023:LMU:H91	0.65	0.60
6:B:154:TRP:CD1	6:B:158:GLN:CG	2.85	0.60
19:A:1780:CLA:H112	19:A:1780:CLA:OBD	2.01	0.60
19:A:1786:CLA:HMB2	19:A:1787:CLA:C2D	2.30	0.60
5:A:22:VAL:HG13	5:A:23:ASP:N	2.15	0.60
5:A:370:ILE:CD1	19:A:1781:CLA:O1D	2.48	0.60
5:A:40:PHE:CZ	5:A:56:ASN:HB3	2.37	0.60
5:A:700:TRP:CZ3	19:A:1813:CLA:O1D	2.54	0.60
5:A:693:LEU:HD11	5:A:738:TYR:CD1	2.37	0.60
19:B:1739:CLA:CMC	22:B:1780:BCR:C28	2.79	0.60
6:B:651:LEU:HB3	19:B:1786:CLA:O2A	2.02	0.60
6:B:393:PHE:CD2	6:B:397:ASP:OD1	2.47	0.60
6:B:551:LYS:CG	6:B:552:ASP:H	2.14	0.60
6:B:534:LEU:HD21	6:B:579:ALA:CB	2.32	0.60
6:B:91:ILE:HG22	19:B:1740:CLA:CAD	2.31	0.60
5:A:257:GLN:O	5:A:258:LEU:HB2	2.02	0.60
5:A:261:SER:O	5:A:262:PHE:CD2	2.55	0.60
5:A:348:GLU:O	5:A:350:LEU:N	2.35	0.60
22:3:1220:BCR:H321	22:3:1220:BCR:HC8	1.84	0.60
5:A:664:VAL:HG23	5:A:665:ILE:HG23	1.82	0.60
6:B:190:TRP:HE3	19:B:1744:CLA:HBB2	1.65	0.60
6:B:8:PHE:O	6:B:35:ASP:CB	2.49	0.60
10:F:20:GLN:O	10:F:21:ALA:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:1056:LMU:H6'	20:R:1056:LMU:H1'	1.67	0.60
6:B:166:SER:O	6:B:168:PHE:N	2.33	0.60
5:A:81:ALA:HB1	19:A:1760:CLA:HMA3	1.78	0.60
19:A:1779:CLA:NC	22:A:1805:BCR:C19	2.56	0.60
19:A:1790:CLA:H2A	19:A:1790:CLA:O1D	2.00	0.60
19:B:1739:CLA:H142	19:B:1739:CLA:C10	2.31	0.60
19:A:1812:CLA:CED	19:B:1785:CLA:H2	2.31	0.60
6:B:464:GLN:HA	6:B:467:HIS:HB2	1.82	0.60
6:B:666:SER:HB3	6:B:671:TRP:NE1	2.12	0.60
9:E:37:LYS:HB2	9:E:49:VAL:HG22	1.82	0.60
5:A:714:LEU:HA	10:F:149:LEU:HD11	1.82	0.60
18:R:35:UNK:N	18:R:38:UNK:CB	2.65	0.60
19:2:1220:CLA:C7	3:3:140:LYS:HZ3	2.15	0.60
20:A:7033:LMU:C1B	20:A:7033:LMU:C6'	2.72	0.60
7:C:28:MET:SD	8:D:122:LYS:C	2.80	0.60
2:2:110:TRP:CE3	19:2:1222:CLA:HED1	2.37	0.60
19:A:1783:CLA:C4	19:A:1783:CLA:HBA1	2.29	0.60
5:A:229:ILE:CG2	5:A:229:ILE:O	2.49	0.60
6:B:412:LEU:O	6:B:415:LYS:HB3	2.02	0.60
6:B:593:TYR:O	6:B:596:TRP:O	2.19	0.60
6:B:652:PHE:O	6:B:656:VAL:HG23	2.00	0.60
19:2:1220:CLA:H62	3:3:140:LYS:HE2	1.83	0.60
20:A:7039:LMU:O2'	20:A:7039:LMU:H5'	2.02	0.60
6:B:482:ASN:OD1	6:B:485:ALA:HB2	2.01	0.60
10:F:151:ASP:OD2	10:F:154:PHE:CD1	2.54	0.60
19:1:1192:CLA:CBC	19:1:1192:CLA:CHD	2.76	0.60
19:A:1770:CLA:CMB	22:A:1803:BCR:H382	2.19	0.60
22:A:1807:BCR:H322	22:A:1808:BCR:H391	1.84	0.60
5:A:412:ALA:HA	5:A:598:VAL:HG21	1.83	0.60
5:A:697:ARG:C	5:A:699:TYR:H	2.04	0.60
5:A:708:VAL:CA	5:A:711:HIS:HD2	2.15	0.60
6:B:282:PHE:HE2	19:B:1746:CLA:H3A	1.66	0.60
6:B:661:PHE:HB2	19:B:1787:CLA:HMC1	1.81	0.60
11:G:26:PHE:HB2	11:G:27:GLN:NE2	2.16	0.60
4:4:122:LYS:HB2	4:4:143:PHE:HD2	1.66	0.60
4:4:122:LYS:CG	4:4:150:LYS:HD2	2.27	0.60
10:F:23:LYS:HB3	10:F:24:LYS:HZ3	1.67	0.60
10:F:10:GLU:OE1	10:F:11:SER:N	2.35	0.60
16:L:135:GLY:O	16:L:138:LYS:HG2	2.01	0.60
12:H:57:LEU:O	12:H:57:LEU:HD13	2.01	0.60
5:A:109:TRP:CH2	5:A:154:ARG:HD3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:122:VAL:HA	5:A:133:ASN:HD21	1.67	0.60
19:A:1760:CLA:HBA2	19:A:1767:CLA:H62	1.84	0.60
5:A:711:HIS:HB3	5:A:717:ALA:CB	2.32	0.60
19:B:1749:CLA:OBD	19:B:1752:CLA:CBC	2.48	0.60
22:B:1778:BCR:C37	10:F:93:ILE:HG22	2.31	0.60
6:B:53:GLN:HA	6:B:53:GLN:OE1	1.91	0.60
6:B:632:ILE:C	6:B:634:GLY:H	2.05	0.60
7:C:49:VAL:HG22	7:C:50:GLY:H	1.67	0.60
7:C:74:THR:O	7:C:77:MET:N	2.30	0.60
8:D:79:ARG:H	8:D:82:GLN:NE2	2.00	0.60
10:F:46:MET:O	10:F:48:LYS:N	2.35	0.60
4:4:193:ILE:HG22	4:4:194:VAL:N	2.17	0.60
19:1:1193:CLA:HAA2	19:1:1193:CLA:CGD	2.32	0.60
18:R:4:UNK:O	18:R:5:UNK:CB	2.50	0.60
6:B:439:HIS:CD2	6:B:453:ILE:HG22	2.37	0.60
3:3:181:LEU:HD13	3:3:184:VAL:HG21	1.82	0.60
6:B:40:GLY:HA2	6:B:165:VAL:HG23	1.82	0.60
5:A:174:PHE:O	5:A:175:ALA:CB	2.49	0.59
19:A:1765:CLA:HMC1	19:A:1765:CLA:HBC3	1.82	0.59
5:A:218:TRP:CA	19:A:1770:CLA:HBB2	2.31	0.59
5:A:736:THR:HG21	19:A:1785:CLA:H91	1.84	0.59
5:A:51:THR:HB	19:A:1795:CLA:HBB2	1.76	0.59
5:A:605:MET:HA	5:A:608:SER:HG	1.64	0.59
6:B:493:TRP:NE1	19:B:1746:CLA:HAC2	2.16	0.59
6:B:277:HIS:HE1	19:B:1748:CLA:NC	2.00	0.59
19:B:1738:CLA:C19	19:B:1757:CLA:H141	2.32	0.59
6:B:357:ALA:O	6:B:358:TYR:CD1	2.54	0.59
5:A:128:GLY:HA3	6:B:446:PHE:CD2	2.37	0.59
6:B:623:TYR:O	6:B:624:LEU:HB2	2.00	0.59
9:E:39:LEU:H	9:E:40:ARG:CZ	2.15	0.59
19:A:1800:CLA:H201	16:L:64:LEU:CD2	2.32	0.59
3:3:74:ALA:HB2	19:3:1215:CLA:C1D	2.32	0.59
11:G:94:ASP:H	11:G:95:PRO:HD2	1.66	0.59
21:B:8059:SUC:HO2	21:B:8059:SUC:C2'	2.13	0.59
8:D:87:GLY:N	8:D:90:LEU:HB3	2.17	0.59
15:K:1:ASP:CA	15:K:5:SER:HB3	2.25	0.59
19:2:1224:CLA:C19	19:2:1224:CLA:H152	2.22	0.59
5:A:535:GLY:O	5:A:539:PHE:HB2	2.01	0.59
6:B:498:LEU:O	6:B:498:LEU:HD12	2.02	0.59
19:A:1765:CLA:CHA	19:A:1765:CLA:HBA2	2.31	0.59
19:A:1793:CLA:CGA	19:A:1793:CLA:CHA	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1741:CLA:O2A	19:B:1741:CLA:HBD	2.01	0.59
6:B:305:LEU:HD22	19:B:1753:CLA:O1D	2.02	0.59
19:B:1757:CLA:HMC1	19:B:1757:CLA:HBC3	1.84	0.59
10:F:103:SER:O	10:F:105:LEU:N	2.34	0.59
19:2:1213:CLA:H2A	19:2:1213:CLA:O1D	2.02	0.59
17:N:39:SER:O	17:N:40:CYS:CB	2.49	0.59
10:F:22:LEU:CA	10:F:25:LEU:HD13	2.32	0.59
21:B:8056:SUC:H1	21:B:8056:SUC:C5'	2.31	0.59
20:A:7021:LMU:C4	20:A:7021:LMU:C6'	2.75	0.59
9:E:56:ASP:HB2	9:E:64:PRO:CB	2.29	0.59
13:I:2:ILE:HG12	13:I:3:ASN:ND2	2.17	0.59
11:G:71:VAL:O	11:G:73:ALA:O	2.20	0.59
19:A:1772:CLA:H2A	19:A:1772:CLA:O2D	1.97	0.59
19:A:1795:CLA:ND	19:B:1735:CLA:HMC3	2.17	0.59
6:B:352:MET:SD	19:B:1758:CLA:OBD	2.60	0.59
6:B:707:LEU:O	6:B:710:LEU:HB3	2.02	0.59
19:G:1099:CLA:HBD	19:G:1099:CLA:HAA2	1.84	0.59
13:I:11:LEU:HG	22:I:1032:BCR:HC7	1.80	0.59
8:D:75:LEU:HD21	16:L:19:PHE:CZ	2.36	0.59
4:4:117:GLN:O	4:4:123:GLN:HA	2.01	0.59
17:N:4:GLU:CD	17:N:5:GLU:HB2	2.22	0.59
6:B:154:TRP:CD1	6:B:158:GLN:HG2	2.37	0.59
3:3:141:GLN:HG2	3:3:142:TYR:N	2.16	0.59
19:A:1771:CLA:HAA1	19:A:1771:CLA:HED2	1.84	0.59
19:A:1773:CLA:H52	19:A:1790:CLA:HBA1	1.84	0.59
5:A:636:HIS:C	5:A:638:THR:H	2.05	0.59
5:A:684:PHE:CD2	5:A:685:VAL:N	2.70	0.59
5:A:737:HIS:HA	5:A:740:LEU:HD23	1.83	0.59
6:B:194:LEU:O	6:B:198:ALA:HB3	2.02	0.59
6:B:330:ILE:HD11	19:B:1737:CLA:C19	2.33	0.59
6:B:436:LEU:O	6:B:437:TYR:HB2	2.02	0.59
11:G:34:GLN:O	11:G:35:VAL:C	2.40	0.59
2:2:169:LEU:CD2	19:2:1215:CLA:CAB	2.75	0.59
19:2:1220:CLA:H42	3:3:140:LYS:HB2	1.84	0.59
19:J:1045:CLA:H2	19:J:1045:CLA:HMA3	1.85	0.59
5:A:527:VAL:CG1	5:A:528:ALA:N	2.66	0.59
6:B:82:PHE:O	6:B:84:VAL:N	2.35	0.59
4:4:169:GLN:OE1	19:4:1199:CLA:HHD	2.01	0.59
5:A:451:ILE:HD11	19:A:1788:CLA:CED	2.32	0.59
5:A:502:THR:H	5:A:504:ALA:HB3	1.68	0.59
5:A:586:ARG:CG	7:C:49:VAL:HG21	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:681:GLY:HA2	5:A:684:PHE:HB3	1.84	0.59
19:B:1743:CLA:C15	19:B:1758:CLA:HMD2	2.29	0.59
19:B:1761:CLA:HBC3	19:B:1761:CLA:HHD	1.80	0.59
6:B:289:LEU:HD22	22:B:1774:BCR:H352	1.83	0.59
6:B:555:TYR:O	6:B:571:SER:HB2	2.02	0.59
8:D:111:TYR:CD2	8:D:114:PRO:CB	2.83	0.59
19:G:1099:CLA:HHD	19:G:1099:CLA:HBC3	1.83	0.59
11:G:45:GLU:O	11:G:46:ALA:CB	2.49	0.59
14:J:26:LEU:HD23	14:J:26:LEU:O	2.02	0.59
19:2:1220:CLA:C6	3:3:140:LYS:CD	2.62	0.59
11:G:93:TYR:C	11:G:95:PRO:HD3	2.22	0.59
11:G:64:VAL:HG12	11:G:64:VAL:O	2.02	0.59
8:D:58:PHE:HD2	8:D:59:GLU:H	1.47	0.59
1:1:25:ASP:HB3	1:1:26:PRO:CD	2.32	0.59
5:A:478:SER:HB3	5:A:644:GLN:CD	2.21	0.59
3:3:90:LEU:HD12	3:3:90:LEU:H	1.67	0.59
6:B:409:ALA:C	6:B:411:MET:N	2.55	0.59
5:A:165:TYR:CD2	5:A:165:TYR:O	2.55	0.59
19:A:1763:CLA:C4B	22:A:1808:BCR:H333	2.32	0.59
5:A:358:LEU:HD21	5:A:413:HIS:ND1	2.17	0.59
5:A:472:ARG:N	5:A:473:PRO:CD	2.64	0.59
6:B:625:TRP:CE3	6:B:626:LEU:N	2.70	0.59
6:B:732:LYS:CG	6:B:733:PHE:HA	2.22	0.59
16:L:124:LYS:C	16:L:126:GLN:N	2.56	0.59
17:N:58:VAL:C	17:N:60:PHE:N	2.52	0.59
17:N:67:LEU:HB2	17:N:68:GLU:HB3	1.85	0.59
15:K:69:ILE:O	15:K:72:VAL:N	2.36	0.59
19:A:1815:CLA:HMA1	19:A:1815:CLA:C2	2.32	0.59
18:R:26:UNK:C	18:R:28:UNK:N	2.66	0.59
1:1:185:TRP:O	1:1:186:HIS:CG	2.55	0.59
16:L:58:LEU:HD21	16:L:153:TRP:CZ2	2.37	0.59
5:A:143:ILE:HD12	5:A:144:GLN:H	1.68	0.59
19:A:1760:CLA:H12	19:A:1767:CLA:H92	1.83	0.59
19:A:1800:CLA:H112	19:A:1800:CLA:H61	1.83	0.59
5:A:396:PHE:O	5:A:396:PHE:CG	2.54	0.59
5:A:582:ASP:HB3	5:A:589:THR:HG22	1.83	0.59
6:B:289:LEU:HD21	19:B:1750:CLA:NA	2.18	0.59
6:B:310:PRO:HB2	6:B:311:PRO:CD	2.33	0.59
6:B:707:LEU:HD11	6:B:711:VAL:HG21	1.84	0.59
7:C:1:MET:CG	7:C:4:SER:HG	2.09	0.59
11:G:42:SER:OG	11:G:44:PHE:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:10:PRO:O	13:I:15:LEU:N	2.35	0.59
16:L:33:ILE:CD1	16:L:36:TYR:HD1	2.16	0.59
18:R:39:UNK:CB	18:R:40:UNK:HA	2.33	0.59
19:2:1215:CLA:HBC2	19:2:1215:CLA:HMC1	1.83	0.59
20:A:7037:LMU:C2	20:A:7037:LMU:H61	2.33	0.59
12:H:21:TRP:N	12:H:22:ASP:CA	2.60	0.59
8:D:61:PRO:HD3	8:D:86:LEU:HD21	1.85	0.59
20:R:1056:LMU:H1B	20:R:1056:LMU:H6B	1.63	0.59
6:B:454:LEU:HD12	6:B:454:LEU:N	2.18	0.59
6:B:657:TRP:O	6:B:660:GLY:N	2.26	0.59
3:3:83:LEU:CD1	19:A:1798:CLA:HED2	2.32	0.59
5:A:295:TRP:HB2	5:A:298:ASP:OD2	2.02	0.59
5:A:680:LEU:HD21	6:B:617:MET:HE3	1.85	0.59
19:B:1739:CLA:H42	19:B:1739:CLA:CHD	2.33	0.59
19:B:1768:CLA:C6	22:B:1779:BCR:H323	2.31	0.59
22:B:1781:BCR:H392	19:I:1031:CLA:C14	2.32	0.59
6:B:212:PHE:CZ	19:B:1744:CLA:HAC1	2.37	0.59
6:B:459:PHE:O	6:B:463:ILE:HD13	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
8:D:46:TYR:CD2	8:D:46:TYR:N	2.70	0.59
11:G:37:GLU:OE2	11:G:42:SER:CA	2.51	0.59
19:1:1200:CLA:HBC2	19:4:1198:CLA:CMB	2.32	0.59
16:L:50:LEU:HG	16:L:51:LEU:HD23	1.85	0.59
19:L:1505:CLA:H41	19:L:1505:CLA:C10	2.33	0.59
19:A:1791:CLA:CAA	19:A:1797:CLA:HBB2	2.33	0.59
22:A:1804:BCR:C23	22:A:1804:BCR:H403	2.14	0.59
5:A:432:LEU:C	5:A:434:ARG:N	2.55	0.59
6:B:55:ALA:HB1	6:B:150:LEU:HD11	1.83	0.59
6:B:50:HIS:HA	6:B:53:GLN:HB2	1.85	0.59
19:4:1196:CLA:O1D	19:4:1196:CLA:H2A	2.03	0.59
12:H:25:GLY:C	12:H:27:ASP:N	2.38	0.59
21:B:8062:SUC:O6	21:B:8062:SUC:C2'	2.50	0.59
20:2:7006:LMU:H3'	20:2:7006:LMU:C5B	2.33	0.59
6:B:156:HIS:O	6:B:163:PRO:HB3	2.03	0.59
3:3:86:GLN:HB2	3:3:88:THR:CB	2.30	0.59
5:A:163:GLN:O	5:A:166:CYS:N	2.36	0.59
19:A:1783:CLA:H18	19:A:1812:CLA:H18	1.85	0.59
5:A:733:VAL:HG11	19:A:1796:CLA:C2D	2.33	0.59
5:A:657:LEU:HD23	19:A:1811:CLA:C1D	2.32	0.59
5:A:44:ILE:O	5:A:46:LYS:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:497:ALA:O	5:A:498:LEU:HB2	2.02	0.59
19:B:1755:CLA:CHB	19:B:1769:CLA:HAA2	2.33	0.59
6:B:190:TRP:CA	19:B:1744:CLA:HBB2	2.33	0.59
6:B:551:LYS:O	6:B:553:PHE:CD2	2.56	0.59
6:B:70:TRP:NE1	6:B:71:GLN:OE1	2.35	0.59
9:E:40:ARG:HH22	9:E:87:VAL:HG22	1.68	0.59
22:I:1032:BCR:H382	22:I:1032:BCR:C40	2.33	0.59
14:J:2:ARG:HB3	14:J:7:TYR:CZ	2.38	0.59
17:N:53:ALA:O	17:N:54:LYS:CD	2.51	0.59
19:4:1196:CLA:HBC3	19:4:1196:CLA:CHD	2.25	0.59
20:A:7037:LMU:C3	20:A:7037:LMU:C7	2.30	0.59
10:F:151:ASP:CA	10:F:154:PHE:HB3	2.33	0.59
9:E:48:ASN:ND2	9:E:71:LYS:HZ2	2.00	0.59
6:B:692:ARG:NH2	6:B:694:ARG:HG2	2.17	0.59
16:L:111:GLU:OE1	20:L:1171:LMU:O6B	2.21	0.59
19:A:1773:CLA:HBC3	19:A:1773:CLA:HMC1	1.83	0.58
5:A:351:THR:HA	19:A:1780:CLA:H191	1.85	0.58
5:A:401:TRP:HB3	19:A:1783:CLA:HMC3	1.85	0.58
5:A:284:ARG:HH22	5:A:507:ALA:C	2.06	0.58
6:B:142:LEU:HD21	22:B:1776:BCR:H333	1.82	0.58
19:B:1737:CLA:OBD	19:B:1737:CLA:H151	2.03	0.58
19:B:1739:CLA:C14	19:B:1739:CLA:H102	2.32	0.58
19:B:1739:CLA:CGA	19:B:1739:CLA:C1A	2.81	0.58
6:B:196:HIS:CE1	19:B:1745:CLA:ND	2.71	0.58
19:B:1747:CLA:CBD	19:B:1756:CLA:HBB2	2.32	0.58
19:B:1738:CLA:H191	19:B:1757:CLA:H141	1.85	0.58
6:B:376:GLN:OE1	6:B:376:GLN:HA	2.03	0.58
6:B:668:ARG:HG3	6:B:700:LEU:O	2.02	0.58
22:B:1778:BCR:H23C	10:F:90:PHE:CD1	2.38	0.58
11:G:30:ASN:HD22	11:G:30:ASN:C	2.05	0.58
20:A:7032:LMU:C4B	20:A:7032:LMU:H31	2.33	0.58
12:H:27:ASP:C	12:H:29:PRO:HD3	2.23	0.58
3:3:194:ILE:HG23	3:3:197:TYR:OH	2.02	0.58
19:A:1781:CLA:HMA1	22:A:1806:BCR:H16C	1.83	0.58
5:A:733:VAL:HG21	19:A:1796:CLA:HMD3	1.84	0.58
5:A:473:PRO:O	5:A:475:ASP:N	2.36	0.58
5:A:691:MET:HB2	19:A:1813:CLA:C1C	2.32	0.58
5:A:79:PHE:HE2	5:A:185:HIS:NE2	1.73	0.58
6:B:615:TYR:HD1	6:B:615:TYR:N	2.01	0.58
6:B:662:MET:HG2	23:B:1773:PQN:O1	2.03	0.58
10:F:80:TRP:HZ3	19:F:1156:CLA:CMC	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1816:CLA:H12	19:A:1816:CLA:HED1	1.78	0.58
17:N:72:LYS:N	17:N:72:LYS:HD3	2.18	0.58
3:3:157:ALA:O	3:3:158:TYR:HB2	2.02	0.58
2:2:181:HIS:CD2	19:2:1214:CLA:C2D	2.86	0.58
5:A:112:ASP:O	5:A:116:ILE:HG12	2.02	0.58
5:A:131:ILE:CG2	5:A:132:LEU:N	2.66	0.58
19:A:1765:CLA:CBD	19:A:1765:CLA:HBA2	2.33	0.58
5:A:691:MET:CE	23:A:1802:PQN:C2M	2.80	0.58
5:A:230:ASN:HA	5:A:233:LEU:HB2	1.85	0.58
5:A:154:ARG:NH2	5:A:233:LEU:HD13	2.18	0.58
5:A:309:LEU:HA	5:A:312:ILE:O	2.02	0.58
7:C:7:ILE:O	7:C:60:THR:HA	2.03	0.58
10:F:78:ARG:O	10:F:80:TRP:HD1	1.86	0.58
11:G:93:TYR:CA	11:G:94:ASP:OD1	2.50	0.58
16:L:108:LYS:O	16:L:132:SER:CB	2.41	0.58
5:A:755:ILE:O	5:A:756:ALA:CB	2.52	0.58
5:A:452:PHE:CD1	19:A:1793:CLA:HBB1	2.32	0.58
23:A:1802:PQN:H272	23:A:1802:PQN:H241	1.86	0.58
5:A:154:ARG:HG3	5:A:383:PRO:HB2	1.85	0.58
5:A:373:ALA:O	5:A:396:PHE:CD1	2.56	0.58
6:B:530:THR:CG2	19:B:1755:CLA:HMC1	2.33	0.58
6:B:710:LEU:C	6:B:712:HIS:N	2.55	0.58
10:F:123:VAL:HG13	14:J:7:TYR:H	1.68	0.58
22:I:1032:BCR:HC22	19:I:1033:CLA:CHD	2.33	0.58
16:L:45:THR:HA	16:L:52:ARG:HH12	1.67	0.58
18:R:35:UNK:C	18:R:36:UNK:O	2.51	0.58
19:4:1198:CLA:O1A	19:4:1198:CLA:H2	2.01	0.58
9:E:69:PHE:CD2	9:E:71:LYS:HG2	2.38	0.58
5:A:207:LEU:HD13	19:A:1776:CLA:HBB2	1.84	0.58
5:A:23:ASP:C	5:A:23:ASP:OD1	2.41	0.58
6:B:458:ILE:HG13	6:B:459:PHE:N	2.16	0.58
13:I:28:VAL:O	13:I:29:GLU:CD	2.42	0.58
19:2:1213:CLA:CBC	19:2:1213:CLA:HHD	2.25	0.58
3:3:92:TRP:HZ2	5:A:250:LEU:HB2	1.68	0.58
15:K:71:GLY:C	15:K:72:VAL:O	2.42	0.58
9:E:51:SER:O	9:E:68:ARG:N	2.27	0.58
19:A:1763:CLA:HHB	19:A:1764:CLA:HMB3	1.85	0.58
19:A:1763:CLA:HBA2	19:A:1765:CLA:C1	2.32	0.58
19:A:1782:CLA:HBA2	22:A:1806:BCR:H12C	1.85	0.58
5:A:239:PRO:CA	5:A:242:ILE:HD11	2.30	0.58
5:A:243:PRO:O	5:A:244:LEU:O	2.20	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:H	1.67	0.58
5:A:98:PHE:HD1	5:A:99:HIS:HD2	1.51	0.58
19:B:1759:CLA:H93	24:B:1783:LMG:H311	1.84	0.58
19:B:1787:CLA:HMC1	19:B:1787:CLA:HBC3	1.86	0.58
6:B:36:ASP:O	6:B:41:ARG:NE	2.37	0.58
6:B:646:TRP:CZ2	6:B:726:ILE:HG21	2.38	0.58
16:L:40:LEU:CB	16:L:41:PRO:CD	2.82	0.58
19:K:1085:CLA:ND	19:K:1142:CLA:HMD3	2.18	0.58
18:R:52:UNK:CB	18:R:53:UNK:CB	2.82	0.58
5:A:157:GLY:O	5:A:158:ILE:HB	2.04	0.58
5:A:225:VAL:HG12	5:A:248:PHE:CD1	2.39	0.58
5:A:413:HIS:ND1	5:A:416:ILE:HD12	2.18	0.58
5:A:42:ARG:C	5:A:44:ILE:N	2.56	0.58
5:A:678:PHE:O	5:A:680:LEU:N	2.36	0.58
5:A:98:PHE:O	5:A:99:HIS:CB	2.51	0.58
19:B:1754:CLA:HMA2	19:B:1754:CLA:H61	1.84	0.58
22:B:1778:BCR:H392	10:F:90:PHE:HA	1.86	0.58
22:B:1781:BCR:H342	19:H:1079:CLA:HAC2	1.85	0.58
19:B:1787:CLA:HED3	19:B:1787:CLA:HBA2	1.85	0.58
6:B:415:LYS:CE	6:B:539:LEU:O	2.51	0.58
6:B:569:ASP:HB3	6:B:574:ASP:HB3	1.86	0.58
6:B:628:SER:O	6:B:631:LEU:HD23	2.03	0.58
19:1:1191:CLA:HHC	19:1:1197:CLA:HBC1	1.86	0.58
3:3:52:LYS:N	3:3:55:ALA:HB3	2.19	0.58
21:3:1221:SUC:C6'	21:3:1221:SUC:H1'1	1.99	0.58
20:A:7030:LMU:H2'	20:A:7030:LMU:H6E	1.84	0.58
10:F:40:LEU:CA	10:F:42:ILE:HG12	2.30	0.58
2:2:79:TRP:CG	2:2:79:TRP:O	2.57	0.58
5:A:122:VAL:HG22	5:A:142:GLY:HA2	1.85	0.58
19:A:1783:CLA:H171	22:A:1808:BCR:H351	1.84	0.58
19:A:1813:CLA:H3A	19:A:1813:CLA:CGA	2.34	0.58
5:A:455:PHE:O	19:A:1789:CLA:CBB	2.52	0.58
6:B:22:TRP:CE2	19:B:1770:CLA:HMB1	2.39	0.58
6:B:187:SER:O	6:B:188:LEU:C	2.41	0.58
6:B:278:LEU:O	6:B:281:ALA:N	2.37	0.58
6:B:304:ILE:HD11	19:B:1749:CLA:HED2	1.82	0.58
6:B:460:ALA:O	6:B:461:GLN:C	2.42	0.58
6:B:561:GLY:CA	7:C:52:LYS:HG2	2.32	0.58
7:C:79:LEU:HD22	7:C:81:TYR:C	2.23	0.58
18:R:37:UNK:C	18:R:42:UNK:O	2.52	0.58
16:L:97:MET:HA	16:L:100:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:103:GLY:HA2	19:2:1222:CLA:HBB2	1.84	0.58
6:B:5:ILE:CB	6:B:6:PRO:HD2	2.30	0.58
5:A:158:ILE:O	5:A:243:PRO:HG2	2.03	0.58
5:A:170:GLY:C	5:A:173:VAL:HG22	2.22	0.58
5:A:185:HIS:O	5:A:188:LYS:N	2.37	0.58
19:B:1735:CLA:NC	19:B:1735:CLA:H52	2.18	0.58
19:B:1758:CLA:C17	22:B:1775:BCR:H363	2.34	0.58
6:B:392:ILE:HG12	6:B:555:TYR:CD1	2.38	0.58
6:B:594:TRP:C	6:B:594:TRP:HD1	2.07	0.58
16:L:56:VAL:HA	19:L:1167:CLA:HED1	1.86	0.58
19:2:1220:CLA:CHD	19:2:1220:CLA:HBC3	2.33	0.58
17:N:62:SER:O	17:N:66:ASP:CG	2.42	0.58
19:K:1085:CLA:NA	19:K:1142:CLA:HMD3	2.18	0.58
17:N:33:TYR:O	17:N:34:THR:CG2	2.51	0.58
10:F:2:ILE:HG22	10:F:3:ALA:N	2.19	0.58
19:4:1199:CLA:H2	19:4:1199:CLA:CED	2.34	0.58
5:A:328:LYS:CG	5:A:332:GLU:CB	2.59	0.58
5:A:390:ALA:CB	5:A:754:ILE:HD13	2.33	0.58
5:A:651:GLY:O	5:A:655:ASP:N	2.37	0.58
5:A:705:GLU:HB3	6:B:545:LYS:NZ	2.18	0.58
6:B:715:VAL:O	6:B:716:GLY:C	2.42	0.58
8:D:31:GLY:HA2	16:L:13:PRO:CB	2.34	0.58
19:J:1044:CLA:H93	19:J:1044:CLA:C4	2.33	0.58
14:J:9:SER:O	14:J:10:VAL:CB	2.51	0.58
6:B:261:PHE:CZ	6:B:500:ALA:HB2	2.39	0.58
2:2:208:PHE:CG	2:2:209:THR:N	2.71	0.58
2:2:77:PRO:O	17:N:3:ILE:CD1	2.52	0.58
3:3:84:ILE:N	19:A:1798:CLA:H41	2.14	0.57
19:A:1788:CLA:HAA1	22:L:1170:BCR:C14	2.34	0.57
5:A:214:GLY:HA3	22:A:1804:BCR:C15	2.34	0.57
5:A:40:PHE:CE1	5:A:53:TRP:HD1	2.17	0.57
5:A:592:VAL:HG23	5:A:593:SER:N	2.19	0.57
6:B:391:PRO:HB3	6:B:538:ALA:CA	2.33	0.57
6:B:422:LEU:CD1	6:B:535:VAL:HG11	2.27	0.57
6:B:594:TRP:CD2	6:B:598:HIS:CE1	2.92	0.57
8:D:29:PHE:O	8:D:30:ALA:HB3	2.04	0.57
17:N:61:LEU:HD13	17:N:63:ASP:CB	2.29	0.57
16:L:161:LEU:HD12	16:L:162:ASP:C	2.22	0.57
4:4:58:MET:O	4:4:60:LEU:N	2.37	0.57
1:1:109:GLU:HB3	19:1:1196:CLA:HMA3	1.84	0.57
19:A:1779:CLA:C1B	22:A:1805:BCR:H15C	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1792:CLA:CBA	19:A:1792:CLA:HBD	2.34	0.57
19:A:1793:CLA:O1D	19:A:1793:CLA:H2A	2.04	0.57
19:A:1795:CLA:O1A	19:A:1795:CLA:C4	2.52	0.57
19:A:1770:CLA:HMC2	22:A:1803:BCR:C15	2.33	0.57
5:A:309:LEU:HD23	5:A:309:LEU:C	2.24	0.57
5:A:708:VAL:O	5:A:711:HIS:HB2	2.04	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
22:B:1781:BCR:HC41	19:B:1787:CLA:H142	1.86	0.57
6:B:665:ILE:HD12	19:B:1787:CLA:HBC1	1.86	0.57
6:B:353:TYR:C	6:B:355:LEU:H	2.07	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
19:A:1800:CLA:H202	16:L:64:LEU:HD21	1.84	0.57
18:R:38:UNK:C	18:R:42:UNK:O	2.52	0.57
19:R:1055:CLA:H111	20:R:1056:LMU:O4'	2.04	0.57
1:1:25:ASP:HB3	1:1:26:PRO:HD3	1.85	0.57
20:A:7038:LMU:C10	20:A:7038:LMU:H61	2.22	0.57
19:4:1201:CLA:C2A	19:4:1201:CLA:O1D	2.52	0.57
5:A:110:LEU:O	5:A:113:PRO:HD3	2.04	0.57
5:A:56:ASN:O	5:A:57:LEU:CB	2.52	0.57
5:A:653:LEU:HD23	19:B:1785:CLA:HBC2	1.86	0.57
5:A:669:GLY:N	6:B:445:ALA:HA	2.15	0.57
19:B:1740:CLA:HBB2	19:B:1786:CLA:C13	2.30	0.57
19:B:1771:CLA:H191	13:I:21:MET:HB2	1.86	0.57
6:B:310:PRO:CB	6:B:311:PRO:CD	2.82	0.57
6:B:557:PHE:HE2	7:C:66:ARG:HE	1.51	0.57
2:2:64:ILE:HD13	19:2:1213:CLA:HMB1	1.86	0.57
17:N:63:ASP:N	17:N:64:ASP:CA	2.55	0.57
3:3:162:PRO:HG2	3:3:164:PHE:CD1	2.40	0.57
5:A:513:LEU:HB3	5:A:529:LEU:HD13	1.85	0.57
19:A:1771:CLA:H42	19:A:1771:CLA:HBA2	1.86	0.57
5:A:691:MET:O	23:A:1802:PQN:O1	2.23	0.57
5:A:595:TRP:HE3	5:A:596:ASP:OD2	1.87	0.57
5:A:691:MET:HE3	23:A:1802:PQN:C2M	2.34	0.57
5:A:131:ILE:HD13	6:B:447:GLY:CA	2.34	0.57
10:F:83:PHE:O	10:F:87:GLY:N	2.38	0.57
11:G:46:ALA:CA	11:G:48:ASP:HB3	2.34	0.57
16:L:125:LYS:C	16:L:127:PRO:HD2	2.24	0.57
19:A:1789:CLA:O1D	16:L:73:PRO:HA	2.05	0.57
19:J:1045:CLA:CMA	19:J:1045:CLA:H2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3011:CLA:CGA	19:3:3011:CLA:H3A	2.34	0.57
8:D:86:LEU:C	8:D:90:LEU:HB3	2.25	0.57
14:J:32:PHE:HE2	14:J:33:PHE:CZ	2.23	0.57
5:A:462:ILE:HD11	19:B:1786:CLA:C5	2.28	0.57
19:B:1747:CLA:C1A	19:B:1747:CLA:H12	2.35	0.57
6:B:674:LEU:HD12	6:B:674:LEU:C	2.25	0.57
14:J:13:VAL:HG12	14:J:15:SER:HB2	1.86	0.57
3:3:92:TRP:HZ2	5:A:250:LEU:HD12	1.69	0.57
17:N:39:SER:OG	17:N:41:LYS:HA	2.04	0.57
17:N:50:GLN:N	17:N:51:ASP:O	2.37	0.57
19:J:1043:CLA:H141	19:J:1044:CLA:HMB3	1.86	0.57
10:F:22:LEU:O	10:F:25:LEU:HD13	2.02	0.57
20:A:7021:LMU:H6D	20:A:7021:LMU:C4	2.35	0.57
20:A:7021:LMU:H3O1	20:A:7021:LMU:C6B	2.14	0.57
2:2:73:ILE:N	2:2:73:ILE:HD12	2.20	0.57
17:N:28:ASN:HA	17:N:30:ALA:H	1.69	0.57
5:A:105:ASN:HB2	5:A:140:PHE:CZ	2.40	0.57
5:A:499:ALA:HB3	19:A:1790:CLA:O2D	2.04	0.57
5:A:193:LEU:O	5:A:194:ALA:C	2.42	0.57
6:B:334:LEU:CB	19:B:1737:CLA:HMD3	2.34	0.57
22:A:1807:BCR:C3	22:B:1778:BCR:H17C	2.34	0.57
6:B:299:HIS:HE1	19:B:1752:CLA:HMD1	1.69	0.57
6:B:649:MET:CE	6:B:723:ALA:HB2	2.35	0.57
8:D:118:VAL:CG1	8:D:119:TYR:H	2.17	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
3:3:121:MET:O	19:3:1218:CLA:HED1	2.05	0.57
20:2:1225:LMU:H41	20:2:1225:LMU:H6D	1.87	0.57
19:A:1787:CLA:H142	19:A:1801:CLA:H43	1.86	0.57
19:A:1795:CLA:C4	19:A:1795:CLA:O2A	2.52	0.57
19:A:1779:CLA:C4B	22:A:1805:BCR:H15C	2.34	0.57
5:A:281:LEU:HD22	19:A:1772:CLA:CMA	2.34	0.57
5:A:746:THR:HG1	19:A:1811:CLA:CGD	2.14	0.57
6:B:432:HIS:CE1	19:B:1762:CLA:NB	2.64	0.57
24:B:1783:LMG:H111	24:B:1783:LMG:HC91	1.87	0.57
22:B:1780:BCR:H351	19:B:1787:CLA:H111	1.85	0.57
6:B:127:ILE:HD13	6:B:193:HIS:CE1	2.40	0.57
7:C:52:LYS:C	7:C:54:CYS:N	2.56	0.57
6:B:564:ARG:NE	7:C:64:SER:OG	2.38	0.57
8:D:49:THR:OG1	8:D:74:LEU:HD12	2.05	0.57
5:A:258:LEU:O	5:A:280:PHE:CE1	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:69:ILE:HG22	4:4:70:ILE:H	1.70	0.57
1:1:54:VAL:O	1:1:56:GLY:N	2.38	0.57
5:A:123:VAL:HB	5:A:129:GLN:OE1	2.04	0.57
19:A:1797:CLA:HMA2	19:A:1797:CLA:O2A	2.03	0.57
5:A:744:ALA:HB2	22:A:1807:BCR:H391	0.67	0.57
19:A:1813:CLA:HMA1	19:A:1813:CLA:H2	1.87	0.57
5:A:402:ILE:C	5:A:404:GLY:H	2.07	0.57
5:A:547:PHE:O	5:A:551:VAL:CG1	2.46	0.57
6:B:212:PHE:HZ	19:B:1744:CLA:HAC1	1.69	0.57
19:A:1811:CLA:H192	19:B:1786:CLA:C2B	2.35	0.57
7:C:6:LYS:N	7:C:65:VAL:HG22	2.20	0.57
8:D:31:GLY:O	8:D:32:SER:CB	2.53	0.57
9:E:32:ARG:NH2	9:E:53:VAL:HA	2.20	0.57
20:A:7042:LMU:C4'	20:A:7042:LMU:O2B	2.52	0.57
9:E:48:ASN:ND2	9:E:71:LYS:HZ1	2.03	0.57
19:4:1204:CLA:HBD	19:4:1204:CLA:HBA2	1.87	0.57
5:A:464:ASN:H	5:A:464:ASN:ND2	2.02	0.57
12:H:36:GLN:O	12:H:36:GLN:HG2	2.04	0.57
19:A:1783:CLA:C11	22:A:1808:BCR:H353	2.35	0.57
5:A:553:VAL:HG22	22:A:1806:BCR:H401	1.86	0.57
19:A:1764:CLA:H142	22:A:1808:BCR:C13	2.35	0.57
5:A:218:TRP:HA	19:A:1770:CLA:HBB2	1.85	0.57
5:A:625:TRP:HB3	5:A:637:ILE:HD11	1.86	0.57
6:B:615:TYR:CD1	6:B:615:TYR:N	2.72	0.57
8:D:45:PHE:C	8:D:46:TYR:HD2	2.07	0.57
11:G:32:ALA:O	11:G:33:LYS:C	2.42	0.57
14:J:18:TRP:CH2	14:J:22:LEU:HD22	2.40	0.57
16:L:14:LEU:CD2	16:L:21:GLY:O	2.53	0.57
16:L:30:SER:C	16:L:32:LEU:N	2.58	0.57
3:3:205:GLY:CA	5:A:252:ARG:NH2	2.62	0.57
19:A:1815:CLA:H61	19:A:1815:CLA:HMA3	1.79	0.57
6:B:48:ALA:CB	6:B:157:LEU:HD22	2.34	0.57
16:L:54:VAL:O	16:L:58:LEU:HB2	2.04	0.57
5:A:109:TRP:HH2	5:A:154:ARG:HD3	1.69	0.57
19:A:1791:CLA:HBC2	22:A:1806:BCR:C3	2.22	0.57
19:B:1745:CLA:O1D	19:B:1745:CLA:H2A	2.05	0.57
19:B:1753:CLA:H2	19:B:1753:CLA:H71	1.82	0.57
19:B:1767:CLA:HBC3	19:B:1767:CLA:CMC	2.25	0.57
6:B:305:LEU:O	6:B:306:GLU:C	2.44	0.57
6:B:34:HIS:O	6:B:36:ASP:N	2.37	0.57
8:D:39:LYS:HG3	8:D:43:GLU:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:1220:CLA:C6	3:3:140:LYS:HE2	2.34	0.57
17:N:80:ASN:OD1	17:N:82:PHE:CA	2.53	0.57
20:A:7032:LMU:H12	20:A:7032:LMU:H2O2	1.66	0.57
4:4:91:PHE:CD2	19:4:1205:CLA:HHD	2.40	0.57
3:3:199:VAL:HG22	19:3:1214:CLA:C4C	2.33	0.57
6:B:399:ASN:O	6:B:401:GLU:N	2.38	0.57
5:A:298:ASP:OD2	5:A:298:ASP:N	2.38	0.56
6:B:257:ILE:HA	6:B:272:ASP:OD2	2.05	0.56
6:B:262:HIS:O	6:B:265:THR:O	2.23	0.56
6:B:493:TRP:CB	19:B:1765:CLA:HED2	2.35	0.56
6:B:545:LYS:CD	6:B:546:LEU:H	2.18	0.56
8:D:101:TYR:CE1	8:D:114:PRO:HD3	2.40	0.56
6:B:542:ARG:NH2	8:D:141:VAL:O	2.38	0.56
8:D:99:GLN:OE1	8:D:101:TYR:OH	2.22	0.56
10:F:76:ASP:O	10:F:78:ARG:N	2.38	0.56
19:2:1218:CLA:C1B	19:2:1218:CLA:H2	2.34	0.56
17:N:80:ASN:C	17:N:82:PHE:N	2.59	0.56
20:A:7016:LMU:H21	20:A:7016:LMU:H61	1.86	0.56
4:4:124:TYR:HB2	4:4:143:PHE:HD1	1.62	0.56
10:F:50:LYS:O	10:F:52:ARG:C	2.43	0.56
5:A:265:GLY:CA	5:A:272:LEU:HD21	2.35	0.56
16:L:17:ASP:OD1	16:L:17:ASP:O	2.23	0.56
15:K:55:PHE:N	15:K:55:PHE:CD1	2.73	0.56
19:A:1796:CLA:H71	19:A:1813:CLA:H171	1.86	0.56
5:A:207:LEU:HA	5:A:211:LEU:HB2	1.86	0.56
5:A:284:ARG:NH1	5:A:507:ALA:HB1	2.19	0.56
5:A:435:VAL:HA	5:A:438:HIS:CE1	2.40	0.56
5:A:583:GLY:O	5:A:585:GLY:N	2.38	0.56
19:B:1738:CLA:H71	24:B:1783:LMG:H381	1.86	0.56
6:B:553:PHE:O	6:B:555:TYR:N	2.38	0.56
16:L:14:LEU:HD21	16:L:20:ILE:HG22	1.87	0.56
16:L:65:VAL:H	16:L:67:PRO:HD2	1.70	0.56
19:2:1215:CLA:C4	19:2:1220:CLA:HBC1	2.34	0.56
17:N:76:LYS:CG	17:N:77:CYS:H	2.07	0.56
4:4:104:ARG:CA	4:4:107:GLN:HB2	2.19	0.56
7:C:31:TRP:CB	7:C:39:ILE:HG21	2.34	0.56
19:1:1188:CLA:CBC	19:1:1188:CLA:HMC1	2.31	0.56
6:B:224:PRO:O	6:B:226:LEU:N	2.38	0.56
19:A:1784:CLA:H51	22:A:1804:BCR:H331	1.87	0.56
19:B:1749:CLA:HBD	19:B:1749:CLA:HBA1	1.87	0.56
19:B:1755:CLA:CHD	19:B:1755:CLA:HBC3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:189:ALA:CB	19:B:1758:CLA:C20	2.66	0.56
6:B:304:ILE:HD11	19:B:1749:CLA:HED3	1.87	0.56
9:E:39:LEU:N	9:E:40:ARG:HH11	1.94	0.56
9:E:41:ARG:HG3	9:E:46:PHE:CE1	2.40	0.56
10:F:131:PHE:O	10:F:133:GLY:N	2.38	0.56
19:A:1796:CLA:C19	14:J:19:PHE:CD2	2.88	0.56
16:L:63:LEU:O	16:L:64:LEU:C	2.42	0.56
5:A:146:THR:HA	5:A:391:THR:HG23	1.85	0.56
19:A:1759:CLA:HMB1	19:A:1767:CLA:H18	1.87	0.56
5:A:309:LEU:O	5:A:310:PHE:CB	2.52	0.56
6:B:707:LEU:HD13	24:B:1783:LMG:H301	1.87	0.56
5:A:567:ARG:NH2	8:D:82:GLN:OE1	2.37	0.56
2:2:56:MET:SD	2:2:169:LEU:HA	2.45	0.56
17:N:80:ASN:O	17:N:82:PHE:HD2	1.89	0.56
20:A:7016:LMU:C3	20:A:7016:LMU:C9	2.62	0.56
3:3:194:ILE:HA	3:3:197:TYR:CE1	2.40	0.56
11:G:60:SER:HG	11:G:63:PRO:HB2	1.70	0.56
6:B:481:THR:O	6:B:482:ASN:HB2	2.05	0.56
6:B:408:LEU:O	6:B:411:MET:HB3	2.04	0.56
6:B:500:ALA:CB	6:B:508:LEU:HD22	2.34	0.56
19:A:1776:CLA:C3C	19:A:1782:CLA:C17	2.77	0.56
19:A:1791:CLA:H3A	19:A:1797:CLA:HBB1	1.87	0.56
5:A:544:ILE:HD11	19:A:1811:CLA:H193	1.88	0.56
5:A:578:ARG:NH1	5:A:578:ARG:HB2	2.20	0.56
5:A:702:GLU:HA	6:B:545:LYS:HE2	1.87	0.56
5:A:95:GLY:HA3	19:A:1763:CLA:C1C	2.35	0.56
6:B:275:HIS:ND1	19:B:1747:CLA:HMB1	2.20	0.56
19:B:1760:CLA:HMB2	19:B:1761:CLA:C4A	2.36	0.56
6:B:266:GLN:HE21	6:B:363:GLN:HG2	1.70	0.56
6:B:442:VAL:HG21	19:B:1763:CLA:CAC	2.32	0.56
6:B:486:LEU:O	6:B:487:ASN:HB3	2.06	0.56
6:B:559:CYS:SG	6:B:560:ASP:N	2.79	0.56
14:J:26:LEU:HA	14:J:29:ILE:HG22	1.88	0.56
4:4:106:TRP:HE3	19:4:1207:CLA:HMA2	1.69	0.56
5:A:40:PHE:H	5:A:44:ILE:HG21	1.71	0.56
6:B:144:PHE:HD2	6:B:144:PHE:O	1.86	0.56
6:B:186:SER:C	6:B:187:SER:O	2.44	0.56
6:B:266:GLN:O	6:B:267:SER:CB	2.45	0.56
6:B:444:LEU:O	6:B:445:ALA:CB	2.54	0.56
6:B:555:TYR:CE2	6:B:573:TRP:HA	2.41	0.56
6:B:722:ALA:O	6:B:726:ILE:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:44:TYR:CD2	9:E:45:TRP:HE3	2.23	0.56
16:L:65:VAL:N	16:L:67:PRO:HD2	2.21	0.56
17:N:45:ASN:HA	17:N:57:LYS:NZ	2.20	0.56
17:N:62:SER:O	17:N:63:ASP:CG	2.44	0.56
21:B:8052:SUC:O5	21:B:8052:SUC:H5'	2.05	0.56
19:J:1044:CLA:C9	19:J:1044:CLA:H151	2.33	0.56
19:J:1044:CLA:O2D	19:J:1045:CLA:C9	2.40	0.56
19:J:1045:CLA:C2	19:J:1045:CLA:O1D	2.54	0.56
19:A:1815:CLA:C3A	19:A:1815:CLA:CGA	2.84	0.56
15:K:43:ARG:NE	15:K:43:ARG:HA	2.21	0.56
19:A:1790:CLA:C1B	22:A:1806:BCR:H333	2.36	0.56
19:A:1795:CLA:CGA	19:A:1795:CLA:C4	2.82	0.56
5:A:716:VAL:O	19:A:1795:CLA:HMD3	2.05	0.56
19:B:1753:CLA:CGD	19:B:1753:CLA:C2A	2.83	0.56
24:B:1783:LMG:H111	24:B:1783:LMG:C9	2.35	0.56
22:B:1780:BCR:C20	19:B:1786:CLA:C15	2.84	0.56
7:C:1:MET:SD	7:C:4:SER:HB2	2.45	0.56
11:G:33:LYS:CA	11:G:33:LYS:CE	2.62	0.56
8:D:75:LEU:HD21	16:L:19:PHE:CE2	2.41	0.56
17:N:47:THR:HG21	17:N:54:LYS:CE	2.30	0.56
17:N:72:LYS:CD	17:N:74:LYS:H	2.19	0.56
10:F:23:LYS:O	10:F:24:LYS:NZ	2.29	0.56
4:4:151:GLU:HG3	4:4:152:LYS:H	1.71	0.56
17:N:25:THR:CG2	17:N:26:GLY:N	2.69	0.56
19:A:1761:CLA:H201	22:A:1804:BCR:C18	2.35	0.56
19:A:1761:CLA:HMC3	19:A:1785:CLA:HMA1	1.87	0.56
19:A:1794:CLA:CMC	19:A:1794:CLA:HBC3	2.25	0.56
19:A:1813:CLA:HBC2	19:A:1813:CLA:HMC1	1.88	0.56
5:A:500:PRO:HB3	5:A:506:GLY:HA2	1.88	0.56
5:A:59:ALA:C	5:A:61:ALA:H	2.09	0.56
5:A:704:ILE:HA	5:A:707:ILE:HG13	1.87	0.56
19:B:1762:CLA:H51	22:B:1779:BCR:C40	2.35	0.56
6:B:510:LEU:HD22	6:B:510:LEU:H	1.70	0.56
6:B:670:TYR:OH	19:B:1787:CLA:CAD	2.53	0.56
10:F:126:ALA:O	10:F:128:SER:N	2.38	0.56
10:F:40:LEU:HD12	10:F:42:ILE:HD11	1.88	0.56
19:1:1192:CLA:O1D	20:1:1202:LMU:O2'	2.23	0.56
5:A:156:SER:O	5:A:158:ILE:N	2.39	0.56
5:A:223:VAL:O	5:A:228:PRO:HD3	2.05	0.56
5:A:362:LEU:HB3	5:A:406:LEU:O	2.05	0.56
5:A:409:GLY:C	5:A:411:ALA:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:132:ASN:OD1	6:B:132:ASN:C	2.44	0.56
19:B:1735:CLA:CBB	19:B:1762:CLA:H43	2.36	0.56
19:B:1735:CLA:HBC3	22:B:1778:BCR:H332	1.88	0.56
19:B:1759:CLA:H62	24:B:1783:LMG:C18	2.35	0.56
24:B:1783:LMG:C11	24:B:1783:LMG:C9	2.84	0.56
6:B:390:GLY:N	6:B:391:PRO:CD	2.69	0.56
19:3:1218:CLA:HHD	19:3:1218:CLA:CBC	2.22	0.56
10:F:22:LEU:CB	10:F:23:LYS:HD3	2.35	0.56
21:B:8056:SUC:H1	21:B:8056:SUC:H5'	1.88	0.56
20:A:7043:LMU:H3O2	20:A:7043:LMU:C1B	2.19	0.56
4:4:169:GLN:NE2	4:4:169:GLN:HA	2.18	0.56
19:A:1771:CLA:HBB1	22:A:1803:BCR:C13	2.36	0.56
19:A:1776:CLA:C1C	19:A:1782:CLA:C17	2.80	0.56
5:A:210:LEU:HD12	19:A:1769:CLA:CMB	2.35	0.56
5:A:232:PHE:CZ	5:A:242:ILE:HG22	2.40	0.56
19:B:1759:CLA:H201	19:B:1771:CLA:HBA1	1.88	0.56
19:B:1760:CLA:HED2	19:B:1760:CLA:HAA2	1.85	0.56
22:B:1775:BCR:C8	22:B:1775:BCR:C33	2.84	0.56
6:B:291:TYR:O	6:B:292:ARG:O	2.24	0.56
7:C:75:ARG:NH1	8:D:110:GLN:OE1	2.37	0.56
9:E:36:VAL:CG2	9:E:52:VAL:HG22	2.36	0.56
18:R:36:UNK:C	18:R:38:UNK:N	2.66	0.56
2:2:53:ARG:HH22	19:2:1212:CLA:HBC1	1.70	0.56
5:A:249:ILE:HG23	5:A:251:ASN:OD1	2.06	0.56
17:N:67:LEU:CB	17:N:68:GLU:CB	2.82	0.56
19:A:1815:CLA:CMA	19:A:1815:CLA:C2	2.83	0.56
8:D:125:PRO:HG2	8:D:127:ARG:HD3	1.87	0.56
11:G:69:VAL:O	11:G:73:ALA:HB3	2.06	0.56
12:H:36:GLN:HE22	19:L:1166:CLA:CAD	2.19	0.56
5:A:150:PHE:H	5:A:153:TRP:HE3	1.49	0.56
5:A:214:GLY:CA	22:A:1804:BCR:H15C	2.36	0.56
5:A:341:GLN:HB3	5:A:434:ARG:NH1	2.21	0.56
5:A:701:GLN:NE2	5:A:701:GLN:HA	2.21	0.56
19:B:1756:CLA:C10	19:B:1756:CLA:H142	2.34	0.56
19:B:1765:CLA:CBB	22:B:1777:BCR:H281	2.35	0.56
19:B:1786:CLA:NB	19:B:1787:CLA:HBB2	2.20	0.56
6:B:321:GLY:O	6:B:325:THR:HG22	2.06	0.56
6:B:388:ALA:HA	6:B:391:PRO:CG	2.36	0.56
10:F:80:TRP:CE3	19:F:1157:CLA:HMC2	2.38	0.56
16:L:25:THR:HB	16:L:26:PRO:HD2	1.88	0.56
20:A:7033:LMU:C6B	20:A:7033:LMU:C2'	2.81	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:455:ILE:HD12	6:B:517:PHE:CZ	2.40	0.56
10:F:7:PRO:HB3	10:F:60:GLY:O	2.06	0.56
19:1:1193:CLA:HBC3	19:1:1193:CLA:CMC	2.33	0.56
3:3:84:ILE:H	19:A:1798:CLA:H41	1.63	0.55
22:A:1807:BCR:H15C	19:A:1812:CLA:H151	1.88	0.55
19:A:1812:CLA:C3D	19:A:1812:CLA:HED2	2.36	0.55
5:A:217:SER:HA	22:A:1803:BCR:C35	2.31	0.55
5:A:361:ASN:HD22	5:A:361:ASN:C	2.09	0.55
5:A:471:GLY:O	5:A:472:ARG:HG2	2.06	0.55
5:A:75:SER:HB3	5:A:354:TRP:CZ2	2.41	0.55
6:B:275:HIS:O	6:B:278:LEU:HB3	2.06	0.55
6:B:630:GLN:HE21	6:B:731:GLY:CA	2.16	0.55
9:E:39:LEU:HA	9:E:46:PHE:CE1	2.41	0.55
11:G:5:SER:O	11:G:7:VAL:HG13	2.05	0.55
6:B:25:ILE:HG22	22:L:1169:BCR:C28	2.25	0.55
17:N:70:GLU:CB	17:N:72:LYS:H	2.15	0.55
19:4:4014:CLA:HED2	19:4:4014:CLA:H2A	0.72	0.55
3:3:49:ILE:HA	3:3:51:PRO:HD2	1.88	0.55
3:3:50:GLU:H	3:3:51:PRO:HD3	1.71	0.55
21:B:8062:SUC:H1	21:B:8062:SUC:O3'	2.07	0.55
6:B:247:THR:CG2	6:B:250:ALA:CB	2.83	0.55
20:A:7013:LMU:H41	20:A:7013:LMU:H1'	1.87	0.55
5:A:337:PRO:CD	19:A:1799:CLA:HHC	2.36	0.55
6:B:341:LEU:O	6:B:345:THR:OG1	2.17	0.55
4:4:161:LEU:HD12	4:4:161:LEU:O	2.07	0.55
19:A:1776:CLA:H43	19:A:1779:CLA:H2	1.88	0.55
5:A:284:ARG:HG3	5:A:295:TRP:CG	2.41	0.55
5:A:361:ASN:ND2	19:A:1761:CLA:HED1	2.18	0.55
5:A:374:GLN:O	5:A:376:MET:N	2.39	0.55
5:A:378:SER:OG	19:A:1782:CLA:HBC2	2.06	0.55
5:A:42:ARG:HA	5:A:44:ILE:HG12	1.88	0.55
5:A:586:ARG:HG3	7:C:49:VAL:CG2	2.36	0.55
5:A:699:TYR:HD1	5:A:700:TRP:CD1	2.24	0.55
5:A:711:HIS:O	5:A:716:VAL:HG22	2.06	0.55
19:B:1754:CLA:C8	19:B:1756:CLA:H43	2.36	0.55
6:B:197:VAL:O	6:B:198:ALA:HB2	2.07	0.55
6:B:586:THR:C	6:B:588:GLY:N	2.54	0.55
6:B:596:TRP:CZ3	6:B:613:SER:HB3	2.41	0.55
19:B:1768:CLA:CBC	10:F:83:PHE:CZ	2.79	0.55
2:2:127:ASN:HB3	14:J:1:MET:O	2.06	0.55
19:2:1220:CLA:H61	3:3:140:LYS:HZ2	1.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:94:ARG:C	3:3:97:PHE:HE1	2.09	0.55
17:N:52:LEU:HB3	17:N:53:ALA:CA	2.36	0.55
3:3:201:ALA:C	3:3:202:LEU:HD22	2.27	0.55
6:B:479:SER:O	6:B:481:THR:N	2.28	0.55
9:E:48:ASN:HD21	9:E:71:LYS:NZ	2.04	0.55
17:N:1:GLY:C	17:N:2:VAL:HG13	2.23	0.55
19:1:1190:CLA:HBA1	19:1:1190:CLA:CHA	2.35	0.55
19:A:1799:CLA:HBA2	19:A:1799:CLA:O2D	2.05	0.55
19:A:1760:CLA:CBA	19:A:1767:CLA:H62	2.36	0.55
19:A:1781:CLA:H162	19:A:1781:CLA:C11	2.36	0.55
5:A:240:LYS:H	5:A:243:PRO:HD3	1.70	0.55
5:A:372:VAL:O	5:A:374:GLN:N	2.39	0.55
5:A:679:PHE:HE1	5:A:749:PHE:HB2	1.70	0.55
19:B:1768:CLA:H121	22:B:1779:BCR:H311	1.88	0.55
6:B:577:TYR:CE2	6:B:578:LEU:HD12	2.41	0.55
6:B:597:LYS:O	6:B:598:HIS:HB2	2.06	0.55
9:E:73:ASN:C	9:E:73:ASN:ND2	2.60	0.55
11:G:46:ALA:CA	11:G:48:ASP:CB	2.81	0.55
22:I:1032:BCR:C3	19:I:1033:CLA:HAC2	2.12	0.55
16:L:25:THR:HB	16:L:26:PRO:CD	2.37	0.55
3:3:202:LEU:HB3	3:3:204:THR:HG23	1.87	0.55
9:E:69:PHE:CD2	9:E:70:ALA:N	2.74	0.55
7:C:44:ARG:NH2	8:D:127:ARG:CB	2.66	0.55
6:B:37:ILE:HD12	6:B:37:ILE:C	2.27	0.55
5:A:133:ASN:HD22	5:A:142:GLY:HA2	1.70	0.55
19:A:1782:CLA:C14	19:A:1782:CLA:H101	2.36	0.55
5:A:545:HIS:ND1	19:A:1792:CLA:CBB	2.52	0.55
5:A:216:LEU:CD1	22:A:1803:BCR:H352	2.37	0.55
5:A:211:LEU:HB3	5:A:310:PHE:CD2	2.42	0.55
5:A:678:PHE:O	5:A:681:GLY:O	2.25	0.55
6:B:707:LEU:HD11	19:B:1759:CLA:C9	2.37	0.55
19:B:1771:CLA:CHD	23:B:1773:PQN:H18	2.36	0.55
6:B:197:VAL:O	6:B:197:VAL:HG12	2.05	0.55
6:B:361:ILE:C	6:B:362:ALA:O	2.44	0.55
6:B:378:ILE:HA	6:B:381:PHE:HB2	1.87	0.55
6:B:421:HIS:CE1	19:B:1761:CLA:C4D	2.89	0.55
5:A:587:GLY:HA3	6:B:668:ARG:CZ	2.36	0.55
6:B:646:TRP:CZ3	6:B:726:ILE:HD13	2.42	0.55
7:C:75:ARG:NH2	8:D:110:GLN:OE1	2.35	0.55
8:D:91:ARG:NH1	8:D:119:TYR:HE1	2.05	0.55
19:A:1801:CLA:HBA1	16:L:33:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:48:GLY:HA3	17:N:49:CYS:C	2.17	0.55
3:3:48:PHE:CD2	3:3:49:ILE:CG2	2.69	0.55
20:A:7030:LMU:C9	20:A:7030:LMU:H51	2.14	0.55
20:A:7038:LMU:H6'	20:A:7038:LMU:C1B	2.18	0.55
5:A:468:SER:HB2	5:A:476:MET:SD	2.47	0.55
6:B:42:LEU:O	6:B:45:ASN:N	2.39	0.55
21:B:8053:SUC:H5	21:B:8053:SUC:O2	2.06	0.55
5:A:100:GLY:HA3	5:A:153:TRP:CZ3	2.42	0.55
5:A:62:HIS:O	19:A:1785:CLA:HAA2	2.06	0.55
5:A:369:THR:HG21	5:A:402:ILE:CG2	2.37	0.55
5:A:64:PHE:HE2	19:A:1761:CLA:HMC1	1.71	0.55
6:B:290:MET:HG3	19:B:1751:CLA:C2C	2.36	0.55
10:F:46:MET:O	10:F:49:THR:N	2.38	0.55
3:3:56:TYR:HD1	3:3:185:LYS:HZ1	1.51	0.55
8:D:69:ARG:O	8:D:70:GLU:CB	2.54	0.55
19:A:1764:CLA:O2D	19:A:1764:CLA:H2A	2.06	0.55
19:A:1787:CLA:H141	19:A:1801:CLA:H93	1.89	0.55
19:A:1788:CLA:H101	19:A:1788:CLA:H142	1.88	0.55
5:A:711:HIS:CG	19:A:1795:CLA:HBC1	2.39	0.55
19:A:1796:CLA:H43	19:A:1796:CLA:ND	2.21	0.55
19:A:1801:CLA:HED1	16:L:32:LEU:CD1	2.34	0.55
5:A:744:ALA:CB	22:A:1807:BCR:C39	2.46	0.55
5:A:88:ILE:CG2	5:A:89:ILE:N	2.70	0.55
6:B:102:GLU:O	6:B:103:ALA:C	2.45	0.55
6:B:597:LYS:HG2	19:B:1767:CLA:HBC1	1.89	0.55
19:B:1786:CLA:H91	19:B:1787:CLA:H92	1.88	0.55
6:B:75:GLU:CB	6:B:132:ASN:HD22	2.19	0.55
8:D:140:ASN:HA	8:D:142:SER:OG	2.06	0.55
13:I:24:LEU:HD21	22:L:1169:BCR:H271	1.89	0.55
3:3:205:GLY:HA3	5:A:252:ARG:NH1	2.21	0.55
17:N:82:PHE:HD2	17:N:82:PHE:H	1.55	0.55
19:J:1043:CLA:C15	19:J:1044:CLA:HMB1	2.37	0.55
12:H:27:ASP:O	12:H:29:PRO:HD3	2.06	0.55
5:A:425:THR:O	5:A:428:TYR:CE1	2.59	0.55
20:R:1056:LMU:O5B	20:R:1056:LMU:H5'	2.07	0.55
6:B:476:ILE:O	6:B:479:SER:OG	2.16	0.55
5:A:478:SER:C	5:A:480:THR:H	2.10	0.55
19:I:1193:CLA:HBA2	19:I:1193:CLA:HMA3	1.88	0.55
15:K:55:PHE:N	15:K:55:PHE:HD1	2.04	0.55
11:G:78:GLY:O	11:G:79:HIS:ND1	2.40	0.55
19:A:1762:CLA:H51	19:A:1785:CLA:C4C	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1781:CLA:HMA2	19:A:1782:CLA:CGA	2.36	0.55
19:A:1789:CLA:O1D	16:L:73:PRO:O	2.25	0.55
5:A:679:PHE:O	5:A:683:HIS:HB2	2.07	0.55
6:B:193:HIS:HD2	19:B:1744:CLA:NC	2.05	0.55
19:B:1768:CLA:H203	22:B:1779:BCR:HC41	1.89	0.55
5:A:705:GLU:CB	6:B:545:LYS:NZ	2.69	0.55
7:C:1:MET:H1	7:C:4:SER:CA	2.20	0.55
11:G:27:GLN:O	11:G:28:ARG:HB3	2.06	0.55
14:J:13:VAL:CG1	14:J:15:SER:HB2	2.37	0.55
17:N:63:ASP:H	17:N:64:ASP:HB2	1.66	0.55
17:N:66:ASP:CA	17:N:67:LEU:HD12	2.33	0.55
20:A:7016:LMU:C1'	20:A:7016:LMU:H31	2.36	0.55
20:2:7006:LMU:H3'	20:2:7006:LMU:O6B	2.06	0.55
16:L:50:LEU:HG	16:L:51:LEU:CD2	2.36	0.55
21:B:8055:SUC:C2'	21:B:8055:SUC:HO2	2.20	0.55
10:F:152:ASN:H	10:F:152:ASN:ND2	2.05	0.55
19:A:1796:CLA:H43	19:A:1796:CLA:C4C	2.36	0.55
5:A:412:ALA:O	5:A:415:ALA:HB3	2.07	0.55
5:A:532:ILE:N	5:A:533:PRO:HD3	2.21	0.55
5:A:603:PHE:HZ	5:A:693:LEU:CD2	2.20	0.55
5:A:82:HIS:O	5:A:84:GLY:N	2.40	0.55
6:B:95:HIS:CE1	19:B:1740:CLA:HMB3	2.41	0.55
6:B:340:SER:O	6:B:344:ILE:HG13	2.07	0.55
6:B:633:ASN:O	6:B:636:THR:HB	2.07	0.55
6:B:654:HIS:HE1	19:B:1785:CLA:NB	2.01	0.55
6:B:574:ASP:OD2	6:B:706:ARG:NE	2.40	0.55
13:I:19:VAL:O	13:I:23:SER:N	2.40	0.55
16:L:41:PRO:HG3	16:L:52:ARG:HD3	1.88	0.55
19:2:1212:CLA:CMC	19:2:1212:CLA:HBC3	2.29	0.55
2:2:60:ALA:HA	2:2:63:PHE:CE2	2.42	0.55
10:F:25:LEU:HD21	10:F:46:MET:HB3	1.84	0.55
5:A:141:ARG:HH21	5:A:141:ARG:CG	2.14	0.55
3:3:134:LYS:O	3:3:135:PRO:C	2.44	0.55
5:A:103:PHE:HE1	19:A:1763:CLA:CGD	2.17	0.55
19:A:1764:CLA:CMB	19:A:1765:CLA:H11	2.37	0.55
19:A:1783:CLA:H171	19:A:1783:CLA:H122	1.89	0.55
5:A:157:GLY:O	5:A:248:PHE:HE1	1.90	0.55
6:B:378:ILE:CA	6:B:381:PHE:HB2	2.37	0.55
6:B:575:ASP:O	6:B:579:ALA:N	2.36	0.55
13:I:12:VAL:CG2	19:I:1031:CLA:O1A	2.52	0.55
19:1:1198:CLA:H101	19:1:1198:CLA:C5	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:154:TRP:O	6:B:157:LEU:N	2.29	0.55
5:A:137:GLY:C	5:A:139:GLY:H	2.10	0.55
5:A:210:LEU:N	5:A:213:LEU:H	2.05	0.55
5:A:358:LEU:O	5:A:361:ASN:HB3	2.06	0.55
5:A:431:LEU:O	5:A:435:VAL:CG1	2.55	0.55
5:A:700:TRP:HZ3	19:A:1813:CLA:O1D	1.90	0.55
6:B:486:LEU:HB2	6:B:489:GLY:O	2.07	0.55
6:B:519:VAL:HG11	6:B:593:TYR:HB2	1.89	0.55
6:B:732:LYS:HG3	6:B:734:GLY:HA2	1.87	0.55
7:C:74:THR:OG1	7:C:75:ARG:N	2.33	0.55
9:E:40:ARG:NH2	9:E:87:VAL:HG22	2.21	0.55
11:G:18:LEU:C	11:G:21:PHE:H	2.10	0.55
19:1:1198:CLA:H92	19:1:1198:CLA:H121	1.86	0.55
17:N:41:LYS:CB	17:N:42:PHE:CA	2.83	0.55
10:F:23:LYS:CA	10:F:24:LYS:NZ	2.70	0.55
12:H:25:GLY:HA3	12:H:27:ASP:CG	2.26	0.55
7:C:39:ILE:HG23	7:C:40:ALA:N	2.22	0.55
20:A:7019:LMU:H32	20:A:7019:LMU:O2'	2.07	0.55
5:A:158:ILE:HG23	5:A:163:GLN:NE2	2.22	0.54
5:A:584:PRO:HG2	7:C:66:ARG:HB2	1.89	0.54
5:A:541:VAL:CG1	5:A:615:HIS:CD2	2.72	0.54
5:A:83:PHE:HA	5:A:86:LEU:HD23	1.89	0.54
11:G:19:GLY:O	11:G:22:VAL:N	2.40	0.54
16:L:88:ALA:O	16:L:90:GLY:N	2.39	0.54
17:N:46:PHE:C	17:N:47:THR:HG23	2.17	0.54
19:1:1187:CLA:HBA2	19:1:1187:CLA:CMA	2.26	0.54
10:F:24:LYS:N	10:F:26:GLN:H	2.05	0.54
19:R:1054:CLA:HBA2	19:R:1054:CLA:HBD	1.89	0.54
15:K:69:ILE:CA	15:K:72:VAL:HG12	2.35	0.54
19:L:1505:CLA:H42	19:L:1505:CLA:HAA1	1.90	0.54
2:2:96:ILE:HG13	2:2:97:VAL:N	2.21	0.54
1:1:111:GLN:HE21	1:1:111:GLN:HA	1.72	0.54
2:2:179:PHE:HD1	2:2:183:TYR:HE2	1.53	0.54
5:A:124:TRP:HA	5:A:124:TRP:CE3	2.42	0.54
19:A:1777:CLA:C2D	19:A:1778:CLA:HMB3	2.37	0.54
5:A:368:LEU:HD12	19:A:1782:CLA:C6	2.38	0.54
5:A:394:SER:HB2	19:A:1783:CLA:CMA	2.28	0.54
19:B:1756:CLA:H72	19:B:1756:CLA:C4	2.37	0.54
19:B:1747:CLA:CAD	19:B:1756:CLA:HBB2	2.36	0.54
22:B:1781:BCR:H342	19:H:1079:CLA:CHD	2.36	0.54
5:A:705:GLU:HB3	6:B:545:LYS:HZ1	1.72	0.54

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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	0.54
16:L:33:ILE:HD11	16:L:36:TYR:HD1	1.72	0.54
5:A:250:LEU:O	5:A:252:ARG:HG2	2.07	0.54
17:N:63:ASP:N	17:N:64:ASP:HB3	2.11	0.54
19:J:1045:CLA:C2	19:J:1045:CLA:CMA	2.84	0.54
20:A:7039:LMU:O2'	20:A:7039:LMU:C5'	2.45	0.54
20:A:7009:LMU:H3O2	20:A:7009:LMU:H5B	1.69	0.54
3:3:156:PRO:O	3:3:157:ALA:C	2.46	0.54
5:A:479:ASP:OD1	5:A:536:THR:O	2.25	0.54
6:B:166:SER:C	6:B:168:PHE:H	2.09	0.54
5:A:527:VAL:CG1	5:A:528:ALA:H	2.19	0.54
6:B:14:GLN:H	6:B:14:GLN:HE21	1.55	0.54
2:2:211:LYS:HA	2:2:211:LYS:HE2	1.89	0.54
4:4:169:GLN:CG	19:4:1199:CLA:CAC	2.80	0.54
5:A:177:LEU:C	5:A:179:LEU:H	2.11	0.54
19:B:1753:CLA:H72	19:B:1753:CLA:C2	2.32	0.54
19:B:1760:CLA:HAA2	19:B:1760:CLA:CED	2.37	0.54
5:A:680:LEU:CD2	6:B:617:MET:HB2	2.37	0.54
6:B:625:TRP:C	6:B:625:TRP:CE3	2.81	0.54
19:I:1033:CLA:H2A	19:I:1033:CLA:O1D	2.07	0.54
16:L:62:PHE:HB2	16:L:154:ALA:HB2	1.88	0.54
19:3:3008:CLA:O1A	19:3:3008:CLA:CGD	2.55	0.54
4:4:107:GLN:HA	19:4:1196:CLA:H2A	1.88	0.54
10:F:23:LYS:HD3	10:F:23:LYS:N	2.19	0.54
2:2:128:ASN:CG	14:J:3:ASP:HB3	2.28	0.54
8:D:124:ASN:HB3	8:D:125:PRO:CD	2.31	0.54
1:1:48:ARG:O	1:1:52:LEU:HB2	2.07	0.54
6:B:224:PRO:HB3	6:B:227:THR:HB	1.89	0.54
3:3:106:TYR:HB3	3:3:107:TRP:HD1	1.71	0.54
19:3:1216:CLA:C2B	19:A:1798:CLA:H2	2.38	0.54
5:A:157:GLY:O	5:A:248:PHE:CE1	2.60	0.54
19:A:1769:CLA:C1	19:A:1769:CLA:HMA2	2.37	0.54
19:A:1783:CLA:H43	19:A:1783:CLA:CGA	2.36	0.54
19:A:1765:CLA:H51	22:A:1808:BCR:C10	2.36	0.54
5:A:229:ILE:HG13	5:A:243:PRO:HB3	1.90	0.54
5:A:287:LEU:N	5:A:295:TRP:HE1	2.05	0.54
5:A:46:LYS:HG3	5:A:48:PRO:HB2	1.88	0.54
19:B:1787:CLA:H41	19:B:1787:CLA:CMB	2.37	0.54
6:B:284:PHE:CE1	19:B:1749:CLA:HHC	2.43	0.54
6:B:633:ASN:HD22	6:B:636:THR:HB	1.73	0.54
6:B:715:VAL:HA	6:B:718:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:46:TYR:CE1	8:D:80:LYS:HE2	2.34	0.54
2:2:169:LEU:HD23	19:2:1215:CLA:HBB2	1.87	0.54
19:2:1220:CLA:H102	19:2:1220:CLA:H51	1.88	0.54
3:3:94:ARG:C	3:3:97:PHE:CE1	2.81	0.54
17:N:50:GLN:OE1	17:N:51:ASP:HA	2.07	0.54
1:1:140:LEU:HG	1:1:142:GLU:N	2.23	0.54
10:F:20:GLN:O	10:F:21:ALA:HB3	2.05	0.54
6:B:456:GLU:HA	6:B:514:PRO:HD3	1.90	0.54
5:A:278:ALA:O	5:A:279:ASP:O	2.26	0.54
5:A:650:ASN:O	5:A:653:LEU:N	2.31	0.54
5:A:731:ARG:O	5:A:735:VAL:HG23	2.08	0.54
6:B:330:ILE:HD11	19:B:1737:CLA:H193	1.89	0.54
19:B:1754:CLA:H61	19:B:1754:CLA:CMA	2.38	0.54
19:B:1756:CLA:C4	19:B:1756:CLA:C7	2.86	0.54
6:B:351:HIS:NE2	19:B:1756:CLA:NC	2.56	0.54
19:B:1759:CLA:C20	19:B:1771:CLA:HBA1	2.37	0.54
19:B:1787:CLA:H41	19:B:1787:CLA:HMB2	1.88	0.54
5:A:547:PHE:CE2	19:B:1787:CLA:O1A	2.59	0.54
6:B:301:ILE:O	6:B:301:ILE:CG2	2.55	0.54
16:L:14:LEU:HD22	16:L:21:GLY:O	2.07	0.54
20:A:7041:LMU:O4'	20:A:7042:LMU:O1'	2.26	0.54
3:3:95:THR:HB	3:3:96:GLY:O	2.08	0.54
17:N:63:ASP:N	17:N:64:ASP:HB2	2.22	0.54
4:4:150:LYS:N	4:4:150:LYS:HE3	2.23	0.54
20:A:7013:LMU:H3O2	20:A:7013:LMU:C1B	2.21	0.54
7:C:19:ARG:NE	8:D:121:GLU:OE2	2.41	0.54
20:1:1202:LMU:H1B	20:1:1202:LMU:C6'	2.36	0.54
8:D:64:GLY:O	8:D:65:ALA:CB	2.56	0.54
7:C:35:LYS:C	7:C:37:LYS:H	2.10	0.54
5:A:162:LEU:C	5:A:165:TYR:HB3	2.28	0.54
19:A:1771:CLA:HMC1	19:A:1771:CLA:CBC	2.35	0.54
19:A:1759:CLA:H41	19:A:1796:CLA:H8	1.89	0.54
19:A:1763:CLA:HMB1	22:A:1808:BCR:HC7	1.89	0.54
5:A:223:VAL:HA	5:A:227:LEU:HB2	1.90	0.54
5:A:23:ASP:OD1	5:A:33:GLN:CG	2.55	0.54
5:A:582:ASP:HB3	5:A:589:THR:CG2	2.38	0.54
5:A:397:THR:HB	5:A:613:ILE:HG12	1.87	0.54
19:B:1755:CLA:C7	19:B:1769:CLA:C3D	2.85	0.54
6:B:50:HIS:HA	6:B:53:GLN:H	1.73	0.54
6:B:16:PRO:HG3	7:C:74:THR:CG2	2.37	0.54
17:N:65:LEU:CG	17:N:65:LEU:O	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:128:ALA:HB2	4:4:143:PHE:CE2	2.43	0.54
20:R:1057:LMU:C6	20:R:1057:LMU:C1	2.76	0.54
6:B:475:ASP:O	6:B:479:SER:OG	2.26	0.54
5:A:262:PHE:O	5:A:264:GLU:N	2.40	0.54
22:3:1220:BCR:C8	22:3:1220:BCR:C31	2.72	0.54
19:A:1759:CLA:H12	19:A:1796:CLA:H61	1.89	0.54
19:A:1781:CLA:HAA2	19:A:1782:CLA:OBD	2.08	0.54
5:A:615:HIS:CE1	19:A:1792:CLA:CBC	2.89	0.54
5:A:207:LEU:HB3	19:A:1776:CLA:CBB	2.38	0.54
5:A:218:TRP:N	19:A:1770:CLA:HBB2	2.22	0.54
5:A:361:ASN:O	5:A:365:LEU:N	2.39	0.54
5:A:451:ILE:HD12	19:A:1788:CLA:CED	2.06	0.54
5:A:619:LYS:HG2	5:A:642:PHE:CE1	2.43	0.54
5:A:622:SER:OG	5:A:642:PHE:HB2	2.07	0.54
5:A:84:GLY:C	5:A:87:SER:O	2.46	0.54
19:B:1747:CLA:H112	19:B:1765:CLA:H3A	1.90	0.54
19:B:1751:CLA:HMA3	19:B:1752:CLA:C4D	2.37	0.54
6:B:310:PRO:CB	6:B:311:PRO:HD2	2.36	0.54
6:B:492:ILE:HD13	6:B:492:ILE:N	2.13	0.54
6:B:76:ALA:O	6:B:79:GLN:N	2.39	0.54
3:3:53:TRP:HA	3:3:56:TYR:HD2	1.73	0.54
8:D:124:ASN:CB	8:D:125:PRO:CD	2.84	0.54
5:A:536:THR:HA	5:A:539:PHE:CB	2.38	0.54
3:3:114:PHE:CE1	19:3:1216:CLA:C3D	2.91	0.54
19:A:1760:CLA:O2D	19:A:1760:CLA:C2A	2.55	0.54
19:A:1811:CLA:HMB3	19:A:1812:CLA:CAD	2.38	0.54
5:A:210:LEU:HD13	19:A:1769:CLA:CMB	2.31	0.54
5:A:328:LYS:CD	5:A:332:GLU:HG3	2.28	0.54
5:A:448:TRP:CD1	19:A:1788:CLA:CED	2.91	0.54
5:A:472:ARG:O	5:A:474:GLN:N	2.41	0.54
5:A:618:TRP:HB2	5:A:656:PHE:CE1	2.43	0.54
5:A:654:ARG:HA	6:B:632:ILE:HD13	1.88	0.54
5:A:706:SER:HB3	6:B:419:ILE:O	2.07	0.54
6:B:124:TRP:CZ2	6:B:135:LEU:HD22	2.43	0.54
6:B:189:ALA:HA	19:B:1745:CLA:HBB1	1.90	0.54
22:B:1777:BCR:C8	22:B:1777:BCR:H311	2.38	0.54
6:B:330:ILE:HD12	6:B:330:ILE:O	2.06	0.54
6:B:550:LYS:CG	6:B:550:LYS:O	2.55	0.54
6:B:649:MET:HE3	6:B:723:ALA:HB2	1.90	0.54
8:D:102:ARG:HH21	8:D:110:GLN:HB2	1.72	0.54
10:F:80:TRP:HB3	19:F:1157:CLA:HHC	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:39:ASN:O	16:L:52:ARG:NH2	2.24	0.54
17:N:52:LEU:HB3	17:N:53:ALA:HA	1.88	0.54
19:J:1043:CLA:H152	19:J:1044:CLA:CMB	2.37	0.54
20:A:7037:LMU:H12	20:A:7037:LMU:C5	1.87	0.54
19:3:1219:CLA:CBC	19:3:1219:CLA:CMC	2.73	0.54
15:K:67:GLY:C	15:K:68:HIS:O	2.45	0.54
10:F:102:ARG:CD	10:F:106:ILE:HD11	2.38	0.54
3:3:66:MET:HG2	3:3:195:LEU:HD11	1.88	0.54
6:B:160:LYS:HE3	6:B:161:TRP:CE2	2.43	0.54
12:H:67:TYR:C	12:H:67:TYR:HD1	2.11	0.54
19:A:1795:CLA:C4D	19:B:1735:CLA:HMC3	2.38	0.54
5:A:308:ILE:O	5:A:311:LEU:HB2	2.07	0.54
5:A:638:THR:OG1	5:A:641:ASN:ND2	2.40	0.54
5:A:83:PHE:CE1	19:A:1769:CLA:HED1	2.43	0.54
5:A:88:ILE:HG22	5:A:89:ILE:H	1.73	0.54
6:B:120:VAL:HA	6:B:123:TRP:HE1	1.66	0.54
5:A:470:LEU:HG	19:B:1740:CLA:HMC3	1.90	0.54
6:B:276:HIS:HB2	19:B:1747:CLA:C1B	2.37	0.54
19:B:1739:CLA:C14	19:B:1757:CLA:H91	2.34	0.54
19:B:1762:CLA:CBB	22:B:1778:BCR:H272	2.36	0.54
22:B:1778:BCR:HC8	22:B:1778:BCR:C33	2.37	0.54
22:B:1781:BCR:HC42	19:B:1787:CLA:H142	1.88	0.54
6:B:363:GLN:HA	6:B:365:PHE:CE1	2.42	0.54
6:B:398:TYR:CD1	6:B:542:ARG:NH2	2.75	0.54
10:F:72:ILE:HG22	10:F:73:VAL:N	2.23	0.54
19:2:1217:CLA:H102	19:2:1217:CLA:H161	1.90	0.54
12:H:14:ILE:HD11	12:H:17:THR:H	1.73	0.54
13:I:2:ILE:HG13	13:I:3:ASN:OD1	2.08	0.54
6:B:20:ARG:HH11	6:B:20:ARG:CG	2.21	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
19:A:1779:CLA:C1C	22:A:1805:BCR:H17C	2.37	0.54
19:A:1796:CLA:NC	19:A:1796:CLA:H41	2.23	0.54
19:A:1800:CLA:C1A	19:A:1800:CLA:CGA	2.86	0.54
19:A:1781:CLA:C3B	22:A:1806:BCR:C21	2.86	0.54
5:A:650:ASN:O	5:A:653:LEU:HD13	2.07	0.54
5:A:672:LEU:HD23	5:A:672:LEU:H	1.71	0.54
5:A:723:ARG:HH11	5:A:723:ARG:HG3	1.68	0.54
6:B:132:ASN:HA	6:B:135:LEU:HG	1.89	0.54
5:A:584:PRO:CB	7:C:67:VAL:HB	2.38	0.54
6:B:25:ILE:HG22	22:L:1169:BCR:H291	1.83	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1788:CLA:H162	22:L:1169:BCR:H362	1.88	0.54
2:2:49:LEU:HB3	19:2:1215:CLA:CAC	2.37	0.54
17:N:59:PRO:C	17:N:61:LEU:O	2.46	0.54
5:A:316:MET:CA	5:A:317:TYR:CB	2.86	0.54
15:K:72:VAL:HG13	15:K:73:GLY:N	2.23	0.54
3:3:194:ILE:HD12	19:3:1212:CLA:HMC2	1.81	0.54
5:A:255:LEU:HD11	5:A:280:PHE:HZ	1.72	0.54
6:B:222:LEU:O	6:B:222:LEU:HD23	2.07	0.54
6:B:117:TYR:O	6:B:367:THR:HG23	2.08	0.54
19:A:1760:CLA:HBB2	19:A:1762:CLA:CAD	2.38	0.53
5:A:224:HIS:HE1	19:A:1771:CLA:C4C	2.20	0.53
5:A:591:GLN:OE1	5:A:600:LEU:HD21	2.08	0.53
19:B:1738:CLA:HBB	19:B:1759:CLA:HBB2	1.90	0.53
22:B:1780:BCR:C33	22:B:1780:BCR:C8	2.85	0.53
6:B:373:THR:O	6:B:377:TYR:N	2.31	0.53
6:B:427:LEU:HB3	19:B:1762:CLA:HED1	1.91	0.53
6:B:463:ILE:O	6:B:464:GLN:CB	2.56	0.53
6:B:573:TRP:O	6:B:577:TYR:N	2.31	0.53
6:B:603:ARG:NH1	6:B:732:LYS:HB3	2.18	0.53
11:G:31:MET:O	11:G:34:GLN:N	2.37	0.53
5:A:253:ASP:O	5:A:256:ALA:CB	2.56	0.53
17:N:62:SER:C	17:N:66:ASP:H	2.10	0.53
4:4:118:ASP:H	4:4:119:PRO:CD	2.21	0.53
1:1:89:VAL:HB	1:1:90:PRO:CD	2.30	0.53
16:L:48:ASN:HB2	16:L:50:LEU:HD22	1.90	0.53
5:A:148:GLY:C	5:A:149:PHE:O	2.43	0.53
5:A:242:ILE:HG12	5:A:243:PRO:HG3	1.90	0.53
5:A:389:TYR:CE1	5:A:625:TRP:CG	2.96	0.53
5:A:78:VAL:O	5:A:82:HIS:CB	2.55	0.53
19:B:1755:CLA:HED2	19:B:1756:CLA:CAD	2.37	0.53
19:B:1758:CLA:H62	22:B:1776:BCR:H321	1.90	0.53
19:B:1768:CLA:C12	22:B:1779:BCR:H311	2.38	0.53
6:B:416:GLU:H	6:B:416:GLU:CD	2.10	0.53
6:B:594:TRP:HD1	6:B:595:HIS:HB2	1.73	0.53
19:1:1191:CLA:CAB	19:1:1197:CLA:CHD	2.87	0.53
19:A:1816:CLA:H2	19:A:1816:CLA:O1A	2.07	0.53
20:A:7023:LMU:C1B	20:A:7023:LMU:O4'	2.55	0.53
4:4:107:GLN:O	19:4:1196:CLA:CMA	2.55	0.53
20:A:7039:LMU:H6B	20:A:7039:LMU:H4'	1.71	0.53
6:B:476:ILE:HG22	6:B:479:SER:OG	2.09	0.53
5:A:629:ASN:HD21	5:A:633:VAL:CG2	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:291:THR:O	5:A:293:GLY:N	2.36	0.53
19:A:1762:CLA:HBA2	19:A:1762:CLA:HED2	1.90	0.53
5:A:29:THR:OG1	5:A:31:PHE:N	2.42	0.53
6:B:302:LYS:O	6:B:303:TYR:CB	2.35	0.53
6:B:533:ILE:O	6:B:537:GLY:N	2.30	0.53
5:A:690:LEU:HD21	6:B:661:PHE:HE1	1.74	0.53
5:A:447:ASN:ND2	6:B:678:LEU:CD2	2.71	0.53
10:F:128:SER:O	10:F:130:LEU:HD23	2.08	0.53
16:L:123:ARG:O	16:L:124:LYS:HE3	2.08	0.53
5:A:253:ASP:O	5:A:256:ALA:HB3	2.09	0.53
3:3:194:ILE:HG13	19:3:1212:CLA:HMC2	1.85	0.53
11:G:13:GLY:O	11:G:16:LEU:HB2	2.07	0.53
17:N:37:PHE:CD2	17:N:37:PHE:N	2.75	0.53
5:A:520:LEU:HD22	20:A:1809:LMU:O1'	2.08	0.53
5:A:420:ARG:HG2	5:A:421:ASP:N	2.22	0.53
19:A:1760:CLA:CHD	19:A:1760:CLA:HBC3	2.37	0.53
19:A:1780:CLA:OBD	19:A:1780:CLA:C9	2.42	0.53
5:A:491:TRP:HE1	19:A:1792:CLA:C1	2.19	0.53
19:B:1740:CLA:H193	19:B:1771:CLA:C4	2.39	0.53
19:B:1746:CLA:CHD	19:B:1746:CLA:HBC2	2.27	0.53
6:B:336:LEU:CD1	19:B:1754:CLA:HBB1	2.37	0.53
6:B:310:PRO:O	19:B:1772:CLA:CHD	2.57	0.53
6:B:437:TYR:CG	6:B:616:LEU:HD22	2.42	0.53
6:B:732:LYS:HG3	6:B:733:PHE:O	2.06	0.53
6:B:78:VAL:HG23	6:B:78:VAL:O	2.08	0.53
9:E:86:GLU:CG	9:E:87:VAL:N	2.30	0.53
9:E:88:GLU:O	9:E:90:VAL:HG23	2.08	0.53
10:F:126:ALA:O	10:F:128:SER:OG	2.17	0.53
16:L:66:GLY:HA2	16:L:69:VAL:HG22	1.91	0.53
16:L:87:ALA:O	16:L:89:ALA:N	2.42	0.53
3:3:56:TYR:O	3:3:60:ILE:HD12	2.07	0.53
2:2:103:GLY:HA2	19:2:1222:CLA:CBB	2.38	0.53
10:F:117:LYS:N	10:F:118:GLU:OE2	2.41	0.53
6:B:15:ASP:O	6:B:20:ARG:CG	2.57	0.53
5:A:131:ILE:HG21	6:B:446:PHE:HA	1.90	0.53
19:A:1794:CLA:HMC1	19:A:1794:CLA:CBC	2.28	0.53
22:A:1805:BCR:C23	22:A:1805:BCR:H382	2.11	0.53
5:A:473:PRO:O	5:A:474:GLN:C	2.47	0.53
5:A:559:GLY:HA2	5:A:597:HIS:ND1	2.23	0.53
19:B:1735:CLA:H52	19:B:1735:CLA:C4C	2.39	0.53
6:B:493:TRP:CH2	19:B:1747:CLA:H122	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:406:ASN:C	6:B:406:ASN:HD22	2.11	0.53
6:B:596:TRP:O	6:B:597:LYS:CB	2.55	0.53
7:C:74:THR:OG1	7:C:80:ALA:HB3	2.07	0.53
19:B:1735:CLA:H191	10:F:104:TYR:CG	2.43	0.53
10:F:123:VAL:HG21	10:F:128:SER:OG	2.08	0.53
17:N:42:PHE:H	17:N:43:PRO:HD2	1.71	0.53
2:2:120:ASN:HA	14:J:5:LYS:CD	2.39	0.53
3:3:49:ILE:HG13	3:3:52:LYS:HB2	1.90	0.53
8:D:86:LEU:HD13	8:D:90:LEU:HG	1.90	0.53
5:A:160:SER:O	5:A:163:GLN:CG	2.38	0.53
5:A:382:TYR:HE2	19:A:1784:CLA:HED3	1.72	0.53
19:A:1762:CLA:O1A	19:A:1785:CLA:HMB2	2.09	0.53
19:A:1789:CLA:HBC3	19:A:1789:CLA:CMC	2.38	0.53
5:A:281:LEU:HB2	5:A:301:HIS:HD2	1.73	0.53
6:B:75:GLU:HB2	6:B:132:ASN:HD22	1.72	0.53
6:B:167:TRP:CZ2	19:B:1741:CLA:HMA1	2.43	0.53
6:B:233:TYR:HB3	6:B:254:ILE:O	2.09	0.53
6:B:338:LEU:O	6:B:339:ALA:HB3	2.08	0.53
7:C:5:VAL:C	7:C:65:VAL:CG2	2.69	0.53
8:D:28:ILE:O	8:D:66:ALA:HB3	2.09	0.53
8:D:75:LEU:HD22	8:D:76:LYS:H	1.74	0.53
11:G:19:GLY:HA2	11:G:22:VAL:H	1.74	0.53
13:I:11:LEU:HD11	22:I:1032:BCR:C10	2.38	0.53
22:B:1781:BCR:H272	22:I:1032:BCR:H352	1.89	0.53
16:L:56:VAL:CA	19:L:1167:CLA:HED2	2.34	0.53
20:A:7023:LMU:C1	20:A:7023:LMU:H91	2.31	0.53
4:4:127:PRO:HB2	4:4:143:PHE:CE1	2.44	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
6:B:20:ARG:CB	6:B:20:ARG:HH11	2.20	0.53
6:B:681:ALA:O	6:B:684:ARG:N	2.33	0.53
19:A:1759:CLA:C1	19:A:1796:CLA:H2	2.39	0.53
19:A:1783:CLA:C17	19:A:1783:CLA:H122	2.37	0.53
6:B:174:ARG:HH12	19:B:1754:CLA:CMD	2.21	0.53
6:B:668:ARG:HH12	6:B:672:GLN:HG2	1.72	0.53
6:B:580:VAL:CG1	6:B:710:LEU:HD21	2.38	0.53
10:F:104:TYR:HD2	10:F:104:TYR:O	1.89	0.53
19:L:1167:CLA:HAC2	22:L:1169:BCR:HC42	1.89	0.53
4:4:119:PRO:HG2	4:4:120:ILE:H	1.74	0.53
18:R:26:UNK:O	18:R:28:UNK:CA	2.57	0.53
6:B:503:GLU:HB3	6:B:507:SER:CA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:2:ILE:HG22	10:F:3:ALA:H	1.74	0.53
5:A:114:THR:O	5:A:525:ASN:ND2	2.42	0.53
5:A:184:PHE:CE2	19:A:1766:CLA:C2D	2.92	0.53
5:A:40:PHE:N	5:A:44:ILE:HG21	2.24	0.53
5:A:567:ARG:NH2	5:A:567:ARG:HB3	2.23	0.53
5:A:55:TRP:CD2	5:A:729:GLN:NE2	2.77	0.53
6:B:91:ILE:HD11	6:B:104:PHE:CE2	2.44	0.53
6:B:196:HIS:NE2	19:B:1745:CLA:ND	2.56	0.53
6:B:188:LEU:HG	6:B:189:ALA:N	2.24	0.53
6:B:294:ASN:CB	11:G:36:PRO:HD2	2.36	0.53
13:I:29:GLU:HA	13:I:29:GLU:OE2	2.09	0.53
14:J:19:PHE:O	14:J:23:ALA:HB3	2.08	0.53
12:H:65:LEU:HD11	16:L:90:GLY:HA2	1.90	0.53
17:N:58:VAL:CG1	17:N:59:PRO:CD	2.87	0.53
17:N:69:CYS:O	17:N:72:LYS:CD	2.57	0.53
4:4:104:ARG:NH1	4:4:105:ARG:HB2	2.16	0.53
19:K:1142:CLA:HHD	19:K:1142:CLA:HBC3	1.91	0.53
9:E:48:ASN:OD1	9:E:48:ASN:C	2.46	0.53
9:E:50:GLY:HA3	9:E:69:PHE:HB2	1.91	0.53
10:F:58:LYS:O	10:F:60:GLY:N	2.42	0.53
2:2:66:GLU:O	2:2:69:THR:HG23	2.09	0.53
19:A:1800:CLA:H92	22:L:1169:BCR:C32	2.36	0.53
5:A:442:ILE:HG23	19:A:1786:CLA:CMC	2.31	0.53
5:A:641:ASN:HD22	5:A:641:ASN:H	1.57	0.53
5:A:710:ALA:CB	19:B:1735:CLA:HED2	2.39	0.53
19:B:1739:CLA:H2	19:B:1739:CLA:H71	1.91	0.53
6:B:172:GLU:C	6:B:176:ASN:HB2	2.29	0.53
22:B:1780:BCR:C19	19:B:1786:CLA:C15	2.80	0.53
8:D:40:ALA:HA	8:D:44:GLU:O	2.08	0.53
10:F:96:TRP:HZ2	19:F:1155:CLA:CAB	2.22	0.53
11:G:47:GLY:N	11:G:48:ASP:HA	2.17	0.53
22:I:1032:BCR:C2	19:I:1033:CLA:C4C	2.66	0.53
17:N:46:PHE:O	17:N:47:THR:CB	2.56	0.53
19:1:1200:CLA:CMA	19:1:1200:CLA:HBA2	2.33	0.53
4:4:154:ILE:O	4:4:157:GLY:N	2.33	0.53
4:4:154:ILE:CG1	4:4:155:ALA:N	2.68	0.53
4:4:136:GLY:O	4:4:137:ILE:HB	2.09	0.53
8:D:87:GLY:H	8:D:90:LEU:H	1.57	0.53
19:1:1192:CLA:CGD	20:1:1202:LMU:O2'	2.57	0.53
5:A:293:GLY:O	5:A:294:LEU:HB3	2.08	0.53
11:G:85:ILE:O	11:G:86:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1782:CLA:CBA	19:A:1782:CLA:O1D	2.46	0.53
19:A:1812:CLA:H101	19:A:1812:CLA:H152	1.90	0.53
5:A:216:LEU:CD1	22:A:1803:BCR:C35	2.86	0.53
5:A:453:LEU:CB	5:A:547:PHE:HB2	2.34	0.53
6:B:308:HIS:HD1	6:B:309:ILE:N	2.06	0.53
6:B:462:TRP:CZ3	19:B:1764:CLA:CBC	2.92	0.53
14:J:25:LEU:HA	14:J:28:GLU:HB2	1.91	0.53
22:L:1169:BCR:H331	22:L:1169:BCR:C8	2.38	0.53
3:3:74:ALA:CB	19:3:1215:CLA:C1D	2.86	0.53
19:2:1212:CLA:HBC2	19:2:1212:CLA:CMC	2.32	0.53
17:N:45:ASN:CA	17:N:57:LYS:NZ	2.72	0.53
1:1:144:LYS:NZ	19:1:1187:CLA:OBD	2.36	0.53
10:F:23:LYS:CA	10:F:24:LYS:HZ3	2.22	0.53
10:F:92:TYR:CD2	10:F:92:TYR:C	2.81	0.53
2:2:40:SER:O	2:2:42:ARG:N	2.40	0.53
5:A:158:ILE:HG23	5:A:163:GLN:HE22	1.74	0.52
19:A:1776:CLA:C9	22:A:1805:BCR:H371	2.22	0.52
5:A:44:ILE:O	5:A:45:ALA:C	2.47	0.52
19:B:1786:CLA:CBB	19:B:1787:CLA:C1B	2.80	0.52
6:B:415:LYS:CG	6:B:416:GLU:OE2	2.57	0.52
18:R:32:UNK:CB	18:R:33:UNK:CA	2.76	0.52
4:4:128:ALA:HB2	4:4:143:PHE:CZ	2.44	0.52
7:C:39:ILE:CG1	7:C:40:ALA:N	2.64	0.52
20:A:7027:LMU:C2B	20:A:7027:LMU:C6B	2.87	0.52
11:G:69:VAL:O	11:G:73:ALA:CB	2.58	0.52
12:H:67:TYR:CD1	12:H:67:TYR:C	2.83	0.52
1:1:29:LEU:O	1:1:31:GLU:N	2.42	0.52
2:2:126:PRO:O	2:2:127:ASN:HB2	2.09	0.52
19:A:1789:CLA:H172	19:A:1793:CLA:H202	1.91	0.52
19:A:1797:CLA:O1A	19:A:1797:CLA:CED	2.57	0.52
19:A:1797:CLA:O1A	19:A:1797:CLA:H2A	1.98	0.52
5:A:214:GLY:O	5:A:215:SER:CB	2.56	0.52
5:A:334:HIS:HB3	19:A:1777:CLA:HMA1	1.90	0.52
5:A:733:VAL:HG11	19:A:1796:CLA:C1D	2.39	0.52
6:B:46:ILE:CD1	19:B:1737:CLA:H192	2.40	0.52
19:B:1738:CLA:C4	24:B:1783:LMG:H321	2.39	0.52
19:B:1755:CLA:CGA	19:B:1769:CLA:HAA1	2.38	0.52
19:B:1764:CLA:C1D	19:B:1765:CLA:HBB2	2.39	0.52
6:B:295:PHE:O	11:G:33:LYS:HB2	2.08	0.52
6:B:596:TRP:O	6:B:597:LYS:HB3	2.08	0.52
6:B:616:LEU:O	6:B:619:TRP:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:40:ARG:H	9:E:46:PHE:HE1	1.56	0.52
6:B:297:ILE:HG21	11:G:21:PHE:HZ	1.75	0.52
11:G:44:PHE:H	11:G:45:GLU:HB3	1.73	0.52
15:K:31:ASN:H	15:K:32:ARG:NH1	2.07	0.52
15:K:32:ARG:HA	15:K:32:ARG:NE	2.24	0.52
16:L:66:GLY:C	19:L:1168:CLA:HMC3	2.29	0.52
19:4:1198:CLA:HBC3	19:4:1198:CLA:HMC1	1.90	0.52
1:1:140:LEU:H	1:1:140:LEU:HD23	1.73	0.52
10:F:44:ALA:HB1	10:F:48:LYS:HB3	1.91	0.52
8:D:86:LEU:CD1	8:D:90:LEU:HG	2.39	0.52
19:2:1224:CLA:H151	19:2:1224:CLA:C8	2.38	0.52
2:2:181:HIS:NE2	19:2:1214:CLA:C2D	2.73	0.52
3:3:208:PRO:HB3	3:3:210:GLN:CD	2.29	0.52
3:3:114:PHE:HE1	19:3:1216:CLA:C3D	2.22	0.52
5:A:144:GLN:CG	5:A:145:ILE:H	2.22	0.52
19:A:1762:CLA:C7	19:A:1762:CLA:H2	2.38	0.52
5:A:187:HIS:NE2	19:A:1767:CLA:C4C	2.50	0.52
5:A:32:GLU:HG3	5:A:33:GLN:N	2.24	0.52
5:A:697:ARG:C	5:A:699:TYR:N	2.62	0.52
6:B:124:TRP:C	6:B:124:TRP:HD1	2.11	0.52
19:B:1762:CLA:CBB	22:B:1778:BCR:C23	2.87	0.52
19:B:1770:CLA:HMC1	19:B:1770:CLA:HBC2	1.91	0.52
6:B:203:ARG:HB3	6:B:270:LEU:HD12	1.91	0.52
6:B:207:VAL:O	6:B:208:ARG:O	2.27	0.52
6:B:378:ILE:HG22	6:B:379:ALA:N	2.24	0.52
6:B:696:LYS:NZ	8:D:39:LYS:HE3	2.25	0.52
11:G:48:ASP:HB3	11:G:49:THR:HG21	1.87	0.52
16:L:66:GLY:N	16:L:67:PRO:CD	2.72	0.52
6:B:475:ASP:HA	6:B:480:SER:C	2.30	0.52
8:D:122:LYS:NZ	8:D:124:ASN:OD1	2.43	0.52
19:A:1790:CLA:C3D	19:A:1791:CLA:CAC	2.87	0.52
22:A:1807:BCR:H17C	19:A:1812:CLA:H172	1.91	0.52
5:A:223:VAL:CG1	5:A:224:HIS:N	2.72	0.52
6:B:127:ILE:CG1	6:B:193:HIS:HE1	2.22	0.52
6:B:525:LEU:HD22	6:B:529:THR:OG1	2.09	0.52
6:B:544:SER:O	6:B:546:LEU:N	2.42	0.52
6:B:564:ARG:NH2	7:C:66:ARG:HH12	2.07	0.52
19:A:1788:CLA:H152	22:L:1169:BCR:H363	1.90	0.52
20:A:7036:LMU:C1B	20:A:7036:LMU:H6E	2.39	0.52
17:N:65:LEU:C	17:N:66:ASP:OD2	2.48	0.52
17:N:67:LEU:N	17:N:67:LEU:CD1	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:126:LEU:N	4:4:127:PRO:CD	2.70	0.52
10:F:22:LEU:C	10:F:25:LEU:HD13	2.29	0.52
3:3:52:LYS:C	3:3:56:TYR:HD2	2.10	0.52
3:3:49:ILE:CG1	3:3:52:LYS:HB2	2.39	0.52
6:B:488:ALA:HB1	19:B:1766:CLA:C1C	2.40	0.52
19:A:1759:CLA:H12	19:A:1796:CLA:C6	2.40	0.52
5:A:353:SER:O	5:A:354:TRP:CB	2.57	0.52
5:A:408:VAL:HG21	5:A:602:LEU:HG	1.90	0.52
5:A:618:TRP:CD1	5:A:618:TRP:O	2.62	0.52
5:A:703:LEU:O	5:A:707:ILE:HG12	2.09	0.52
6:B:143:LEU:C	6:B:145:LEU:N	2.62	0.52
19:B:1753:CLA:H12	19:B:1753:CLA:CAA	2.23	0.52
19:B:1762:CLA:CBB	22:B:1778:BCR:H23C	2.39	0.52
6:B:545:LYS:HG2	9:E:74:TYR:CE2	2.44	0.52
6:B:551:LYS:O	6:B:553:PHE:CE2	2.62	0.52
7:C:69:LEU:HD23	7:C:70:TRP:N	2.24	0.52
8:D:113:HIS:HD2	8:D:118:VAL:HG21	1.72	0.52
6:B:551:LYS:CD	8:D:143:PRO:HA	2.39	0.52
13:I:17:PRO:O	13:I:18:ALA:C	2.48	0.52
13:I:8:PHE:CE1	19:I:1031:CLA:H43	2.44	0.52
19:2:1218:CLA:HBA1	20:2:7003:LMU:H51	1.91	0.52
2:2:120:ASN:CA	14:J:5:LYS:CD	2.86	0.52
6:B:98:GLN:O	6:B:98:GLN:NE2	2.43	0.52
5:A:163:GLN:O	5:A:166:CYS:SG	2.67	0.52
19:A:1779:CLA:NB	22:A:1805:BCR:H15C	2.24	0.52
5:A:40:PHE:HZ	5:A:56:ASN:HB3	1.73	0.52
5:A:389:TYR:CD1	5:A:625:TRP:CG	2.97	0.52
5:A:656:PHE:O	5:A:659:ALA:N	2.42	0.52
19:B:1753:CLA:HMD2	19:B:1754:CLA:HBB2	1.89	0.52
6:B:330:ILE:CD1	6:B:330:ILE:O	2.58	0.52
8:D:36:LEU:HD21	8:D:45:PHE:CZ	2.44	0.52
10:F:96:TRP:CE3	10:F:134:PHE:N	2.78	0.52
11:G:45:GLU:CA	11:G:49:THR:CG2	2.76	0.52
20:A:7042:LMU:C6'	20:A:7042:LMU:C4	2.88	0.52
17:N:42:PHE:N	17:N:43:PRO:HD3	2.22	0.52
17:N:76:LYS:O	17:N:77:CYS:O	2.27	0.52
12:H:23:VAL:O	12:H:24:TYR:C	2.48	0.52
3:3:60:ILE:HA	3:3:63:ARG:HD2	1.92	0.52
20:A:7010:LMU:C2B	20:A:7010:LMU:H3'	2.36	0.52
5:A:631:GLN:O	5:A:632:GLY:C	2.48	0.52
5:A:265:GLY:HA2	5:A:272:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:74:LEU:O	2:2:75:ASN:HB2	2.10	0.52
5:A:331:LEU:CD1	5:A:346:LEU:CB	2.61	0.52
5:A:438:HIS:HB2	5:A:441:ALA:HB3	1.92	0.52
19:B:1735:CLA:HBC3	19:B:1735:CLA:HHD	1.92	0.52
19:B:1736:CLA:CHD	22:I:1032:BCR:H401	2.40	0.52
6:B:546:LEU:HD11	6:B:567:THR:CG2	2.38	0.52
5:A:680:LEU:HD21	6:B:617:MET:HB2	1.91	0.52
9:E:90:VAL:O	9:E:91:ALA:O	2.28	0.52
20:A:7036:LMU:H22	20:A:7036:LMU:C9	2.38	0.52
3:3:132:TRP:CZ3	3:3:155:GLU:OE1	2.57	0.52
18:R:39:UNK:CA	18:R:41:UNK:CB	2.88	0.52
2:2:64:ILE:HG13	2:2:68:LEU:HD13	1.91	0.52
4:4:107:GLN:C	19:4:1196:CLA:HMA3	2.02	0.52
21:3:1221:SUC:O1'	21:3:1221:SUC:C5'	2.56	0.52
1:1:25:ASP:N	6:B:314:ARG:HH22	1.99	0.52
12:H:47:PHE:CD2	16:L:141:GLY:HA2	2.45	0.52
12:H:34:SER:OG	12:H:36:GLN:NE2	2.42	0.52
16:L:58:LEU:HA	16:L:146:GLY:O	2.10	0.52
2:2:126:PRO:HD2	2:2:129:LYS:HB2	1.90	0.52
5:A:365:LEU:CD2	19:A:1761:CLA:CED	2.67	0.52
5:A:361:ASN:OD1	19:A:1761:CLA:OBD	2.28	0.52
19:A:1764:CLA:HBB2	19:A:1765:CLA:C4D	2.39	0.52
5:A:242:ILE:HG12	5:A:243:PRO:CG	2.39	0.52
5:A:310:PHE:H	5:A:313:ALA:HB3	1.74	0.52
5:A:378:SER:OG	5:A:378:SER:O	2.28	0.52
5:A:707:ILE:C	5:A:711:HIS:HD2	2.13	0.52
19:B:1738:CLA:H43	24:B:1783:LMG:H321	1.92	0.52
22:B:1780:BCR:C19	19:B:1786:CLA:H112	2.29	0.52
5:A:709:TRP:CZ3	6:B:417:ALA:HA	2.45	0.52
8:D:31:GLY:O	8:D:32:SER:HB2	2.10	0.52
11:G:28:ARG:CG	11:G:29:GLU:HB2	2.39	0.52
19:A:1788:CLA:C15	22:L:1169:BCR:H361	2.38	0.52
16:L:8:TYR:HE1	16:L:11:ILE:CG2	2.20	0.52
17:N:70:GLU:O	17:N:72:LYS:N	2.40	0.52
3:3:47:GLY:C	3:3:49:ILE:H	2.10	0.52
12:H:58:ILE:CD1	16:L:97:MET:SD	2.84	0.52
17:N:5:GLU:OE2	17:N:6:TYR:CA	2.57	0.52
5:A:527:VAL:HG13	5:A:528:ALA:H	1.75	0.52
3:3:104:TYR:CB	3:3:106:TYR:H	2.22	0.52
3:3:106:TYR:CB	3:3:107:TRP:CD1	2.92	0.52
5:A:375:HIS:HE1	19:A:1782:CLA:NC	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:455:PHE:CD1	19:A:1788:CLA:HMA2	2.44	0.52
5:A:435:VAL:O	5:A:438:HIS:ND1	2.39	0.52
6:B:304:ILE:CD1	19:B:1749:CLA:CED	2.86	0.52
6:B:326:ILE:O	6:B:326:ILE:HG12	2.09	0.52
6:B:546:LEU:HD12	6:B:570:ILE:HD13	1.91	0.52
6:B:87:ILE:O	6:B:121:TYR:HE2	1.92	0.52
6:B:8:PHE:O	6:B:35:ASP:CG	2.48	0.52
4:4:106:TRP:NE1	19:4:1196:CLA:HED3	2.19	0.52
4:4:91:PHE:O	4:4:95:PHE:CD1	2.63	0.52
6:B:513:GLY:O	6:B:515:GLY:N	2.42	0.52
16:L:5:LYS:N	16:L:6:PRO:CD	2.73	0.52
19:A:1799:CLA:CED	19:A:1799:CLA:CBA	2.88	0.52
5:A:149:PHE:O	5:A:150:PHE:HB2	2.09	0.52
5:A:351:THR:O	19:A:1780:CLA:H201	2.10	0.52
19:A:1776:CLA:CAA	19:A:1780:CLA:HBB2	2.38	0.52
19:A:1783:CLA:C1A	19:A:1783:CLA:CGA	2.88	0.52
5:A:299:ILE:HD11	19:A:1774:CLA:HMA3	1.91	0.52
5:A:701:GLN:OE1	9:E:74:TYR:CE1	2.63	0.52
6:B:70:TRP:HB3	6:B:136:TYR:OH	2.08	0.52
19:B:1755:CLA:C2B	22:B:1777:BCR:C35	2.88	0.52
19:B:1755:CLA:H52	19:B:1769:CLA:HBD	1.91	0.52
19:B:1786:CLA:C12	19:B:1786:CLA:H71	2.39	0.52
19:H:1079:CLA:HMA2	19:H:1079:CLA:C1	2.39	0.52
16:L:33:ILE:O	16:L:36:TYR:N	2.43	0.52
12:H:20:GLN:C	12:H:22:ASP:HB3	2.31	0.52
4:4:154:ILE:CD1	19:4:1202:CLA:CHA	2.84	0.52
19:A:1815:CLA:H3A	19:A:1815:CLA:CGA	2.33	0.52
19:1:1193:CLA:HAA2	19:1:1193:CLA:CBD	2.40	0.52
2:2:189:ILE:O	2:2:190:ASP:HB3	2.10	0.52
11:G:14:LEU:HG	11:G:14:LEU:O	2.09	0.52
19:A:1781:CLA:CBA	19:A:1794:CLA:CED	2.81	0.51
19:A:1779:CLA:ND	22:A:1805:BCR:C19	2.73	0.51
5:A:209:GLY:C	5:A:213:LEU:HB2	2.30	0.51
5:A:197:GLN:OE1	5:A:351:THR:O	2.28	0.51
5:A:40:PHE:H	5:A:44:ILE:CG2	2.23	0.51
5:A:473:PRO:C	5:A:475:ASP:N	2.61	0.51
6:B:729:THR:CG2	6:B:729:THR:O	2.29	0.51
11:G:43:HIS:O	11:G:45:GLU:CA	2.57	0.51
22:I:1032:BCR:C38	22:I:1032:BCR:C40	2.75	0.51
17:N:44:GLU:C	17:N:46:PHE:H	2.13	0.51
19:3:1219:CLA:O1A	19:3:1219:CLA:C3A	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:194:ILE:CG1	19:3:1212:CLA:CMC	2.84	0.51
11:G:13:GLY:C	11:G:16:LEU:HG	2.31	0.51
4:4:161:LEU:O	4:4:162:ALA:HB2	2.11	0.51
5:A:747:TRP:HB2	19:A:1783:CLA:HBB1	1.92	0.51
19:A:1787:CLA:HMB1	19:A:1800:CLA:HAA2	1.92	0.51
5:A:466:THR:O	5:A:470:LEU:CG	2.59	0.51
5:A:379:MET:SD	5:A:512:SER:HB2	2.50	0.51
5:A:584:PRO:HB2	7:C:67:VAL:HB	1.92	0.51
5:A:603:PHE:CZ	5:A:735:VAL:HG22	2.45	0.51
6:B:323:TYR:CD1	19:B:1754:CLA:CBC	2.93	0.51
6:B:531:THR:CG2	19:B:1755:CLA:HMC2	2.07	0.51
6:B:593:TYR:CZ	19:B:1767:CLA:HBC2	2.45	0.51
19:B:1768:CLA:C6	22:B:1779:BCR:C32	2.87	0.51
6:B:273:VAL:O	6:B:277:HIS:CD2	2.62	0.51
6:B:274:ALA:O	6:B:278:LEU:HB2	2.09	0.51
6:B:362:ALA:C	6:B:364:ASP:H	2.14	0.51
19:A:1813:CLA:H93	6:B:431:PHE:CD1	2.46	0.51
6:B:536:LYS:O	6:B:537:GLY:C	2.48	0.51
6:B:551:LYS:HE2	8:D:143:PRO:CA	2.39	0.51
6:B:626:LEU:O	6:B:627:ASN:HB2	2.10	0.51
6:B:715:VAL:O	6:B:719:PHE:N	2.33	0.51
8:D:43:GLU:HG3	8:D:44:GLU:H	1.75	0.51
10:F:149:LEU:HD23	10:F:153:ASN:ND2	2.24	0.51
18:R:39:UNK:CA	18:R:42:UNK:CB	2.85	0.51
19:2:1212:CLA:C3A	19:2:1212:CLA:CGA	2.87	0.51
2:2:53:ARG:O	2:2:57:LEU:HB3	2.10	0.51
7:C:9:ASP:CB	25:C:1083:SF4:S3	2.98	0.51
5:A:316:MET:CA	5:A:317:TYR:HD1	2.20	0.51
4:4:154:ILE:CG1	4:4:155:ALA:H	2.16	0.51
20:A:7043:LMU:H102	20:A:7043:LMU:H61	1.80	0.51
20:A:7026:LMU:C2B	20:A:7026:LMU:O3'	2.56	0.51
3:3:157:ALA:O	3:3:158:TYR:CD2	2.63	0.51
1:1:42:SER:HA	1:1:45:ILE:HG12	1.92	0.51
12:H:32:TYR:OH	16:L:44:ARG:NE	2.22	0.51
6:B:440:ASN:ND2	6:B:453:ILE:O	2.44	0.51
3:3:153:SER:OG	3:3:154:GLY:N	2.43	0.51
5:A:224:HIS:HE1	19:A:1771:CLA:CHD	2.22	0.51
19:A:1773:CLA:H12	19:A:1773:CLA:C4A	2.41	0.51
5:A:183:TRP:O	5:A:185:HIS:N	2.44	0.51
5:A:211:LEU:HB3	5:A:310:PHE:CE2	2.44	0.51
5:A:430:ASP:H	5:A:433:ASP:CG	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1755:CLA:H11	19:B:1769:CLA:HBD	1.92	0.51
6:B:190:TRP:HE3	19:B:1744:CLA:CAB	2.23	0.51
6:B:55:ALA:HB1	6:B:150:LEU:HD12	1.91	0.51
6:B:563:GLY:C	6:B:564:ARG:O	2.46	0.51
5:A:588:GLY:N	6:B:668:ARG:NH1	2.57	0.51
16:L:96:SER:HG	16:L:143:PHE:HD2	1.50	0.51
16:L:163:LEU:O	16:L:164:PRO:O	2.29	0.51
18:R:38:UNK:O	18:R:42:UNK:C	2.59	0.51
17:N:38:GLY:HA3	17:N:46:PHE:CD1	2.46	0.51
17:N:42:PHE:CD1	17:N:43:PRO:CA	2.93	0.51
17:N:61:LEU:HG	17:N:62:SER:N	2.14	0.51
17:N:63:ASP:OD1	17:N:66:ASP:OD2	2.29	0.51
6:B:247:THR:O	6:B:248:GLN:O	2.27	0.51
7:C:31:TRP:HD1	7:C:32:GLY:N	2.08	0.51
17:N:34:THR:C	17:N:36:GLU:N	2.64	0.51
12:H:77:LEU:HB3	12:H:78:PRO:HD2	1.93	0.51
19:A:1781:CLA:CHC	22:A:1806:BCR:H371	2.39	0.51
5:A:356:ALA:O	5:A:360:ILE:HG22	2.10	0.51
5:A:393:LEU:O	5:A:397:THR:CG2	2.55	0.51
5:A:619:LYS:O	5:A:621:GLN:N	2.43	0.51
6:B:130:ARG:NH1	6:B:130:ARG:CG	2.71	0.51
6:B:724:PHE:CE1	19:B:1785:CLA:HMD1	2.45	0.51
6:B:202:SER:CB	6:B:270:LEU:HD21	2.41	0.51
6:B:292:ARG:NE	6:B:297:ILE:O	2.44	0.51
6:B:337:ALA:O	6:B:339:ALA:O	2.29	0.51
6:B:529:THR:HA	6:B:532:LEU:HD23	1.91	0.51
6:B:231:ASN:OD1	11:G:5:SER:HB2	2.10	0.51
17:N:53:ALA:HB3	17:N:55:GLN:NE2	2.25	0.51
19:J:1043:CLA:NA	19:J:1043:CLA:HED3	2.12	0.51
8:D:58:PHE:CD2	8:D:59:GLU:N	2.78	0.51
4:4:95:PHE:CZ	19:4:1208:CLA:C1C	2.94	0.51
20:A:7017:LMU:O3'	20:A:7017:LMU:C1B	2.55	0.51
5:A:630:ASP:C	5:A:632:GLY:N	2.60	0.51
4:4:171:ASN:O	4:4:172:VAL:CB	2.58	0.51
12:H:70:ALA:O	12:H:71:ASN:HB2	2.10	0.51
5:A:224:HIS:CE1	19:A:1771:CLA:NC	2.78	0.51
5:A:281:LEU:HD22	19:A:1772:CLA:HMA3	1.93	0.51
6:B:556:SER:O	24:B:1783:LMG:HC2	2.11	0.51
19:B:1786:CLA:C14	19:H:1079:CLA:HBC3	2.40	0.51
6:B:188:LEU:HG	6:B:189:ALA:H	1.75	0.51
6:B:18:THR:O	6:B:21:ILE:N	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:309:ILE:HD12	6:B:312:GLY:HA3	1.92	0.51
6:B:599:ILE:O	6:B:734:GLY:C	2.48	0.51
7:C:1:MET:SD	7:C:4:SER:OG	2.68	0.51
10:F:73:VAL:HG11	10:F:83:PHE:HB2	1.90	0.51
16:L:128:ASP:CG	16:L:129:GLN:N	2.63	0.51
19:2:1220:CLA:H62	3:3:140:LYS:HZ3	1.74	0.51
2:2:59:ALA:HB1	2:2:172:LEU:HD22	1.91	0.51
17:N:69:CYS:O	17:N:70:GLU:O	2.28	0.51
3:3:63:ARG:NH2	3:3:189:LEU:HD23	2.19	0.51
5:A:335:LYS:CG	5:A:336:GLY:N	2.60	0.51
6:B:160:LYS:HG3	6:B:161:TRP:N	2.20	0.51
11:G:96:SER:C	11:G:98:PHE:H	2.13	0.51
5:A:187:HIS:CD2	19:A:1767:CLA:C1C	2.94	0.51
19:A:1788:CLA:H11	19:A:1800:CLA:H43	1.92	0.51
5:A:207:LEU:HA	5:A:211:LEU:CB	2.40	0.51
5:A:725:LEU:HD12	5:A:725:LEU:N	2.26	0.51
19:B:1740:CLA:H143	19:B:1757:CLA:H18	1.93	0.51
19:B:1755:CLA:OBD	19:B:1767:CLA:HBB1	2.11	0.51
6:B:17:THR:HA	6:B:696:LYS:N	2.26	0.51
6:B:700:LEU:N	6:B:700:LEU:CD2	2.73	0.51
6:B:730:SER:O	6:B:731:GLY:O	2.29	0.51
6:B:74:PHE:C	6:B:76:ALA:H	2.13	0.51
7:C:51:CYS:N	25:C:1082:SF4:S2	2.78	0.51
7:C:5:VAL:HB	7:C:65:VAL:HG22	1.91	0.51
7:C:73:THR:OG1	7:C:76:SER:OG	2.29	0.51
8:D:30:ALA:O	16:L:18:PRO:CB	2.54	0.51
5:A:130:GLU:HG3	10:F:45:THR:HG21	1.92	0.51
11:G:28:ARG:HH21	11:G:29:GLU:N	2.06	0.51
18:R:37:UNK:O	18:R:42:UNK:O	2.29	0.51
19:J:1045:CLA:C2	19:J:1045:CLA:HMA2	2.41	0.51
20:A:7030:LMU:H2'	20:A:7030:LMU:C6'	2.41	0.51
16:L:108:LYS:C	16:L:108:LYS:HE2	2.31	0.51
7:C:12:ILE:O	7:C:38:GLN:HG2	2.10	0.51
1:1:160:GLY:C	19:1:1189:CLA:HBB2	2.31	0.51
5:A:536:THR:HA	5:A:539:PHE:HB3	1.93	0.51
6:B:44:GLN:CD	6:B:163:PRO:HB2	2.30	0.51
1:1:32:VAL:HG12	1:1:36:LEU:HD12	1.92	0.51
3:3:116:PHE:O	3:3:120:LEU:HB2	2.10	0.51
3:3:85:PRO:HB2	3:3:104:TYR:HA	1.91	0.51
19:A:1782:CLA:C10	19:A:1782:CLA:H143	2.40	0.51
5:A:450:CYS:O	5:A:453:LEU:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:509:ALA:O	5:A:510:SER:OG	2.17	0.51
5:A:63:ASP:HA	19:A:1785:CLA:HED2	1.92	0.51
6:B:375:HIS:CE1	19:B:1758:CLA:NC	2.76	0.51
6:B:197:VAL:O	6:B:198:ALA:CB	2.59	0.51
6:B:464:GLN:OE1	6:B:469:LYS:CD	2.55	0.51
6:B:606:VAL:C	6:B:608:GLN:H	2.14	0.51
6:B:710:LEU:C	6:B:712:HIS:H	2.12	0.51
8:D:50:TRP:N	8:D:50:TRP:CD1	2.79	0.51
9:E:40:ARG:N	9:E:46:PHE:HE1	2.09	0.51
5:A:701:GLN:OE1	9:E:74:TYR:HE1	1.93	0.51
11:G:32:ALA:C	11:G:34:GLN:N	2.64	0.51
16:L:102:TYR:C	16:L:104:ILE:H	2.14	0.51
16:L:123:ARG:C	16:L:124:LYS:HE3	2.31	0.51
16:L:60:HIS:HD2	19:L:1167:CLA:CED	2.24	0.51
19:A:1816:CLA:C7	19:A:1816:CLA:H2	2.41	0.51
17:N:72:LYS:HZ3	17:N:74:LYS:HA	1.76	0.51
10:F:23:LYS:O	10:F:24:LYS:HE2	2.08	0.51
15:K:69:ILE:O	15:K:70:MET:O	2.29	0.51
10:F:50:LYS:C	10:F:52:ARG:N	2.63	0.51
10:F:91:LEU:O	10:F:94:ALA:O	2.28	0.51
5:A:439:ARG:HG2	5:A:562:PHE:CE2	2.45	0.51
19:B:1752:CLA:O1A	11:G:54:TYR:OH	2.28	0.51
6:B:486:LEU:HD12	19:B:1765:CLA:OBD	2.10	0.51
6:B:271:THR:OG1	6:B:272:ASP:N	2.43	0.51
6:B:290:MET:HG2	6:B:290:MET:O	2.10	0.51
6:B:305:LEU:O	6:B:308:HIS:N	2.25	0.51
6:B:376:GLN:HB3	6:B:587:ILE:HD12	1.93	0.51
6:B:420:SER:O	6:B:424:TRP:N	2.35	0.51
6:B:428:PHE:HA	19:B:1762:CLA:O1D	2.11	0.51
6:B:549:ASP:OD1	7:C:63:LEU:HB3	2.11	0.51
6:B:560:ASP:OD1	7:C:52:LYS:NZ	2.40	0.51
11:G:38:GLN:O	11:G:40:GLY:O	2.28	0.51
22:I:1032:BCR:H271	22:I:1032:BCR:H403	1.92	0.51
19:A:1800:CLA:HMB2	19:L:1167:CLA:CBC	2.38	0.51
18:R:30:UNK:O	18:R:32:UNK:N	2.43	0.51
17:N:47:THR:O	17:N:48:GLY:O	2.29	0.51
17:N:51:ASP:N	17:N:51:ASP:OD2	2.30	0.51
20:A:7039:LMU:O6B	20:A:7039:LMU:O3'	2.29	0.51
21:B:8062:SUC:O6	21:B:8062:SUC:O2'	2.29	0.51
18:R:27:UNK:C	18:R:29:UNK:N	2.74	0.51
17:N:35:VAL:HG12	17:N:37:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:4:GLU:CD	17:N:4:GLU:C	2.70	0.51
2:2:179:PHE:HD1	2:2:183:TYR:CE2	2.28	0.51
5:A:104:SER:HG	5:A:161:GLU:CD	2.14	0.51
19:A:1770:CLA:C4B	22:A:1803:BCR:C20	2.87	0.51
19:A:1783:CLA:HAA1	19:A:1783:CLA:HBD	1.92	0.51
19:A:1783:CLA:H92	22:A:1807:BCR:H373	1.92	0.51
5:A:584:PRO:HG3	6:B:559:CYS:SG	2.50	0.51
5:A:401:TRP:CZ3	5:A:609:ILE:HB	2.45	0.51
5:A:685:VAL:O	5:A:688:PHE:HB3	2.11	0.51
6:B:167:TRP:HB2	11:G:41:MET:HE3	1.91	0.51
19:B:1735:CLA:HBB2	19:B:1735:CLA:C11	2.41	0.51
19:B:1755:CLA:HBD	19:B:1767:CLA:HMB3	1.92	0.51
6:B:387:PHE:O	6:B:391:PRO:HG3	2.10	0.51
8:D:48:ILE:HG12	8:D:49:THR:N	2.23	0.51
10:F:80:TRP:CH2	19:F:1156:CLA:HAC2	2.46	0.51
10:F:124:PRO:C	10:F:126:ALA:H	2.14	0.51
11:G:33:LYS:O	11:G:34:GLN:O	2.28	0.51
19:A:1787:CLA:H93	16:L:36:TYR:HE1	1.76	0.51
19:1:1198:CLA:HAA2	19:1:1198:CLA:HBD	1.93	0.51
19:2:1215:CLA:HED2	19:2:1220:CLA:HBB1	1.92	0.51
17:N:45:ASN:CA	17:N:57:LYS:HZ2	2.24	0.51
19:J:1043:CLA:CBC	19:J:1043:CLA:CHD	2.85	0.51
12:H:26:SER:O	12:H:27:ASP:O	2.29	0.51
19:3:3011:CLA:C12	19:3:3011:CLA:H172	2.30	0.51
10:F:53:PHE:C	10:F:55:ASN:N	2.63	0.51
7:C:12:ILE:HG21	7:C:39:ILE:C	2.31	0.51
7:C:34:CYS:SG	7:C:39:ILE:HD12	2.51	0.51
6:B:92:TRP:CZ2	13:I:6:SER:HB2	2.45	0.51
2:2:77:PRO:O	17:N:3:ILE:HD12	2.10	0.51
22:A:1808:BCR:C23	22:A:1808:BCR:C39	2.66	0.51
5:A:592:VAL:O	5:A:597:HIS:CD2	2.64	0.51
5:A:685:VAL:HG12	5:A:741:GLY:CA	2.40	0.51
5:A:746:THR:O	5:A:750:PHE:N	2.38	0.51
5:A:750:PHE:O	5:A:752:ALA:N	2.44	0.51
6:B:185:VAL:CG2	22:B:1775:BCR:H272	2.41	0.51
6:B:561:GLY:HA3	7:C:52:LYS:CB	2.41	0.51
19:F:1156:CLA:O1D	19:F:1156:CLA:H2A	2.11	0.51
11:G:7:VAL:HG23	11:G:8:ILE:H	1.64	0.51
17:N:42:PHE:HD1	17:N:43:PRO:CA	2.24	0.51
17:N:45:ASN:ND2	17:N:45:ASN:O	2.44	0.51
17:N:62:SER:O	17:N:66:ASP:OD2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:82:PHE:HD2	17:N:82:PHE:N	2.08	0.51
19:J:1044:CLA:OBD	19:J:1045:CLA:C4	2.54	0.51
17:N:27:ALA:O	17:N:28:ASN:O	2.29	0.51
3:3:86:GLN:CB	3:3:88:THR:HB	2.37	0.50
5:A:118:PRO:HB3	5:A:150:PHE:CD2	2.46	0.50
19:A:1776:CLA:HMC1	19:A:1776:CLA:HBC2	1.92	0.50
19:A:1781:CLA:HAA1	19:A:1781:CLA:HED2	1.92	0.50
19:A:1791:CLA:HBD	19:A:1791:CLA:HAA1	1.94	0.50
5:A:23:ASP:HA	5:A:24:ARG:HD2	1.87	0.50
5:A:327:ILE:O	5:A:328:LYS:O	2.29	0.50
5:A:462:ILE:HG21	19:A:1789:CLA:CMC	2.41	0.50
5:A:379:MET:SD	5:A:511:THR:O	2.69	0.50
6:B:231:ASN:O	6:B:233:TYR:N	2.44	0.50
6:B:436:LEU:O	6:B:437:TYR:CB	2.59	0.50
6:B:626:LEU:HD12	6:B:627:ASN:N	2.26	0.50
6:B:726:ILE:C	6:B:728:SER:H	2.13	0.50
7:C:7:ILE:CG2	7:C:65:VAL:HG21	2.42	0.50
18:R:38:UNK:C	18:R:42:UNK:C	2.89	0.50
3:3:92:TRP:O	3:3:95:THR:HG23	2.11	0.50
17:N:49:CYS:O	17:N:51:ASP:O	2.29	0.50
17:N:49:CYS:O	17:N:50:GLN:O	2.30	0.50
17:N:62:SER:O	17:N:66:ASP:OD1	2.29	0.50
20:A:7016:LMU:H71	20:A:7016:LMU:H111	1.92	0.50
7:C:9:ASP:HB3	25:C:1083:SF4:S3	2.51	0.50
3:3:182:LYS:O	3:3:185:LYS:HB3	2.11	0.50
8:D:132:LEU:HD23	8:D:133:ASN:O	2.10	0.50
7:C:28:MET:SD	8:D:122:LYS:O	2.70	0.50
6:B:440:ASN:CG	6:B:614:THR:O	2.49	0.50
4:4:160:MET:CG	19:4:1201:CLA:CBB	2.87	0.50
19:A:1789:CLA:H172	19:A:1793:CLA:C20	2.41	0.50
19:A:1796:CLA:H62	19:A:1813:CLA:C19	2.41	0.50
19:A:1800:CLA:C11	19:A:1800:CLA:H61	2.40	0.50
5:A:212:GLY:C	5:A:214:GLY:H	2.14	0.50
5:A:227:LEU:HD23	5:A:231:GLN:NE2	2.25	0.50
5:A:23:ASP:OD1	5:A:23:ASP:O	2.29	0.50
5:A:329:ASP:O	5:A:332:GLU:O	2.29	0.50
5:A:665:ILE:HD13	6:B:621:ARG:HG3	1.93	0.50
5:A:741:GLY:O	5:A:743:ILE:N	2.44	0.50
6:B:182:LEU:HA	19:B:1743:CLA:HMB2	1.93	0.50
19:B:1768:CLA:C12	22:B:1779:BCR:H312	2.33	0.50
6:B:392:ILE:HD13	19:B:1759:CLA:HED1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:393:PHE:CE1	6:B:394:PHE:CE2	2.99	0.50
6:B:648:TRP:CZ2	19:B:1786:CLA:H62	2.46	0.50
6:B:77:TRP:CE2	6:B:81:PRO:HB3	2.46	0.50
6:B:295:PHE:HE2	11:G:38:GLN:NE2	2.09	0.50
3:3:74:ALA:CB	3:3:75:PRO:HD3	2.26	0.50
18:R:35:UNK:O	18:R:42:UNK:O	2.30	0.50
17:N:62:SER:O	17:N:63:ASP:OD1	2.29	0.50
19:K:1146:CLA:HBC2	19:K:1146:CLA:CMC	2.20	0.50
9:E:69:PHE:HD2	9:E:71:LYS:HG2	1.77	0.50
7:C:29:ILE:CG2	8:D:126:GLY:CA	2.89	0.50
5:A:274:TRP:NE1	5:A:277:TYR:CE2	2.79	0.50
19:A:1799:CLA:HBA1	19:A:1799:CLA:CED	2.41	0.50
5:A:281:LEU:CD2	19:A:1772:CLA:HMA2	2.41	0.50
19:A:1781:CLA:H111	19:A:1781:CLA:H162	1.93	0.50
5:A:462:ILE:HG21	19:A:1789:CLA:HMC3	1.94	0.50
19:A:1770:CLA:CAB	22:A:1803:BCR:H19C	2.33	0.50
5:A:672:LEU:C	5:A:674:ALA:H	2.08	0.50
5:A:89:ILE:O	5:A:93:LEU:HG	2.11	0.50
6:B:54:LEU:HD11	19:B:1743:CLA:HBA2	1.91	0.50
6:B:343:VAL:CG1	19:B:1756:CLA:H2	2.41	0.50
19:B:1759:CLA:C9	24:B:1783:LMG:H311	2.42	0.50
6:B:535:VAL:HG13	6:B:536:LYS:H	1.76	0.50
9:E:80:ASN:HB3	9:E:82:TYR:CE2	2.46	0.50
9:E:63:TYR:HA	9:E:83:ALA:HB2	1.93	0.50
20:A:7023:LMU:C1B	20:A:7023:LMU:H4O1	2.23	0.50
2:2:56:MET:HG2	2:2:172:LEU:HB2	1.93	0.50
17:N:80:ASN:O	17:N:80:ASN:OD1	2.30	0.50
15:K:58:ALA:HB1	19:K:1085:CLA:HMD3	1.92	0.50
19:K:1142:CLA:O1D	19:K:1142:CLA:H2A	2.11	0.50
10:F:28:SER:O	10:F:29:LEU:O	2.29	0.50
19:4:4014:CLA:HAA2	19:4:4014:CLA:HBD	1.94	0.50
20:A:7020:LMU:O1B	20:A:7020:LMU:O6'	2.29	0.50
20:A:7022:LMU:O3B	20:A:7022:LMU:O6B	2.30	0.50
3:3:182:LYS:HG2	3:3:182:LYS:O	2.12	0.50
21:3:1221:SUC:O6	21:3:1221:SUC:H5'	2.10	0.50
3:3:157:ALA:O	3:3:158:TYR:CB	2.59	0.50
19:1:1188:CLA:HED2	19:1:1188:CLA:CAD	2.42	0.50
18:R:44:UNK:O	18:R:45:UNK:O	2.30	0.50
6:B:31:PHE:O	6:B:32:GLU:C	2.49	0.50
1:1:54:VAL:C	1:1:56:GLY:H	2.15	0.50
22:3:1220:BCR:H361	19:A:1798:CLA:H92	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:86:GLN:HB2	3:3:88:THR:N	2.26	0.50
4:4:164:LEU:O	4:4:165:GLY:C	2.50	0.50
19:A:1762:CLA:CED	19:A:1762:CLA:HBA2	2.41	0.50
19:A:1781:CLA:H43	19:A:1793:CLA:HBA1	1.92	0.50
19:A:1791:CLA:HMA2	19:A:1797:CLA:CHC	2.42	0.50
5:A:341:GLN:O	5:A:344:LYS:HB2	2.12	0.50
5:A:38:GLY:O	5:A:39:HIS:HB3	2.11	0.50
5:A:409:GLY:C	5:A:411:ALA:N	2.65	0.50
5:A:734:GLY:O	5:A:736:THR:N	2.45	0.50
5:A:685:VAL:CG1	5:A:741:GLY:HA2	2.41	0.50
6:B:136:TYR:O	6:B:140:ILE:HD11	2.12	0.50
19:B:1735:CLA:HAA1	19:B:1735:CLA:HBD	1.93	0.50
8:D:113:HIS:N	8:D:114:PRO:CD	2.74	0.50
5:A:571:ASP:OD2	8:D:88:THR:HG21	2.12	0.50
10:F:144:LEU:HG	10:F:145:LEU:HD23	1.94	0.50
11:G:21:PHE:O	11:G:23:PHE:N	2.44	0.50
11:G:43:HIS:O	11:G:45:GLU:OE1	2.29	0.50
22:I:1032:BCR:H291	22:L:1169:BCR:H281	1.92	0.50
16:L:99:LEU:HD11	22:L:1169:BCR:C7	2.40	0.50
3:3:64:TYR:HB2	19:3:1218:CLA:H42	1.87	0.50
19:2:1213:CLA:CBC	19:2:1213:CLA:CHD	2.88	0.50
17:N:58:VAL:HG12	17:N:59:PRO:HD3	1.93	0.50
17:N:82:PHE:CD2	17:N:82:PHE:N	2.78	0.50
17:N:5:GLU:OE2	17:N:6:TYR:N	2.45	0.50
6:B:681:ALA:O	6:B:683:GLU:N	2.45	0.50
2:2:182:ILE:O	2:2:205:PHE:HB3	2.11	0.50
5:A:163:GLN:C	5:A:165:TYR:N	2.64	0.50
19:A:1776:CLA:H101	19:A:1779:CLA:H93	1.94	0.50
19:A:1781:CLA:HHB	22:A:1806:BCR:H363	1.88	0.50
5:A:354:TRP:O	5:A:358:LEU:N	2.44	0.50
5:A:472:ARG:NE	5:A:474:GLN:HG3	2.15	0.50
5:A:655:ASP:O	5:A:660:GLN:NE2	2.45	0.50
5:A:88:ILE:C	5:A:90:PHE:N	2.63	0.50
6:B:50:HIS:CA	6:B:53:GLN:HB2	2.41	0.50
6:B:560:ASP:HB2	7:C:66:ARG:CZ	2.40	0.50
9:E:85:ASP:OD1	9:E:85:ASP:O	2.30	0.50
10:F:83:PHE:C	10:F:86:PRO:HD2	2.32	0.50
16:L:123:ARG:HB3	16:L:126:GLN:CG	2.41	0.50
16:L:136:TRP:O	16:L:140:THR:HG23	2.12	0.50
18:R:38:UNK:O	18:R:39:UNK:O	2.30	0.50
19:2:1215:CLA:H43	19:2:1220:CLA:CBC	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:59:PRO:O	17:N:61:LEU:O	2.29	0.50
19:4:1196:CLA:O2D	19:4:1196:CLA:OBD	2.30	0.50
8:D:131:GLY:O	8:D:132:LEU:HB2	2.10	0.50
8:D:116:ASP:HB3	8:D:127:ARG:HH12	1.75	0.50
8:D:120:PRO:O	8:D:121:GLU:HB3	2.11	0.50
15:K:40:LEU:O	15:K:41:GLU:HG3	2.12	0.50
3:3:106:TYR:CD2	3:3:107:TRP:CG	2.99	0.50
3:3:109:ASP:O	3:3:110:SER:O	2.28	0.50
19:A:1773:CLA:H51	19:A:1782:CLA:HMB1	1.94	0.50
5:A:733:VAL:CG1	19:A:1796:CLA:C3D	2.89	0.50
19:A:1811:CLA:HMB3	19:A:1812:CLA:HMD1	1.94	0.50
5:A:746:THR:OG1	19:A:1811:CLA:O1D	2.19	0.50
5:A:216:LEU:O	5:A:219:ALA:N	2.44	0.50
5:A:334:HIS:HB3	19:A:1777:CLA:HMA3	1.93	0.50
5:A:620:MET:SD	5:A:624:VAL:HG21	2.52	0.50
5:A:72:GLU:HB3	5:A:76:ARG:NH2	2.27	0.50
23:B:1773:PQN:C29	24:B:1783:LMG:H201	2.41	0.50
19:B:1787:CLA:HMC1	19:B:1787:CLA:HBC2	1.93	0.50
6:B:290:MET:HG3	19:B:1751:CLA:HMC3	1.94	0.50
6:B:320:LYS:O	6:B:322:LEU:N	2.44	0.50
6:B:382:ILE:O	6:B:385:GLY:N	2.42	0.50
6:B:662:MET:HE2	23:B:1773:PQN:H2M3	1.93	0.50
9:E:89:GLU:O	9:E:90:VAL:CB	2.59	0.50
11:G:43:HIS:O	11:G:45:GLU:N	2.45	0.50
2:2:63:PHE:CD1	2:2:64:ILE:N	2.80	0.50
17:N:46:PHE:O	17:N:47:THR:OG1	2.30	0.50
20:A:7016:LMU:H72	20:A:7016:LMU:H112	1.91	0.50
19:R:1054:CLA:C4D	19:R:1054:CLA:HED3	2.36	0.50
20:A:7021:LMU:C2	20:A:7021:LMU:C6	2.72	0.50
7:C:11:CYS:C	7:C:13:GLY:H	2.14	0.50
19:A:1765:CLA:CHA	19:A:1765:CLA:CBA	2.89	0.50
19:A:1786:CLA:CBB	19:A:1794:CLA:HBB2	2.40	0.50
5:A:462:ILE:CG2	19:A:1789:CLA:HMC3	2.42	0.50
5:A:51:THR:CG2	19:A:1795:CLA:HBB1	2.06	0.50
19:A:1776:CLA:H18	22:A:1805:BCR:H383	1.94	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
5:A:571:ASP:HB3	7:C:53:ARG:HH12	1.76	0.50
5:A:594:ALA:O	5:A:598:VAL:HG23	2.11	0.50
19:B:1756:CLA:H101	22:B:1777:BCR:H14C	1.93	0.50
19:B:1757:CLA:CGA	19:B:1757:CLA:H3A	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1775:BCR:C8	22:B:1775:BCR:H331	2.41	0.50
6:B:406:ASN:ND2	6:B:406:ASN:C	2.65	0.50
6:B:595:HIS:CE1	6:B:599:ILE:HD11	2.46	0.50
7:C:72:GLU:O	7:C:73:THR:O	2.29	0.50
7:C:73:THR:O	7:C:76:SER:OG	2.30	0.50
8:D:41:GLN:HG3	16:L:125:LYS:HZ2	1.77	0.50
8:D:46:TYR:HD1	8:D:80:LYS:HB3	1.76	0.50
11:G:19:GLY:C	11:G:21:PHE:HA	2.32	0.50
8:D:33:THR:HG23	16:L:23:LEU:HD12	1.94	0.50
5:A:254:LEU:C	5:A:256:ALA:N	2.64	0.50
21:B:8062:SUC:O1	21:B:8062:SUC:O6	2.30	0.50
11:G:16:LEU:CD2	11:G:68:ILE:HG21	2.42	0.50
16:L:48:ASN:CB	16:L:49:PRO:HD2	2.34	0.50
8:D:24:THR:OG1	8:D:24:THR:O	2.30	0.50
3:3:84:ILE:HD13	3:3:84:ILE:O	2.12	0.50
5:A:394:SER:OG	5:A:395:LEU:N	2.44	0.50
5:A:93:LEU:O	5:A:97:TYR:HD2	1.94	0.50
6:B:190:TRP:CD2	19:B:1748:CLA:HMD3	2.47	0.50
19:B:1764:CLA:HMC3	19:B:1767:CLA:H2	1.94	0.50
6:B:655:LEU:HD22	19:B:1771:CLA:CAB	2.41	0.50
24:B:1783:LMG:C11	24:B:1783:LMG:HC91	2.40	0.50
5:A:654:ARG:HH21	6:B:637:PRO:HD2	1.76	0.50
5:A:588:GLY:HA3	6:B:668:ARG:HB3	1.93	0.50
9:E:88:GLU:O	9:E:90:VAL:CG2	2.59	0.50
9:E:88:GLU:O	9:E:90:VAL:N	2.44	0.50
18:R:34:UNK:O	18:R:36:UNK:O	2.30	0.50
19:2:1212:CLA:O1A	19:2:1212:CLA:C4A	2.59	0.50
17:N:47:THR:O	17:N:52:LEU:O	2.30	0.50
16:L:160:VAL:O	16:L:161:LEU:O	2.29	0.50
11:G:92:GLY:O	11:G:93:TYR:O	2.30	0.50
20:A:7022:LMU:H2O2	20:A:7022:LMU:H5'	1.76	0.50
21:3:1221:SUC:C5'	21:3:1221:SUC:O6	2.60	0.50
11:G:68:ILE:H	11:G:68:ILE:HD12	1.77	0.50
7:C:31:TRP:CD1	7:C:32:GLY:N	2.80	0.50
16:L:115:ALA:N	16:L:116:PRO:CD	2.70	0.50
3:3:80:LYS:HD3	3:3:105:ASN:HB3	1.91	0.50
6:B:160:LYS:O	6:B:162:LYS:N	2.44	0.50
5:A:519:ASP:C	5:A:520:LEU:HG	2.31	0.50
5:A:635:THR:HG22	5:A:635:THR:O	2.12	0.50
5:A:398:HIS:HD2	19:A:1783:CLA:ND	2.09	0.50
19:A:1787:CLA:H12	6:B:686:PRO:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:24:ARG:O	5:A:25:ASP:O	2.29	0.50
5:A:332:GLU:HA	5:A:344:LYS:HG2	1.93	0.50
5:A:430:ASP:O	5:A:434:ARG:HB2	2.12	0.50
5:A:744:ALA:HA	5:A:747:TRP:HB3	1.93	0.50
6:B:141:PHE:O	6:B:144:PHE:N	2.45	0.50
19:B:1741:CLA:HAA2	19:B:1741:CLA:H12	1.94	0.50
19:B:1746:CLA:HMA2	19:B:1746:CLA:O2A	2.12	0.50
19:B:1755:CLA:HED1	19:B:1756:CLA:HMD2	1.88	0.50
19:B:1758:CLA:H171	22:B:1775:BCR:H363	1.93	0.50
6:B:346:SER:O	6:B:350:GLN:N	2.43	0.50
6:B:586:THR:O	6:B:589:TRP:N	2.44	0.50
6:B:707:LEU:HD12	6:B:711:VAL:CG2	2.42	0.50
18:R:35:UNK:O	18:R:36:UNK:O	2.30	0.50
20:A:7023:LMU:O1B	20:A:7023:LMU:O4'	2.29	0.50
5:A:249:ILE:N	5:A:251:ASN:OD1	2.45	0.50
4:4:108:ASP:OD1	4:4:120:ILE:HG12	2.11	0.50
10:F:25:LEU:O	10:F:26:GLN:O	2.30	0.50
1:1:45:ILE:HG22	1:1:48:ARG:HD2	1.94	0.50
16:L:112:PRO:O	16:L:113:SER:HB3	2.12	0.50
3:3:84:ILE:N	19:A:1798:CLA:C3	2.62	0.49
5:A:438:HIS:HB2	5:A:441:ALA:CB	2.42	0.49
6:B:122:GLN:O	6:B:126:THR:CB	2.59	0.49
19:B:1735:CLA:H2A	19:B:1735:CLA:CED	2.27	0.49
19:B:1736:CLA:HBC2	19:B:1736:CLA:HMC1	1.94	0.49
6:B:655:LEU:CD2	19:B:1771:CLA:CAB	2.90	0.49
19:B:1735:CLA:CBC	22:B:1778:BCR:C33	2.90	0.49
5:A:462:ILE:HD13	19:B:1786:CLA:H72	1.93	0.49
6:B:353:TYR:HB2	6:B:594:TRP:HH2	1.77	0.49
6:B:441:ASP:OD1	6:B:617:MET:HB3	2.12	0.49
20:A:7036:LMU:O5B	20:A:7036:LMU:O6'	2.30	0.49
20:A:7042:LMU:H5'	20:A:7042:LMU:C2B	2.41	0.49
18:R:38:UNK:O	18:R:42:UNK:O	2.30	0.49
19:2:1212:CLA:H43	19:2:1212:CLA:CGA	2.34	0.49
17:N:42:PHE:O	17:N:43:PRO:O	2.29	0.49
17:N:59:PRO:O	17:N:66:ASP:OD1	2.30	0.49
21:B:8062:SUC:O3'	21:B:8062:SUC:C1	2.60	0.49
4:4:35:GLU:O	4:4:37:LEU:N	2.34	0.49
21:2:1226:SUC:O2	21:2:1226:SUC:O4'	2.30	0.49
5:A:527:VAL:HG12	5:A:528:ALA:N	2.27	0.49
19:A:1781:CLA:HAA1	19:A:1781:CLA:HBD	1.93	0.49
5:A:369:THR:HG21	5:A:402:ILE:HG22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:441:ALA:HA	5:A:444:SER:HB3	1.94	0.49
5:A:575:LEU:CD1	5:A:576:GLY:H	2.25	0.49
6:B:707:LEU:HD11	19:B:1759:CLA:H91	1.93	0.49
19:B:1755:CLA:C4A	19:B:1769:CLA:HAA2	2.42	0.49
6:B:661:PHE:HB3	19:B:1787:CLA:HMC1	1.93	0.49
5:A:668:TYR:CE1	6:B:445:ALA:HB2	2.47	0.49
7:C:72:GLU:C	7:C:73:THR:O	2.46	0.49
10:F:123:VAL:HG13	14:J:7:TYR:N	2.26	0.49
11:G:37:GLU:O	11:G:38:GLN:O	2.29	0.49
5:A:249:ILE:HD13	5:A:250:LEU:HB2	1.93	0.49
4:4:150:LYS:HG2	4:4:150:LYS:O	2.12	0.49
3:3:157:ALA:O	3:3:158:TYR:HD2	1.95	0.49
11:G:58:LEU:O	11:G:60:SER:N	2.44	0.49
15:K:24:PHE:HB3	15:K:52:PRO:CG	2.40	0.49
2:2:206:ALA:O	2:2:207:ALA:CB	2.59	0.49
3:3:86:GLN:HB2	3:3:88:THR:H	1.76	0.49
19:A:1784:CLA:H52	19:A:1784:CLA:CMD	2.42	0.49
5:A:648:THR:O	5:A:649:ILE:HG22	2.12	0.49
6:B:292:ARG:HH22	19:B:1750:CLA:HED1	1.76	0.49
19:B:1768:CLA:C16	22:B:1779:BCR:H311	2.38	0.49
19:B:1759:CLA:HMD2	24:B:1783:LMG:H341	1.95	0.49
6:B:667:TRP:O	6:B:669:GLY:N	2.45	0.49
9:E:55:VAL:CG2	9:E:65:VAL:HB	2.40	0.49
14:J:22:LEU:O	14:J:23:ALA:C	2.51	0.49
17:N:38:GLY:O	17:N:39:SER:O	2.30	0.49
4:4:124:TYR:HA	4:4:145:PRO:HD3	1.94	0.49
19:J:1045:CLA:O1A	19:J:1045:CLA:O1D	2.30	0.49
20:A:7037:LMU:O1B	20:A:7037:LMU:O2'	2.30	0.49
20:K:1086:LMU:O4'	20:K:1086:LMU:O6B	2.30	0.49
20:A:7032:LMU:O1'	20:A:7032:LMU:O5B	2.29	0.49
19:R:1054:CLA:C4D	19:R:1054:CLA:CED	2.90	0.49
19:A:1817:CLA:HAA1	19:A:1817:CLA:CGD	2.43	0.49
1:1:160:GLY:C	1:1:162:CYS:H	2.14	0.49
12:H:45:ALA:C	12:H:48:THR:H	2.09	0.49
10:F:116:GLN:O	10:F:118:GLU:N	2.45	0.49
6:B:232:LEU:HD21	6:B:235:GLN:OE1	2.12	0.49
6:B:509:PHE:CD2	6:B:509:PHE:N	2.81	0.49
19:A:1783:CLA:O1D	19:A:1783:CLA:H2A	2.12	0.49
19:A:1793:CLA:HMB2	19:A:1794:CLA:C2D	2.42	0.49
5:A:393:LEU:HD13	5:A:750:PHE:CE1	2.45	0.49
19:B:1750:CLA:HMA1	11:G:21:PHE:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:289:LEU:HA	19:B:1750:CLA:O1D	2.12	0.49
6:B:50:HIS:HB2	6:B:53:GLN:HB2	1.94	0.49
8:D:72:PRO:HB2	8:D:74:LEU:HB2	1.95	0.49
19:G:1099:CLA:HBC3	19:G:1099:CLA:CHD	2.42	0.49
11:G:47:GLY:N	11:G:48:ASP:HB3	2.10	0.49
19:J:1044:CLA:OBD	19:J:1044:CLA:O2D	2.29	0.49
20:A:7013:LMU:O3'	20:A:7013:LMU:O5B	2.29	0.49
12:H:54:LEU:CD1	12:H:55:LYS:HG3	2.42	0.49
6:B:48:ALA:HB3	6:B:157:LEU:HD22	1.93	0.49
16:L:78:GLU:HG3	16:L:78:GLU:O	2.13	0.49
19:A:1774:CLA:CBB	19:A:1774:CLA:H8	2.43	0.49
5:A:729:GLN:HE21	19:A:1796:CLA:HMD1	1.77	0.49
22:A:1805:BCR:C23	22:A:1805:BCR:C38	2.74	0.49
19:A:1781:CLA:C3B	22:A:1806:BCR:C37	2.90	0.49
5:A:298:ASP:O	5:A:301:HIS:N	2.45	0.49
5:A:549:ILE:O	5:A:552:THR:O	2.30	0.49
5:A:694:PHE:HZ	6:B:661:PHE:CD1	2.30	0.49
19:B:1762:CLA:H13	19:B:1762:CLA:HMD2	1.94	0.49
6:B:193:HIS:CD2	19:B:1744:CLA:NB	2.80	0.49
6:B:278:LEU:HD12	19:B:1746:CLA:HMA1	1.90	0.49
6:B:377:TYR:O	6:B:378:ILE:HB	2.13	0.49
6:B:521:HIS:CE1	19:B:1768:CLA:C4A	2.96	0.49
6:B:535:VAL:CG2	6:B:539:LEU:HD23	2.42	0.49
11:G:42:SER:OG	11:G:43:HIS:O	2.30	0.49
21:B:8054:SUC:O1'	21:B:8054:SUC:O2	2.29	0.49
3:3:98:ILE:O	17:N:63:ASP:C	2.46	0.49
17:N:38:GLY:C	17:N:39:SER:O	2.49	0.49
17:N:45:ASN:O	17:N:46:PHE:O	2.30	0.49
17:N:60:PHE:N	17:N:61:LEU:O	2.45	0.49
21:B:8062:SUC:O6'	21:B:8062:SUC:O1'	2.30	0.49
10:F:151:ASP:HA	10:F:154:PHE:CB	2.43	0.49
2:2:98:GLU:O	2:2:102:ILE:HG12	2.12	0.49
1:1:161:PHE:O	1:1:164:GLN:HB2	2.12	0.49
10:F:17:ARG:O	10:F:18:GLU:C	2.51	0.49
16:L:5:LYS:N	16:L:6:PRO:HD3	2.28	0.49
5:A:354:TRP:CZ2	19:A:1780:CLA:H171	2.48	0.49
19:A:1797:CLA:O1A	19:A:1797:CLA:O2D	2.30	0.49
19:A:1783:CLA:C20	22:A:1808:BCR:C16	2.88	0.49
5:A:79:PHE:HZ	5:A:185:HIS:HE2	1.57	0.49
5:A:302:HIS:HE1	19:A:1774:CLA:C1B	2.25	0.49
5:A:44:ILE:O	5:A:46:LYS:CA	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:497:ALA:HA	5:A:510:SER:OG	2.12	0.49
5:A:538:ASP:O	5:A:542:HIS:HB2	2.11	0.49
5:A:569:ILE:HB	5:A:572:LYS:HG3	1.94	0.49
5:A:598:VAL:HG12	5:A:598:VAL:O	2.13	0.49
19:B:1751:CLA:HMA3	19:B:1752:CLA:C3D	2.42	0.49
19:B:1753:CLA:H43	19:B:1753:CLA:CHA	2.38	0.49
19:B:1758:CLA:H172	22:B:1775:BCR:H363	1.94	0.49
19:B:1758:CLA:H62	22:B:1776:BCR:C32	2.43	0.49
19:B:1740:CLA:C9	22:B:1781:BCR:H361	2.41	0.49
6:B:492:ILE:O	6:B:493:TRP:HB2	2.13	0.49
6:B:606:VAL:C	6:B:608:GLN:N	2.64	0.49
8:D:75:LEU:HD21	16:L:19:PHE:CE1	2.48	0.49
19:4:1196:CLA:HAA1	19:4:1196:CLA:HBD	1.93	0.49
20:A:7021:LMU:H6'1	20:A:7021:LMU:O3B	2.10	0.49
5:A:141:ARG:NH2	5:A:141:ARG:HG3	2.16	0.49
5:A:464:ASN:O	5:A:468:SER:N	2.40	0.49
4:4:48:GLY:N	4:4:161:LEU:HD23	2.27	0.49
3:3:133:ALA:O	3:3:134:LYS:HB2	2.12	0.49
5:A:402:ILE:HD11	19:A:1784:CLA:CBB	2.40	0.49
5:A:411:ALA:O	5:A:412:ALA:C	2.51	0.49
5:A:435:VAL:HA	5:A:438:HIS:HE1	1.76	0.49
5:A:473:PRO:C	5:A:475:ASP:H	2.16	0.49
5:A:90:PHE:HE2	5:A:178:MET:SD	2.34	0.49
19:A:1795:CLA:NC	19:B:1735:CLA:HBC2	2.27	0.49
6:B:304:ILE:HG22	19:B:1752:CLA:O1D	2.10	0.49
6:B:356:PRO:HB2	6:B:361:ILE:CG2	2.43	0.49
6:B:419:ILE:C	6:B:420:SER:OG	2.47	0.49
5:A:705:GLU:HG2	6:B:545:LYS:HZ2	1.76	0.49
6:B:580:VAL:HG11	6:B:710:LEU:HD21	1.94	0.49
9:E:52:VAL:HA	9:E:67:VAL:HA	1.95	0.49
11:G:8:ILE:CG1	11:G:8:ILE:O	2.56	0.49
19:1:1191:CLA:CHC	19:1:1197:CLA:HBC1	2.43	0.49
2:2:59:ALA:HB3	2:2:172:LEU:HD13	1.94	0.49
17:N:77:CYS:O	17:N:79:SER:O	2.29	0.49
4:4:146:THR:HG22	4:4:147:LEU:HD12	1.93	0.49
7:C:15:THR:N	7:C:17:CYS:SG	2.85	0.49
10:F:22:LEU:HB2	10:F:23:LYS:HD3	1.94	0.49
10:F:26:GLN:O	10:F:28:SER:OG	2.29	0.49
19:3:1217: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
4:4:36:ASN:HB2	4:4:39:TRP:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:259:TYR:HB3	5:A:260:PRO:CD	2.31	0.49
12:H:40:PHE:O	12:H:43:PHE:N	2.46	0.49
5:A:68:THR:O	5:A:70:ASP:N	2.43	0.49
2:2:192:LEU:HG	2:2:193:PHE:H	1.78	0.49
22:A:1807:BCR:C15	19:A:1812:CLA:H151	2.43	0.49
5:A:188:LYS:O	5:A:190:ALA:N	2.46	0.49
5:A:283:PHE:O	5:A:284:ARG:NH1	2.45	0.49
5:A:366:GLY:O	5:A:403:GLY:HA2	2.12	0.49
5:A:681:GLY:C	5:A:683:HIS:H	2.15	0.49
6:B:255:LEU:HD12	19:B:1746:CLA:O2D	2.13	0.49
23:B:1773:PQN:H141	22:B:1780:BCR:H331	1.94	0.49
6:B:255:LEU:N	6:B:255:LEU:HD23	2.28	0.49
6:B:662:MET:O	6:B:663:PHE:C	2.50	0.49
7:C:7:ILE:HA	7:C:60:THR:OG1	2.13	0.49
19:K:1085:CLA:C1B	19:K:1142:CLA:OBD	2.61	0.49
20:A:7033:LMU:O6B	20:A:7033:LMU:O2'	2.29	0.49
6:B:517:PHE:O	6:B:517:PHE:CG	2.61	0.49
4:4:192:THR:HG22	4:4:193:ILE:N	2.26	0.49
5:A:338:PHE:CE1	19:A:1799:CLA:HBB1	2.48	0.49
6:B:681:ALA:O	6:B:682:HIS:C	2.51	0.49
3:3:129:PHE:O	3:3:129:PHE:CD1	2.66	0.49
2:2:124:ILE:HD12	2:2:129:LYS:O	2.13	0.49
19:A:1761:CLA:C4	22:A:1804:BCR:C31	2.90	0.49
19:A:1774:CLA:HAC2	22:A:1804:BCR:H352	1.95	0.49
19:A:1776:CLA:HBC2	19:A:1782:CLA:H18	1.93	0.49
5:A:368:LEU:HD12	19:A:1782:CLA:H61	1.93	0.49
19:A:1779:CLA:CAB	22:A:1805:BCR:H353	2.34	0.49
5:A:382:TYR:HB2	5:A:385:LEU:HD11	1.94	0.49
5:A:589:THR:HG22	5:A:589:THR:O	2.13	0.49
19:B:1759:CLA:HBC3	19:B:1759:CLA:CMC	2.37	0.49
19:B:1786:CLA:H122	19:B:1786:CLA:H71	1.95	0.49
6:B:29:HIS:CE1	19:B:1759:CLA:H43	2.48	0.49
10:F:104:TYR:C	10:F:104:TYR:CD2	2.86	0.49
11:G:46:ALA:N	11:G:48:ASP:CG	2.60	0.49
17:N:61:LEU:HD21	17:N:64:ASP:N	2.28	0.49
4:4:106:TRP:HA	4:4:109:ILE:HG13	1.94	0.49
6:B:247:THR:HB	6:B:248:GLN:OE1	2.12	0.49
20:A:7038:LMU:C6'	20:A:7038:LMU:C1B	2.90	0.49
2:2:116:PRO:O	2:2:131:THR:HB	2.13	0.49
5:A:92:TRP:CD1	19:A:1763:CLA:CBB	2.96	0.49
19:A:1779:CLA:NC	22:A:1805:BCR:C17	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:683:HIS:O	19:A:1812:CLA:HAA2	2.13	0.49
5:A:73:GLU:HA	5:A:76:ARG:HD2	1.94	0.49
19:B:1736:CLA:HBC3	19:B:1759:CLA:H41	1.95	0.49
19:B:1747:CLA:O1D	19:B:1748:CLA:HMA1	2.12	0.49
19:B:1771:CLA:H51	23:B:1773:PQN:H251	1.93	0.49
6:B:420:SER:H	6:B:422:LEU:H	1.61	0.49
6:B:568:CYS:O	6:B:570:ILE:HG23	2.12	0.49
6:B:564:ARG:CZ	7:C:64:SER:OG	2.61	0.49
8:D:28:ILE:O	8:D:66:ALA:CB	2.61	0.49
8:D:67:ILE:O	8:D:68:MET:HG3	2.12	0.49
19:L:1167:CLA:CAC	22:L:1169:BCR:HC42	2.43	0.49
16:L:126:GLN:O	16:L:127:PRO:O	2.31	0.49
17:N:61:LEU:O	17:N:62:SER:O	2.30	0.49
1:1:142:GLU:OE1	19:1:1187:CLA:HMD3	2.13	0.49
10:F:28:SER:O	10:F:30:LYS:O	2.29	0.49
6:B:317:ARG:NH2	6:B:410:ARG:HG2	2.28	0.49
6:B:224:PRO:HB3	6:B:227:THR:CB	2.43	0.49
13:I:4:LEU:O	13:I:4:LEU:HG	2.13	0.49
5:A:396:PHE:O	5:A:396:PHE:CD1	2.65	0.48
5:A:506:GLY:O	5:A:507:ALA:HB3	2.12	0.48
5:A:58:HIS:CE1	19:A:1759:CLA:C4D	2.96	0.48
19:B:1755:CLA:O2D	19:B:1756:CLA:OBD	2.30	0.48
6:B:385:GLY:N	19:B:1759:CLA:HBC3	2.28	0.48
6:B:299:HIS:NE2	6:B:304:ILE:HG21	2.28	0.48
6:B:461:GLN:N	6:B:512:ILE:HD12	2.28	0.48
6:B:510:LEU:CD2	6:B:510:LEU:H	2.25	0.48
6:B:646:TRP:CZ3	6:B:726:ILE:CD1	2.96	0.48
10:F:104:TYR:HD2	10:F:104:TYR:C	2.16	0.48
19:2:1215:CLA:H43	19:2:1220:CLA:HHD	1.95	0.48
4:4:121:PHE:CD1	4:4:143:PHE:CE2	3.01	0.48
11:G:17:PHE:O	11:G:20:ARG:CB	2.57	0.48
4:4:91:PHE:HA	4:4:94:GLU:HB3	1.95	0.48
6:B:601:LEU:O	6:B:601:LEU:HD22	2.12	0.48
5:A:104:SER:OG	5:A:161:GLU:OE1	2.31	0.48
5:A:165:TYR:HD2	5:A:165:TYR:O	1.95	0.48
19:A:1764:CLA:HBC3	19:A:1764:CLA:HHD	1.95	0.48
19:A:1793:CLA:C1B	19:A:1794:CLA:HMD3	2.43	0.48
5:A:415:ALA:HB2	5:A:560:VAL:HG12	1.94	0.48
5:A:661:ALA:O	5:A:665:ILE:HG13	2.13	0.48
5:A:679:PHE:CE2	5:A:683:HIS:CD2	2.98	0.48
6:B:145:LEU:HD22	6:B:148:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1762:CLA:CBB	22:B:1778:BCR:C26	2.92	0.48
19:B:1770:CLA:HBA1	22:L:1169:BCR:H362	1.94	0.48
19:B:1762:CLA:C5	22:B:1779:BCR:C40	2.91	0.48
6:B:724:PHE:CD1	19:B:1785:CLA:HMD1	2.49	0.48
19:B:1787:CLA:O2A	19:B:1787:CLA:C3A	2.57	0.48
6:B:471:THR:CG2	6:B:502:ASN:ND2	2.76	0.48
6:B:531:THR:O	6:B:535:VAL:CG1	2.54	0.48
6:B:570:ILE:O	6:B:570:ILE:HG13	2.13	0.48
6:B:67:HIS:O	6:B:88:ALA:O	2.31	0.48
8:D:101:TYR:CD1	8:D:114:PRO:CD	2.95	0.48
9:E:41:ARG:NE	9:E:46:PHE:CZ	2.81	0.48
6:B:295:PHE:CE2	11:G:38:GLN:NE2	2.81	0.48
6:B:302:LYS:HD3	11:G:49:THR:HA	1.94	0.48
6:B:228:GLY:HA3	11:G:8:ILE:HB	1.95	0.48
16:L:56:VAL:HG22	19:L:1167:CLA:HED2	1.95	0.48
16:L:96:SER:OG	16:L:143:PHE:CD2	2.60	0.48
19:3:3008:CLA:O1A	19:3:3008:CLA:O2D	2.30	0.48
17:N:47:THR:OG1	17:N:52:LEU:O	2.30	0.48
19:1:1200:CLA:HMA3	19:1:1200:CLA:HBA2	1.94	0.48
19:1:1187:CLA:CMA	19:1:1187:CLA:HBA1	2.17	0.48
20:A:7032:LMU:H2B	20:A:7032:LMU:C4	2.43	0.48
2:2:120:ASN:ND2	14:J:5:LYS:CD	2.75	0.48
11:G:16:LEU:CD1	11:G:17:PHE:CE2	2.93	0.48
6:B:317:ARG:HD3	6:B:410:ARG:HG2	1.95	0.48
12:H:42:THR:O	12:H:45:ALA:N	2.47	0.48
5:A:484:LEU:N	5:A:485:GLN:OE1	2.40	0.48
5:A:176:GLY:O	5:A:180:PHE:HB2	2.13	0.48
5:A:131:ILE:HG23	5:A:132:LEU:N	2.29	0.48
19:A:1782:CLA:HBD	19:A:1782:CLA:CBA	2.43	0.48
19:A:1764:CLA:HAA2	19:A:1783:CLA:HED3	1.95	0.48
19:A:1811:CLA:HBB2	19:A:1812:CLA:HED1	1.95	0.48
5:A:242:ILE:HD13	5:A:242:ILE:N	2.28	0.48
5:A:24:ARG:O	5:A:25:ASP:C	2.50	0.48
5:A:553:VAL:O	5:A:557:LEU:HB2	2.12	0.48
5:A:578:ARG:O	5:A:593:SER:OG	2.27	0.48
5:A:684:PHE:HB2	19:A:1812:CLA:HAA1	1.95	0.48
5:A:580:PRO:HB3	5:A:727:ILE:HG21	1.94	0.48
6:B:86:PRO:C	6:B:115:ASN:HB3	2.34	0.48
6:B:124:TRP:HZ2	6:B:135:LEU:HB2	1.78	0.48
6:B:389:HIS:HE1	19:B:1759:CLA:NC	2.12	0.48
19:B:1747:CLA:H8	19:B:1765:CLA:HMA1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1762:CLA:HBB2	22:B:1778:BCR:C25	2.43	0.48
6:B:22:TRP:HA	6:B:25:ILE:HD11	1.93	0.48
6:B:331:HIS:CE1	6:B:392:ILE:CG2	2.92	0.48
6:B:577:TYR:CE1	6:B:706:ARG:HB3	2.48	0.48
8:D:118:VAL:HG13	8:D:119:TYR:H	1.76	0.48
8:D:34:GLY:HA3	8:D:62:THR:HB	1.94	0.48
9:E:43:SER:CB	9:E:82:TYR:HE1	2.22	0.48
11:G:34:GLN:O	11:G:36:PRO:HD3	2.12	0.48
19:A:1788:CLA:H152	22:L:1169:BCR:H361	1.93	0.48
17:N:52:LEU:CB	17:N:53:ALA:CA	2.91	0.48
17:N:84:LYS:HZ2	17:N:84:LYS:HG2	1.43	0.48
4:4:137:ILE:HG22	4:4:138:PHE:HD2	1.77	0.48
6:B:247:THR:O	6:B:248:GLN:C	2.51	0.48
20:A:7040:LMU:O6B	20:A:7040:LMU:O4'	2.29	0.48
1:1:57:ILE:HG23	1:1:58:LEU:N	2.19	0.48
21:B:8055:SUC:O4'	21:B:8055:SUC:O1	2.30	0.48
5:A:574:ASN:OD1	5:A:574:ASN:N	2.45	0.48
5:A:103:PHE:H	5:A:103:PHE:HD2	1.60	0.48
5:A:172:LEU:O	5:A:175:ALA:O	2.31	0.48
5:A:331:LEU:CD2	5:A:343:HIS:C	2.62	0.48
5:A:53:TRP:CA	5:A:56:ASN:HB2	2.38	0.48
5:A:657:LEU:HD13	19:A:1811:CLA:H93	1.96	0.48
5:A:679:PHE:O	5:A:683:HIS:CB	2.62	0.48
19:B:1785:CLA:H161	19:B:1785:CLA:H193	1.52	0.48
6:B:272:ASP:C	6:B:274:ALA:H	2.17	0.48
6:B:502:ASN:OD1	6:B:511:THR:HG21	2.13	0.48
19:4:1199:CLA:CBA	19:F:1157:CLA:H42	2.43	0.48
16:L:11:ILE:O	16:L:12:GLN:HG3	2.13	0.48
19:1:1197:CLA:OBD	19:1:1197:CLA:CMD	2.54	0.48
3:3:94:ARG:CB	3:3:97:PHE:HE1	2.26	0.48
15:K:4:GLY:HA2	15:K:7:THR:CB	2.42	0.48
21:B:8055:SUC:O6'	21:B:8055:SUC:O3'	2.30	0.48
12:H:70:ALA:O	12:H:71:ASN:CB	2.61	0.48
5:A:151:GLN:HA	5:A:154:ARG:HG2	1.95	0.48
19:A:1768:CLA:C4D	19:A:1769:CLA:HMC3	2.43	0.48
5:A:351:THR:CA	19:A:1780:CLA:H191	2.43	0.48
19:A:1788:CLA:CBC	19:A:1793:CLA:CBC	2.91	0.48
5:A:284:ARG:HB2	5:A:298:ASP:OD1	2.12	0.48
5:A:385:LEU:O	5:A:386:ALA:HB3	2.13	0.48
5:A:40:PHE:N	5:A:44:ILE:CG2	2.77	0.48
5:A:618:TRP:CZ2	5:A:655:ASP:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:693:LEU:HD23	5:A:734:GLY:HA3	1.96	0.48
5:A:697:ARG:NH1	5:A:724:ALA:HB3	2.27	0.48
6:B:396:ARG:HH11	19:B:1759:CLA:HED2	1.79	0.48
6:B:447:GLY:O	6:B:449:PRO:CD	2.62	0.48
5:A:567:ARG:HH11	8:D:35:GLY:N	2.11	0.48
14:J:21:SER:O	14:J:22:LEU:C	2.52	0.48
17:N:83:TRP:O	17:N:83:TRP:CE3	2.64	0.48
21:B:8052:SUC:O1	21:B:8052:SUC:O4	2.29	0.48
21:B:8059:SUC:HO6	21:B:8059:SUC:H1	1.73	0.48
21:B:8059:SUC:O2	21:B:8059:SUC:O2'	2.29	0.48
7:C:28:MET:HA	7:C:38:GLN:HB2	1.95	0.48
6:B:110:LEU:CD1	6:B:111:GLY:H	2.19	0.48
21:2:1226:SUC:O2'	21:2:1226:SUC:H2	2.13	0.48
5:A:159:THR:O	5:A:163:GLN:OE1	2.31	0.48
3:3:83:LEU:C	19:A:1798:CLA:H43	2.32	0.48
5:A:312:ILE:O	5:A:313:ALA:CB	2.61	0.48
5:A:312:ILE:O	5:A:313:ALA:HB2	2.13	0.48
5:A:330:ILE:O	5:A:330:ILE:CG2	2.61	0.48
5:A:430:ASP:HA	5:A:434:ARG:HH21	1.78	0.48
5:A:73:GLU:HA	5:A:76:ARG:HB2	1.95	0.48
6:B:124:TRP:CE2	6:B:129:LEU:HD22	2.48	0.48
6:B:58:PHE:CE2	6:B:145:LEU:HD12	2.47	0.48
6:B:348:VAL:HG21	19:B:1758:CLA:HHD	1.94	0.48
22:B:1780:BCR:H331	22:B:1780:BCR:C8	2.44	0.48
6:B:21:ILE:HD12	6:B:21:ILE:N	2.29	0.48
6:B:180:SER:CB	6:B:288:GLY:HA3	2.41	0.48
6:B:36:ASP:O	6:B:41:ARG:CZ	2.62	0.48
6:B:462:TRP:HZ3	19:B:1764:CLA:HBC1	1.77	0.48
16:L:9:GLN:HG3	16:L:10:VAL:H	1.79	0.48
6:B:690:LEU:HD21	16:L:129:GLN:HA	1.95	0.48
2:2:57:LEU:O	2:2:60:ALA:HB3	2.13	0.48
17:N:61:LEU:O	17:N:66:ASP:OD1	2.30	0.48
4:4:118:ASP:H	4:4:119:PRO:HD2	1.77	0.48
10:F:22:LEU:CD1	10:F:22:LEU:N	2.32	0.48
10:F:23:LYS:O	10:F:24:LYS:CE	2.61	0.48
20:A:7030:LMU:C2'	20:A:7030:LMU:H6E	2.37	0.48
5:A:258:LEU:HG	5:A:280:PHE:CD1	2.48	0.48
5:A:630:ASP:O	5:A:632:GLY:N	2.46	0.48
6:B:238:SER:OG	6:B:239:SER:N	2.46	0.48
5:A:308:ILE:HG13	19:A:1772:CLA:HBB1	1.95	0.48
19:A:1783:CLA:C10	22:A:1807:BCR:C37	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1807:BCR:H17C	19:A:1812:CLA:C17	2.44	0.48
5:A:185:HIS:O	5:A:187:HIS:N	2.47	0.48
5:A:499:ALA:N	5:A:500:PRO:CD	2.76	0.48
5:A:665:ILE:CD1	5:A:665:ILE:C	2.82	0.48
5:A:705:GLU:O	5:A:708:VAL:N	2.46	0.48
19:B:1741:CLA:HBD	19:B:1741:CLA:C1	2.43	0.48
19:B:1737:CLA:HAC1	19:B:1759:CLA:HMA1	1.94	0.48
19:B:1751:CLA:HMD2	22:B:1774:BCR:C32	2.43	0.48
6:B:390:GLY:CA	22:B:1777:BCR:HC22	2.43	0.48
6:B:464:GLN:CG	6:B:469:LYS:HD3	2.43	0.48
22:B:1779:BCR:C33	19:F:1156:CLA:HMA1	2.43	0.48
11:G:19:GLY:N	11:G:21:PHE:H	2.11	0.48
11:G:44:PHE:C	11:G:46:ALA:HB2	2.34	0.48
19:3:1218:CLA:CHD	19:3:1218:CLA:CBC	2.75	0.48
17:N:61:LEU:HG	17:N:64:ASP:HB2	1.95	0.48
10:F:19:LYS:O	10:F:23:LYS:HB2	2.13	0.48
21:3:1221:SUC:O1'	21:3:1221:SUC:O6'	2.30	0.48
11:G:57:LEU:O	11:G:61:ASN:OD1	2.31	0.48
20:A:7013:LMU:H22	20:A:7013:LMU:O5'	2.13	0.48
1:1:45:ILE:CD1	19:1:1195:CLA:CMD	2.91	0.48
19:1:1188:CLA:HMA2	19:1:1188:CLA:HBA1	1.96	0.48
6:B:503:GLU:CB	6:B:507:SER:HB2	2.42	0.48
8:D:96:ILE:O	8:D:97:LYS:HB2	2.13	0.48
5:A:127:VAL:CG2	19:A:1765:CLA:HBB2	2.44	0.48
5:A:159:THR:O	5:A:160:SER:CB	2.62	0.48
5:A:169:ILE:O	5:A:173:VAL:HG13	2.14	0.48
5:A:185:HIS:O	5:A:188:LYS:HG3	2.14	0.48
5:A:229:ILE:HG12	5:A:243:PRO:CB	2.42	0.48
5:A:679:PHE:O	5:A:679:PHE:CD2	2.67	0.48
6:B:178:HIS:C	6:B:180:SER:N	2.65	0.48
6:B:309:ILE:HD11	6:B:313:GLY:H	1.79	0.48
6:B:672:GLN:NE2	6:B:672:GLN:CA	2.59	0.48
6:B:577:TYR:CD1	6:B:706:ARG:HB3	2.48	0.48
20:A:7042:LMU:H91	20:A:7042:LMU:H121	1.49	0.48
7:C:17:CYS:SG	7:C:18:VAL:N	2.87	0.48
12:H:23:VAL:O	12:H:23:VAL:HG13	2.13	0.48
6:B:479:SER:C	6:B:481:THR:H	2.15	0.48
20:A:7013:LMU:H42	20:A:7013:LMU:H11	1.54	0.48
10:F:113:LYS:NZ	10:F:115:THR:HG21	2.28	0.48
19:4:1201:CLA:CMA	19:4:1201:CLA:O2A	2.61	0.48
19:A:1762:CLA:H51	19:A:1785:CLA:NC	2.29	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
19:A:1796:CLA:H11	19:A:1796:CLA:C4D	2.44	0.48
19:A:1791:CLA:CMA	19:A:1797:CLA:CBB	2.92	0.48
5:A:229:ILE:O	5:A:229:ILE:HG22	2.14	0.48
5:A:53:TRP:HA	5:A:56:ASN:CG	2.34	0.48
19:B:1740:CLA:H192	22:B:1781:BCR:H19C	1.96	0.48
6:B:290:MET:HB2	19:B:1751:CLA:HMC3	1.96	0.48
6:B:486:LEU:HD13	19:B:1765:CLA:HMD3	1.96	0.48
6:B:587:ILE:HA	6:B:587:ILE:HD13	1.68	0.48
6:B:353:TYR:CD1	6:B:594:TRP:HZ3	2.30	0.48
11:G:43:HIS:C	11:G:45:GLU:CB	2.61	0.48
18:R:38:UNK:O	18:R:39:UNK:C	2.62	0.48
2:2:56:MET:HA	2:2:59:ALA:HB3	1.96	0.48
9:E:69:PHE:CG	9:E:70:ALA:N	2.81	0.48
5:A:529:LEU:H	5:A:529:LEU:HD12	1.79	0.48
19:A:1762:CLA:H12	19:A:1762:CLA:HED2	1.94	0.48
19:A:1783:CLA:H193	19:A:1783:CLA:H162	1.75	0.48
19:A:1788:CLA:HBC1	19:A:1793:CLA:HBC2	1.95	0.48
5:A:364:MET:CE	19:A:1782:CLA:H2	2.44	0.48
19:B:1744:CLA:H111	19:B:1744:CLA:H71	1.41	0.48
6:B:628:SER:O	6:B:629:SER:C	2.51	0.48
9:E:38:ILE:HB	9:E:46:PHE:O	2.14	0.48
9:E:41:ARG:CD	9:E:46:PHE:CZ	2.97	0.48
21:B:8052:SUC:O3'	21:B:8052:SUC:O1'	2.30	0.48
20:A:7037:LMU:O4'	20:A:7037:LMU:O6B	2.29	0.48
19:3:1219:CLA:OBD	19:3:1219:CLA:O1D	2.30	0.48
8:D:132:LEU:O	8:D:135:ARG:O	2.32	0.48
12:H:75:ASP:CB	12:H:77:LEU:HG	2.43	0.48
16:L:57:GLY:HA3	16:L:146:GLY:HA3	1.96	0.48
7:C:30:PRO:HB3	7:C:37:LYS:O	2.14	0.48
14:J:36:ALA:O	14:J:37:LEU:HB2	2.13	0.48
5:A:182:GLY:C	19:A:1767:CLA:HAC1	2.34	0.47
22:A:1804:BCR:C8	22:A:1804:BCR:H311	2.44	0.47
5:A:502:THR:C	5:A:504:ALA:N	2.68	0.47
5:A:558:LYS:HZ2	6:B:674:LEU:CB	2.24	0.47
5:A:606:TYR:OH	19:A:1811:CLA:HED3	2.14	0.47
5:A:703:LEU:HD13	5:A:707:ILE:HD11	1.96	0.47
6:B:693:TRP:CD1	19:B:1770:CLA:HMD3	2.48	0.47
6:B:335:GLY:HA2	6:B:338:LEU:HB2	1.96	0.47
6:B:339:ALA:O	6:B:340:SER:CB	2.62	0.47
16:L:36:TYR:O	16:L:37:LEU:CB	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:1218:CLA:H121	19:3:1218:CLA:C9	2.28	0.47
19:A:1816:CLA:O1A	19:A:1816:CLA:HED1	2.03	0.47
20:A:7016:LMU:H1'	20:A:7016:LMU:O6'	1.90	0.47
10:F:22:LEU:HB3	10:F:25:LEU:HD13	1.96	0.47
19:4:4014:CLA:O1A	19:4:4014:CLA:H2A	2.14	0.47
12:H:20:GLN:HB2	12:H:22:ASP:CB	2.39	0.47
3:3:195:LEU:HA	3:3:198:PHE:HB2	1.96	0.47
5:A:539:PHE:HE2	5:A:543:HIS:CE1	2.31	0.47
20:A:7031:LMU:H4'	20:A:7031:LMU:H3B	1.95	0.47
5:A:338:PHE:O	5:A:339:THR:O	2.31	0.47
6:B:600:THR:O	6:B:605:ASN:O	2.32	0.47
19:A:1762:CLA:HAA2	19:A:1762:CLA:HBD	1.96	0.47
19:A:1781:CLA:HBB2	19:A:1794:CLA:C3A	2.43	0.47
22:A:1807:BCR:C35	19:A:1812:CLA:H41	2.44	0.47
5:A:23:ASP:CB	5:A:24:ARG:CZ	2.80	0.47
5:A:650:ASN:O	5:A:654:ARG:N	2.36	0.47
19:B:1742:CLA:H61	19:B:1742:CLA:C1	2.43	0.47
22:B:1781:BCR:H342	19:H:1079:CLA:HHD	1.95	0.47
6:B:292:ARG:CZ	6:B:297:ILE:H	2.27	0.47
6:B:81:PRO:HG2	6:B:360:PHE:CE1	2.49	0.47
6:B:414:HIS:NE2	19:B:1760:CLA:NA	2.63	0.47
19:3:1215:CLA:HHC	19:3:1218:CLA:H11	1.95	0.47
19:3:1218:CLA:O2D	19:3:1218:CLA:OBD	2.31	0.47
19:2:1213:CLA:HAA2	19:2:1218:CLA:HED2	1.94	0.47
4:4:105:ARG:O	4:4:109:ILE:HG13	2.14	0.47
20:A:7039:LMU:O1B	20:A:7039:LMU:O2'	2.29	0.47
11:G:20:ARG:NH2	11:G:61:ASN:CA	2.77	0.47
10:F:43:LYS:HE3	10:F:43:LYS:N	2.29	0.47
2:2:103:GLY:CA	19:2:1222:CLA:CBB	2.89	0.47
12:H:72:ALA:HA	21:H:1080:SUC:O6'	2.14	0.47
11:G:80:ILE:O	11:G:80:ILE:HD12	2.14	0.47
3:3:181:LEU:HD13	3:3:184:VAL:CG2	2.44	0.47
3:3:83:LEU:HD13	19:3:1216:CLA:C3B	2.44	0.47
19:A:1774:CLA:HBB2	19:A:1774:CLA:H8	1.97	0.47
5:A:197:GLN:NE2	5:A:351:THR:O	2.47	0.47
5:A:347:TYR:HE1	5:A:417:PHE:HZ	1.61	0.47
6:B:96:PHE:HZ	6:B:104:PHE:CE2	2.32	0.47
19:B:1735:CLA:HBB1	19:B:1762:CLA:H43	1.96	0.47
19:B:1738:CLA:O1D	19:B:1738:CLA:C2A	2.55	0.47
6:B:427:LEU:C	19:B:1762:CLA:HED2	2.35	0.47
19:B:1755:CLA:O1A	19:B:1769:CLA:HAA1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1770:CLA:H91	22:B:1781:BCR:H333	1.95	0.47
5:A:680:LEU:CG	6:B:617:MET:HB2	2.44	0.47
9:E:43:SER:HB2	9:E:82:TYR:CE1	2.36	0.47
10:F:123:VAL:O	10:F:126:ALA:N	2.47	0.47
16:L:23:LEU:O	16:L:25:THR:N	2.47	0.47
17:N:70:GLU:HB3	17:N:72:LYS:HA	1.94	0.47
21:B:8059:SUC:O2'	21:B:8059:SUC:O5	2.30	0.47
21:3:1221:SUC:O2'	21:3:1221:SUC:O5	2.30	0.47
7:C:31:TRP:CD1	7:C:31:TRP:C	2.87	0.47
11:G:80:ILE:O	11:G:81:VAL:O	2.31	0.47
19:B:1766:CLA:HBA2	19:B:1766:CLA:H3A	1.70	0.47
20:3:7005:LMU:H101	20:3:7005:LMU:H62	1.96	0.47
5:A:747:TRP:HB2	19:A:1783:CLA:CBB	2.45	0.47
5:A:733:VAL:HG11	19:A:1796:CLA:C3D	2.43	0.47
19:A:1796:CLA:H192	14:J:19:PHE:HD2	1.79	0.47
6:B:167:TRP:O	6:B:167:TRP:CG	2.67	0.47
19:B:1739:CLA:C9	19:B:1739:CLA:CBB	2.68	0.47
6:B:459:PHE:CD2	19:B:1768:CLA:C3D	2.97	0.47
6:B:653:GLY:HA3	6:B:720:THR:OG1	2.13	0.47
9:E:37:LYS:N	9:E:49:VAL:HG13	2.29	0.47
19:1:1197:CLA:C4	19:1:1198:CLA:O1D	2.62	0.47
4:4:36:ASN:HB2	4:4:39:TRP:CD2	2.48	0.47
2:2:181:HIS:CD2	19:2:1214:CLA:ND	2.82	0.47
5:A:337:PRO:HD2	19:A:1799:CLA:HHC	1.95	0.47
10:F:152:ASN:HD22	10:F:152:ASN:N	2.12	0.47
1:1:33:PRO:HG2	1:1:137:PRO:HG3	1.96	0.47
19:A:1761:CLA:H161	19:A:1761:CLA:H141	1.64	0.47
19:A:1800:CLA:HMC3	19:B:1770:CLA:ND	2.29	0.47
5:A:197:GLN:HE22	5:A:351:THR:CB	2.22	0.47
5:A:434:ARG:O	5:A:437:ARG:N	2.47	0.47
5:A:452:PHE:O	5:A:456:HIS:ND1	2.28	0.47
5:A:599:PHE:CZ	5:A:731:ARG:HB3	2.47	0.47
6:B:125:TYR:CE1	6:B:130:ARG:NH1	2.83	0.47
19:B:1764:CLA:H2A	19:B:1764:CLA:O1D	2.15	0.47
19:B:1764:CLA:CMD	19:B:1765:CLA:C1C	2.92	0.47
6:B:697:PRO:HB3	19:B:1770:CLA:CBC	2.41	0.47
22:B:1778:BCR:C33	22:B:1778:BCR:C8	2.91	0.47
6:B:361:ILE:HG22	6:B:361:ILE:O	2.14	0.47
19:B:1740:CLA:HED1	19:I:1031:CLA:HMA2	1.96	0.47
16:L:65:VAL:C	16:L:67:PRO:CD	2.83	0.47
16:L:95:LEU:O	16:L:99:LEU:HD13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:58:VAL:CG1	17:N:59:PRO:HD3	2.44	0.47
20:A:7033:LMU:O3'	20:A:7033:LMU:O6B	2.29	0.47
3:3:59:ILE:HB	3:3:63:ARG:HH21	1.79	0.47
4:4:94:GLU:OE2	19:4:1208:CLA:NB	2.47	0.47
6:B:475:ASP:HA	6:B:480:SER:CA	2.45	0.47
2:2:98:GLU:CD	19:2:1223:CLA:CHD	2.83	0.47
4:4:58:MET:O	4:4:60:LEU:HD23	2.14	0.47
21:2:1226:SUC:O2'	21:2:1226:SUC:O2	2.30	0.47
6:B:31:PHE:O	6:B:37:ILE:HG21	2.13	0.47
5:A:553:VAL:CG2	22:A:1806:BCR:H401	2.43	0.47
19:B:1785:CLA:HBA2	19:B:1785:CLA:H3A	1.40	0.47
6:B:292:ARG:NH1	6:B:293:THR:H	2.13	0.47
6:B:631:LEU:HG	6:B:632:ILE:HG23	1.97	0.47
7:C:63:LEU:CG	7:C:64:SER:N	2.51	0.47
7:C:6:LYS:O	7:C:63:LEU:HD21	2.14	0.47
6:B:560:ASP:CB	7:C:66:ARG:NE	2.61	0.47
9:E:83:ALA:O	9:E:85:ASP:N	2.47	0.47
11:G:30:ASN:ND2	11:G:31:MET:O	2.48	0.47
16:L:46:ALA:CB	16:L:52:ARG:NH2	2.77	0.47
17:N:68:GLU:O	17:N:69:CYS:HB2	2.13	0.47
17:N:81:VAL:C	17:N:83:TRP:N	2.68	0.47
20:A:7020:LMU:O2B	20:A:7020:LMU:O6'	2.32	0.47
18:R:46:UNK:CB	18:R:47:UNK:CA	2.92	0.47
20:2:7006:LMU:H3'	20:2:7006:LMU:H5B	1.95	0.47
1:1:39:TYR:HB2	19:1:1196:CLA:OBD	2.12	0.47
5:A:70:ASP:O	5:A:71:LEU:O	2.33	0.47
5:A:420:ARG:HB3	5:A:420:ARG:CZ	2.45	0.47
20:3:7005:LMU:O3'	20:3:7005:LMU:H1B	2.12	0.47
2:2:161:THR:HG22	2:2:165:LYS:HD2	1.96	0.47
5:A:81:ALA:CA	19:A:1760:CLA:HMA1	2.38	0.47
19:A:1782:CLA:O2D	19:A:1782:CLA:OBD	2.32	0.47
19:A:1813:CLA:CMA	19:A:1813:CLA:H2	2.44	0.47
5:A:302:HIS:CD2	19:A:1773:CLA:NB	2.82	0.47
5:A:409:GLY:O	5:A:411:ALA:N	2.47	0.47
5:A:553:VAL:N	5:A:556:LEU:HD12	2.26	0.47
5:A:568:LEU:O	5:A:586:ARG:HD3	2.14	0.47
5:A:669:GLY:H	6:B:445:ALA:CA	2.21	0.47
5:A:78:VAL:O	5:A:82:HIS:CD2	2.67	0.47
6:B:415:LYS:HG2	6:B:416:GLU:OE2	2.13	0.47
6:B:535:VAL:CG1	6:B:536:LYS:N	2.76	0.47
6:B:720:THR:O	6:B:724:PHE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:732:LYS:CD	6:B:734:GLY:CA	2.93	0.47
8:D:36:LEU:HB2	16:L:19:PHE:O	2.14	0.47
11:G:28:ARG:HG2	11:G:29:GLU:HB2	1.96	0.47
13:I:9:VAL:H	13:I:10:PRO:CD	2.27	0.47
13:I:12:VAL:HG21	19:I:1031:CLA:CGA	2.45	0.47
16:L:101:MET:SD	16:L:104:ILE:HG12	2.55	0.47
16:L:63:LEU:O	16:L:65:VAL:N	2.48	0.47
19:A:1786:CLA:HMB2	19:A:1787:CLA:C3D	2.45	0.47
5:A:449:VAL:CG2	19:A:1794:CLA:HMC3	2.44	0.47
5:A:210:LEU:CD1	19:A:1769:CLA:HHB	2.45	0.47
5:A:302:HIS:HD2	19:A:1773:CLA:NB	2.11	0.47
5:A:377:TYR:HD1	5:A:616:PHE:HE1	1.59	0.47
5:A:392:GLN:O	5:A:392:GLN:CG	2.63	0.47
5:A:457:SER:OG	5:A:544:ILE:HA	2.15	0.47
5:A:508:THR:O	5:A:509:ALA:HB3	2.14	0.47
5:A:603:PHE:CE1	5:A:735:VAL:HA	2.50	0.47
22:B:1776:BCR:H15C	22:B:1776:BCR:H351	1.80	0.47
19:B:1758:CLA:H62	22:B:1776:BCR:HC7	1.96	0.47
6:B:448:THR:O	6:B:448:THR:OG1	2.31	0.47
13:I:7:LEU:HD12	22:I:1032:BCR:H333	0.83	0.47
16:L:99:LEU:O	16:L:136:TRP:HZ3	1.98	0.47
20:A:7041:LMU:H111	20:A:7041:LMU:H82	1.48	0.47
17:N:47:THR:O	17:N:48:GLY:C	2.52	0.47
4:4:118:ASP:OD2	4:4:123:GLN:HB2	2.15	0.47
7:C:14:CYS:SG	7:C:17:CYS:SG	3.13	0.47
20:A:7033:LMU:H6E	20:A:7033:LMU:H2B	1.96	0.47
12:H:19:GLY:O	12:H:20:GLN:HB2	2.15	0.47
20:A:7039:LMU:H6'2	20:A:7039:LMU:H1B	1.40	0.47
19:3:3011:CLA:H93	19:3:3011:CLA:H52	1.97	0.47
11:G:64:VAL:HG13	11:G:67:ASN:HB2	1.94	0.47
4:4:91:PHE:O	4:4:94:GLU:HB3	2.14	0.47
4:4:95:PHE:HZ	19:4:1208:CLA:C4C	2.25	0.47
7:C:12:ILE:N	7:C:12:ILE:CD1	2.73	0.47
2:2:98:GLU:OE1	19:2:1223:CLA:CHD	2.63	0.47
20:A:7027:LMU:H31	20:A:7027:LMU:H62	1.62	0.47
7:C:25:VAL:HA	7:C:43:PRO:CD	2.45	0.47
16:L:5:LYS:CA	16:L:5:LYS:HE2	2.37	0.47
19:L:1166:CLA:HBC2	19:L:1166:CLA:HHD	1.96	0.47
11:G:79:HIS:NE2	11:G:82:ALA:HB2	2.30	0.47
10:F:136:TRP:HB2	10:F:139:ALA:CB	2.45	0.47
3:3:166:PRO:HB2	3:3:167:LEU:H	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:132:LEU:HD13	5:A:671:SER:O	2.15	0.47
5:A:144:GLN:C	5:A:145:ILE:HG12	2.36	0.47
19:A:1772:CLA:H93	19:A:1772:CLA:H61	1.58	0.47
19:A:1787:CLA:HBB1	19:A:1793:CLA:C19	2.39	0.47
19:A:1787:CLA:C9	19:A:1801:CLA:H2	2.44	0.47
5:A:248:PHE:HD2	5:A:248:PHE:N	1.93	0.47
5:A:41:SER:O	5:A:44:ILE:CA	2.61	0.47
5:A:467:MET:HE1	5:A:475:ASP:O	2.15	0.47
5:A:605:MET:O	5:A:608:SER:N	2.48	0.47
19:B:1752:CLA:HBA2	19:B:1752:CLA:H3A	1.46	0.47
19:B:1753:CLA:O1D	19:B:1753:CLA:OBD	2.31	0.47
6:B:311:PRO:HD3	19:B:1772:CLA:C3C	2.44	0.47
6:B:182:LEU:HD13	19:B:1743:CLA:HHB	1.97	0.47
6:B:183:PHE:HB3	6:B:284:PHE:HD2	1.80	0.47
6:B:269:TRP:CD1	6:B:497:TRP:HH2	2.33	0.47
6:B:289:LEU:O	19:B:1751:CLA:HMC1	2.15	0.47
6:B:459:PHE:CD2	19:B:1768:CLA:C2D	2.98	0.47
6:B:471:THR:HB	6:B:472:TYR:CE1	2.50	0.47
7:C:66:ARG:NH2	7:C:66:ARG:CG	2.69	0.47
8:D:138:GLY:O	8:D:140:ASN:N	2.48	0.47
16:L:123:ARG:HB3	16:L:126:GLN:HG3	1.96	0.47
19:3:1218:CLA:HAA2	19:3:1218:CLA:O1D	2.15	0.47
17:N:70:GLU:CA	17:N:72:LYS:H	2.26	0.47
19:4:1200:CLA:HBD	19:4:1200:CLA:HAA2	1.97	0.47
4:4:124:TYR:O	4:4:125:SER:HB2	2.15	0.47
8:D:58:PHE:HE2	8:D:60:MET:HA	1.80	0.47
6:B:478:LEU:O	6:B:479:SER:HB3	2.15	0.47
17:N:6:TYR:HA	17:N:6:TYR:HD2	1.68	0.47
2:2:189:ILE:O	2:2:190:ASP:CB	2.63	0.47
8:D:89:ARG:O	8:D:92:SER:N	2.48	0.47
5:A:628:ILE:HG13	5:A:632:GLY:CA	2.42	0.47
5:A:539:PHE:CD2	5:A:539:PHE:C	2.88	0.47
10:F:116:GLN:C	10:F:118:GLU:N	2.58	0.47
1:1:38:ARG:HA	1:1:41:GLU:HG3	1.97	0.47
19:A:1781:CLA:H11	19:A:1794:CLA:CAD	2.45	0.47
5:A:202:MET:HB3	19:A:1780:CLA:HMD3	1.97	0.47
19:B:1749:CLA:H61	19:B:1749:CLA:H41	1.66	0.47
19:B:1756:CLA:H122	22:B:1777:BCR:C12	2.45	0.47
6:B:431:PHE:HE2	19:B:1762:CLA:CED	2.28	0.47
19:B:1767:CLA:CBC	19:B:1767:CLA:HMC1	2.24	0.47
6:B:724:PHE:CE2	19:B:1785:CLA:CMD	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1785:CLA:HMB3	19:B:1786:CLA:CAD	2.44	0.47
6:B:30:ASP:O	6:B:34:HIS:HD2	1.98	0.47
6:B:647:ALA:O	6:B:651:LEU:HD22	2.15	0.47
7:C:70:TRP:O	7:C:71:HIS:C	2.53	0.47
7:C:77:MET:C	7:C:79:LEU:H	2.12	0.47
18:R:34:UNK:CB	18:R:35:UNK:CA	2.80	0.47
3:3:189:LEU:C	3:3:191:MET:H	2.18	0.47
7:C:29:ILE:HG23	8:D:126:GLY:CA	2.39	0.47
6:B:454:LEU:H	6:B:454:LEU:HD12	1.80	0.47
4:4:76:TYR:HB2	19:4:1204:CLA:CGD	2.45	0.47
16:L:55:GLU:HG3	19:L:1166:CLA:C1A	2.45	0.47
20:A:7031:LMU:H21	20:A:7031:LMU:H52	1.70	0.47
6:B:63:GLY:HA2	6:B:66:PHE:HB3	1.97	0.47
6:B:211:ASN:ND2	6:B:214:ASP:OD1	2.48	0.47
3:3:127:ARG:C	3:3:129:PHE:H	2.18	0.47
3:3:171:LYS:HE3	3:3:171:LYS:N	2.29	0.47
5:A:241:GLU:OE1	5:A:241:GLU:O	2.32	0.47
19:A:1774:CLA:H71	19:A:1774:CLA:CAB	2.45	0.47
19:A:1795:CLA:OBD	10:F:105:LEU:HD11	2.15	0.47
5:A:298:ASP:O	5:A:300:ALA:N	2.48	0.47
5:A:417:PHE:C	5:A:417:PHE:CD1	2.89	0.47
5:A:581:CYS:HB3	5:A:590:CYS:O	2.14	0.47
6:B:135:LEU:HD12	6:B:135:LEU:O	2.15	0.47
19:B:1753:CLA:C15	19:B:1753:CLA:C10	2.55	0.47
6:B:230:TRP:O	6:B:231:ASN:C	2.52	0.47
6:B:309:ILE:HG22	6:B:319:HIS:CD2	2.50	0.47
6:B:9:SER:HA	6:B:35:ASP:OD1	2.15	0.47
6:B:580:VAL:HG11	6:B:710:LEU:HD11	1.97	0.47
10:F:95:GLY:O	10:F:99:TRP:CB	2.62	0.47
14:J:15:SER:HA	14:J:18:TRP:HB3	1.97	0.47
19:1:1200:CLA:HMC1	19:4:1198:CLA:CMB	2.44	0.47
1:1:135:LYS:HB3	1:1:136:ASP:H	1.54	0.47
3:3:197:TYR:OH	19:3:1212:CLA:CHC	2.63	0.47
19:1:1190:CLA:CMC	19:1:1196:CLA:CAC	2.92	0.47
5:A:629:ASN:CG	5:A:630:ASP:N	2.68	0.47
3:3:164:PHE:O	3:3:165:ASN:C	2.53	0.47
3:3:141:GLN:O	3:3:142:TYR:HB2	2.14	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:109:TRP:HA	5:A:116:ILE:CG1	2.44	0.46
19:A:1761:CLA:HMB3	19:A:1762:CLA:HAA1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:185:HIS:O	5:A:186:TYR:C	2.53	0.46
5:A:354:TRP:O	5:A:357:GLN:N	2.48	0.46
5:A:603:PHE:CZ	5:A:693:LEU:CD2	2.98	0.46
5:A:613:ILE:HG22	5:A:614:PHE:N	2.29	0.46
5:A:636:HIS:O	5:A:637:ILE:C	2.53	0.46
5:A:660:GLN:HE21	5:A:660:GLN:H	1.62	0.46
5:A:99:HIS:C	5:A:101:ALA:H	2.17	0.46
19:B:1758:CLA:H101	22:B:1776:BCR:C34	2.43	0.46
22:B:1779:BCR:H24C	22:B:1779:BCR:H371	1.52	0.46
6:B:293:THR:C	6:B:294:ASN:CG	2.66	0.46
6:B:350:GLN:O	6:B:353:TYR:CD1	2.69	0.46
6:B:377:TYR:O	6:B:378:ILE:CB	2.62	0.46
6:B:387:PHE:HE2	19:B:1755:CLA:HHC	1.79	0.46
6:B:552:ASP:OD1	6:B:553:PHE:HD2	1.98	0.46
6:B:556:SER:CA	6:B:558:PRO:HD2	2.45	0.46
7:C:81:TYR:CD1	7:C:81:TYR:N	2.83	0.46
8:D:48:ILE:CG1	8:D:49:THR:N	2.77	0.46
9:E:88:GLU:O	9:E:89:GLU:C	2.53	0.46
11:G:37:GLU:O	11:G:38:GLN:C	2.52	0.46
16:L:40:LEU:HD12	16:L:40:LEU:H	1.80	0.46
16:L:56:VAL:HG13	19:L:1167:CLA:HED3	1.94	0.46
3:3:63:ARG:NH1	3:3:189:LEU:H	2.13	0.46
15:K:69:ILE:HG12	15:K:72:VAL:HG12	1.96	0.46
3:3:58:GLU:HG2	19:3:1217:CLA:C1D	2.45	0.46
1:1:40:LYS:O	1:1:44:LEU:HG	2.15	0.46
15:K:52:PRO:O	15:K:56:THR:HG22	2.15	0.46
19:A:1782:CLA:H151	19:A:1782:CLA:H111	1.56	0.46
19:A:1796:CLA:HBD	19:A:1796:CLA:HAA1	1.97	0.46
19:A:1791:CLA:HMA2	19:A:1797:CLA:CBB	2.45	0.46
19:A:1781:CLA:H93	22:A:1806:BCR:C10	2.45	0.46
5:A:83:PHE:CE2	5:A:185:HIS:CD2	3.03	0.46
5:A:218:TRP:CZ3	19:A:1770:CLA:HMB3	2.50	0.46
5:A:223:VAL:HG12	5:A:224:HIS:H	1.79	0.46
5:A:281:LEU:CD2	19:A:1772:CLA:CMA	2.94	0.46
5:A:616:PHE:O	5:A:620:MET:HB2	2.15	0.46
5:A:733:VAL:HG12	5:A:737:HIS:CE1	2.50	0.46
6:B:127:ILE:O	6:B:128:GLY:C	2.53	0.46
22:B:1779:BCR:H311	22:B:1779:BCR:HC8	1.97	0.46
24:B:1783:LMG:O8	24:B:1783:LMG:H111	2.15	0.46
6:B:292:ARG:NH2	19:B:1750:CLA:HED1	2.31	0.46
6:B:594:TRP:CD1	6:B:595:HIS:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:N:59:PRO:CA	17:N:66:ASP:OD1	2.63	0.46
17:N:80:ASN:OD1	17:N:80:ASN:C	2.54	0.46
10:F:41:ALA:O	10:F:44:ALA:O	2.33	0.46
3:3:56:TYR:HD1	3:3:185:LYS:CE	2.29	0.46
19:1:1188:CLA:CGA	19:1:1188:CLA:HMA2	2.45	0.46
18:R:6:UNK:CB	18:R:10:UNK:CB	2.92	0.46
6:B:154:TRP:O	6:B:155:LEU:C	2.53	0.46
17:N:28:ASN:CA	17:N:30:ALA:H	2.28	0.46
5:A:265:GLY:HA3	5:A:272:LEU:HD21	1.97	0.46
10:F:34:ASP:O	10:F:34:ASP:OD2	2.33	0.46
5:A:154:ARG:O	5:A:155:ALA:C	2.54	0.46
19:A:1776:CLA:H43	19:A:1779:CLA:C2	2.45	0.46
19:A:1776:CLA:HBC3	19:A:1776:CLA:HMC1	1.95	0.46
19:A:1778:CLA:HAA1	15:K:32:ARG:NE	2.30	0.46
19:A:1776:CLA:HMC2	19:A:1782:CLA:H193	1.96	0.46
19:A:1790:CLA:H3A	19:A:1790:CLA:HBA2	1.53	0.46
5:A:110:LEU:CD1	5:A:239:PRO:HG2	2.38	0.46
5:A:281:LEU:C	5:A:283:PHE:N	2.68	0.46
5:A:452:PHE:CD2	5:A:456:HIS:CE1	3.03	0.46
5:A:86:LEU:H	5:A:86:LEU:HD22	1.81	0.46
6:B:164:SER:HB2	6:B:167:TRP:CE3	2.50	0.46
6:B:334:LEU:HA	19:B:1737:CLA:HMD3	1.97	0.46
6:B:172:GLU:O	6:B:173:SER:C	2.54	0.46
6:B:719:PHE:CZ	19:B:1757:CLA:H71	2.50	0.46
19:B:1756:CLA:CED	19:B:1764:CLA:CBB	2.91	0.46
19:B:1764:CLA:HBA2	19:B:1764:CLA:H3A	1.46	0.46
19:B:1767:CLA:OBD	19:B:1767:CLA:O2D	2.33	0.46
6:B:176:ASN:ND2	6:B:293:THR:OG1	2.47	0.46
6:B:596:TRP:CZ3	6:B:613:SER:CB	2.98	0.46
6:B:721:TYR:HA	6:B:724:PHE:HB3	1.96	0.46
10:F:131:PHE:C	10:F:133:GLY:N	2.68	0.46
11:G:34:GLN:O	11:G:36:PRO:N	2.47	0.46
17:N:53:ALA:O	17:N:54:LYS:CB	2.62	0.46
17:N:62:SER:OG	17:N:66:ASP:HB3	2.15	0.46
20:A:7016:LMU:O6'	20:A:7016:LMU:H31	2.13	0.46
19:K:1085:CLA:CMC	19:K:1085:CLA:HBC2	2.41	0.46
20:A:7039:LMU:O5'	20:A:7039:LMU:O3'	2.29	0.46
19:A:1815:CLA:CMC	19:A:1815:CLA:CBC	2.89	0.46
21:B:8059:SUC:H1'2	21:B:8059:SUC:H6'2	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:426:THR:HG23	5:A:428:TYR:OH	2.15	0.46
15:K:74:ILE:CG2	15:K:75:VAL:HG22	2.37	0.46
1:1:29:LEU:C	1:1:33:PRO:HD3	2.36	0.46
5:A:308:ILE:HG21	19:A:1772:CLA:HMC2	1.98	0.46
5:A:740:LEU:HD13	19:A:1796:CLA:HMA1	1.98	0.46
5:A:76:ARG:C	5:A:186:TYR:HD2	2.19	0.46
5:A:361:ASN:C	5:A:361:ASN:ND2	2.68	0.46
5:A:385:LEU:O	5:A:386:ALA:HB2	2.13	0.46
5:A:458:PHE:C	5:A:458:PHE:CD1	2.89	0.46
22:B:1775:BCR:H15C	22:B:1775:BCR:H351	1.71	0.46
6:B:395:ILE:HG22	6:B:551:LYS:HG3	1.97	0.46
6:B:396:ARG:NH1	19:B:1759:CLA:HED2	2.30	0.46
6:B:442:VAL:O	6:B:446:PHE:HB2	2.16	0.46
7:C:52:LYS:C	7:C:54:CYS:H	2.17	0.46
10:F:80:TRP:CH2	19:F:1156:CLA:CAC	2.98	0.46
19:H:1079:CLA:HMB1	13:I:9:VAL:HG13	1.97	0.46
12:H:62:GLY:O	13:I:15:LEU:HD22	2.15	0.46
5:A:249:ILE:CG2	5:A:251:ASN:OD1	2.64	0.46
17:N:59:PRO:HG2	17:N:73:ASP:O	2.15	0.46
4:4:106:TRP:CG	19:4:1196:CLA:HED2	2.50	0.46
11:G:20:ARG:NH1	11:G:64:VAL:C	2.69	0.46
11:G:57:LEU:O	11:G:57:LEU:HD22	2.16	0.46
6:B:454:LEU:HD22	10:F:70:HIS:CD2	2.50	0.46
12:H:73:PRO:HG3	21:H:1080:SUC:H5'	0.89	0.46
20:A:7017:LMU:H1B	20:A:7017:LMU:H6'2	1.44	0.46
5:A:350:LEU:HD23	5:A:350:LEU:HA	1.51	0.46
12:H:57:LEU:HD13	12:H:57:LEU:C	2.36	0.46
8:D:77:LEU:HD23	8:D:77:LEU:HA	1.66	0.46
5:A:531:PRO:O	5:A:532:ILE:HG23	2.15	0.46
5:A:550:HIS:C	5:A:552:THR:O	2.53	0.46
6:B:280:ILE:HD13	19:B:1748:CLA:HBB2	1.96	0.46
6:B:348:VAL:HG22	19:B:1758:CLA:HMD3	1.97	0.46
5:A:131:ILE:HD13	6:B:447:GLY:HA3	1.97	0.46
6:B:717:TYR:O	19:B:1785:CLA:HED3	2.15	0.46
9:E:60:LYS:CG	9:E:61:THR:N	2.72	0.46
12:H:66:THR:N	12:H:69:SER:HB3	2.29	0.46
19:A:1816:CLA:CAA	19:A:1816:CLA:CED	2.92	0.46
19:K:1142:CLA:HBC3	19:K:1142:CLA:CHD	2.46	0.46
20:A:7020:LMU:O5B	20:A:7020:LMU:O6'	2.30	0.46
20:A:7021:LMU:C4	20:A:7021:LMU:H1'	2.43	0.46
20:R:1056:LMU:H102	20:R:1056:LMU:H71	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:LEU:O	1:1:48:ARG:N	2.49	0.46
3:3:165:ASN:HA	3:3:165:ASN:HD22	1.59	0.46
5:A:720:THR:O	5:A:720:THR:CG2	2.62	0.46
5:A:207:LEU:CD1	19:A:1776:CLA:HBB2	2.46	0.46
19:A:1762:CLA:H11	19:A:1785:CLA:O2A	2.16	0.46
19:A:1797:CLA:H143	19:A:1797:CLA:H111	1.73	0.46
5:A:205:HIS:ND1	19:A:1769:CLA:HMC2	2.30	0.46
5:A:208:ALA:HB2	5:A:314:GLY:CA	2.38	0.46
19:B:1755:CLA:CAD	19:B:1767:CLA:CBB	2.91	0.46
6:B:22:TRP:CZ2	19:B:1770:CLA:HMB1	2.51	0.46
6:B:255:LEU:HA	6:B:271:THR:HB	1.98	0.46
6:B:256:THR:HG22	6:B:271:THR:OG1	2.16	0.46
11:G:30:ASN:ND2	11:G:34:GLN:H	2.14	0.46
11:G:50:ARG:HB2	11:G:51:ALA:HB2	1.96	0.46
19:H:1079:CLA:H41	16:L:87:ALA:HB1	1.98	0.46
20:A:7036:LMU:O5B	20:A:7036:LMU:C5'	2.62	0.46
3:3:74:ALA:CB	19:3:1215:CLA:ND	2.78	0.46
17:N:59:PRO:CB	17:N:75:TYR:CE1	2.96	0.46
19:K:1085:CLA:HAA2	19:K:1085:CLA:HBD	1.97	0.46
19:K:1142:CLA:HAA2	19:K:1142:CLA:HBD	1.96	0.46
20:A:7010:LMU:O3'	20:A:7010:LMU:C2B	2.64	0.46
11:G:16:LEU:HB2	11:G:17:PHE:CD2	2.51	0.46
16:L:108:LYS:HD3	16:L:132:SER:HB3	1.98	0.46
18:R:1:UNK:O	18:R:2:UNK:O	2.34	0.46
3:3:84:ILE:HG23	3:3:84:ILE:O	2.16	0.46
5:A:365:LEU:HD22	19:A:1761:CLA:HED3	1.91	0.46
19:A:1779:CLA:CBB	22:A:1805:BCR:H352	2.29	0.46
19:A:1796:CLA:H143	19:A:1796:CLA:H111	1.72	0.46
19:A:1797:CLA:HBD	19:A:1797:CLA:HAA2	1.96	0.46
5:A:218:TRP:HZ3	19:A:1770:CLA:HMB3	1.80	0.46
19:B:1739:CLA:H162	19:B:1757:CLA:H192	1.97	0.46
19:B:1771:CLA:H2	23:B:1773:PQN:H251	1.97	0.46
23:B:1773:PQN:H143	22:B:1780:BCR:H322	1.97	0.46
5:A:462:ILE:HD13	19:B:1786:CLA:H93	1.97	0.46
19:B:1785:CLA:HMB3	19:B:1786:CLA:OBD	2.16	0.46
6:B:544:SER:O	6:B:547:MET:C	2.54	0.46
11:G:28:ARG:CG	11:G:29:GLU:CB	2.94	0.46
22:I:1032:BCR:H11C	22:I:1032:BCR:H341	1.72	0.46
16:L:126:GLN:N	16:L:127:PRO:CD	2.78	0.46
19:A:1787:CLA:C4	16:L:33:ILE:CG1	2.93	0.46
2:2:68:LEU:HD21	19:2:1217:CLA:C17	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:158:MET:CG	16:L:159:TYR:N	2.75	0.46
6:B:399:ASN:O	6:B:399:ASN:OD1	2.34	0.46
10:F:37:ALA:N	10:F:38:PRO:HD3	2.31	0.46
19:A:1781:CLA:CED	19:A:1782:CLA:HMD2	2.38	0.46
5:A:401:TRP:CB	19:A:1783:CLA:HMC3	2.46	0.46
19:A:1796:CLA:H62	19:A:1813:CLA:C17	2.46	0.46
19:A:1783:CLA:H202	22:A:1808:BCR:C16	2.46	0.46
5:A:660:GLN:O	5:A:661:ALA:HB3	2.15	0.46
19:A:1795:CLA:C2C	19:B:1735:CLA:HBC2	2.45	0.46
6:B:645:VAL:HA	19:B:1740:CLA:HAC1	1.97	0.46
19:B:1748:CLA:C15	19:B:1749:CLA:H71	2.46	0.46
19:B:1743:CLA:H192	19:B:1748:CLA:OBD	2.16	0.46
19:B:1771:CLA:HHD	23:B:1773:PQN:H18	1.97	0.46
6:B:322:LEU:O	6:B:326:ILE:HG22	2.16	0.46
6:B:568:CYS:C	6:B:570:ILE:HG23	2.36	0.46
6:B:527:LEU:CD1	6:B:586:THR:HG21	2.43	0.46
8:D:102:ARG:NH2	8:D:110:GLN:HB2	2.30	0.46
11:G:39:ASN:HA	11:G:40:GLY:O	2.16	0.46
14:J:2:ARG:CG	14:J:2:ARG:HH11	2.29	0.46
2:2:55:ALA:HB3	2:2:56:MET:HE2	1.96	0.46
4:4:107:GLN:HA	19:4:1196:CLA:C2A	2.46	0.46
10:F:26:GLN:O	10:F:28:SER:N	2.48	0.46
10:F:44:ALA:C	10:F:46:MET:N	2.69	0.46
3:3:56:TYR:HD1	3:3:185:LYS:NZ	2.12	0.46
19:4:1204:CLA:HBA2	19:4:1204:CLA:CBD	2.46	0.46
11:G:66:PHE:O	11:G:69:VAL:HG12	2.16	0.46
3:3:162:PRO:HG2	3:3:164:PHE:CG	2.50	0.46
6:B:31:PHE:HB2	6:B:42:LEU:HD12	1.97	0.46
5:A:265:GLY:HA2	5:A:272:LEU:CD2	2.46	0.46
8:D:146:VAL:HG21	8:D:152:GLN:HG3	1.98	0.46
19:A:1761:CLA:H161	19:A:1761:CLA:H202	1.63	0.46
5:A:296:LEU:C	5:A:298:ASP:N	2.67	0.46
5:A:302:HIS:O	5:A:306:ILE:CG1	2.51	0.46
5:A:313:ALA:C	5:A:315:HIS:H	2.19	0.46
5:A:606:TYR:HH	19:A:1811:CLA:HED3	1.81	0.46
5:A:660:GLN:O	5:A:661:ALA:HB2	2.14	0.46
6:B:138:GLY:H	6:B:140:ILE:HG12	1.80	0.46
19:B:1745:CLA:HMA1	22:B:1776:BCR:H372	1.98	0.46
6:B:290:MET:SD	6:B:291:TYR:CE1	3.08	0.46
17:N:62:SER:HB3	17:N:66:ASP:N	2.30	0.46
4:4:98:SER:HA	4:4:101:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:142:ASN:O	4:4:143:PHE:HB2	2.16	0.46
2:2:91:THR:O	2:2:94:LEU:HB3	2.15	0.46
5:A:258:LEU:O	5:A:259:TYR:HB2	2.15	0.46
5:A:258:LEU:HG	5:A:280:PHE:CE1	2.51	0.46
12:H:53:LEU:HG	12:H:54:LEU:N	2.22	0.46
6:B:244:PHE:CD2	6:B:244:PHE:C	2.89	0.46
5:A:68:THR:C	5:A:70:ASP:N	2.68	0.46
6:B:224:PRO:CA	6:B:227:THR:OG1	2.63	0.46
17:N:27:ALA:O	17:N:28:ASN:C	2.54	0.46
2:2:206:ALA:O	2:2:207:ALA:HB3	2.16	0.46
3:3:106:TYR:O	3:3:107:TRP:C	2.54	0.46
3:3:112:THR:C	3:3:114:PHE:N	2.69	0.46
19:A:1763:CLA:H3A	19:A:1763:CLA:HBA2	1.48	0.46
19:A:1781:CLA:H93	22:A:1806:BCR:H10C	1.98	0.46
5:A:355:HIS:ND1	5:A:416:ILE:HG22	2.24	0.46
5:A:434:ARG:O	5:A:435:VAL:C	2.54	0.46
5:A:457:SER:HG	5:A:544:ILE:HA	1.80	0.46
5:A:637:ILE:HG12	5:A:637:ILE:H	1.52	0.46
5:A:708:VAL:N	5:A:711:HIS:HD2	2.14	0.46
19:B:1743:CLA:H41	19:B:1748:CLA:CBC	2.46	0.46
6:B:530:THR:HG22	19:B:1755:CLA:CMC	2.46	0.46
22:B:1774:BCR:H15C	22:B:1774:BCR:H351	1.77	0.46
10:F:124:PRO:O	10:F:125:LEU:HB2	2.15	0.46
11:G:43:HIS:CA	11:G:44:PHE:CB	2.62	0.46
17:N:42:PHE:N	17:N:43:PRO:CD	2.58	0.46
5:A:316:MET:CA	5:A:317:TYR:CD1	2.99	0.46
3:3:188:ARG:HA	3:3:191:MET:HB2	1.97	0.46
6:B:500:ALA:C	6:B:501:ILE:HG12	2.36	0.46
5:A:47:GLY:O	10:F:115:THR:HB	2.16	0.46
10:F:115:THR:O	10:F:116:GLN:CB	2.63	0.46
6:B:15:ASP:OD2	6:B:15:ASP:C	2.55	0.46
6:B:638:LEU:N	6:B:638:LEU:HD22	2.31	0.46
4:4:169:GLN:HE22	19:4:1199:CLA:CHD	2.26	0.45
19:A:1761:CLA:H3A	19:A:1761:CLA:HBA1	1.66	0.45
5:A:678:PHE:CZ	19:A:1783:CLA:H142	2.51	0.45
19:A:1800:CLA:HMC3	19:B:1770:CLA:C1D	2.46	0.45
19:A:1790:CLA:C2B	22:A:1806:BCR:H333	2.46	0.45
5:A:709:TRP:O	5:A:712:ASN:N	2.49	0.45
5:A:693:LEU:HD11	5:A:738:TYR:HD1	1.78	0.45
5:A:685:VAL:CG1	5:A:741:GLY:CA	2.94	0.45
5:A:64:PHE:CE1	5:A:74:ILE:HG22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:98:PHE:HD1	5:A:99:HIS:CD2	2.33	0.45
6:B:125:TYR:HE1	6:B:130:ARG:NH1	2.14	0.45
19:B:1755:CLA:H11	19:B:1769:CLA:CAD	2.45	0.45
19:B:1755:CLA:C2B	22:B:1777:BCR:H352	2.46	0.45
6:B:551:LYS:HG2	6:B:552:ASP:H	1.79	0.45
9:E:58:ASP:OD1	9:E:58:ASP:N	2.30	0.45
19:A:1795:CLA:C6	10:F:121:ILE:HD12	2.46	0.45
13:I:8:PHE:HE1	22:I:1032:BCR:C9	2.28	0.45
3:3:132:TRP:HZ3	3:3:155:GLU:CD	1.82	0.45
21:B:8054:SUC:H3'	21:B:8054:SUC:H1	1.50	0.45
5:A:316:MET:HA	5:A:317:TYR:HD1	1.82	0.45
19:A:1799:CLA:HBA2	19:A:1799:CLA:CED	2.46	0.45
4:4:156:ASN:O	4:4:160:MET:HG3	2.17	0.45
5:A:126:ILE:O	5:A:129:GLN:HB2	2.16	0.45
19:A:1767:CLA:H202	19:A:1767:CLA:H152	1.98	0.45
5:A:193:LEU:O	5:A:195:TRP:N	2.50	0.45
5:A:358:LEU:HD11	5:A:413:HIS:HB2	1.90	0.45
19:B:1735:CLA:HBC1	22:B:1778:BCR:C33	2.46	0.45
6:B:50:HIS:HB3	19:B:1737:CLA:CHB	2.47	0.45
19:B:1748:CLA:CGA	19:B:1748:CLA:C4A	2.94	0.45
6:B:527:LEU:CD1	19:B:1755:CLA:C1D	2.88	0.45
6:B:557:PHE:O	6:B:557:PHE:CD2	2.69	0.45
6:B:80:ASP:HA	6:B:81:PRO:HD3	1.56	0.45
8:D:137:ILE:HG13	8:D:137:ILE:H	1.44	0.45
9:E:60:LYS:HG3	9:E:61:THR:OG1	2.16	0.45
11:G:48:ASP:CB	11:G:49:THR:CB	2.92	0.45
8:D:31:GLY:CA	16:L:13:PRO:HB3	2.44	0.45
16:L:63:LEU:HD13	16:L:64:LEU:HG	1.98	0.45
19:2:1215:CLA:C3	19:2:1220:CLA:HBC3	2.42	0.45
17:N:42:PHE:CG	17:N:43:PRO:N	2.80	0.45
4:4:106:TRP:C	4:4:108:ASP:H	2.19	0.45
3:3:66:MET:CE	3:3:69:ALA:HB3	2.46	0.45
5:A:257:GLN:O	5:A:258:LEU:CB	2.64	0.45
6:B:216:LEU:O	6:B:218:TYR:O	2.34	0.45
3:3:90:LEU:HD12	3:3:90:LEU:N	2.31	0.45
4:4:161:LEU:O	4:4:162:ALA:CB	2.64	0.45
1:1:85:LEU:HD13	1:1:85:LEU:H	1.82	0.45
19:A:1759:CLA:HHD	19:A:1759:CLA:HBC3	1.99	0.45
19:A:1764:CLA:ND	19:A:1783:CLA:C4	2.79	0.45
19:A:1781:CLA:CBB	19:A:1794:CLA:HMA1	2.47	0.45
19:A:1783:CLA:H191	19:A:1812:CLA:H13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1793:CLA:HMB2	19:A:1794:CLA:C1D	2.46	0.45
19:A:1798:CLA:H11	19:A:1798:CLA:H52	1.75	0.45
5:A:374:GLN:O	5:A:377:TYR:CD2	2.64	0.45
5:A:672:LEU:HD23	5:A:673:SER:H	1.80	0.45
19:B:1738:CLA:H161	19:B:1738:CLA:H91	1.97	0.45
6:B:176:ASN:ND2	6:B:291:TYR:O	2.48	0.45
23:B:1773:PQN:H2M1	23:B:1773:PQN:H111	1.67	0.45
6:B:180:SER:O	6:B:181:GLY:C	2.54	0.45
6:B:573:TRP:O	6:B:576:PHE:HB3	2.16	0.45
6:B:700:LEU:H	6:B:700:LEU:HD23	1.80	0.45
6:B:77:TRP:O	6:B:81:PRO:HG3	2.17	0.45
19:L:1168:CLA:HHD	19:L:1168:CLA:HBC2	1.88	0.45
16:L:63:LEU:CD2	16:L:64:LEU:N	2.75	0.45
19:1:1197:CLA:CBD	19:1:1197:CLA:HAA2	2.44	0.45
3:3:73:ILE:O	19:3:1215:CLA:C3D	2.65	0.45
10:F:23:LYS:HB3	10:F:24:LYS:NZ	2.19	0.45
21:B:8056:SUC:H3'	21:B:8056:SUC:HO2	1.68	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
6:B:470:THR:OG1	6:B:501:ILE:HG23	2.16	0.45
8:D:26:SER:N	8:D:27:PRO:HD3	2.30	0.45
2:2:50:VAL:O	2:2:50:VAL:HG12	2.17	0.45
19:4:1201:CLA:O2D	19:4:1201:CLA:HAA2	2.14	0.45
5:A:107:GLU:O	5:A:110:LEU:HG	2.17	0.45
19:A:1764:CLA:HBB2	19:A:1765:CLA:C3D	2.47	0.45
19:A:1781:CLA:HMB3	22:A:1806:BCR:C17	2.46	0.45
19:A:1792:CLA:O1A	19:A:1792:CLA:C2	2.64	0.45
5:A:205:HIS:CG	19:A:1769:CLA:HMC2	2.51	0.45
5:A:284:ARG:HG3	5:A:295:TRP:CB	2.47	0.45
5:A:374:GLN:C	5:A:376:MET:N	2.68	0.45
5:A:680:LEU:HD21	6:B:617:MET:SD	2.55	0.45
5:A:707:ILE:H	5:A:707:ILE:HG12	1.53	0.45
5:A:707:ILE:HG22	5:A:711:HIS:CD2	2.49	0.45
5:A:714:LEU:HD13	22:B:1779:BCR:H393	1.92	0.45
19:B:1737:CLA:H92	19:B:1754:CLA:O1A	2.17	0.45
6:B:260:GLY:HA2	6:B:497:TRP:CE2	2.52	0.45
6:B:535:VAL:O	6:B:539:LEU:HB2	2.17	0.45
6:B:652:PHE:CZ	6:B:656:VAL:HG21	2.52	0.45
10:F:145:LEU:C	10:F:146:ASN:ND2	2.70	0.45
16:L:40:LEU:CB	16:L:41:PRO:HD3	2.38	0.45
19:1:1198:CLA:H91	19:1:1198:CLA:H122	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:44:GLU:HB3	17:N:45:ASN:H	1.43	0.45
17:N:45:ASN:CG	17:N:57:LYS:NZ	2.70	0.45
4:4:107:GLN:C	19:4:1196:CLA:HMA1	2.24	0.45
21:2:1226:SUC:C6	21:2:1226:SUC:C2	2.87	0.45
5:A:70:ASP:O	5:A:71:LEU:C	2.54	0.45
19:A:1778:CLA:HAA2	19:A:1778:CLA:CGD	2.47	0.45
19:A:1781:CLA:H43	19:A:1793:CLA:CBA	2.47	0.45
5:A:678:PHE:HZ	19:A:1783:CLA:H142	1.82	0.45
5:A:53:TRP:HA	5:A:56:ASN:ND2	2.32	0.45
5:A:680:LEU:HD22	5:A:680:LEU:N	2.31	0.45
5:A:73:GLU:O	5:A:76:ARG:HB2	2.16	0.45
19:B:1747:CLA:H12	19:B:1747:CLA:NA	2.31	0.45
6:B:431:PHE:HE2	19:B:1762:CLA:HED3	1.81	0.45
19:B:1755:CLA:CAB	19:B:1769:CLA:HMA1	2.47	0.45
6:B:319:HIS:O	6:B:320:LYS:O	2.34	0.45
6:B:53:GLN:NE2	19:B:1736:CLA:HBB1	2.30	0.45
8:D:113:HIS:O	8:D:113:HIS:HD2	2.00	0.45
6:B:398:TYR:O	8:D:143:PRO:HG2	2.16	0.45
9:E:83:ALA:O	9:E:86:GLU:CG	2.50	0.45
19:2:1213:CLA:OBD	19:2:1213:CLA:O2D	2.35	0.45
17:N:38:GLY:HA3	17:N:46:PHE:HD1	1.80	0.45
4:4:101:VAL:C	4:4:104:ARG:HD3	2.37	0.45
11:G:57:LEU:CD2	11:G:57:LEU:O	2.64	0.45
11:G:62:ASP:CB	11:G:63:PRO:HD3	2.42	0.45
5:A:425:THR:O	5:A:427:ARG:CD	2.65	0.45
7:C:44:ARG:NH2	8:D:127:ARG:NE	2.63	0.45
2:2:70:LYS:HG3	2:2:73:ILE:HG12	1.95	0.45
21:B:8055:SUC:H1'1	21:B:8055:SUC:HO2	1.80	0.45
5:A:539:PHE:CD2	5:A:539:PHE:O	2.65	0.45
6:B:439:HIS:NE2	6:B:443:MET:SD	2.89	0.45
5:A:493:GLN:OE1	5:A:534:LEU:HD11	2.16	0.45
19:A:1781:CLA:CMA	19:A:1782:CLA:CGA	2.94	0.45
5:A:207:LEU:HD11	5:A:313:ALA:HB1	1.98	0.45
5:A:397:THR:HB	5:A:613:ILE:HG13	1.97	0.45
5:A:347:TYR:HE1	5:A:417:PHE:CZ	2.34	0.45
5:A:645:SER:O	5:A:651:GLY:HA3	2.16	0.45
5:A:701:GLN:O	5:A:703:LEU:N	2.49	0.45
5:A:73:GLU:O	5:A:76:ARG:CA	2.64	0.45
6:B:212:PHE:CE1	19:B:1744:CLA:HHD	2.36	0.45
6:B:323:TYR:O	6:B:327:ASN:HB2	2.17	0.45
8:D:99:GLN:HG2	8:D:101:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:36:VAL:HG23	9:E:52:VAL:HG22	1.99	0.45
9:E:62:ARG:O	9:E:83:ALA:CB	2.65	0.45
10:F:149:LEU:CD2	10:F:153:ASN:HD21	2.29	0.45
19:B:1762:CLA:NB	10:F:90:PHE:CE1	2.85	0.45
11:G:34:GLN:O	11:G:36:PRO:CD	2.65	0.45
14:J:7:TYR:HB3	14:J:8:LEU:H	1.61	0.45
19:4:1198:CLA:HBC3	19:4:1198:CLA:CMC	2.46	0.45
7:C:18:VAL:HB	7:C:58:CYS:HB2	1.99	0.45
14:J:31:ARG:HH22	19:J:1043:CLA:C3B	2.10	0.45
19:A:1815:CLA:HBA1	19:A:1815:CLA:H3A	1.74	0.45
8:D:132:LEU:HD12	8:D:136:SER:OG	2.17	0.45
10:F:102:ARG:NH1	10:F:106:ILE:HD12	2.31	0.45
5:A:141:ARG:CD	10:F:40:LEU:H	2.30	0.45
17:N:7:LEU:O	17:N:8:GLU:HB2	2.16	0.45
6:B:513:GLY:O	6:B:516:ASP:OD1	2.35	0.45
5:A:476:MET:O	5:A:477:PHE:HB2	2.17	0.45
3:3:164:PHE:HA	3:3:164:PHE:HD1	1.71	0.45
12:H:75:ASP:HB3	12:H:77:LEU:HG	1.99	0.45
22:A:1805:BCR:H11C	22:A:1805:BCR:H341	1.71	0.45
22:A:1807:BCR:H341	22:A:1807:BCR:H11C	1.72	0.45
5:A:347:TYR:CE1	5:A:417:PHE:HZ	2.34	0.45
5:A:499:ALA:O	5:A:501:GLY:N	2.38	0.45
6:B:167:TRP:O	6:B:167:TRP:CD2	2.70	0.45
19:B:1735:CLA:CHD	19:B:1735:CLA:HBC3	2.46	0.45
19:B:1738:CLA:CBC	19:B:1757:CLA:CMD	2.95	0.45
6:B:467:HIS:NE2	19:B:1764:CLA:CHA	2.80	0.45
6:B:188:LEU:HD21	22:B:1775:BCR:H281	1.99	0.45
6:B:347:LEU:HD13	6:B:351:HIS:ND1	2.29	0.45
6:B:540:ASP:OD1	6:B:540:ASP:N	2.48	0.45
6:B:707:LEU:CD1	24:B:1783:LMG:H301	2.47	0.45
6:B:708:VAL:C	6:B:710:LEU:O	2.55	0.45
8:D:139:LYS:HZ3	9:E:41:ARG:NH1	2.15	0.45
19:A:1786:CLA:H2A	16:L:25:THR:HG21	1.99	0.45
3:3:94:ARG:HG2	3:3:97:PHE:CD1	2.52	0.45
20:A:7022:LMU:O3B	20:A:7022:LMU:H6'2	2.13	0.45
17:N:2:VAL:CG2	17:N:2:VAL:O	2.63	0.45
1:1:89:VAL:O	11:G:77:ILE:HD13	2.16	0.45
20:L:1171:LMU:H52	20:L:1171:LMU:H82	1.78	0.45
2:2:96:ILE:HG13	2:2:97:VAL:H	1.80	0.45
1:1:34:ALA:O	1:1:38:ARG:N	2.39	0.45
19:A:1767:CLA:C4A	19:A:1767:CLA:CBA	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1768:CLA:O1D	19:A:1769:CLA:HMC1	2.17	0.45
19:A:1779:CLA:NB	22:A:1805:BCR:C15	2.79	0.45
5:A:555:ILE:HG12	5:A:555:ILE:H	1.46	0.45
5:A:709:TRP:CE3	5:A:710:ALA:N	2.85	0.45
5:A:83:PHE:HA	5:A:86:LEU:CD2	2.47	0.45
6:B:279:ALA:HA	19:B:1746:CLA:HMA1	1.99	0.45
19:B:1755:CLA:C2	19:B:1768:CLA:HBA2	2.46	0.45
22:B:1775:BCR:HC8	22:B:1775:BCR:H331	1.96	0.45
19:B:1787:CLA:H202	19:B:1787:CLA:H162	1.72	0.45
6:B:198:ALA:H	6:B:200:PRO:HG2	1.82	0.45
6:B:47:PHE:CZ	6:B:51:PHE:HE1	2.35	0.45
6:B:518:LEU:O	6:B:521:HIS:N	2.42	0.45
6:B:623:TYR:H	6:B:626:LEU:HB3	1.81	0.45
7:C:81:TYR:HD1	7:C:81:TYR:N	2.15	0.45
11:G:33:LYS:O	11:G:34:GLN:HG2	2.15	0.45
14:J:26:LEU:H	14:J:28:GLU:H	1.65	0.45
19:A:1816:CLA:HED3	19:A:1816:CLA:H72	1.98	0.45
7:C:17:CYS:O	7:C:58:CYS:HB2	2.16	0.45
11:G:16:LEU:CA	11:G:68:ILE:HG13	2.45	0.45
19:R:1055:CLA:H122	20:R:1056:LMU:O4'	2.17	0.45
19:2:1224:CLA:H71	19:2:1224:CLA:H111	1.59	0.45
6:B:514:PRO:HG2	10:F:70:HIS:CE1	2.51	0.45
6:B:216:LEU:O	6:B:217:PRO:C	2.55	0.45
1:1:184:PRO:HA	1:1:185:TRP:O	2.16	0.45
10:F:152:ASN:N	10:F:152:ASN:ND2	2.64	0.45
5:A:614:PHE:HE1	19:A:1811:CLA:H62	1.82	0.45
5:A:365:LEU:HD23	19:A:1761:CLA:HED2	1.91	0.45
5:A:593:SER:O	5:A:594:ALA:HB2	2.16	0.45
5:A:656:PHE:O	5:A:658:TRP:N	2.50	0.45
5:A:663:GLN:OE1	5:A:753:ARG:NE	2.50	0.45
5:A:72:GLU:HB2	5:A:73:GLU:H	1.56	0.45
5:A:82:HIS:CE1	19:A:1761:CLA:HAA1	2.51	0.45
6:B:29:HIS:HB2	19:B:1759:CLA:HBA1	1.99	0.45
22:B:1780:BCR:C38	22:B:1780:BCR:C23	2.74	0.45
6:B:560:ASP:O	25:B:1784:SF4:S3	2.75	0.45
6:B:461:GLN:HE21	6:B:461:GLN:HB3	1.63	0.45
6:B:558:PRO:HB3	6:B:706:ARG:HH21	1.80	0.45
10:F:62:LEU:HG	10:F:72:ILE:HD11	1.96	0.45
16:L:154:ALA:O	16:L:155:CYS:C	2.55	0.45
17:N:45:ASN:O	17:N:46:PHE:C	2.50	0.45
19:K:1085:CLA:HMB1	19:K:1142:CLA:HED2	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:4014:CLA:HBC3	19:4:4014:CLA:CMC	2.12	0.45
5:A:260:PRO:HG3	5:A:277:TYR:CZ	2.51	0.45
3:3:111:TYR:HB2	3:3:112:THR:H	1.68	0.45
19:A:1759:CLA:H12	19:A:1796:CLA:C5	2.47	0.45
19:A:1760:CLA:HMC3	19:A:1762:CLA:CED	2.47	0.45
19:A:1776:CLA:H121	22:A:1806:BCR:H23C	1.98	0.45
19:A:1797:CLA:H41	19:A:1797:CLA:H62	1.45	0.45
5:A:327:ILE:O	5:A:328:LYS:C	2.55	0.45
5:A:463:HIS:NE2	5:A:467:MET:SD	2.90	0.45
5:A:541:VAL:HG12	5:A:545:HIS:NE2	2.32	0.45
5:A:684:PHE:HD2	5:A:685:VAL:CA	2.29	0.45
5:A:73:GLU:O	5:A:74:ILE:C	2.55	0.45
19:B:1749:CLA:CHA	19:B:1749:CLA:HBA1	2.46	0.45
6:B:304:ILE:CD1	19:B:1749:CLA:HED3	2.47	0.45
6:B:347:LEU:HD21	6:B:351:HIS:CE1	2.40	0.45
6:B:493:TRP:CZ2	19:B:1747:CLA:H122	2.52	0.45
8:D:139:LYS:HG2	8:D:141:VAL:HG22	1.98	0.45
22:L:1169:BCR:H341	22:L:1169:BCR:H11C	1.83	0.45
7:C:9:ASP:HB2	25:C:1083:SF4:S3	2.57	0.45
14:J:31:ARG:O	14:J:34:PRO:HG3	2.17	0.45
12:H:24:TYR:HB3	12:H:25:GLY:H	1.60	0.45
12:H:29:PRO:O	12:H:30:SER:OG	2.30	0.45
6:B:218:TYR:HB3	6:B:219:PRO:HD2	1.99	0.45
12:H:40:PHE:O	12:H:41:GLU:C	2.56	0.45
5:A:132:LEU:O	5:A:143:ILE:HB	2.17	0.44
5:A:187:HIS:CE1	19:A:1767:CLA:CHA	2.96	0.44
19:A:1780:CLA:HMD2	19:A:1780:CLA:C14	2.33	0.44
22:A:1803:BCR:C34	22:A:1803:BCR:C12	2.88	0.44
5:A:462:ILE:O	5:A:466:THR:OG1	2.33	0.44
5:A:488:PHE:CZ	5:A:533:PRO:HB3	2.52	0.44
5:A:400:MET:HE3	5:A:612:VAL:HG11	1.99	0.44
19:B:1738:CLA:HBA1	19:B:1738:CLA:H3A	1.71	0.44
6:B:17:THR:OG1	6:B:18:THR:N	2.50	0.44
6:B:275:HIS:HD2	19:B:1746:CLA:HMA3	1.83	0.44
8:D:74:LEU:HG	8:D:74:LEU:O	2.16	0.44
14:J:21:SER:O	14:J:23:ALA:N	2.50	0.44
20:A:7032:LMU:H52	20:A:7032:LMU:H81	1.36	0.44
20:R:1056:LMU:H22	20:R:1056:LMU:O2'	2.17	0.44
17:N:22:LEU:HD23	17:N:22:LEU:O	2.17	0.44
6:B:318:GLY:HA3	6:B:405:ASP:OD2	2.17	0.44
1:1:57:ILE:CG2	1:1:58:LEU:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:131:THR:HG23	2:2:132:GLY:N	2.30	0.44
6:B:679:ALA:O	6:B:683:GLU:OE2	2.35	0.44
3:3:114:PHE:CE1	19:3:1216:CLA:C4D	3.01	0.44
5:A:113:PRO:O	5:A:115:HIS:CD2	2.70	0.44
5:A:122:VAL:HG22	5:A:142:GLY:CA	2.47	0.44
5:A:163:GLN:C	5:A:165:TYR:H	2.19	0.44
19:A:1759:CLA:HBC3	19:A:1759:CLA:CHD	2.47	0.44
19:A:1762:CLA:C7	19:A:1762:CLA:C2	2.95	0.44
19:A:1786:CLA:HMB2	19:A:1787:CLA:C4D	2.48	0.44
5:A:451:ILE:HD13	19:A:1788:CLA:HED1	1.98	0.44
22:A:1804:BCR:C8	22:A:1804:BCR:C31	2.95	0.44
5:A:680:LEU:HB3	19:A:1812:CLA:C2	2.47	0.44
5:A:436:LEU:C	5:A:438:HIS:O	2.56	0.44
5:A:472:ARG:O	5:A:474:GLN:CB	2.65	0.44
5:A:665:ILE:HD12	5:A:666:GLN:N	2.32	0.44
19:B:1747:CLA:H3A	19:B:1747:CLA:HBA2	1.33	0.44
19:B:1756:CLA:H202	19:B:1756:CLA:H162	1.64	0.44
6:B:343:VAL:HG11	19:B:1756:CLA:H2	1.98	0.44
19:B:1738:CLA:CBB	19:B:1758:CLA:HHC	2.47	0.44
23:B:1773:PQN:C2M	23:B:1773:PQN:H142	2.46	0.44
6:B:415:LYS:HG3	6:B:416:GLU:OE2	2.17	0.44
6:B:629:SER:O	6:B:630:GLN:C	2.54	0.44
7:C:62:PHE:CE2	9:E:42:GLU:CD	2.82	0.44
6:B:564:ARG:HH12	7:C:63:LEU:HA	1.82	0.44
8:D:41:GLN:CD	8:D:41:GLN:C	2.76	0.44
22:B:1778:BCR:H372	10:F:93:ILE:HG22	1.99	0.44
5:A:251:ASN:O	5:A:253:ASP:HB3	2.17	0.44
3:3:49:ILE:CG1	3:3:52:LYS:CB	2.94	0.44
11:G:16:LEU:CD1	11:G:17:PHE:CZ	3.00	0.44
8:D:93:LYS:CB	8:D:93:LYS:HZ2	2.27	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
16:L:107:PHE:CB	16:L:109:GLU:OE1	2.62	0.44
20:3:7005:LMU:H6D	20:3:7005:LMU:H1'	1.74	0.44
3:3:86:GLN:HB2	3:3:88:THR:CA	2.48	0.44
19:A:1766:CLA:HBB2	19:A:1769:CLA:HMA3	1.98	0.44
19:A:1773:CLA:C4C	19:A:1773:CLA:H62	2.47	0.44
19:A:1788:CLA:HED1	19:A:1800:CLA:O1A	2.16	0.44
5:A:732:ALA:HB1	19:A:1796:CLA:HED2	1.99	0.44
22:A:1803:BCR:C31	22:A:1803:BCR:C8	2.67	0.44
19:A:1764:CLA:H111	22:A:1808:BCR:C10	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:223:VAL:CG1	5:A:224:HIS:H	2.29	0.44
5:A:369:THR:O	5:A:372:VAL:HG23	2.18	0.44
5:A:432:LEU:O	5:A:435:VAL:N	2.50	0.44
5:A:514:THR:HA	5:A:530:LEU:O	2.17	0.44
5:A:581:CYS:HB2	5:A:590:CYS:O	2.16	0.44
5:A:705:GLU:CG	6:B:545:LYS:HZ2	2.31	0.44
6:B:120:VAL:HG22	6:B:123:TRP:HE1	1.83	0.44
6:B:194:LEU:O	6:B:199:ILE:HG13	2.17	0.44
6:B:353:TYR:C	6:B:355:LEU:N	2.70	0.44
6:B:535:VAL:CG1	6:B:536:LYS:H	2.30	0.44
7:C:53:ARG:O	7:C:55:GLU:O	2.36	0.44
19:F:1157:CLA:OBD	19:F:1157:CLA:O2D	2.31	0.44
14:J:2:ARG:HH22	14:J:8:LEU:HD22	1.81	0.44
19:A:1800:CLA:H93	22:L:1169:BCR:H321	1.97	0.44
16:L:65:VAL:C	16:L:69:VAL:HG22	2.36	0.44
19:2:1218:CLA:CGA	19:2:1218:CLA:C1A	2.96	0.44
4:4:104:ARG:HE	4:4:105:ARG:N	2.15	0.44
4:4:103:ILE:HG23	19:4:1207:CLA:HMB3	2.00	0.44
20:A:7033:LMU:H61	20:A:7033:LMU:H31	1.59	0.44
10:F:24:LYS:HE3	10:F:24:LYS:N	2.25	0.44
20:1:7004:LMU:H2O2	20:1:7004:LMU:H11	1.74	0.44
20:A:7010:LMU:H22	20:A:7010:LMU:H51	1.40	0.44
11:G:60:SER:O	11:G:62:ASP:N	2.50	0.44
12:H:42:THR:HG22	12:H:45:ALA:CB	2.44	0.44
18:R:5:UNK:O	18:R:6:UNK:CB	2.65	0.44
5:A:49:ASP:HB2	5:A:720:THR:HA	1.98	0.44
6:B:158:GLN:O	6:B:159:PRO:O	2.36	0.44
5:A:174:PHE:HE2	19:A:1761:CLA:H152	1.79	0.44
5:A:143:ILE:HG12	19:A:1764:CLA:HBC2	2.00	0.44
5:A:79:PHE:CD2	5:A:185:HIS:CD2	2.97	0.44
5:A:430:ASP:C	5:A:432:LEU:H	2.21	0.44
5:A:64:PHE:CD1	5:A:74:ILE:HG22	2.53	0.44
5:A:711:HIS:CB	5:A:717:ALA:HB2	2.41	0.44
19:B:1738:CLA:CBC	19:B:1757:CLA:HMD3	2.48	0.44
19:B:1768:CLA:HBD	19:B:1768:CLA:HAA1	1.99	0.44
6:B:431:PHE:CE2	19:B:1762:CLA:CED	3.00	0.44
6:B:57:ILE:HG22	6:B:58:PHE:CD1	2.52	0.44
6:B:60:TRP:CD1	19:B:1738:CLA:HBC1	2.52	0.44
6:B:693:TRP:CZ2	6:B:697:PRO:HG3	2.52	0.44
6:B:710:LEU:O	6:B:712:HIS:N	2.51	0.44
6:B:718:ILE:HD11	19:B:1757:CLA:HHC	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:139:LYS:NZ	9:E:41:ARG:NH1	2.65	0.44
10:F:104:TYR:OH	10:F:121:ILE:HA	2.17	0.44
3:3:93:PHE:HD2	3:3:95:THR:N	2.12	0.44
17:N:59:PRO:HA	17:N:66:ASP:OD1	2.16	0.44
7:C:58:CYS:HA	7:C:59:PRO:HD2	1.65	0.44
20:A:7033:LMU:H2O2	20:A:7033:LMU:C6B	2.19	0.44
20:A:7020:LMU:C6'	20:A:7020:LMU:C1B	2.95	0.44
19:A:1817:CLA:HAA1	19:A:1817:CLA:O1D	2.15	0.44
4:4:35:GLU:HB2	4:4:36:ASN:H	1.52	0.44
9:E:69:PHE:CE2	9:E:70:ALA:HB3	2.53	0.44
7:C:28:MET:HB2	8:D:121:GLU:HA	1.99	0.44
20:1:1202:LMU:H5'	20:1:1202:LMU:O5B	2.15	0.44
8:D:94:TYR:O	8:D:95:LYS:NZ	2.33	0.44
10:F:33:ALA:C	10:F:35:ASP:H	2.20	0.44
19:L:1166:CLA:HBA2	19:L:1166:CLA:H3A	1.54	0.44
12:H:11:LEU:HA	12:H:11:LEU:HD22	1.85	0.44
8:D:21:ASP:HB3	8:D:22:PRO:HD3	1.99	0.44
19:A:1760:CLA:HBA2	19:A:1767:CLA:C6	2.47	0.44
19:A:1767:CLA:H171	19:A:1767:CLA:H141	1.98	0.44
19:A:1774:CLA:ND	19:A:1784:CLA:H72	2.33	0.44
5:A:55:TRP:CH2	19:A:1795:CLA:HMB1	2.53	0.44
5:A:472:ARG:HG2	6:B:97:GLY:HA3	2.00	0.44
5:A:575:LEU:HD12	5:A:575:LEU:H	1.82	0.44
19:B:1741:CLA:H51	19:B:1741:CLA:H8	1.59	0.44
19:B:1763:CLA:H3A	19:B:1763:CLA:HBA1	1.67	0.44
6:B:700:LEU:N	23:B:1773:PQN:O4	2.44	0.44
22:B:1775:BCR:H341	22:B:1775:BCR:H11C	1.70	0.44
19:B:1735:CLA:H61	22:B:1778:BCR:H12C	1.99	0.44
6:B:183:PHE:HE1	19:B:1743:CLA:H71	1.83	0.44
6:B:290:MET:HA	19:B:1751:CLA:C3C	2.47	0.44
6:B:365:PHE:HB3	6:B:602:TRP:CZ2	2.52	0.44
6:B:544:SER:N	6:B:547:MET:O	2.47	0.44
6:B:590:VAL:O	6:B:593:TYR:HB3	2.18	0.44
6:B:74:PHE:C	6:B:76:ALA:N	2.70	0.44
7:C:60:THR:HG21	7:C:64:SER:HB3	1.98	0.44
10:F:72:ILE:O	10:F:73:VAL:HG12	2.18	0.44
11:G:28:ARG:NH2	11:G:28:ARG:CG	2.72	0.44
16:L:61:GLY:O	16:L:63:LEU:N	2.51	0.44
16:L:95:LEU:HA	16:L:98:CYS:CB	2.42	0.44
19:J:1044:CLA:C8	19:J:1044:CLA:C4	2.76	0.44
5:A:316:MET:HA	5:A:317:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7043:LMU:C7	20:A:7043:LMU:H111	2.22	0.44
21:B:8062:SUC:O4	21:B:8062:SUC:O2	2.29	0.44
20:A:7030:LMU:H42	20:A:7030:LMU:H11	1.76	0.44
14:J:10:VAL:CG2	14:J:14:LEU:HD12	2.47	0.44
1:1:27:LEU:H	6:B:314:ARG:HH12	1.66	0.44
5:A:349:ILE:HD13	5:A:422:TYR:HB3	1.99	0.44
2:2:37:ASP:HA	2:2:38:PRO:HD3	1.85	0.44
6:B:694:ARG:HE	16:L:105:ALA:CA	2.28	0.44
6:B:509:PHE:N	6:B:509:PHE:HD2	2.15	0.44
6:B:673:GLU:O	6:B:676:GLU:HB2	2.18	0.44
19:A:1765:CLA:HBC3	19:A:1765:CLA:CMC	2.48	0.44
19:A:1764:CLA:H161	19:A:1785:CLA:C20	2.48	0.44
19:A:1787:CLA:H122	19:A:1787:CLA:H161	1.60	0.44
19:A:1787:CLA:O1A	6:B:686:PRO:HD3	2.18	0.44
22:A:1805:BCR:H321	22:A:1805:BCR:C8	2.48	0.44
5:A:363:ALA:O	5:A:367:SER:CB	2.65	0.44
5:A:377:TYR:CD1	5:A:616:PHE:CE1	3.04	0.44
5:A:400:MET:CE	5:A:612:VAL:HG11	2.48	0.44
6:B:103:ALA:HA	6:B:105:THR:O	2.18	0.44
6:B:167:TRP:HD1	11:G:41:MET:HE1	1.82	0.44
19:B:1747:CLA:H2	19:B:1756:CLA:HBB1	1.98	0.44
22:B:1774:BCR:H343	11:G:21:PHE:CE1	2.51	0.44
6:B:288:GLY:O	6:B:289:LEU:HB2	2.17	0.44
6:B:395:ILE:HG13	6:B:395:ILE:H	1.72	0.44
6:B:668:ARG:NH1	6:B:672:GLN:HG2	2.32	0.44
6:B:726:ILE:C	6:B:728:SER:N	2.70	0.44
8:D:41:GLN:HG3	16:L:125:LYS:NZ	2.33	0.44
9:E:44:TYR:HB3	9:E:45:TRP:CZ3	2.53	0.44
20:A:7042:LMU:H61	20:A:7042:LMU:H31	1.48	0.44
19:2:1213:CLA:H42	19:2:1213:CLA:CHD	2.48	0.44
19:2:1220:CLA:H11	19:2:1220:CLA:H51	1.85	0.44
17:N:62:SER:OG	17:N:66:ASP:HA	2.18	0.44
17:N:72:LYS:HA	17:N:72:LYS:HD2	1.57	0.44
20:A:7016:LMU:H42	20:A:7016:LMU:H72	1.51	0.44
19:J:1045:CLA:CBA	19:J:1045:CLA:CHA	2.87	0.44
1:1:141:GLU:O	1:1:143:LEU:O	2.36	0.44
20:A:7039:LMU:H82	20:A:7039:LMU:H112	1.38	0.44
3:3:50:GLU:OE1	3:3:54:LEU:HB2	2.17	0.44
11:G:58:LEU:HB2	11:G:59:LYS:H	1.42	0.44
1:1:45:ILE:CD1	19:1:1195:CLA:HMD2	2.38	0.44
19:1:1188:CLA:HMA2	19:1:1188:CLA:CBA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:154:TRP:CD1	6:B:154:TRP:C	2.91	0.44
26:B:8057:UNL:O3'	26:B:8057:UNL:O1'	2.29	0.44
3:3:111:TYR:HB2	3:3:112:THR:HG22	2.00	0.44
3:3:86:GLN:CB	3:3:88:THR:H	2.31	0.44
5:A:301:HIS:NE2	19:A:1772:CLA:CHA	2.81	0.44
19:A:1780:CLA:HMC1	19:A:1780:CLA:HBC2	1.98	0.44
19:A:1793:CLA:HBD	19:A:1793:CLA:HAA1	1.99	0.44
22:A:1806:BCR:H341	22:A:1806:BCR:H11C	1.71	0.44
5:A:203:LEU:O	5:A:207:LEU:HD23	2.17	0.44
5:A:334:HIS:CB	19:A:1777:CLA:HMA3	2.48	0.44
5:A:458:PHE:C	5:A:460:LEU:N	2.70	0.44
5:A:461:TYR:CD2	5:A:649:ILE:HD12	2.52	0.44
6:B:141:PHE:CG	19:B:1744:CLA:H12	2.53	0.44
6:B:431:PHE:CE2	19:B:1762:CLA:HED3	2.53	0.44
6:B:431:PHE:CD2	19:B:1762:CLA:HMA3	2.52	0.44
5:A:680:LEU:HG	6:B:617:MET:HB2	1.98	0.44
7:C:77:MET:C	7:C:79:LEU:N	2.69	0.44
8:D:113:HIS:O	8:D:113:HIS:CD2	2.70	0.44
10:F:84:ILE:HD13	10:F:84:ILE:N	2.33	0.44
19:H:1079:CLA:O1D	19:H:1079:CLA:H2A	2.17	0.44
11:G:92:GLY:O	11:G:94:ASP:OD1	2.36	0.44
20:A:7009:LMU:O6B	20:A:7009:LMU:H3'	2.18	0.44
2:2:189:ILE:H	2:2:189:ILE:CD1	2.20	0.44
7:C:26:LEU:O	7:C:43:PRO:HB3	2.18	0.44
6:B:332:PHE:HE1	6:B:408:LEU:CD2	2.30	0.44
15:K:47:ILE:HG23	15:K:48:GLN:N	2.28	0.44
8:D:152:GLN:HA	8:D:153:PRO:HD2	1.73	0.44
5:A:173:VAL:O	5:A:175:ALA:O	2.36	0.44
19:A:1768:CLA:HBD	19:A:1768:CLA:HAA1	1.98	0.44
19:A:1782:CLA:H91	19:A:1782:CLA:H112	1.61	0.44
19:A:1792:CLA:HBD	19:A:1792:CLA:HBA1	1.99	0.44
19:A:1793:CLA:H71	19:A:1793:CLA:H112	1.70	0.44
19:A:1796:CLA:C4	19:A:1796:CLA:C4C	2.94	0.44
5:A:212:GLY:O	5:A:214:GLY:N	2.51	0.44
5:A:42:ARG:O	5:A:44:ILE:HG13	2.17	0.44
5:A:554:LEU:CD2	19:B:1787:CLA:O2D	2.66	0.44
5:A:560:VAL:O	5:A:563:ALA:HB2	2.16	0.44
5:A:665:ILE:O	6:B:621:ARG:HD3	2.18	0.44
19:B:1744:CLA:HBA2	19:B:1744:CLA:H3A	1.58	0.44
19:B:1743:CLA:C14	19:B:1748:CLA:H2	2.39	0.44
19:B:1749:CLA:C2	19:B:1754:CLA:H92	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1777:BCR:C23	22:B:1777:BCR:C38	2.66	0.44
24:B:1783:LMG:O3	7:C:70:TRP:HZ2	1.88	0.44
6:B:309:ILE:HA	6:B:310:PRO:HD3	1.82	0.44
6:B:535:VAL:HG23	6:B:539:LEU:HD23	1.98	0.44
6:B:353:TYR:CB	6:B:594:TRP:CH2	3.00	0.44
6:B:67:HIS:CD2	6:B:71:GLN:HE22	2.35	0.44
9:E:46:PHE:CD2	9:E:47:LYS:N	2.86	0.44
16:L:151:VAL:O	16:L:154:ALA:HB3	2.17	0.44
3:3:132:TRP:CE3	3:3:155:GLU:HG2	2.26	0.44
18:R:34:UNK:C	18:R:36:UNK:O	2.66	0.44
19:3:1219:CLA:CED	19:3:1219:CLA:H2A	2.48	0.44
18:R:8:UNK:CB	19:R:1054:CLA:O2D	2.66	0.44
19:3:3011:CLA:H62	19:3:3011:CLA:H41	1.73	0.44
4:4:38:ARG:O	4:4:39:TRP:CD1	2.68	0.44
10:F:61:LEU:HD23	10:F:69:PRO:HB3	1.96	0.44
6:B:5:ILE:CB	6:B:6:PRO:CD	2.86	0.44
2:2:186:THR:O	2:2:187:GLY:C	2.56	0.44
1:1:137:PRO:O	1:1:139:LYS:N	2.51	0.44
1:1:105:ILE:HG22	1:1:105:ILE:O	2.18	0.44
5:A:144:GLN:HG3	5:A:145:ILE:H	1.82	0.44
19:A:1811:CLA:H122	19:A:1811:CLA:H162	1.68	0.44
5:A:388:ASP:OD1	5:A:391:THR:HB	2.18	0.44
5:A:596:ASP:HA	5:A:599:PHE:CB	2.39	0.44
6:B:120:VAL:C	6:B:123:TRP:HD1	2.20	0.44
6:B:196:HIS:CE1	19:B:1745:CLA:C4D	3.00	0.44
19:B:1768:CLA:C8	19:B:1768:CLA:HBB2	2.42	0.44
6:B:457:PRO:O	6:B:460:ALA:HB3	2.18	0.44
6:B:727:ALA:O	6:B:728:SER:OG	2.29	0.44
6:B:564:ARG:NH1	7:C:63:LEU:HA	2.33	0.44
16:L:123:ARG:CA	16:L:123:ARG:NE	2.72	0.44
3:3:92:TRP:CZ2	5:A:250:LEU:HB2	2.51	0.44
20:A:7032:LMU:C1B	20:A:7032:LMU:C1	2.96	0.44
12:H:25:GLY:HA3	12:H:27:ASP:OD2	2.11	0.44
11:G:16:LEU:HD12	11:G:17:PHE:CZ	2.51	0.44
10:F:89:LEU:HA	10:F:89:LEU:HD12	1.88	0.44
19:A:1783:CLA:H18	19:A:1783:CLA:H122	1.99	0.43
19:A:1801:CLA:H41	19:A:1801:CLA:H62	1.63	0.43
5:A:570:PRO:C	5:A:572:LYS:H	2.21	0.43
5:A:651:GLY:O	5:A:655:ASP:HB2	2.18	0.43
5:A:92:TRP:CD1	19:A:1763:CLA:HBB2	2.53	0.43
6:B:460:ALA:O	6:B:462:TRP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:583:MET:CE	6:B:583:MET:O	2.66	0.43
6:B:714:SER:O	6:B:718:ILE:HG22	2.18	0.43
8:D:79:ARG:H	8:D:82:GLN:HE21	1.63	0.43
6:B:458:ILE:HD11	19:F:1156:CLA:HED1	2.00	0.43
19:B:1762:CLA:C4B	10:F:90:PHE:CE1	3.01	0.43
17:N:42:PHE:CD1	17:N:43:PRO:CD	3.01	0.43
17:N:69:CYS:O	17:N:72:LYS:HD2	2.17	0.43
17:N:84:LYS:HA	17:N:85:TRP:HA	1.46	0.43
20:A:7037:LMU:H4B	20:A:7037:LMU:H1B	1.50	0.43
18:R:50:UNK:HA	18:R:51:UNK:HA	1.70	0.43
18:R:27:UNK:O	18:R:29:UNK:C	2.65	0.43
8:D:125:PRO:HG2	8:D:127:ARG:HH11	1.82	0.43
5:A:631:GLN:HG2	5:A:633:VAL:HG13	1.98	0.43
5:A:220:ARG:O	5:A:221:HIS:CB	2.62	0.43
2:2:161:THR:HA	2:2:165:LYS:HB2	2.00	0.43
16:L:92:VAL:HG11	16:L:147:GLY:CA	2.47	0.43
19:A:1772:CLA:H121	19:A:1772:CLA:H8	1.87	0.43
19:A:1781:CLA:HMB3	22:A:1806:BCR:C19	2.48	0.43
19:A:1793:CLA:O1A	19:A:1793:CLA:CB	2.67	0.43
5:A:711:HIS:NE2	19:A:1795:CLA:CB	2.79	0.43
22:A:1807:BCR:C8	19:A:1813:CLA:H142	2.48	0.43
5:A:222:GLN:O	5:A:227:LEU:HD12	2.19	0.43
5:A:25:ASP:HB3	5:A:26:PRO:HD3	2.00	0.43
5:A:567:ARG:HH11	8:D:34:GLY:C	2.22	0.43
5:A:569:ILE:HG12	5:A:586:ARG:NH1	2.33	0.43
5:A:705:GLU:O	5:A:706:SER:C	2.57	0.43
6:B:141:PHE:O	6:B:142:LEU:C	2.57	0.43
6:B:434:LEU:O	6:B:438:VAL:HG13	2.18	0.43
6:B:560:ASP:CG	7:C:66:ARG:CZ	2.86	0.43
5:A:558:LYS:HZ1	6:B:674:LEU:HD23	1.82	0.43
8:D:29:PHE:HA	8:D:66:ALA:HB2	2.00	0.43
7:C:75:ARG:NH1	8:D:46:TYR:OH	2.51	0.43
10:F:123:VAL:CB	10:F:126:ALA:O	2.66	0.43
16:L:127:PRO:O	16:L:128:ASP:O	2.37	0.43
4:4:143:PHE:O	4:4:144:ALA:CB	2.65	0.43
19:3:1219:CLA:HBC3	19:3:1219:CLA:CMC	2.12	0.43
11:G:10:LEU:HD23	11:G:13:GLY:HA3	2.00	0.43
5:A:478:SER:HB2	5:A:481:ALA:H	1.83	0.43
19:4:1204:CLA:C8	19:4:1204:CLA:H41	2.48	0.43
8:D:94:TYR:O	8:D:95:LYS:HB3	2.18	0.43
16:L:43:TYR:O	16:L:44:ARG:CB	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:74:TRP:CZ3	1:1:81:GLN:HA	2.54	0.43
5:A:34:TRP:O	5:A:35:ALA:CB	2.66	0.43
4:4:83:TYR:HB3	4:4:84:PHE:H	1.64	0.43
19:4:1201:CLA:CHD	19:4:1201:CLA:HBC3	2.48	0.43
3:3:84:ILE:N	19:A:1798:CLA:H51	2.33	0.43
5:A:310:PHE:H	5:A:313:ALA:CB	2.32	0.43
5:A:390:ALA:HA	5:A:393:LEU:HD21	1.98	0.43
5:A:568:LEU:HD21	5:A:586:ARG:HB3	1.99	0.43
19:B:1758:CLA:H3A	19:B:1758:CLA:HBA2	1.55	0.43
6:B:651:LEU:HB3	19:B:1786:CLA:C1	2.48	0.43
6:B:297:ILE:HG21	11:G:21:PHE:CZ	2.54	0.43
6:B:460:ALA:O	6:B:463:ILE:N	2.52	0.43
6:B:556:SER:HA	6:B:558:PRO:HD3	2.00	0.43
6:B:365:PHE:HB3	6:B:602:TRP:CH2	2.53	0.43
6:B:621:ARG:HB3	6:B:621:ARG:HE	1.57	0.43
6:B:626:LEU:O	6:B:627:ASN:CB	2.66	0.43
8:D:40:ALA:O	8:D:45:PHE:CD2	2.71	0.43
9:E:80:ASN:OD1	9:E:81:ASN:N	2.49	0.43
13:I:25:PHE:CE2	13:I:28:VAL:HG21	2.53	0.43
16:L:33:ILE:HG23	16:L:34:ALA:N	2.34	0.43
19:3:1218:CLA:HBA2	19:3:1218:CLA:H3A	1.69	0.43
2:2:55:ALA:HB3	2:2:56:MET:CE	2.48	0.43
17:N:62:SER:CB	17:N:66:ASP:HA	2.48	0.43
4:4:102:GLU:C	4:4:104:ARG:H	2.21	0.43
4:4:117:GLN:HB3	4:4:121:PHE:CE2	2.53	0.43
3:3:50:GLU:OE2	3:3:54:LEU:HD13	2.17	0.43
19:A:1817:CLA:CBC	19:A:1817:CLA:CMC	2.81	0.43
10:F:51:LYS:O	10:F:53:PHE:N	2.46	0.43
9:E:69:PHE:HD2	9:E:71:LYS:H	1.61	0.43
16:L:77:THR:OG1	16:L:82:ALA:HB3	2.19	0.43
20:A:7038:LMU:O1B	20:A:7038:LMU:O6'	2.30	0.43
2:2:211:LYS:HA	2:2:211:LYS:CE	2.48	0.43
19:A:1776:CLA:HBA1	19:A:1780:CLA:CBB	2.48	0.43
19:A:1784:CLA:H52	19:A:1784:CLA:HMD2	2.00	0.43
19:A:1796:CLA:H41	19:A:1796:CLA:C1C	2.48	0.43
5:A:213:LEU:O	22:A:1804:BCR:C17	2.66	0.43
19:A:1783:CLA:C11	22:A:1808:BCR:C35	2.96	0.43
5:A:27:ILE:C	5:A:28:LYS:HG3	2.24	0.43
5:A:400:MET:HG3	5:A:609:ILE:HG23	2.00	0.43
5:A:363:ALA:N	5:A:410:ALA:CB	2.81	0.43
5:A:656:PHE:O	5:A:657:LEU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:385:GLY:CA	19:B:1759:CLA:HBC3	2.48	0.43
23:B:1773:PQN:H192	22:B:1780:BCR:HC8	1.97	0.43
6:B:659:THR:OG1	19:B:1787:CLA:C3B	2.67	0.43
6:B:662:MET:O	6:B:664:LEU:N	2.52	0.43
9:E:42:GLU:CG	9:E:43:SER:N	2.70	0.43
9:E:65:VAL:HG23	9:E:66:VAL:O	2.19	0.43
19:2:1215:CLA:HED2	19:2:1220:CLA:CBB	2.48	0.43
2:2:171:MET:SD	2:2:172:LEU:HG	2.57	0.43
17:N:40:CYS:N	17:N:41:LYS:CA	2.81	0.43
19:4:1196:CLA:H41	19:4:1196:CLA:H62	1.60	0.43
4:4:119:PRO:HG2	4:4:120:ILE:HG13	2.01	0.43
4:4:143:PHE:O	4:4:144:ALA:HB2	2.19	0.43
20:A:7026:LMU:H1B	20:A:7026:LMU:H4B	1.07	0.43
11:G:60:SER:O	11:G:61:ASN:C	2.56	0.43
10:F:63:CYS:CA	10:F:69:PRO:HA	2.45	0.43
12:H:53:LEU:CG	12:H:54:LEU:N	2.77	0.43
8:D:56:GLN:OE1	8:D:94:TYR:CE2	2.71	0.43
5:A:539:PHE:HE2	5:A:543:HIS:HE1	1.66	0.43
17:N:25:THR:HG22	17:N:26:GLY:N	2.33	0.43
17:N:25:THR:HG22	17:N:26:GLY:H	1.83	0.43
5:A:128:GLY:HA3	6:B:446:PHE:HD2	1.80	0.43
19:A:1761:CLA:H122	22:A:1803:BCR:C39	2.48	0.43
5:A:503:THR:HG21	19:A:1791:CLA:NB	2.33	0.43
19:A:1796:CLA:H11	19:A:1796:CLA:ND	2.33	0.43
22:A:1807:BCR:C12	19:A:1812:CLA:H122	2.48	0.43
5:A:284:ARG:CZ	5:A:284:ARG:CA	2.91	0.43
5:A:370:ILE:CG2	5:A:400:MET:CA	2.87	0.43
5:A:379:MET:HB2	5:A:379:MET:HE2	1.80	0.43
5:A:506:GLY:O	5:A:507:ALA:CB	2.66	0.43
5:A:603:PHE:CE2	6:B:665:ILE:HG21	2.54	0.43
6:B:144:PHE:O	6:B:148:ILE:HD11	2.18	0.43
19:B:1750:CLA:O2A	19:B:1750:CLA:NA	2.52	0.43
6:B:589:TRP:CD1	19:B:1785:CLA:H152	2.54	0.43
6:B:190:TRP:CE2	19:B:1748:CLA:CMD	3.01	0.43
6:B:183:PHE:HB3	6:B:284:PHE:CD2	2.53	0.43
6:B:351:HIS:HB3	19:B:1747:CLA:CED	2.35	0.43
6:B:458:ILE:HG13	6:B:459:PHE:CD1	2.54	0.43
6:B:57:ILE:HG12	19:B:1738:CLA:HMC2	2.00	0.43
6:B:674:LEU:O	6:B:678:LEU:HB2	2.18	0.43
7:C:5:VAL:CA	7:C:65:VAL:HG22	2.46	0.43
13:I:15:LEU:HD12	13:I:18:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:249:ILE:C	5:A:251:ASN:N	2.65	0.43
20:A:7030:LMU:H6D	20:A:7030:LMU:H1'	1.18	0.43
10:F:53:PHE:O	10:F:55:ASN:N	2.52	0.43
6:B:473:GLY:O	6:B:474:PHE:HB3	2.19	0.43
16:L:49:PRO:HG3	16:L:131:GLN:NE2	2.34	0.43
8:D:92:SER:O	8:D:93:LYS:HG3	2.19	0.43
16:L:107:PHE:HA	16:L:133:ALA:HB2	2.00	0.43
10:F:116:GLN:HA	10:F:118:GLU:OE1	2.18	0.43
12:H:77:LEU:HD23	12:H:78:PRO:CD	2.48	0.43
1:1:180:HIS:O	4:4:88:SER:OG	2.27	0.43
2:2:124:ILE:HG22	2:2:124:ILE:O	2.18	0.43
5:A:725:LEU:HD21	19:A:1796:CLA:HMD3	1.99	0.43
19:A:1783:CLA:C20	22:A:1808:BCR:C15	2.95	0.43
19:A:1763:CLA:CHC	22:A:1808:BCR:H333	2.49	0.43
5:A:680:LEU:HB3	19:A:1812:CLA:C1	2.48	0.43
5:A:703:LEU:O	5:A:707:ILE:CG1	2.67	0.43
5:A:98:PHE:O	5:A:99:HIS:CD2	2.71	0.43
19:B:1736:CLA:H3A	19:B:1736:CLA:HBA2	1.53	0.43
19:B:1744:CLA:H162	19:B:1744:CLA:H143	1.75	0.43
6:B:289:LEU:CD2	19:B:1750:CLA:C1A	2.96	0.43
19:B:1750:CLA:H43	19:B:1750:CLA:C1C	2.49	0.43
19:B:1757:CLA:H161	19:B:1757:CLA:H193	1.88	0.43
6:B:179:LEU:O	6:B:284:PHE:O	2.36	0.43
6:B:361:ILE:O	6:B:362:ALA:O	2.36	0.43
6:B:672:GLN:HE22	6:B:698:VAL:HA	1.84	0.43
9:E:37:LYS:CB	9:E:49:VAL:HG22	2.47	0.43
9:E:65:VAL:CG2	9:E:66:VAL:O	2.66	0.43
6:B:458:ILE:HD11	19:F:1156:CLA:CED	2.48	0.43
22:B:1781:BCR:C34	19:H:1079:CLA:CHD	2.96	0.43
17:N:53:ALA:O	17:N:54:LYS:CG	2.67	0.43
19:R:1054:CLA:H62	19:R:1054:CLA:H41	1.87	0.43
10:F:151:ASP:O	10:F:154:PHE:N	2.52	0.43
5:A:163:GLN:O	5:A:165:TYR:N	2.51	0.43
19:A:1776:CLA:H111	19:A:1776:CLA:C16	2.47	0.43
5:A:281:LEU:HD21	19:A:1772:CLA:HMA2	1.99	0.43
5:A:347:TYR:CE1	5:A:417:PHE:CZ	3.06	0.43
5:A:378:SER:HG	5:A:512:SER:HG	1.65	0.43
5:A:530:LEU:HD11	5:A:624:VAL:HA	2.01	0.43
5:A:606:TYR:HB2	5:A:739:LEU:HD22	2.00	0.43
5:A:620:MET:C	5:A:623:ASP:O	2.57	0.43
5:A:682:ALA:HA	5:A:685:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1771:CLA:C2	23:B:1773:PQN:H251	2.49	0.43
6:B:190:TRP:O	6:B:191:ALA:C	2.57	0.43
6:B:203:ARG:CG	6:B:204:GLY:N	2.70	0.43
6:B:594:TRP:HD1	6:B:595:HIS:N	2.16	0.43
8:D:46:TYR:HD2	8:D:46:TYR:N	2.13	0.43
9:E:73:ASN:ND2	9:E:78:SER:HB2	2.33	0.43
9:E:88:GLU:O	9:E:90:VAL:HA	2.14	0.43
19:3:1218:CLA:CAA	19:3:1218:CLA:O1D	2.66	0.43
19:2:1220:CLA:C11	3:3:137:SER:OG	2.67	0.43
17:N:47:THR:CG2	17:N:54:LYS:HZ2	2.16	0.43
17:N:72:LYS:HZ2	17:N:74:LYS:HG2	1.59	0.43
4:4:105:ARG:O	4:4:108:ASP:HB3	2.18	0.43
20:A:7039:LMU:H4B	20:A:7039:LMU:H1B	1.58	0.43
20:2:7006:LMU:H71	20:2:7006:LMU:H41	1.81	0.43
5:A:479:ASP:HA	5:A:536:THR:CG2	2.46	0.43
12:H:63:SER:O	12:H:67:TYR:HB3	2.17	0.43
6:B:680:TRP:O	6:B:681:ALA:O	2.37	0.43
2:2:117:GLY:O	2:2:119:VAL:HG22	2.18	0.43
19:A:1764:CLA:H122	19:A:1764:CLA:H161	1.73	0.43
19:A:1767:CLA:CMC	19:A:1767:CLA:HBC3	2.37	0.43
5:A:499:ALA:CB	19:A:1790:CLA:O2D	2.66	0.43
19:A:1793:CLA:HMC1	19:A:1793:CLA:HBC2	2.00	0.43
5:A:208:ALA:CA	5:A:310:PHE:O	2.43	0.43
5:A:552:THR:O	5:A:553:VAL:HB	2.19	0.43
5:A:57:LEU:HD22	5:A:58:HIS:CD2	2.54	0.43
5:A:648:THR:HG23	5:A:650:ASN:H	1.83	0.43
5:A:655:ASP:O	5:A:659:ALA:HB3	2.18	0.43
19:B:1736:CLA:H2A	19:B:1736:CLA:O1D	2.18	0.43
6:B:278:LEU:CD1	19:B:1746:CLA:HMA2	2.42	0.43
19:B:1755:CLA:HBB1	19:B:1769:CLA:HHB	1.95	0.43
6:B:414:HIS:O	6:B:414:HIS:CD2	2.71	0.43
6:B:421:HIS:O	19:B:1769:CLA:HMC3	2.18	0.43
6:B:555:TYR:HE2	6:B:573:TRP:HD1	1.67	0.43
19:A:1811:CLA:HBB1	6:B:624:LEU:HD11	2.00	0.43
6:B:715:VAL:O	6:B:719:PHE:HB2	2.18	0.43
6:B:91:ILE:HD12	19:B:1740:CLA:HMD3	2.00	0.43
19:A:1789:CLA:HMD2	6:B:95:HIS:HD2	1.84	0.43
19:4:1199:CLA:HAA1	19:F:1157:CLA:H12	2.00	0.43
16:L:64:LEU:CD2	16:L:91:LEU:HD22	2.48	0.43
5:A:249:ILE:CD1	5:A:250:LEU:HB2	2.48	0.43
20:A:7016:LMU:O6'	20:A:7016:LMU:H41	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:22:LEU:CB	10:F:25:LEU:HD13	2.48	0.43
20:A:7032:LMU:C6B	20:A:7032:LMU:H22	2.44	0.43
12:H:27:ASP:O	12:H:29:PRO:CD	2.67	0.43
4:4:152:LYS:HA	4:4:152:LYS:HD2	1.81	0.43
20:A:7026:LMU:C4	20:A:7026:LMU:H82	2.29	0.43
10:F:52:ARG:N	10:F:52:ARG:HD2	2.33	0.43
7:C:12:ILE:HD12	7:C:12:ILE:H	1.81	0.43
20:A:7019:LMU:H72	20:A:7019:LMU:H101	1.67	0.43
20:A:7034:LMU:H1B	20:A:7034:LMU:H5'	1.47	0.43
19:A:1759:CLA:O1A	19:A:1796:CLA:H52	2.19	0.43
5:A:545:HIS:HB3	19:A:1792:CLA:CBB	2.30	0.43
5:A:551:VAL:HG21	5:A:604:TRP:CZ2	2.54	0.43
5:A:554:LEU:HD21	19:B:1787:CLA:O2D	2.18	0.43
6:B:175:LEU:O	6:B:179:LEU:CG	2.66	0.43
23:B:1773:PQN:H2M1	23:B:1773:PQN:C14	2.47	0.43
8:D:75:LEU:HD11	16:L:19:PHE:CD1	2.54	0.43
8:D:83:CYS:O	8:D:83:CYS:SG	2.77	0.43
8:D:84:LEU:HD12	8:D:100:PHE:CZ	2.50	0.43
9:E:44:TYR:HD2	9:E:45:TRP:HE3	1.66	0.43
5:A:48:PRO:HB3	9:E:72:VAL:HG22	2.01	0.43
11:G:42:SER:HG	11:G:45:GLU:CB	2.31	0.43
11:G:88:THR:HG23	11:G:91:ASN:O	2.18	0.43
5:A:141:ARG:HE	10:F:40:LEU:H	1.67	0.43
1:1:161:PHE:CD1	19:1:1189:CLA:CBB	3.01	0.43
1:1:55:PRO:HA	1:1:58:LEU:HB2	2.01	0.43
15:K:51:ASP:CB	15:K:52:PRO:CD	2.91	0.43
6:B:42:LEU:O	6:B:43:TYR:O	2.37	0.43
19:L:1505:CLA:HAA2	19:L:1505:CLA:HBD	2.00	0.43
14:J:32:PHE:HE2	14:J:33:PHE:CE1	2.37	0.43
14:J:32:PHE:CE2	14:J:33:PHE:CZ	3.05	0.43
8:D:149:THR:O	8:D:151:LYS:N	2.51	0.43
5:A:105:ASN:HB3	5:A:150:PHE:HZ	1.84	0.43
5:A:154:ARG:NE	5:A:154:ARG:HA	2.33	0.43
5:A:154:ARG:NH2	5:A:233:LEU:CD1	2.81	0.43
5:A:304:LEU:CD2	19:A:1772:CLA:CBB	2.70	0.43
19:A:1796:CLA:HBA2	19:A:1796:CLA:H3A	1.48	0.43
19:A:1797:CLA:C12	19:A:1797:CLA:H71	2.09	0.43
5:A:361:ASN:O	5:A:364:MET:N	2.52	0.43
5:A:413:HIS:CG	5:A:416:ILE:HD12	2.54	0.43
5:A:78:VAL:O	5:A:82:HIS:CG	2.72	0.43
6:B:114:ASN:O	6:B:115:ASN:OD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1767:CLA:HAA1	19:B:1768:CLA:HAA2	2.00	0.43
6:B:400:PRO:HG2	8:D:141:VAL:C	2.39	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:17:THR:CA	6:B:696:LYS:H	2.31	0.43
10:F:104:TYR:N	10:F:129:LEU:HD13	2.34	0.43
11:G:48:ASP:HB3	11:G:49:THR:CB	2.44	0.43
19:A:1778:CLA:HAA1	15:K:32:ARG:HD3	2.01	0.43
20:A:7042:LMU:H4'	20:A:7042:LMU:H1'	1.56	0.43
17:N:78:GLY:O	17:N:82:PHE:CE2	2.72	0.43
3:3:192:LEU:C	3:3:194:ILE:H	2.23	0.43
11:G:62:ASP:HB2	11:G:63:PRO:CD	2.45	0.43
14:J:10:VAL:HG13	14:J:14:LEU:CG	2.42	0.43
8:D:126:GLY:C	8:D:127:ARG:CG	2.86	0.43
4:4:70:ILE:O	4:4:72:VAL:N	2.52	0.43
4:4:73:PRO:O	4:4:74:LYS:HB2	2.19	0.43
19:A:1772:CLA:HBD	19:A:1772:CLA:HAA1	2.00	0.42
5:A:219:ALA:O	5:A:222:GLN:N	2.48	0.42
5:A:40:PHE:O	5:A:40:PHE:CD1	2.72	0.42
5:A:114:THR:HG1	5:A:525:ASN:HB2	1.77	0.42
6:B:167:TRP:CD1	11:G:41:MET:CE	3.02	0.42
6:B:188:LEU:CD1	19:B:1745:CLA:CBB	2.92	0.42
19:B:1758:CLA:H122	22:B:1775:BCR:C14	2.49	0.42
22:B:1777:BCR:H15C	22:B:1777:BCR:H351	1.82	0.42
19:B:1785:CLA:HAA2	19:B:1785:CLA:H11	2.01	0.42
6:B:182:LEU:HG	6:B:183:PHE:H	1.84	0.42
6:B:182:LEU:HG	6:B:183:PHE:N	2.33	0.42
6:B:393:PHE:CE2	6:B:398:TYR:HB2	2.54	0.42
6:B:685:THR:HA	6:B:686:PRO:HD3	1.92	0.42
3:3:194:ILE:HG13	19:3:1212:CLA:C2C	2.49	0.42
6:B:332:PHE:HE1	6:B:408:LEU:HD21	1.85	0.42
20:L:1171:LMU:O6'	20:L:1171:LMU:H81	2.18	0.42
3:3:84:ILE:CA	19:A:1798:CLA:C5	2.86	0.42
5:A:149:PHE:C	5:A:151:GLN:N	2.71	0.42
19:A:1773:CLA:HBA2	19:A:1773:CLA:H3A	1.24	0.42
19:A:1789:CLA:C4	16:L:64:LEU:CD2	2.93	0.42
19:A:1792:CLA:CBA	19:A:1792:CLA:CB D	2.97	0.42
5:A:700:TRP:CE2	23:A:1802:PQN:H2M3	2.53	0.42
19:A:1812:CLA:C9	19:A:1812:CLA:H122	2.46	0.42
5:A:227:LEU:O	5:A:231:GLN:HB2	2.18	0.42
5:A:654:ARG:HG3	5:A:655:ASP:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:723:ARG:H	19:A:1795:CLA:CBB	2.31	0.42
5:A:748:ALA:O	5:A:749:PHE:C	2.57	0.42
5:A:86:LEU:HA	5:A:89:ILE:HD12	2.00	0.42
5:A:96:MET:N	5:A:98:PHE:O	2.51	0.42
6:B:172:GLU:O	6:B:176:ASN:N	2.51	0.42
19:B:1741:CLA:HBD	19:B:1741:CLA:CGA	2.49	0.42
19:B:1747:CLA:H141	19:B:1747:CLA:HMC2	2.01	0.42
6:B:724:PHE:CZ	19:B:1785:CLA:HMD1	2.54	0.42
6:B:531:THR:O	6:B:535:VAL:N	2.49	0.42
9:E:40:ARG:N	9:E:46:PHE:CE1	2.82	0.42
10:F:128:SER:C	10:F:130:LEU:HD23	2.40	0.42
10:F:99:TRP:CZ3	10:F:140:ALA:HB2	2.55	0.42
22:I:1032:BCR:C39	22:L:1169:BCR:C40	2.96	0.42
22:L:1170:BCR:HC7	22:L:1170:BCR:H342	1.53	0.42
4:4:103:ILE:HG13	19:4:1197:CLA:CMD	2.45	0.42
10:F:26:GLN:HB3	10:F:27:ALA:H	1.69	0.42
3:3:49:ILE:O	3:3:49:ILE:HG23	2.19	0.42
19:3:3011:CLA:H142	19:3:3011:CLA:H101	2.01	0.42
17:N:4:GLU:OE2	17:N:5:GLU:N	2.52	0.42
6:B:440:ASN:OD1	6:B:452:GLN:NE2	2.52	0.42
3:3:127:ARG:HG2	3:3:131:ASP:OD1	2.18	0.42
8:D:20:LEU:O	8:D:21:ASP:C	2.58	0.42
5:A:173:VAL:HG23	5:A:174:PHE:N	2.34	0.42
19:A:1764:CLA:CGA	19:A:1783:CLA:H11	2.49	0.42
19:A:1779:CLA:HBC1	22:A:1805:BCR:H393	2.02	0.42
5:A:515:TRP:CZ2	19:A:1782:CLA:HMC3	2.54	0.42
5:A:306:ILE:O	5:A:309:LEU:N	2.52	0.42
5:A:29:THR:OG1	5:A:31:PHE:HB2	2.19	0.42
5:A:343:HIS:O	5:A:346:LEU:HB2	2.19	0.42
5:A:388:ASP:O	5:A:390:ALA:N	2.52	0.42
5:A:541:VAL:O	5:A:544:ILE:HG22	2.18	0.42
5:A:588:GLY:N	6:B:668:ARG:CD	2.73	0.42
5:A:591:GLN:HA	5:A:591:GLN:NE2	2.26	0.42
5:A:693:LEU:CD2	5:A:734:GLY:HA3	2.49	0.42
5:A:64:PHE:HZ	5:A:77:LYS:CE	2.32	0.42
19:B:1745:CLA:C4B	22:B:1774:BCR:H291	2.49	0.42
19:B:1751:CLA:HBA2	19:B:1752:CLA:O1A	2.18	0.42
19:B:1757:CLA:H71	19:B:1757:CLA:H41	2.01	0.42
6:B:175:LEU:HD11	19:B:1749:CLA:CMA	2.49	0.42
19:B:1768:CLA:CBB	19:B:1768:CLA:C9	2.54	0.42
19:B:1770:CLA:H191	13:I:21:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:25:ILE:H	6:B:25:ILE:HG13	1.56	0.42
6:B:260:GLY:O	6:B:262:HIS:NE2	2.51	0.42
6:B:262:HIS:HA	6:B:263:PRO:HD2	1.92	0.42
6:B:278:LEU:O	6:B:279:ALA:C	2.58	0.42
6:B:176:ASN:ND2	6:B:292:ARG:O	2.52	0.42
6:B:393:PHE:CZ	6:B:398:TYR:CD2	3.07	0.42
5:A:694:PHE:CZ	6:B:661:PHE:CD1	3.07	0.42
6:B:674:LEU:CD1	6:B:674:LEU:C	2.88	0.42
10:F:96:TRP:HZ3	10:F:134:PHE:CB	2.21	0.42
19:L:1168:CLA:CAA	19:L:1168:CLA:O1D	2.63	0.42
16:L:12:GLN:HA	16:L:13:PRO:HD3	1.82	0.42
19:2:1212:CLA:CMC	19:2:1212:CLA:CBC	2.63	0.42
19:3:1219:CLA:HBD	19:3:1219:CLA:HAA2	2.00	0.42
19:A:1815:CLA:C5	19:A:1815:CLA:HMA1	2.49	0.42
11:G:60:SER:C	11:G:62:ASP:N	2.71	0.42
19:1:1189:CLA:O1A	19:1:1189:CLA:C2	2.66	0.42
21:B:8055:SUC:O4'	21:B:8055:SUC:O5	2.36	0.42
1:1:181:LEU:O	1:1:182:ALA:HB2	2.19	0.42
5:A:179:LEU:HD13	5:A:179:LEU:O	2.19	0.42
22:A:1804:BCR:H15C	22:A:1804:BCR:H351	1.81	0.42
5:A:281:LEU:HB2	5:A:301:HIS:CD2	2.52	0.42
5:A:374:GLN:C	5:A:376:MET:H	2.21	0.42
5:A:570:PRO:C	5:A:572:LYS:N	2.72	0.42
5:A:59:ALA:C	5:A:61:ALA:N	2.72	0.42
5:A:97:TYR:HA	5:A:153:TRP:HZ2	1.85	0.42
6:B:123:TRP:CZ3	19:B:1743:CLA:C19	2.99	0.42
19:B:1764:CLA:ND	19:B:1765:CLA:CBB	2.82	0.42
19:B:1787:CLA:C3A	19:B:1787:CLA:CGA	2.92	0.42
6:B:632:ILE:C	6:B:634:GLY:N	2.72	0.42
6:B:8:PHE:CD2	6:B:34:HIS:ND1	2.87	0.42
11:G:28:ARG:HG2	11:G:29:GLU:CB	2.50	0.42
11:G:5:SER:O	11:G:7:VAL:CG1	2.67	0.42
19:A:1800:CLA:H201	16:L:64:LEU:CG	2.50	0.42
19:2:1217:CLA:H41	19:2:1217:CLA:H72	2.01	0.42
4:4:106:TRP:HE3	19:4:1207:CLA:HMA1	1.84	0.42
19:K:1146:CLA:C3A	19:K:1146:CLA:CGA	2.96	0.42
10:F:22:LEU:HA	10:F:25:LEU:CD1	2.49	0.42
19:A:1815:CLA:H2	19:A:1815:CLA:H61	1.82	0.42
21:B:8060:SUC:H1'2	21:B:8060:SUC:C5	2.47	0.42
3:3:66:MET:HE1	3:3:69:ALA:HB3	2.01	0.42
4:4:193:ILE:CG2	4:4:194:VAL:H	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:25:ASP:CB	1:1:26:PRO:CD	2.97	0.42
5:A:422:TYR:N	5:A:422:TYR:HD1	2.11	0.42
11:G:75:GLY:O	11:G:80:ILE:HG23	2.19	0.42
5:A:536:THR:HA	5:A:539:PHE:HB2	2.01	0.42
8:D:151:LYS:HB3	8:D:151:LYS:NZ	2.33	0.42
5:A:164:LEU:HA	5:A:167:THR:CG2	2.46	0.42
19:A:1759:CLA:H42	19:A:1796:CLA:C8	2.46	0.42
5:A:90:PHE:HB3	5:A:175:ALA:HB2	2.01	0.42
5:A:382:TYR:CD2	19:A:1784:CLA:HED3	2.54	0.42
19:A:1787:CLA:H72	19:A:1801:CLA:CBA	2.50	0.42
19:A:1789:CLA:H41	19:A:1789:CLA:H61	1.64	0.42
5:A:183:TRP:C	5:A:185:HIS:H	2.23	0.42
5:A:729:GLN:O	5:A:732:ALA:HB3	2.19	0.42
6:B:145:LEU:HA	6:B:145:LEU:HD22	1.83	0.42
19:B:1737:CLA:HMC3	19:B:1759:CLA:H3A	2.00	0.42
19:B:1759:CLA:HHD	24:B:1783:LMG:H352	2.01	0.42
24:B:1783:LMG:H112	24:B:1783:LMG:H292	2.00	0.42
6:B:199:ILE:N	6:B:200:PRO:HD2	2.34	0.42
6:B:336:LEU:HD13	19:B:1754:CLA:CBB	2.48	0.42
6:B:269:TRP:CG	6:B:497:TRP:HH2	2.37	0.42
6:B:603:ARG:HB3	6:B:734:GLY:H	1.84	0.42
6:B:542:ARG:HH21	8:D:143:PRO:HG3	1.80	0.42
16:L:62:PHE:HE2	19:L:1168:CLA:H2A	1.84	0.42
16:L:99:LEU:HB3	16:L:140:THR:HG21	2.02	0.42
19:2:1217:CLA:HED2	19:2:1217:CLA:OBD	2.19	0.42
17:N:62:SER:HA	17:N:64:ASP:HB3	2.02	0.42
20:A:7016:LMU:H6'	20:A:7016:LMU:H12	1.84	0.42
20:A:7037:LMU:H12	20:A:7037:LMU:H41	1.45	0.42
20:A:7021:LMU:O6'	20:A:7021:LMU:H22	2.14	0.42
20:R:1056:LMU:H62	20:R:1056:LMU:H32	1.69	0.42
6:B:477:PRO:O	6:B:478:LEU:HD22	2.19	0.42
6:B:470:THR:H	6:B:501:ILE:HG23	1.84	0.42
19:L:1166:CLA:H11	19:L:1166:CLA:C4D	2.49	0.42
1:1:60:PRO:O	1:1:61:GLU:HB3	2.19	0.42
1:1:113:SER:O	1:1:114:MET:HG3	2.20	0.42
6:B:505:SER:O	6:B:506:ASN:HB3	2.19	0.42
6:B:641:ASN:HB3	6:B:642:SER:H	1.72	0.42
15:K:35:THR:HG23	15:K:36:ALA:H	1.84	0.42
22:3:1220:BCR:H11C	22:3:1220:BCR:H341	1.56	0.42
5:A:372:VAL:HG22	19:A:1774:CLA:C4	2.49	0.42
19:A:1774:CLA:HBA2	19:A:1774:CLA:H3A	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1792:CLA:HBA2	19:A:1792:CLA:CBD	2.49	0.42
22:A:1805:BCR:H351	22:A:1805:BCR:H15C	1.84	0.42
22:A:1806:BCR:H351	22:A:1806:BCR:H15C	1.87	0.42
5:A:299:ILE:HA	5:A:299:ILE:HD12	1.69	0.42
5:A:467:MET:HE1	5:A:475:ASP:C	2.40	0.42
5:A:650:ASN:C	5:A:652:TRP:N	2.71	0.42
6:B:16:PRO:HG3	7:C:74:THR:HG22	2.01	0.42
19:B:1739:CLA:HMB3	19:I:1031:CLA:HMA1	2.00	0.42
6:B:354:SER:OG	19:B:1756:CLA:HBC3	2.19	0.42
19:B:1738:CLA:H192	19:B:1757:CLA:H141	2.02	0.42
19:B:1765:CLA:CBB	22:B:1777:BCR:C28	2.98	0.42
6:B:649:MET:CG	22:B:1780:BCR:H272	2.49	0.42
6:B:274:ALA:HA	6:B:277:HIS:HB2	2.00	0.42
6:B:494:LEU:HD12	19:B:1765:CLA:CED	2.48	0.42
6:B:561:GLY:H	7:C:66:ARG:HB3	1.85	0.42
8:D:41:GLN:NE2	8:D:42:VAL:HA	2.34	0.42
9:E:87:VAL:C	9:E:89:GLU:N	2.67	0.42
16:L:149:SER:C	16:L:151:VAL:N	2.72	0.42
16:L:65:VAL:O	16:L:69:VAL:N	2.53	0.42
18:R:38:UNK:C	18:R:42:UNK:CA	2.97	0.42
3:3:182:LYS:O	3:3:186:ASN:N	2.33	0.42
21:B:8062:SUC:HO6	21:B:8062:SUC:C2'	2.31	0.42
7:C:27:GLU:OE1	7:C:40:ALA:HB3	2.19	0.42
20:2:7006:LMU:H3'	20:2:7006:LMU:C6B	2.50	0.42
20:A:1810:LMU:H12	20:A:1810:LMU:H41	1.71	0.42
12:H:36:GLN:O	12:H:36:GLN:CG	2.68	0.42
6:B:242:HIS:CE1	6:B:244:PHE:HA	2.55	0.42
4:4:70:ILE:HG13	4:4:71:ASN:N	2.35	0.42
16:L:135:GLY:HA2	16:L:138:LYS:HE2	2.02	0.42
6:B:684:ARG:HA	6:B:684:ARG:HD3	1.74	0.42
6:B:543:GLY:HA3	6:B:548:PRO:O	2.20	0.42
5:A:419:VAL:HG21	5:A:577:PHE:HB2	2.01	0.42
5:A:150:PHE:O	5:A:151:GLN:HG3	2.20	0.42
19:A:1763:CLA:HMB2	22:A:1808:BCR:H342	2.01	0.42
19:A:1777:CLA:H3A	19:A:1777:CLA:HBA2	1.63	0.42
19:A:1778:CLA:HED2	19:A:1778:CLA:CBA	2.49	0.42
19:A:1788:CLA:H192	19:B:1770:CLA:HMB2	2.01	0.42
19:A:1800:CLA:CHA	19:A:1800:CLA:CGA	2.98	0.42
5:A:408:VAL:O	5:A:411:ALA:HB3	2.20	0.42
5:A:579:PHE:HA	5:A:580:PRO:HD2	1.66	0.42
5:A:648:THR:C	5:A:650:ASN:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:79:PHE:CE2	5:A:185:HIS:CG	2.93	0.42
5:A:82:HIS:CE1	19:A:1761:CLA:C1A	3.02	0.42
8:D:49:THR:C	8:D:50:TRP:HD1	2.23	0.42
9:E:36:VAL:CG2	9:E:52:VAL:CG2	2.97	0.42
10:F:126:ALA:HB1	10:F:129:LEU:HD12	2.02	0.42
10:F:78:ARG:O	10:F:80:TRP:CD1	2.69	0.42
11:G:32:ALA:O	11:G:34:GLN:C	2.57	0.42
16:L:98:CYS:SG	22:L:1169:BCR:C12	3.08	0.42
19:1:1200:CLA:H3A	19:1:1200:CLA:HBA1	1.42	0.42
10:F:44:ALA:O	10:F:46:MET:HG2	2.20	0.42
6:B:454:LEU:HD13	10:F:69:PRO:O	2.15	0.42
5:A:132:LEU:HD23	6:B:446:PHE:HE1	1.85	0.42
5:A:163:GLN:HA	5:A:166:CYS:SG	2.60	0.42
19:A:1777:CLA:H52	19:A:1777:CLA:C1C	2.50	0.42
5:A:210:LEU:N	5:A:213:LEU:N	2.68	0.42
5:A:244:LEU:H	5:A:244:LEU:HD12	1.85	0.42
5:A:315:HIS:HB2	19:A:1778:CLA:HBC1	2.02	0.42
5:A:500:PRO:HA	5:A:504:ALA:HB1	2.01	0.42
5:A:575:LEU:HD13	5:A:576:GLY:H	1.85	0.42
19:B:1743:CLA:HHD	19:B:1743:CLA:HAC2	1.84	0.42
6:B:587:ILE:CG2	6:B:587:ILE:O	2.67	0.42
6:B:661:PHE:O	6:B:662:MET:O	2.37	0.42
11:G:45:GLU:C	11:G:49:THR:CG2	2.62	0.42
11:G:50:ARG:HB2	11:G:51:ALA:CA	2.50	0.42
16:L:149:SER:C	16:L:151:VAL:H	2.23	0.42
20:A:7041:LMU:H4B	20:A:7041:LMU:H1B	1.52	0.42
20:2:7003:LMU:O2'	20:2:7003:LMU:H22	2.20	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:HZ3	1.84	0.42
20:K:1086:LMU:H52	19:K:1146:CLA:HMD2	2.02	0.42
8:D:133:ASN:C	8:D:134:MET:SD	2.94	0.42
11:G:20:ARG:NH2	11:G:61:ASN:C	2.73	0.42
9:E:69:PHE:CD2	9:E:71:LYS:N	2.82	0.42
20:2:7006:LMU:C2	20:2:7006:LMU:H2'	2.48	0.42
6:B:216:LEU:HD22	6:B:218:TYR:H	1.85	0.42
4:4:60:LEU:HG	4:4:61:PRO:HD3	2.02	0.42
12:H:50:ARG:NH1	12:H:53:LEU:C	2.63	0.42
15:K:24:PHE:CB	15:K:52:PRO:HG2	2.43	0.42
3:3:106:TYR:CB	3:3:107:TRP:HD1	2.32	0.42
5:A:163:GLN:CG	5:A:164:LEU:N	2.82	0.42
5:A:90:PHE:CD1	19:A:1761:CLA:H91	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:204:ASN:HA	5:A:314:GLY:O	2.20	0.42
5:A:452:PHE:HE1	19:A:1793:CLA:CAB	2.27	0.42
5:A:621:GLN:HG2	5:A:637:ILE:CD1	2.39	0.42
5:A:664:VAL:HG11	5:A:749:PHE:HA	2.01	0.42
5:A:98:PHE:C	5:A:98:PHE:CD1	2.93	0.42
6:B:175:LEU:HD11	19:B:1749:CLA:HMA1	2.02	0.42
19:B:1753:CLA:H43	19:B:1753:CLA:C2A	2.41	0.42
6:B:269:TRP:HA	6:B:269:TRP:CE3	2.55	0.42
6:B:373:THR:C	6:B:376:GLN:H	2.23	0.42
6:B:588:GLY:O	6:B:592:PHE:CB	2.51	0.42
8:D:100:PHE:O	8:D:113:HIS:HB2	2.20	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
20:A:7037:LMU:H3O2	20:A:7037:LMU:C6'	2.20	0.42
3:3:52:LYS:O	3:3:56:TYR:CB	2.68	0.42
20:R:1057:LMU:H3'	20:R:1057:LMU:H1B	1.31	0.42
19:4:1209:CLA:O1D	19:4:1209:CLA:C3D	2.57	0.42
5:A:277:TYR:CD2	5:A:278:ALA:N	2.88	0.42
14:J:38:THR:O	14:J:39:PHE:CB	2.68	0.42
21:B:8055:SUC:O1'	21:B:8055:SUC:O3'	2.30	0.42
6:B:503:GLU:CA	6:B:507:SER:HB2	2.50	0.42
3:3:207:GLY:O	3:3:208:PRO:C	2.58	0.42
4:4:52:MET:C	4:4:54:GLY:H	2.23	0.42
19:A:1777:CLA:O2D	19:A:1777:CLA:OBD	2.38	0.42
3:3:83:LEU:C	19:A:1798:CLA:C4	2.88	0.42
23:A:1802:PQN:H251	19:B:1735:CLA:HMC1	2.01	0.42
5:A:210:LEU:HD23	5:A:211:LEU:N	2.35	0.42
5:A:302:HIS:HE2	19:A:1774:CLA:HMB3	1.84	0.42
5:A:368:LEU:HD12	19:A:1782:CLA:H62	2.01	0.42
5:A:372:VAL:HG22	19:A:1774:CLA:H41	2.01	0.42
5:A:51:THR:OG1	19:A:1795:CLA:CAB	2.68	0.42
5:A:672:LEU:CD2	5:A:672:LEU:H	2.33	0.42
19:B:1758:CLA:C19	22:B:1776:BCR:H14C	2.50	0.42
19:B:1756:CLA:H201	19:B:1769:CLA:C2	2.50	0.42
6:B:721:TYR:N	19:B:1785:CLA:O1D	2.53	0.42
6:B:199:ILE:HG22	6:B:203:ARG:CZ	2.50	0.42
6:B:310:PRO:CG	6:B:311:PRO:CD	2.87	0.42
6:B:350:GLN:HG3	6:B:372:TYR:HE1	1.84	0.42
6:B:593:TYR:CD1	19:B:1767:CLA:HMC2	2.55	0.42
6:B:693:TRP:CD1	19:B:1770:CLA:CMD	3.03	0.42
7:C:5:VAL:HG23	7:C:65:VAL:HG21	1.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:43:HIS:C	11:G:45:GLU:CA	2.88	0.42
16:L:64:LEU:CA	16:L:67:PRO:HG2	2.46	0.42
21:B:8054:SUC:H1'1	21:B:8054:SUC:HO2	1.80	0.42
3:3:94:ARG:CA	3:3:97:PHE:HE1	2.33	0.42
17:N:72:LYS:HB3	17:N:74:LYS:HB2	1.98	0.42
14:J:31:ARG:HH21	19:J:1043:CLA:C3B	2.32	0.42
10:F:44:ALA:O	10:F:46:MET:N	2.52	0.42
20:A:7026:LMU:O3B	21:B:8062:SUC:C6'	2.58	0.42
17:N:29:PHE:O	17:N:33:TYR:N	2.53	0.42
4:4:193:ILE:CG2	14:J:42:PHE:CD1	2.87	0.42
2:2:103:GLY:HA2	19:2:1222:CLA:CAB	2.49	0.42
2:2:70:LYS:O	2:2:73:ILE:N	2.52	0.42
6:B:541:ALA:HB2	6:B:572:ALA:CB	2.50	0.42
2:2:197:LEU:HD21	5:A:162:LEU:CD2	2.45	0.41
3:3:114:PHE:HD1	19:3:1216:CLA:CHA	2.31	0.41
19:A:1761:CLA:C4B	19:A:1785:CLA:HMB2	2.50	0.41
19:A:1781:CLA:HAA1	19:A:1781:CLA:CED	2.50	0.41
5:A:183:TRP:C	5:A:185:HIS:N	2.74	0.41
5:A:207:LEU:HD11	5:A:313:ALA:CB	2.50	0.41
5:A:159:THR:OG1	5:A:239:PRO:HB3	2.20	0.41
5:A:302:HIS:NE2	19:A:1774:CLA:HMB3	2.34	0.41
5:A:345:GLY:C	5:A:347:TYR:N	2.66	0.41
5:A:538:ASP:O	5:A:542:HIS:CD2	2.73	0.41
5:A:681:GLY:O	5:A:682:ALA:HB3	2.19	0.41
5:A:87:SER:HA	5:A:90:PHE:HB2	2.02	0.41
5:A:92:TRP:C	5:A:94:SER:H	2.22	0.41
6:B:120:VAL:O	6:B:123:TRP:HD1	2.02	0.41
19:B:1749:CLA:HBB2	19:B:1754:CLA:C4	2.48	0.41
19:B:1753:CLA:H141	19:B:1753:CLA:H161	1.65	0.41
6:B:518:LEU:O	6:B:519:VAL:C	2.59	0.41
9:E:36:VAL:CG1	9:E:87:VAL:HG11	2.49	0.41
19:A:1795:CLA:H43	10:F:121:ILE:HD13	2.01	0.41
10:F:147:GLY:O	10:F:149:LEU:O	2.38	0.41
11:G:46:ALA:C	11:G:48:ASP:CB	2.82	0.41
14:J:2:ARG:HB3	14:J:7:TYR:CE1	2.55	0.41
6:B:691:ILE:HA	16:L:102:TYR:OH	2.20	0.41
19:3:1218:CLA:CAA	19:3:1218:CLA:CBD	2.98	0.41
19:A:1816:CLA:CGD	19:A:1816:CLA:C2A	2.88	0.41
2:2:163:GLU:O	2:2:167:GLY:N	2.52	0.41
5:A:254:LEU:HD13	5:A:254:LEU:HA	1.66	0.41
4:4:127:PRO:C	4:4:143:PHE:HZ	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:93:TYR:CB	11:G:94:ASP:HB2	2.43	0.41
19:3:3011:CLA:H112	19:3:3011:CLA:H71	1.55	0.41
19:3:3011:CLA:H11	19:3:3011:CLA:HBA2	1.91	0.41
11:G:83:TYR:O	11:G:83:TYR:CD1	2.72	0.41
3:3:111:TYR:HB2	3:3:112:THR:CG2	2.51	0.41
3:3:88:THR:H	22:3:1220:BCR:H383	1.79	0.41
3:3:84:ILE:H	19:A:1798:CLA:C5	2.30	0.41
19:A:1767:CLA:H111	19:A:1767:CLA:H72	1.50	0.41
19:A:1774:CLA:H2	19:A:1774:CLA:HMB2	2.02	0.41
5:A:21:LEU:HD13	5:A:21:LEU:O	2.16	0.41
5:A:599:PHE:CD1	5:A:600:LEU:HD23	2.36	0.41
5:A:620:MET:HG3	5:A:625:TRP:CD2	2.54	0.41
5:A:662:SER:HA	5:A:665:ILE:CD1	2.50	0.41
22:B:1780:BCR:H353	19:B:1787:CLA:H122	2.02	0.41
6:B:292:ARG:NE	6:B:292:ARG:CA	2.65	0.41
6:B:392:ILE:CD1	19:B:1759:CLA:O2D	2.68	0.41
6:B:429:LEU:HD11	19:B:1768:CLA:CMB	2.50	0.41
5:A:677:LEU:HD11	6:B:442:VAL:HG13	2.01	0.41
5:A:690:LEU:HD22	6:B:661:PHE:HE1	1.84	0.41
6:B:75:GLU:HB2	6:B:132:ASN:CB	2.42	0.41
8:D:48:ILE:HA	8:D:100:PHE:HB3	2.01	0.41
11:G:28:ARG:HG3	11:G:29:GLU:CB	2.50	0.41
20:A:7042:LMU:H11	20:A:7042:LMU:H71	2.00	0.41
17:N:57:LYS:O	17:N:60:PHE:HD1	2.00	0.41
20:A:7033:LMU:C2'	20:A:7033:LMU:O6B	2.68	0.41
5:A:67:HIS:O	5:A:68:THR:HB	2.21	0.41
11:G:79:HIS:CG	11:G:79:HIS:O	2.72	0.41
5:A:35:ALA:O	5:A:36:LYS:HB2	2.20	0.41
8:D:53:PRO:HB2	8:D:54:LYS:H	1.63	0.41
5:A:177:LEU:HA	5:A:177:LEU:HD22	1.90	0.41
5:A:733:VAL:HG13	19:A:1796:CLA:C3D	2.50	0.41
5:A:207:LEU:CB	19:A:1776:CLA:CBB	2.86	0.41
5:A:75:SER:HB3	5:A:354:TRP:HZ2	1.83	0.41
5:A:499:ALA:HB3	19:A:1790:CLA:CED	2.50	0.41
5:A:547:PHE:CD1	5:A:547:PHE:C	2.90	0.41
19:B:1737:CLA:HBA1	19:B:1743:CLA:HBA1	2.02	0.41
19:B:1737:CLA:H162	19:B:1743:CLA:OBD	2.20	0.41
19:B:1760:CLA:HBA2	19:B:1760:CLA:H3A	1.49	0.41
19:B:1768:CLA:H203	19:B:1768:CLA:H161	1.91	0.41
6:B:378:ILE:H	6:B:381:PHE:HD1	1.69	0.41
6:B:534:LEU:CD2	6:B:579:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:625:TRP:C	6:B:625:TRP:CD2	2.92	0.41
6:B:658:ALA:O	6:B:661:PHE:CD2	2.69	0.41
6:B:707:LEU:HD23	24:B:1783:LMG:H132	2.02	0.41
16:L:68:PHE:CD1	16:L:68:PHE:N	2.89	0.41
19:2:1220:CLA:C4	3:3:140:LYS:HE2	2.46	0.41
17:N:45:ASN:HA	17:N:57:LYS:HZ2	1.84	0.41
17:N:72:LYS:CD	17:N:74:LYS:HG3	2.43	0.41
4:4:104:ARG:HB2	4:4:107:GLN:HE21	1.85	0.41
20:A:7032:LMU:H31	20:A:7032:LMU:H4B	2.03	0.41
20:1:7004:LMU:O3'	20:1:7004:LMU:C1B	2.68	0.41
3:3:153:SER:C	3:3:161:GLY:HA2	2.41	0.41
1:1:38:ARG:O	1:1:41:GLU:HB2	2.21	0.41
5:A:113:PRO:C	5:A:115:HIS:N	2.71	0.41
5:A:705:GLU:OE1	5:A:708:VAL:HG12	2.20	0.41
6:B:190:TRP:CE3	19:B:1744:CLA:HBB2	2.51	0.41
6:B:340:SER:CA	19:B:1756:CLA:H51	2.29	0.41
19:B:1764:CLA:HMD2	19:B:1765:CLA:CMC	2.50	0.41
6:B:707:LEU:O	6:B:710:LEU:CB	2.68	0.41
22:B:1779:BCR:C5	19:F:1156:CLA:HMA1	2.50	0.41
11:G:24:PHE:HB3	11:G:28:ARG:HH11	1.86	0.41
16:L:33:ILE:O	16:L:35:TRP:N	2.53	0.41
19:3:1215:CLA:C3B	19:3:1218:CLA:H11	2.50	0.41
19:2:1213:CLA:C4	19:2:1213:CLA:CHD	2.98	0.41
19:2:1213:CLA:HBA2	19:2:1213:CLA:H3A	1.80	0.41
20:2:7003:LMU:H3B	21:B:8054:SUC:O4'	2.20	0.41
17:N:72:LYS:CB	17:N:74:LYS:H	2.22	0.41
4:4:107:GLN:O	19:4:1196:CLA:HMA1	2.20	0.41
19:J:1045:CLA:H61	19:J:1045:CLA:H93	1.63	0.41
20:A:7039:LMU:H61	20:A:7039:LMU:H92	1.71	0.41
4:4:193:ILE:CG2	4:4:194:VAL:N	2.83	0.41
5:A:536:THR:O	5:A:537:ALA:HB3	2.20	0.41
6:B:32:GLU:N	6:B:42:LEU:HD13	2.36	0.41
1:1:51:MET:SD	1:1:54:VAL:HB	2.61	0.41
1:1:34:ALA:O	1:1:35:ASN:C	2.59	0.41
5:A:561:LEU:HA	5:A:561:LEU:HD23	1.76	0.41
5:A:667:SER:O	5:A:667:SER:OG	2.38	0.41
17:N:9:LYS:HB3	17:N:9:LYS:HE2	1.86	0.41
4:4:160:MET:HG2	19:4:1201:CLA:HBB2	2.02	0.41
5:A:156:SER:HB2	5:A:159:THR:H	1.86	0.41
19:A:1759:CLA:HBB2	19:A:1760:CLA:C1C	2.50	0.41
19:A:1776:CLA:HMB2	19:A:1780:CLA:HMA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1813:CLA:H162	19:A:1813:CLA:H203	1.79	0.41
5:A:405:PHE:O	19:A:1785:CLA:HMC1	2.20	0.41
5:A:553:VAL:O	5:A:557:LEU:CB	2.68	0.41
5:A:749:PHE:CG	19:A:1811:CLA:HMD1	2.55	0.41
5:A:88:ILE:O	5:A:92:TRP:N	2.44	0.41
6:B:174:ARG:HH12	19:B:1754:CLA:HMD2	1.85	0.41
6:B:393:PHE:CZ	6:B:398:TYR:HD2	2.37	0.41
6:B:416:GLU:N	6:B:416:GLU:CD	2.74	0.41
6:B:448:THR:OG1	6:B:451:LYS:HB2	2.20	0.41
5:A:697:ARG:CD	6:B:566:GLY:O	2.67	0.41
7:C:55:GLU:HG3	7:C:60:THR:HG22	2.02	0.41
10:F:104:TYR:OH	10:F:122:ASP:N	2.34	0.41
13:I:8:PHE:CD1	19:I:1031:CLA:H12	2.54	0.41
16:L:10:VAL:HG13	16:L:12:GLN:HE22	1.86	0.41
16:L:127:PRO:C	16:L:128:ASP:O	2.59	0.41
16:L:90:GLY:O	16:L:94:ILE:N	2.49	0.41
20:A:7016:LMU:H1'	20:A:7016:LMU:H6D	1.43	0.41
4:4:150:LYS:H	4:4:150:LYS:CE	2.33	0.41
19:K:1146:CLA:HMA2	19:K:1146:CLA:H43	2.01	0.41
10:F:23:LYS:HA	10:F:23:LYS:HD2	1.60	0.41
3:3:158:TYR:C	3:3:160:GLY:N	2.70	0.41
17:N:32:ALA:CB	17:N:35:VAL:HA	2.50	0.41
5:A:277:TYR:HD2	5:A:278:ALA:N	2.19	0.41
17:N:6:TYR:H	17:N:8:GLU:HA	1.85	0.41
6:B:332:PHE:CE1	6:B:408:LEU:HD21	2.55	0.41
7:C:42:ALA:O	8:D:129:GLY:HA3	2.21	0.41
10:F:65:SER:C	10:F:67:GLY:H	2.23	0.41
19:A:1764:CLA:H3A	19:A:1764:CLA:HBA2	1.39	0.41
19:A:1781:CLA:C5	19:A:1782:CLA:CED	2.86	0.41
22:A:1807:BCR:C23	22:A:1807:BCR:C39	2.74	0.41
5:A:358:LEU:HD11	5:A:413:HIS:CD2	2.53	0.41
5:A:378:SER:OG	19:A:1782:CLA:CBC	2.69	0.41
5:A:509:ALA:O	5:A:510:SER:CB	2.68	0.41
5:A:412:ALA:CB	5:A:598:VAL:HG11	2.33	0.41
5:A:74:ILE:O	5:A:78:VAL:HG13	2.20	0.41
6:B:174:ARG:C	6:B:176:ASN:H	2.24	0.41
23:B:1773:PQN:H161	23:B:1773:PQN:H141	1.42	0.41
6:B:334:LEU:HB2	19:B:1737:CLA:CMD	2.46	0.41
6:B:377:TYR:OH	6:B:717:TYR:HE1	2.04	0.41
7:C:74:THR:HB	7:C:80:ALA:HB2	1.97	0.41
8:D:102:ARG:CZ	8:D:110:GLN:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:100:VAL:C	10:F:103:SER:HG	2.23	0.41
16:L:127:PRO:O	16:L:128:ASP:C	2.59	0.41
16:L:33:ILE:HG13	16:L:37:LEU:HD21	2.03	0.41
16:L:68:PHE:HD1	16:L:68:PHE:H	1.68	0.41
19:2:1212:CLA:CGA	19:2:1212:CLA:C4A	2.99	0.41
17:N:69:CYS:O	17:N:72:LYS:HE3	2.20	0.41
19:3:1219:CLA:H61	19:3:1219:CLA:H41	1.54	0.41
18:R:27:UNK:C	18:R:29:UNK:C	2.98	0.41
20:A:7038:LMU:H62	20:A:7038:LMU:H91	1.93	0.41
12:H:54:LEU:O	12:H:54:LEU:HD22	2.21	0.41
2:2:187:GLY:O	2:2:189:ILE:HG12	2.20	0.41
5:A:523:VAL:HG13	5:A:524:GLY:N	2.36	0.41
20:A:1810:LMU:H1'	20:A:1810:LMU:H21	1.60	0.41
16:L:159:TYR:O	16:L:159:TYR:CG	2.74	0.41
15:K:59:ASP:HA	15:K:62:ALA:HB3	2.01	0.41
5:A:126:ILE:HG13	5:A:126:ILE:H	1.59	0.41
19:A:1761:CLA:H41	22:A:1804:BCR:C31	2.51	0.41
5:A:225:VAL:C	5:A:228:PRO:HD2	2.41	0.41
5:A:436:LEU:O	5:A:438:HIS:O	2.37	0.41
5:A:452:PHE:HB2	19:A:1788:CLA:OBD	2.21	0.41
5:A:396:PHE:CE2	5:A:616:PHE:CB	2.94	0.41
19:B:1764:CLA:ND	19:B:1765:CLA:HBB2	2.35	0.41
19:B:1743:CLA:H11	22:B:1775:BCR:C10	2.51	0.41
22:B:1781:BCR:H342	22:B:1781:BCR:HC7	1.63	0.41
6:B:307:ALA:O	6:B:308:HIS:O	2.38	0.41
6:B:534:LEU:HD21	6:B:579:ALA:HB2	2.01	0.41
6:B:707:LEU:HG	6:B:708:VAL:N	2.36	0.41
6:B:70:TRP:H	6:B:70:TRP:HD1	1.67	0.41
7:C:60:THR:HG21	7:C:63:LEU:O	2.18	0.41
7:C:69:LEU:O	7:C:71:HIS:N	2.53	0.41
8:D:112:LEU:N	8:D:114:PRO:HG2	2.36	0.41
16:L:123:ARG:C	16:L:124:LYS:HD3	2.41	0.41
16:L:46:ALA:N	16:L:52:ARG:HH12	2.18	0.41
3:3:205:GLY:CA	5:A:252:ARG:NH1	2.79	0.41
17:N:57:LYS:CG	17:N:58:VAL:N	2.26	0.41
19:J:1044:CLA:HED2	19:J:1045:CLA:C2	2.41	0.41
6:B:475:ASP:CB	6:B:480:SER:HA	2.51	0.41
19:4:1204:CLA:HBC2	19:4:1204:CLA:CHD	2.51	0.41
6:B:112:PRO:O	6:B:113:VAL:HG13	2.21	0.41
3:3:112:THR:HG1	3:3:113:LEU:H	1.60	0.41
2:2:211:LYS:HG2	3:3:113:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:112:ASP:N	5:A:113:PRO:HD3	2.36	0.41
5:A:132:LEU:HD21	5:A:674:ALA:HB2	2.03	0.41
19:A:1774:CLA:H152	19:A:1774:CLA:H8	2.02	0.41
19:A:1776:CLA:H112	19:A:1776:CLA:H91	1.83	0.41
5:A:462:ILE:CG2	19:A:1789:CLA:CMC	2.99	0.41
19:A:1795:CLA:C2	19:A:1795:CLA:O1A	2.68	0.41
19:A:1800:CLA:H152	22:L:1170:BCR:C35	2.47	0.41
19:A:1784:CLA:C4C	22:A:1804:BCR:H333	2.50	0.41
5:A:583:GLY:O	5:A:589:THR:HB	2.21	0.41
5:A:690:LEU:O	5:A:694:PHE:N	2.42	0.41
5:A:705:GLU:HG2	6:B:545:LYS:NZ	2.36	0.41
6:B:22:TRP:HA	6:B:25:ILE:CD1	2.51	0.41
6:B:180:SER:OG	6:B:285:LEU:HA	2.20	0.41
6:B:301:ILE:O	6:B:301:ILE:HG23	2.21	0.41
6:B:336:LEU:CD1	19:B:1754:CLA:CBB	2.99	0.41
6:B:387:PHE:CB	6:B:534:LEU:HD13	2.50	0.41
6:B:447:GLY:C	6:B:449:PRO:HD3	2.40	0.41
6:B:527:LEU:O	19:B:1769:CLA:HMA3	2.20	0.41
6:B:568:CYS:HB3	6:B:569:ASP:H	1.67	0.41
5:A:558:LYS:HZ1	6:B:674:LEU:HB3	1.81	0.41
6:B:710:LEU:HA	6:B:710:LEU:HD22	1.94	0.41
7:C:51:CYS:HB2	7:C:53:ARG:H	1.85	0.41
6:B:11:GLY:CA	7:C:71:HIS:CD2	2.94	0.41
8:D:111:TYR:CD2	8:D:114:PRO:CG	3.04	0.41
11:G:18:LEU:HD23	11:G:18:LEU:N	2.36	0.41
16:L:15:ASN:N	16:L:24:GLU:OE1	2.54	0.41
16:L:14:LEU:HD21	16:L:21:GLY:O	2.20	0.41
3:3:47:GLY:O	3:3:48:PHE:CD2	2.74	0.41
3:3:49:ILE:CA	3:3:51:PRO:HD2	2.51	0.41
20:A:7043:LMU:H6'2	20:A:7043:LMU:O3B	2.21	0.41
4:4:34:PRO:HB2	4:4:137:ILE:HA	2.02	0.41
20:A:7026:LMU:C4	20:A:7026:LMU:H81	2.40	0.41
3:3:158:TYR:CB	3:3:159:PRO:CD	2.82	0.41
20:R:1056:LMU:H6D	20:R:1056:LMU:C5B	2.50	0.41
5:A:349:ILE:CD1	5:A:422:TYR:HB3	2.51	0.41
13:I:1:MET:O	13:I:2:ILE:CG2	2.59	0.41
12:H:55:LYS:O	12:H:56:PHE:HB2	2.21	0.41
17:N:11:LYS:HE2	17:N:11:LYS:HB3	1.85	0.41
3:3:120:LEU:O	3:3:123:PHE:HB3	2.21	0.41
5:A:34:TRP:O	5:A:35:ALA:HB3	2.21	0.41
4:4:114:SER:O	4:4:116:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:52:MET:HE3	4:4:156:ASN:HB3	2.03	0.41
5:A:124:TRP:HE3	5:A:124:TRP:HA	1.84	0.41
19:A:1764:CLA:H112	19:A:1783:CLA:H91	2.01	0.41
22:A:1807:BCR:H24C	22:A:1807:BCR:H371	1.79	0.41
5:A:541:VAL:HA	5:A:544:ILE:HG22	2.03	0.41
5:A:714:LEU:CD1	19:B:1735:CLA:HMA1	2.51	0.41
5:A:747:TRP:CE3	22:A:1807:BCR:H402	2.53	0.41
19:B:1752:CLA:HBB1	19:B:1752:CLA:H72	1.99	0.41
19:B:1768:CLA:H62	19:B:1768:CLA:H101	1.98	0.41
6:B:289:LEU:CD2	22:B:1774:BCR:H352	2.49	0.41
6:B:290:MET:HG3	19:B:1751:CLA:CMC	2.50	0.41
6:B:309:ILE:CD1	6:B:312:GLY:HA3	2.51	0.41
6:B:366:THR:C	6:B:368:GLN:N	2.74	0.41
6:B:393:PHE:CE2	6:B:398:TYR:HD2	2.38	0.41
6:B:325:THR:HG21	6:B:403:ASN:HD21	1.86	0.41
6:B:416:GLU:O	6:B:420:SER:OG	2.39	0.41
6:B:693:TRP:HE1	19:B:1770:CLA:HHD	1.86	0.41
6:B:603:ARG:HB2	6:B:732:LYS:HD3	2.03	0.41
13:I:20:ALA:O	13:I:24:LEU:N	2.54	0.41
5:A:131:ILE:HD13	6:B:446:PHE:O	2.21	0.41
5:A:158:ILE:HA	5:A:243:PRO:O	2.20	0.41
19:A:1781:CLA:H202	19:A:1781:CLA:H161	1.85	0.41
19:A:1781:CLA:HBB2	19:A:1794:CLA:CMA	2.50	0.41
5:A:379:MET:CE	19:A:1782:CLA:HMC2	2.51	0.41
6:B:138:GLY:O	6:B:139:ALA:C	2.59	0.41
19:B:1736:CLA:HMC3	19:B:1738:CLA:OBD	2.21	0.41
19:B:1768:CLA:HBC1	10:F:83:PHE:CE1	2.49	0.41
19:B:1742:CLA:HMC2	22:B:1775:BCR:H373	2.00	0.41
6:B:185:VAL:HG22	22:B:1775:BCR:H272	2.03	0.41
6:B:126:THR:HG21	6:B:358:TYR:HD1	1.86	0.41
7:C:3:HIS:ND1	7:C:69:LEU:HD12	2.36	0.41
9:E:37:LYS:HD2	9:E:47:LYS:HE3	2.03	0.41
17:N:45:ASN:ND2	17:N:54:LYS:CD	2.73	0.41
17:N:53:ALA:C	17:N:54:LYS:HD2	2.41	0.41
17:N:45:ASN:CG	17:N:57:LYS:HZ1	2.17	0.41
17:N:57:LYS:O	17:N:58:VAL:C	2.58	0.41
17:N:72:LYS:CA	17:N:73:ASP:C	2.89	0.41
19:J:1043:CLA:CHA	19:J:1043:CLA:HED2	2.45	0.41
1:1:143:LEU:HB2	1:1:144:LYS:HZ3	1.85	0.41
3:3:56:TYR:CD1	3:3:185:LYS:NZ	2.84	0.41
10:F:39:ALA:O	10:F:42:ILE:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:112:PRO:O	16:L:113:SER:CB	2.68	0.41
2:2:181:HIS:CE1	19:2:1214:CLA:C4D	3.04	0.41
11:G:80:ILE:O	11:G:81:VAL:C	2.59	0.41
8:D:70:GLU:OE1	8:D:71:GLY:O	2.39	0.41
6:B:213:LEU:HD12	6:B:214:ASP:H	1.85	0.41
5:A:527:VAL:HG12	5:A:528:ALA:O	2.21	0.41
5:A:338:PHE:C	5:A:338:PHE:CD2	2.94	0.41
1:1:74:TRP:CH2	1:1:81:GLN:HA	2.56	0.41
3:3:84:ILE:N	3:3:85:PRO:HD3	2.36	0.41
5:A:77:LYS:NZ	19:A:1760:CLA:CED	2.84	0.41
19:A:1764:CLA:HBC3	19:A:1764:CLA:CHD	2.50	0.41
19:A:1789:CLA:HBC2	19:H:1079:CLA:HBC1	2.03	0.41
19:A:1795:CLA:HBA1	19:A:1795:CLA:H3A	1.68	0.41
19:A:1796:CLA:HAC1	23:A:1802:PQN:H152	2.03	0.41
22:A:1805:BCR:C32	22:A:1805:BCR:C8	2.98	0.41
5:A:242:ILE:CG1	5:A:243:PRO:HD3	2.44	0.41
5:A:344:LYS:HE2	5:A:344:LYS:HB3	1.90	0.41
5:A:57:LEU:O	5:A:61:ALA:HB2	2.21	0.41
5:A:586:ARG:H	7:C:49:VAL:HG22	1.86	0.41
5:A:607:ASN:HD22	5:A:607:ASN:HA	1.68	0.41
5:A:663:GLN:OE1	5:A:753:ARG:CZ	2.69	0.41
6:B:122:GLN:HB2	6:B:358:TYR:HB3	2.01	0.41
6:B:58:PHE:HE2	6:B:145:LEU:HD12	1.86	0.41
19:B:1755:CLA:HBA2	19:B:1755:CLA:H3A	1.40	0.41
23:B:1773:PQN:H192	22:B:1780:BCR:C9	2.47	0.41
6:B:266:GLN:NE2	6:B:363:GLN:HG2	2.35	0.41
6:B:54:LEU:HD11	19:B:1743:CLA:CBA	2.51	0.41
6:B:557:PHE:HE2	7:C:66:ARG:NE	2.16	0.41
6:B:556:SER:CA	6:B:558:PRO:CD	2.99	0.41
7:C:62:PHE:CZ	9:E:42:GLU:CB	3.04	0.41
10:F:96:TRP:HE3	10:F:134:PHE:N	2.16	0.41
10:F:144:LEU:CD1	10:F:149:LEU:HD13	2.51	0.41
19:B:1736:CLA:C4C	22:I:1032:BCR:H401	2.51	0.41
16:L:104:ILE:HD12	16:L:104:ILE:C	2.42	0.41
19:1:1191:CLA:CMC	19:1:1194:CLA:CHD	2.70	0.41
19:3:1218:CLA:H2	19:3:1218:CLA:O1A	2.21	0.41
20:A:7020:LMU:H62	20:A:7020:LMU:H92	1.25	0.41
3:3:189:LEU:C	3:3:191:MET:N	2.74	0.41
3:3:50:GLU:HG3	3:3:51:PRO:N	2.35	0.41
11:G:17:PHE:N	11:G:17:PHE:CD2	2.88	0.41
11:G:20:ARG:NH2	11:G:61:ASN:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:47:GLU:N	10:F:50:LYS:HB2	2.36	0.41
19:R:1055:CLA:C11	20:R:1056:LMU:O4'	2.67	0.41
10:F:151:ASP:OD2	10:F:154:PHE:CG	2.73	0.41
5:A:277:TYR:HD2	5:A:279:ASP:H	1.68	0.41
8:D:93:LYS:HB3	8:D:93:LYS:HZ2	1.80	0.41
5:A:630:ASP:C	5:A:632:GLY:H	2.22	0.41
10:F:17:ARG:CA	10:F:17:ARG:NE	2.83	0.41
6:B:52:GLY:O	6:B:56:ILE:HG12	2.21	0.41
20:B:1782:LMU:H3'	20:B:1782:LMU:H1B	1.49	0.41
19:4:1201:CLA:CGD	19:4:1201:CLA:C2A	2.97	0.40
19:A:1766:CLA:HBB1	19:A:1769:CLA:NA	2.36	0.40
19:A:1793:CLA:H18	19:A:1793:CLA:H151	1.76	0.40
5:A:733:VAL:CG1	19:A:1796:CLA:C4D	2.99	0.40
19:A:1796:CLA:C7	19:A:1813:CLA:H171	2.51	0.40
5:A:392:GLN:CD	5:A:392:GLN:O	2.60	0.40
5:A:40:PHE:O	5:A:40:PHE:CG	2.74	0.40
5:A:604:TRP:O	5:A:605:MET:C	2.60	0.40
5:A:650:ASN:HD22	6:B:635:ILE:CD1	2.34	0.40
19:B:1755:CLA:H42	19:B:1768:CLA:CBA	2.51	0.40
22:B:1776:BCR:C8	22:B:1776:BCR:C33	2.86	0.40
6:B:197:VAL:HG22	6:B:207:VAL:HG11	2.03	0.40
6:B:262:HIS:ND1	6:B:265:THR:O	2.42	0.40
6:B:330:ILE:HA	6:B:333:GLN:NE2	2.36	0.40
6:B:522:ALA:O	6:B:589:TRP:HE3	2.04	0.40
6:B:17:THR:HA	6:B:696:LYS:CB	2.51	0.40
6:B:696:LYS:HE2	6:B:696:LYS:HB2	1.83	0.40
17:N:58:VAL:O	17:N:59:PRO:C	2.59	0.40
4:4:127:PRO:HB2	4:4:143:PHE:HE1	1.83	0.40
11:G:58:LEU:HA	11:G:61:ASN:OD1	2.21	0.40
20:R:1056:LMU:O2'	20:R:1056:LMU:C2	2.69	0.40
17:N:4:GLU:OE2	17:N:5:GLU:CB	2.62	0.40
12:H:45:ALA:HA	12:H:48:THR:OG1	2.21	0.40
15:K:10:ILE:HG23	15:K:13:THR:OG1	2.21	0.40
5:A:472:ARG:HH22	16:L:74:LEU:CD2	2.29	0.40
5:A:575:LEU:HD13	5:A:579:PHE:HB3	2.03	0.40
5:A:714:LEU:HB2	5:A:716:VAL:HG13	2.02	0.40
5:A:733:VAL:HG11	19:A:1796:CLA:C4D	2.51	0.40
6:B:91:ILE:CG2	19:B:1740:CLA:CAD	2.96	0.40
22:B:1774:BCR:H341	22:B:1774:BCR:H11C	1.73	0.40
19:B:1762:CLA:C7	22:B:1779:BCR:H402	2.50	0.40
6:B:228:GLY:HA3	11:G:8:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:362:ALA:HA	6:B:365:PHE:H	1.85	0.40
7:C:73:THR:HB	7:C:74:THR:H	1.17	0.40
8:D:109:VAL:O	8:D:110:GLN:HG3	2.21	0.40
10:F:123:VAL:O	10:F:126:ALA:CA	2.69	0.40
11:G:24:PHE:C	11:G:26:PHE:N	2.71	0.40
11:G:44:PHE:HA	11:G:46:ALA:HB2	2.03	0.40
16:L:14:LEU:CA	16:L:24:GLU:HG3	2.41	0.40
19:A:1816:CLA:HBA2	19:A:1816:CLA:O2D	2.19	0.40
2:2:167:GLY:O	2:2:171:MET:N	2.53	0.40
20:K:1086:LMU:H122	20:K:1086:LMU:H91	1.27	0.40
19:L:1166:CLA:HED2	19:L:1166:CLA:CAA	2.48	0.40
6:B:488:ALA:HB2	19:B:1766:CLA:C3C	2.51	0.40
1:1:18:ALA:N	1:1:19:PRO:HD2	2.36	0.40
5:A:430:ASP:O	5:A:432:LEU:N	2.55	0.40
6:B:140:ILE:N	6:B:140:ILE:HD13	2.32	0.40
6:B:139:ALA:O	6:B:141:PHE:N	2.54	0.40
6:B:167:TRP:HD1	11:G:41:MET:CE	2.34	0.40
24:B:1783:LMG:O8	24:B:1783:LMG:C11	2.69	0.40
6:B:387:PHE:O	6:B:391:PRO:CD	2.67	0.40
6:B:471:THR:HG23	6:B:502:ASN:HD21	1.83	0.40
6:B:381:PHE:HA	6:B:583:MET:SD	2.62	0.40
8:D:47:VAL:O	8:D:100:PHE:HB2	2.22	0.40
11:G:42:SER:OG	11:G:45:GLU:CG	2.69	0.40
13:I:8:PHE:CE1	22:I:1032:BCR:C9	3.04	0.40
19:A:1789:CLA:HAA2	16:L:71:ALA:O	2.21	0.40
20:A:7042:LMU:H81	20:A:7042:LMU:H52	1.58	0.40
19:2:1220:CLA:H52	19:2:1220:CLA:H92	0.61	0.40
3:3:92:TRP:O	3:3:95:THR:CG2	2.68	0.40
4:4:106:TRP:HB3	19:4:1196:CLA:HED2	2.03	0.40
4:4:119:PRO:CG	4:4:120:ILE:H	2.34	0.40
5:A:316:MET:CA	5:A:317:TYR:HB2	2.39	0.40
1:1:136:ASP:HB2	1:1:140:LEU:HB3	2.03	0.40
11:G:67:ASN:HA	11:G:70:ASP:CG	2.40	0.40
4:4:38:ARG:CG	4:4:38:ARG:NH1	2.70	0.40
4:4:94:GLU:OE2	19:4:1208:CLA:C1B	2.69	0.40
6:B:160:LYS:NZ	6:B:160:LYS:HB2	2.32	0.40
20:A:7031:LMU:H4'	20:A:7031:LMU:C3B	2.46	0.40
8:D:152:GLN:O	8:D:154:TYR:N	2.55	0.40
5:A:36:LYS:HA	5:A:37:PRO:HD3	1.97	0.40
5:A:639:ALA:O	5:A:640:GLY:C	2.59	0.40
2:2:126:PRO:CG	2:2:129:LYS:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1785:CLA:HBD	19:A:1785:CLA:HAA1	2.03	0.40
19:A:1801:CLA:HMA3	16:L:27:VAL:CA	2.19	0.40
22:A:1808:BCR:C8	22:A:1808:BCR:H311	2.51	0.40
5:A:334:HIS:CD2	19:A:1777:CLA:NB	2.90	0.40
5:A:375:HIS:CE1	19:A:1782:CLA:C1C	3.04	0.40
5:A:396:PHE:CE2	5:A:616:PHE:CD1	3.09	0.40
5:A:413:HIS:HA	5:A:416:ILE:HD12	2.03	0.40
5:A:44:ILE:HG13	5:A:44:ILE:H	1.59	0.40
5:A:457:SER:O	5:A:544:ILE:CD1	2.64	0.40
5:A:652:TRP:CE2	19:A:1811:CLA:H142	2.56	0.40
5:A:698:GLY:CA	6:B:570:ILE:HG21	2.52	0.40
5:A:704:ILE:HG12	19:A:1795:CLA:CMC	2.52	0.40
6:B:122:GLN:HG3	6:B:361:ILE:CG1	2.44	0.40
6:B:193:HIS:O	6:B:194:LEU:C	2.57	0.40
6:B:303:TYR:H	6:B:306:GLU:HB2	1.85	0.40
6:B:355:LEU:HD21	19:B:1756:CLA:HMC2	2.03	0.40
6:B:429:LEU:HA	6:B:429:LEU:HD23	1.66	0.40
6:B:462:TRP:CZ3	19:B:1764:CLA:HBC1	2.55	0.40
6:B:557:PHE:N	6:B:558:PRO:HD3	2.31	0.40
6:B:583:MET:HE2	6:B:583:MET:O	2.21	0.40
7:C:63:LEU:CD1	7:C:65:VAL:H	2.35	0.40
9:E:34:SER:O	9:E:35:LYS:CB	2.66	0.40
10:F:125:LEU:O	10:F:126:ALA:HB3	2.21	0.40
11:G:44:PHE:CA	11:G:46:ALA:HB2	2.50	0.40
19:B:1786:CLA:H141	19:H:1079:CLA:HBC3	2.02	0.40
20:A:7036:LMU:H101	20:A:7036:LMU:H72	1.68	0.40
17:N:54:LYS:HA	17:N:54:LYS:HD2	1.29	0.40
17:N:64:ASP:HB3	17:N:65:LEU:H	1.44	0.40
4:4:124:TYR:HB3	4:4:127:PRO:HG2	2.03	0.40
4:4:121:PHE:HD1	4:4:143:PHE:CE2	2.40	0.40
1:1:142:GLU:O	1:1:143:LEU:HB2	2.21	0.40
11:G:20:ARG:NH2	11:G:61:ASN:O	2.55	0.40
4:4:38:ARG:HG3	4:4:39:TRP:N	2.27	0.40
19:1:1189:CLA:HMA2	19:1:1189:CLA:O1A	2.22	0.40
1:1:28:GLY:CA	19:1:1199:CLA:C3C	2.95	0.40
6:B:98:GLN:N	6:B:99:PRO:HD2	2.37	0.40
20:A:1809:LMU:H51	20:A:1809:LMU:H22	1.66	0.40
5:A:150:PHE:N	5:A:153:TRP:HE3	2.19	0.40
5:A:158:ILE:HG21	19:A:1770:CLA:O1D	2.21	0.40
5:A:173:VAL:HG23	5:A:174:PHE:H	1.86	0.40
19:A:1776:CLA:H92	22:A:1805:BCR:H373	0.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1779:CLA:CAB	22:A:1805:BCR:H15C	2.52	0.40
19:A:1781:CLA:CBB	19:A:1794:CLA:CMA	3.00	0.40
19:A:1789:CLA:HBA1	19:A:1789:CLA:H3A	1.84	0.40
22:A:1807:BCR:C17	19:A:1812:CLA:H172	2.51	0.40
5:A:193:LEU:HA	5:A:196:PHE:HE2	1.82	0.40
5:A:193:LEU:O	5:A:196:PHE:CD2	2.75	0.40
5:A:567:ARG:CB	5:A:567:ARG:HH21	2.35	0.40
5:A:581:CYS:HB2	5:A:590:CYS:C	2.42	0.40
5:A:686:TRP:C	5:A:688:PHE:H	2.24	0.40
5:A:97:TYR:HA	5:A:153:TRP:CZ2	2.57	0.40
6:B:178:HIS:CE1	19:B:1743:CLA:NC	2.85	0.40
6:B:347:LEU:O	6:B:351:HIS:HB2	2.21	0.40
6:B:471:THR:O	6:B:472:TYR:C	2.60	0.40
7:C:49:VAL:O	25:C:1082:SF4:S2	2.79	0.40
9:E:36:VAL:HG11	9:E:87:VAL:HG11	2.04	0.40
11:G:50:ARG:CB	11:G:51:ALA:CA	2.99	0.40
3:3:205:GLY:HA2	5:A:252:ARG:HH12	1.85	0.40
17:N:67:LEU:CB	17:N:68:GLU:HB3	2.48	0.40
4:4:142:ASN:O	4:4:143:PHE:CB	2.69	0.40
3:3:157:ALA:HB1	3:3:158:TYR:CD2	2.57	0.40
20:A:7013:LMU:O3'	20:A:7013:LMU:C1B	2.66	0.40
2:2:51:HIS:O	2:2:54:TRP:HB2	2.22	0.40
3:3:172:ASP:H	3:3:173:GLU:CB	2.34	0.40
1:1:26:PRO:HD2	6:B:314:ARG:NH1	2.36	0.40
19:1:1192:CLA:H62	19:1:1192:CLA:H41	1.78	0.40
6:B:227:THR:HG1	11:G:97:PHE:HD2	1.68	0.40
12:H:77:LEU:CD2	12:H:78:PRO:HD2	2.52	0.40
6:B:151:LEU:HD23	6:B:151:LEU:HA	1.91	0.40

All (21) 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)
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.92	1.28
11:G:31:MET:CE	17:N:85:TRP:CE2[2_546]	1.19	1.01
11:G:31:MET:SD	17:N:85:TRP:CE2[2_546]	1.46	0.74
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	1.50	0.70
11:G:31:MET:SD	17:N:85:TRP:CD2[2_546]	1.65	0.55
4:4:126:LEU:O	16:L:78:GLU:N[1_655]	1.77	0.43
4:4:129:GLY:CA	16:L:77:THR:O[1_655]	1.87	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:78:PRO:O	3:3:45:THR:CG2[1_554]	1.89	0.31
11:G:31:MET:CE	17:N:85:TRP:CZ2[2_546]	1.92	0.28
19:1:1193:CLA:CED	19:K:1142:CLA:O2A[1_654]	1.94	0.26
11:G:31:MET:SD	17:N:85:TRP:CZ2[2_546]	1.95	0.25
4:4:121:PHE:CD2	16:L:78:GLU:OE1[1_655]	1.99	0.21
4:4:128:ALA:N	16:L:76:ASN:O[1_655]	2.02	0.18
4:4:121:PHE:CE2	16:L:78:GLU:CD[1_655]	2.11	0.09
11:G:31:MET:CE	17:N:85:TRP:CD1[2_546]	2.11	0.09
4:4:121:PHE:CD2	16:L:78:GLU:CD[1_655]	2.12	0.08
4:4:127:PRO:C	16:L:76:ASN:O[1_655]	2.13	0.07
6:B:205:GLU:OE2	15:K:23:ARG:NH1[1_554]	2.15	0.05
4:4:121:PHE:CD2	16:L:78:GLU:OE2[1_655]	2.18	0.02
20:2:1225:LMU:O2B	19:A:1791:CLA:CMB[1_655]	2.18	0.02
4:4:121:PHE:CZ	16:L:78:GLU:OE2[1_655]	2.19	0.01

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	161/241 (67%)	83 (52%)	43 (27%)	35 (22%)	0	0
2	2	174/269 (65%)	88 (51%)	56 (32%)	30 (17%)	0	1
3	3	156/276 (56%)	78 (50%)	43 (28%)	35 (22%)	0	0
4	4	164/251 (65%)	79 (48%)	47 (29%)	38 (23%)	0	0
5	A	726/758 (96%)	334 (46%)	200 (28%)	192 (26%)	0	0
6	B	731/734 (100%)	361 (49%)	189 (26%)	181 (25%)	0	0
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	48 (35%)	42 (31%)	46 (34%)	0	0
9	E	63/143 (44%)	29 (46%)	14 (22%)	20 (32%)	0	0
10	F	152/231 (66%)	67 (44%)	44 (29%)	41 (27%)	0	0
11	G	93/167 (56%)	35 (38%)	28 (30%)	30 (32%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	49 (60%)	15 (18%)	18 (22%)	0	0
16	L	159/216 (74%)	66 (42%)	47 (30%)	46 (29%)	0	0
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0
All	All	3094/4108 (75%)	1419 (46%)	853 (28%)	822 (27%)	0	0

All (822) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	29	LEU
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU
1	1	90	PRO
1	1	118	PRO
1	1	130	PRO
1	1	137	PRO
1	1	161	PHE
1	1	183	ASP
1	1	184	PRO
2	2	37	ASP
2	2	42	ARG
2	2	70	LYS
2	2	71	LEU
2	2	73	ILE
2	2	125	PHE
2	2	127	ASN
2	2	149	GLY
2	2	188	PRO
2	2	189	ILE
2	2	190	ASP
2	2	200	PRO
2	2	204	ILE
2	2	206	ALA
3	3	48	PHE
3	3	49	ILE
3	3	85	PRO

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Mol	Chain	Res	Type
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
3	3	166	PRO
3	3	167	LEU
3	3	172	ASP
3	3	206	VAL
3	3	210	GLN
4	4	34	PRO
4	4	36	ASN
4	4	83	TYR
4	4	115	VAL
4	4	119	PRO
4	4	125	SER
4	4	143	PHE
4	4	144	ALA
4	4	172	VAL
4	4	188	PRO
5	A	22	VAL
5	A	28	LYS
5	A	29	THR
5	A	30	SER
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

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Mol	Chain	Res	Type
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	329	ASP
5	A	333	ALA
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	610	ASN
6	B	629	SER

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	35	THR
15	K	41	GLU
15	K	47	ILE
15	K	51	ASP
15	K	52	PRO
15	K	68	HIS
15	K	69	ILE
15	K	72	VAL
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

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Mol	Chain	Res	Type
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	161	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
17	N	74	LYS
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	178	ALA
1	1	182	ALA
1	1	185	TRP

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Mol	Chain	Res	Type
2	2	41	LEU
2	2	128	ASN
2	2	129	LYS
2	2	193	PHE
2	2	207	ALA
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	58	MET
4	4	59	LEU
4	4	69	ILE
4	4	141	LEU
4	4	162	ALA
4	4	177	PRO
5	A	39	HIS
5	A	41	SER
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	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	266	ALA
5	A	278	ALA
5	A	290	LEU
5	A	292	GLY
5	A	308	ILE
5	A	313	ALA
5	A	317	TYR

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Mol	Chain	Res	Type
5	A	328	LYS
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
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	178	HIS
6	B	188	LEU
6	B	207	VAL
6	B	222	LEU
6	B	224	PRO
6	B	230	TRP
6	B	232	LEU

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Mol	Chain	Res	Type
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
6	B	592	PHE
6	B	605	ASN
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	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

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Mol	Chain	Res	Type
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
13	I	25	PHE
14	J	23	ALA
14	J	26	LEU
14	J	37	LEU
15	K	27	ALA
15	K	32	ARG
15	K	70	MET
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
17	N	35	VAL
17	N	42	PHE
17	N	48	GLY
17	N	54	LYS
17	N	56	LYS
17	N	69	CYS
17	N	71	GLY
17	N	78	GLY
1	1	21	ASP
1	1	57	ILE
1	1	65	TYR

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Mol	Chain	Res	Type
1	1	124	PRO
1	1	135	LYS
1	1	138	LYS
1	1	177	LEU
1	1	179	THR
2	2	91	THR
2	2	116	PRO
2	2	148	TRP
2	2	186	THR
2	2	194	ALA
3	3	88	THR
3	3	91	PRO
3	3	153	SER
3	3	157	ALA
4	4	65	THR
4	4	71	ASN
4	4	108	ASP
4	4	122	LYS
4	4	123	GLN
4	4	148	GLU
4	4	178	PHE
5	A	31	PHE
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	149	PHE
5	A	151	GLN
5	A	200	GLU
5	A	225	VAL
5	A	263	ALA
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

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Mol	Chain	Res	Type
6	B	41	ARG
6	B	43	TYR
6	B	71	GLN
6	B	161	TRP
6	B	173	SER
6	B	179	LEU
6	B	189	ALA
6	B	223	GLY
6	B	225	LEU
6	B	228	GLY
6	B	239	SER
6	B	240	SER
6	B	270	LEU
6	B	272	ASP
6	B	273	VAL
6	B	278	LEU
6	B	281	ALA
6	B	309	ILE
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	43	PRO
8	D	55	GLU
8	D	93	LYS
8	D	128	GLN
9	E	84	LEU
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

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Mol	Chain	Res	Type
13	I	2	ILE
14	J	9	SER
14	J	38	THR
15	K	40	LEU
15	K	48	GLN
16	L	113	SER
16	L	147	GLY
17	N	9	LYS
17	N	21	ARG
17	N	81	VAL
1	1	122	LYS
1	1	134	SER
2	2	83	GLY
2	2	141	LEU
2	2	154	GLN
3	3	75	PRO
3	3	141	GLN
3	3	156	PRO
3	3	169	PHE
4	4	38	ARG
4	4	77	ALA
4	4	114	SER
4	4	118	ASP
4	4	139	ASN
4	4	187	ASP
5	A	37	PRO
5	A	135	ASP
5	A	230	ASN
5	A	276	LYS
5	A	305	ALA
5	A	422	TYR
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	335	GLY
6	B	354	SER
6	B	361	ILE

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Mol	Chain	Res	Type
6	B	379	ALA
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
7	C	9	ASP
7	C	12	ILE
7	C	28	MET
7	C	30	PRO
7	C	37	LYS
8	D	46	TYR
8	D	60	MET
8	D	106	SER
8	D	143	PRO
9	E	61	THR
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	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	78	PRO

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Mol	Chain	Res	Type
1	1	84	TYR
2	2	187	GLY
4	4	88	SER
4	4	127	PRO
5	A	26	PRO
5	A	86	LEU
5	A	95	GLY
5	A	186	TYR
5	A	235	ALA
5	A	269	PHE
5	A	306	ILE
5	A	353	SER
5	A	375	HIS
5	A	410	ALA
5	A	472	ARG
5	A	503	THR
5	A	571	ASP
5	A	580	PRO
5	A	709	TRP
6	B	139	ALA
6	B	206	TYR
6	B	212	PHE
6	B	360	PHE
6	B	421	HIS
6	B	451	LYS
6	B	460	ALA
6	B	550	LYS
6	B	559	CYS
6	B	586	THR
6	B	593	TYR
6	B	598	HIS
6	B	704	GLN
7	C	35	LYS
7	C	52	LYS
7	C	55	GLU
7	C	58	CYS
7	C	73	THR
8	D	22	PRO
8	D	34	GLY
8	D	40	ALA
8	D	104	PHE
8	D	125	PRO

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Mol	Chain	Res	Type
8	D	148	PHE
9	E	52	VAL
10	F	73	VAL
10	F	102	ARG
12	H	16	ASN
12	H	74	GLN
13	I	5	PRO
16	L	50	LEU
16	L	61	GLY
16	L	135	GLY
16	L	157	LEU
17	N	34	THR
17	N	50	GLN
17	N	62	SER
1	1	32	VAL
1	1	55	PRO
1	1	99	ALA
1	1	143	LEU
1	1	160	GLY
2	2	76	THR
2	2	136	GLY
4	4	73	PRO
4	4	126	LEU
4	4	147	LEU
4	4	185	ILE
5	A	179	LEU
5	A	239	PRO
5	A	259	TYR
5	A	500	PRO
5	A	584	PRO
5	A	696	GLY
5	A	721	GLN
6	B	162	LYS
6	B	219	PRO
6	B	391	PRO
6	B	472	TYR
6	B	498	LEU
6	B	630	GLN
6	B	708	VAL
10	F	37	ALA
11	G	91	ASN
12	H	72	ALA

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Mol	Chain	Res	Type
15	K	34	ALA
16	L	69	VAL
1	1	79	GLY
1	1	145	VAL
4	4	136	GLY
5	A	48	PRO
5	A	223	VAL
5	A	229	ILE
5	A	531	PRO
5	A	570	PRO
5	A	754	ILE
6	B	94	PRO
6	B	557	PHE
6	B	711	VAL
16	L	150	GLY
17	N	59	PRO
5	A	190	ALA
5	A	716	VAL
6	B	606	VAL
8	D	67	ILE
9	E	55	VAL
11	G	64	VAL
16	L	53	GLY
16	L	72	GLY
1	1	28	GLY
8	D	28	ILE
11	G	71	VAL
13	I	12	VAL
4	4	137	ILE
4	4	168	ILE
5	A	718	PRO
6	B	87	ILE
6	B	113	VAL
6	B	463	ILE
11	G	35	VAL
12	H	60	GLY
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	127/190 (67%)	102 (80%)	25 (20%)	1	7
2	2	140/216 (65%)	107 (76%)	33 (24%)	1	3
3	3	120/215 (56%)	82 (68%)	38 (32%)	0	1
4	4	138/201 (69%)	103 (75%)	35 (25%)	1	2
5	A	592/618 (96%)	392 (66%)	200 (34%)	0	1
6	B	598/600 (100%)	367 (61%)	231 (39%)	0	0
7	C	70/70 (100%)	40 (57%)	30 (43%)	0	0
8	D	118/173 (68%)	75 (64%)	43 (36%)	0	1
9	E	56/114 (49%)	37 (66%)	19 (34%)	0	1
10	F	127/190 (67%)	73 (58%)	54 (42%)	0	0
11	G	79/144 (55%)	46 (58%)	33 (42%)	0	0
12	H	57/115 (50%)	26 (46%)	31 (54%)	0	0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0	1
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	1
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	1
16	L	124/169 (73%)	81 (65%)	43 (35%)	0	1
17	N	74/139 (53%)	33 (45%)	41 (55%)	0	0
All	All	2543/3331 (76%)	1650 (65%)	893 (35%)	0	1

All (893) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	27	LEU
1	1	31	GLU
1	1	49	TRP
1	1	52	LEU
1	1	57	ILE
1	1	58	LEU
1	1	59	VAL
1	1	61	GLU
1	1	84	TYR
1	1	85	LEU
1	1	93	THR

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Mol	Chain	Res	Type
1	1	103	LEU
1	1	110	HIS
1	1	111	GLN
1	1	120	LYS
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	152	ARG
1	1	179	THR
1	1	181	LEU
1	1	186	HIS
2	2	39	GLU
2	2	43	TRP
2	2	46	GLN
2	2	51	HIS
2	2	57	LEU
2	2	70	LYS
2	2	71	LEU
2	2	73	ILE
2	2	89	THR
2	2	94	LEU
2	2	95	PHE
2	2	100	VAL
2	2	101	PHE
2	2	109	ARG
2	2	110	TRP
2	2	113	ILE
2	2	115	ASN
2	2	119	VAL
2	2	125	PHE
2	2	129	LYS
2	2	130	LEU
2	2	137	TYR
2	2	158	GLU
2	2	159	LEU
2	2	162	LYS
2	2	164	ILE
2	2	169	LEU
2	2	179	PHE

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Mol	Chain	Res	Type
2	2	189	ILE
2	2	193	PHE
2	2	196	HIS
2	2	199	ASP
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
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	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

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Mol	Chain	Res	Type
3	3	210	GLN
4	4	32	GLU
4	4	33	ASP
4	4	35	GLU
4	4	38	ARG
4	4	39	TRP
4	4	50	TRP
4	4	52	MET
4	4	53	LEU
4	4	59	LEU
4	4	60	LEU
4	4	64	PHE
4	4	69	ILE
4	4	71	ASN
4	4	83	TYR
4	4	90	LEU
4	4	103	ILE
4	4	104	ARG
4	4	116	ASN
4	4	118	ASP
4	4	120	ILE
4	4	124	TYR
4	4	126	LEU
4	4	131	VAL
4	4	139	ASN
4	4	147	LEU
4	4	150	LYS
4	4	159	LEU
4	4	163	PHE
4	4	169	GLN
4	4	173	THR
4	4	175	LYS
4	4	189	TRP
4	4	190	HIS
4	4	194	VAL
4	4	195	GLN
5	A	21	LEU
5	A	22	VAL
5	A	23	ASP
5	A	24	ARG
5	A	25	ASP
5	A	29	THR

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Mol	Chain	Res	Type
5	A	30	SER
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
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

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Mol	Chain	Res	Type
5	A	203	LEU
5	A	207	LEU
5	A	213	LEU
5	A	217	SER
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
5	A	299	ILE
5	A	304	LEU
5	A	308	ILE
5	A	309	LEU
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	358	LEU
5	A	361	ASN

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Mol	Chain	Res	Type
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
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	520	LEU
5	A	521	VAL
5	A	529	LEU

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
5	A	657	LEU
5	A	660	GLN
5	A	662	SER
5	A	663	GLN
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
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

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Mol	Chain	Res	Type
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	80	ASP
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	118	SER
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	31	LYS
9	E	32	ARG
9	E	35	LYS
9	E	36	VAL
9	E	39	LEU
9	E	40	ARG

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	152	ASN
10	F	153	ASN
10	F	154	PHE
11	G	7	VAL
11	G	10	LEU
11	G	12	THR
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

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Mol	Chain	Res	Type
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	59	LYS
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
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

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Mol	Chain	Res	Type
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	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	18	MET
15	K	19	LEU
15	K	20	PHE
15	K	23	ARG
15	K	32	ARG
15	K	39	LYS
15	K	40	LEU
15	K	41	GLU
15	K	43	ARG
15	K	45	SER
15	K	48	GLN
15	K	52	PRO
15	K	55	PHE
15	K	68	HIS
15	K	69	ILE
15	K	70	MET
15	K	72	VAL

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Mol	Chain	Res	Type
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
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	164	PRO

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Mol	Chain	Res	Type
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
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 (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	46	HIS
1	1	72	GLN
1	1	111	GLN
2	2	120	ASN
2	2	128	ASN
3	3	105	ASN
3	3	126	HIS
3	3	165	ASN
4	4	71	ASN
4	4	107	GLN
4	4	111	ASN
4	4	169	GLN
5	A	33	GLN
5	A	58	HIS
5	A	99	HIS
5	A	121	GLN
5	A	129	GLN
5	A	144	GLN
5	A	187	HIS
5	A	197	GLN
5	A	224	HIS
5	A	230	ASN
5	A	231	GLN
5	A	246	HIS
5	A	302	HIS
5	A	303	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

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Mol	Chain	Res	Type
5	A	683	HIS
5	A	701	GLN
5	A	711	HIS
5	A	729	GLN
6	B	14	GLN
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
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

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Mol	Chain	Res	Type
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	27	GLN
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
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 256 ligands modelled in this entry, 1 is unknown - leaving 255 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	1187	1	36,54,73	2.53	13 (36%)	41,90,113	5.54	26 (63%)
19	CLA	1	1188	-	37,55,73	2.36	9 (24%)	42,91,113	4.62	20 (47%)
19	CLA	1	1189	-	37,55,73	2.43	10 (27%)	42,91,113	5.15	18 (42%)
19	CLA	1	1190	-	36,54,73	2.54	11 (30%)	41,90,113	4.44	17 (41%)
19	CLA	1	1191	-	24,44,73	2.97	8 (33%)	28,78,113	4.64	13 (46%)
19	CLA	1	1192	-	51,69,73	2.16	10 (19%)	56,108,113	3.72	17 (30%)
19	CLA	1	1193	19	41,59,73	2.46	13 (31%)	44,96,113	4.89	21 (47%)
19	CLA	1	1194	-	16,32,73	1.82	4 (25%)	21,54,113	3.21	12 (57%)
19	CLA	1	1195	-	24,44,73	3.25	12 (50%)	28,78,113	5.60	14 (50%)
19	CLA	1	1196	1	24,44,73	2.83	8 (33%)	28,78,113	4.37	11 (39%)
19	CLA	1	1197	19	41,59,73	2.87	18 (43%)	44,96,113	5.37	22 (50%)
19	CLA	1	1198	19	51,69,73	2.06	11 (21%)	56,108,113	4.58	20 (35%)
19	CLA	1	1199	-	16,32,73	1.83	4 (25%)	21,54,113	3.32	12 (57%)
19	CLA	1	1200	-	41,59,73	2.45	13 (31%)	44,96,113	6.51	24 (54%)
19	CLA	1	1201	-	16,32,73	1.77	3 (18%)	21,54,113	3.78	11 (52%)
20	LMU	1	1202	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
20	LMU	1	7004	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
19	CLA	2	1212	-	41,59,73	2.25	10 (24%)	44,96,113	5.18	17 (38%)
19	CLA	2	1213	-	46,64,73	2.20	10 (21%)	50,102,113	4.06	21 (42%)
19	CLA	2	1214	-	16,32,73	1.67	4 (25%)	21,54,113	3.24	11 (52%)
19	CLA	2	1215	-	40,58,73	2.27	11 (27%)	44,95,113	4.50	17 (38%)
19	CLA	2	1216	-	16,32,73	1.90	7 (43%)	21,54,113	3.52	12 (57%)
19	CLA	2	1217	-	55,73,73	2.08	10 (18%)	61,113,113	4.26	16 (26%)
19	CLA	2	1218	19	55,73,73	2.03	9 (16%)	61,113,113	4.09	21 (34%)
19	CLA	2	1219	-	16,32,73	1.69	3 (18%)	21,54,113	3.16	12 (57%)
19	CLA	2	1220	19	46,64,73	2.20	12 (26%)	50,102,113	5.06	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	1221	-	16,32,73	1.79	3 (18%)	21,54,113	3.22	12 (57%)
19	CLA	2	1222	2	40,58,73	2.39	9 (22%)	44,95,113	4.32	19 (43%)
19	CLA	2	1223	-	40,58,73	2.38	10 (25%)	44,95,113	5.01	16 (36%)
19	CLA	2	1224	-	55,73,73	2.02	11 (20%)	61,113,113	4.45	21 (34%)
20	LMU	2	1225	-	36,36,36	0.87	1 (2%)	47,47,47	0.95	2 (4%)
21	SUC	2	1226	-	23,23,24	1.02	1 (4%)	35,35,36	2.23	13 (37%)
19	CLA	2	1227	-	16,32,73	1.88	7 (43%)	21,54,113	3.52	11 (52%)
19	CLA	2	2010	-	16,32,73	1.85	4 (25%)	21,54,113	2.79	8 (38%)
20	LMU	2	7003	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
20	LMU	2	7006	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
19	CLA	3	1212	-	24,44,73	2.77	8 (33%)	28,78,113	4.11	14 (50%)
19	CLA	3	1213	-	16,32,73	1.89	6 (37%)	21,54,113	3.35	12 (57%)
19	CLA	3	1214	-	16,32,73	1.89	5 (31%)	21,54,113	3.27	12 (57%)
19	CLA	3	1215	-	16,32,73	1.87	5 (31%)	21,54,113	3.29	12 (57%)
19	CLA	3	1216	-	16,32,73	1.65	3 (18%)	21,54,113	3.03	11 (52%)
19	CLA	3	1217	-	16,32,73	1.99	5 (31%)	21,54,113	3.52	12 (57%)
19	CLA	3	1218	-	55,73,73	2.19	14 (25%)	61,113,113	4.96	19 (31%)
19	CLA	3	1219	-	55,73,73	1.94	11 (20%)	61,113,113	4.40	17 (27%)
22	BCR	3	1220	-	41,41,41	2.05	5 (12%)	56,56,56	5.89	21 (37%)
21	SUC	3	1221	-	24,24,24	0.78	0	36,36,36	2.21	9 (25%)
19	CLA	3	3001	-	16,32,73	1.91	4 (25%)	21,54,113	3.29	11 (52%)
19	CLA	3	3002	-	16,32,73	1.80	4 (25%)	21,54,113	2.97	11 (52%)
19	CLA	3	3007	-	32,50,73	2.39	8 (25%)	36,85,113	5.45	17 (47%)
19	CLA	3	3008	-	40,58,73	2.26	12 (30%)	44,95,113	5.36	19 (43%)
19	CLA	3	3011	-	55,73,73	1.90	10 (18%)	61,113,113	4.01	18 (29%)
19	CLA	3	3014	-	16,32,73	1.77	4 (25%)	21,54,113	3.61	12 (57%)
19	CLA	3	3015	-	16,32,73	1.80	4 (25%)	21,54,113	2.96	10 (47%)
20	LMU	3	7005	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
19	CLA	4	1196	-	45,63,73	2.16	11 (24%)	49,101,113	4.90	17 (34%)
19	CLA	4	1197	-	24,44,73	2.95	8 (33%)	28,78,113	4.83	15 (53%)
19	CLA	4	1198	-	55,73,73	2.22	15 (27%)	61,113,113	4.54	25 (40%)
19	CLA	4	1199	-	45,63,73	2.17	9 (20%)	49,101,113	4.29	17 (34%)
19	CLA	4	1200	-	40,58,73	2.42	10 (25%)	44,95,113	4.74	18 (40%)
19	CLA	4	1201	-	42,60,73	2.62	19 (45%)	45,97,113	5.77	31 (68%)
19	CLA	4	1202	-	16,32,73	1.81	4 (25%)	21,54,113	3.32	12 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	1203	-	16,32,73	1.92	4 (25%)	21,54,113	3.12	11 (52%)
19	CLA	4	1204	-	45,63,73	2.31	9 (20%)	49,101,113	4.47	17 (34%)
19	CLA	4	1205	-	16,32,73	1.77	4 (25%)	21,54,113	3.22	12 (57%)
19	CLA	4	1206	-	16,32,73	1.65	2 (12%)	21,54,113	3.29	13 (61%)
19	CLA	4	1207	-	24,44,73	2.72	7 (29%)	28,78,113	5.16	17 (60%)
19	CLA	4	1208	4	16,32,73	1.73	4 (25%)	21,54,113	2.62	11 (52%)
19	CLA	4	1209	-	36,54,73	2.58	13 (36%)	41,90,113	5.08	15 (36%)
20	LMU	4	1210	-	36,36,36	0.84	1 (2%)	47,47,47	1.24	4 (8%)
19	CLA	4	4003	-	16,32,73	1.73	4 (25%)	21,54,113	2.83	11 (52%)
19	CLA	4	4007	-	42,60,73	2.36	10 (23%)	45,97,113	4.88	19 (42%)
19	CLA	4	4014	20	37,55,73	2.38	11 (29%)	42,91,113	5.25	16 (38%)
19	CLA	A	1759	-	40,58,73	2.29	10 (25%)	44,95,113	5.02	20 (45%)
19	CLA	A	1760	-	45,63,73	2.31	11 (24%)	49,101,113	3.52	18 (36%)
19	CLA	A	1761	-	55,73,73	2.04	11 (20%)	61,113,113	3.99	19 (31%)
19	CLA	A	1762	-	47,65,73	2.18	10 (21%)	50,103,113	4.84	19 (38%)
19	CLA	A	1763	-	36,54,73	2.34	9 (25%)	41,90,113	5.56	19 (46%)
19	CLA	A	1764	5	55,73,73	2.04	13 (23%)	61,113,113	4.10	21 (34%)
19	CLA	A	1765	-	45,63,73	2.12	9 (20%)	49,101,113	4.31	19 (38%)
19	CLA	A	1766	-	32,53,73	2.53	9 (28%)	37,89,113	5.25	18 (48%)
19	CLA	A	1767	5	55,73,73	2.09	11 (20%)	61,113,113	3.99	22 (36%)
19	CLA	A	1768	5	44,62,73	2.19	11 (25%)	47,99,113	4.10	15 (31%)
19	CLA	A	1769	-	44,62,73	2.05	10 (22%)	47,99,113	4.02	20 (42%)
19	CLA	A	1770	-	32,53,73	2.59	9 (28%)	37,89,113	4.65	15 (40%)
19	CLA	A	1771	5	40,58,73	2.42	10 (25%)	44,95,113	4.68	19 (43%)
19	CLA	A	1772	5	55,73,73	1.97	12 (21%)	61,113,113	4.31	22 (36%)
19	CLA	A	1773	-	42,60,73	2.34	10 (23%)	45,97,113	4.99	16 (35%)
19	CLA	A	1774	-	55,73,73	1.98	11 (20%)	61,113,113	3.64	20 (32%)
19	CLA	A	1775	-	24,44,73	2.82	8 (33%)	28,78,113	4.58	13 (46%)
19	CLA	A	1776	-	55,73,73	2.00	9 (16%)	61,113,113	4.01	20 (32%)
19	CLA	A	1777	-	41,59,73	2.32	10 (24%)	44,96,113	4.91	17 (38%)
19	CLA	A	1778	5	32,50,73	2.54	10 (31%)	36,85,113	5.20	17 (47%)
19	CLA	A	1779	-	45,63,73	2.23	11 (24%)	49,101,113	4.57	19 (38%)
19	CLA	A	1780	-	55,73,73	1.87	9 (16%)	61,113,113	3.62	19 (31%)
19	CLA	A	1781	-	55,73,73	1.95	11 (20%)	61,113,113	4.40	17 (27%)
19	CLA	A	1782	19	55,73,73	1.94	10 (18%)	61,113,113	4.41	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1783	-	55,73,73	2.02	10 (18%)	61,113,113	4.31	20 (32%)
19	CLA	A	1784	5	45,63,73	2.26	11 (24%)	49,101,113	4.57	16 (32%)
19	CLA	A	1785	-	55,73,73	2.02	11 (20%)	61,113,113	4.04	22 (36%)
19	CLA	A	1786	-	40,58,73	2.30	10 (25%)	44,95,113	5.05	22 (50%)
19	CLA	A	1787	5	55,73,73	2.07	9 (16%)	61,113,113	4.08	20 (32%)
19	CLA	A	1788	-	55,73,73	2.01	11 (20%)	61,113,113	4.29	18 (29%)
19	CLA	A	1789	-	55,73,73	2.02	11 (20%)	61,113,113	4.30	22 (36%)
19	CLA	A	1790	19,5	40,58,73	2.25	9 (22%)	44,95,113	4.52	16 (36%)
19	CLA	A	1791	5	32,53,73	2.42	10 (31%)	37,89,113	5.57	15 (40%)
19	CLA	A	1792	-	41,59,73	2.26	11 (26%)	44,96,113	5.17	17 (38%)
19	CLA	A	1793	-	55,73,73	1.95	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	A	1794	-	37,55,73	2.37	11 (29%)	42,91,113	5.26	16 (38%)
19	CLA	A	1795	-	41,59,73	2.26	11 (26%)	44,96,113	5.18	17 (38%)
19	CLA	A	1796	-	55,73,73	1.95	11 (20%)	61,113,113	4.40	17 (27%)
19	CLA	A	1797	-	55,73,73	1.95	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	A	1798	-	45,63,73	2.25	10 (22%)	49,101,113	4.67	18 (36%)
19	CLA	A	1799	-	40,58,73	2.31	9 (22%)	44,95,113	5.03	17 (38%)
19	CLA	A	1800	-	55,73,73	1.99	11 (20%)	61,113,113	4.46	20 (32%)
19	CLA	A	1801	-	45,63,73	2.36	9 (20%)	49,101,113	4.21	19 (38%)
23	PQN	A	1802	-	34,34,34	1.57	3 (8%)	44,45,45	1.41	5 (11%)
22	BCR	A	1803	5	41,41,41	1.93	3 (7%)	56,56,56	5.90	19 (33%)
22	BCR	A	1804	-	41,41,41	1.92	3 (7%)	56,56,56	5.90	19 (33%)
22	BCR	A	1805	-	41,41,41	1.93	3 (7%)	56,56,56	5.91	19 (33%)
22	BCR	A	1806	-	41,41,41	1.93	3 (7%)	56,56,56	5.91	19 (33%)
22	BCR	A	1807	-	41,41,41	1.93	3 (7%)	56,56,56	5.90	19 (33%)
22	BCR	A	1808	-	41,41,41	1.92	3 (7%)	56,56,56	5.91	19 (33%)
20	LMU	A	1809	-	36,36,36	0.92	0	47,47,47	1.42	8 (17%)
20	LMU	A	1810	-	36,36,36	0.92	1 (2%)	47,47,47	1.73	11 (23%)
19	CLA	A	1811	-	55,73,73	2.03	12 (21%)	61,113,113	4.48	20 (32%)
19	CLA	A	1812	-	55,73,73	2.05	13 (23%)	61,113,113	4.20	19 (31%)
19	CLA	A	1813	-	55,73,73	2.14	12 (21%)	61,113,113	4.39	19 (31%)
19	CLA	A	1815	-	45,63,73	2.28	11 (24%)	49,101,113	5.11	19 (38%)
19	CLA	A	1816	-	45,63,73	2.32	13 (28%)	49,101,113	4.74	20 (40%)
19	CLA	A	1817	-	36,54,73	2.73	13 (36%)	42,90,113	4.93	26 (61%)
20	LMU	A	7009	-	35,35,36	0.40	0	46,46,47	0.71	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	A	7010	-	36,36,36	0.40	0	47,47,47	0.71	1 (2%)
20	LMU	A	7013	-	36,36,36	0.44	0	47,47,47	1.65	11 (23%)
20	LMU	A	7015	-	36,36,36	0.91	1 (2%)	47,47,47	1.45	7 (14%)
20	LMU	A	7016	-	36,36,36	0.61	1 (2%)	47,47,47	1.97	12 (25%)
20	LMU	A	7017	-	36,36,36	0.69	2 (5%)	47,47,47	2.36	15 (31%)
20	LMU	A	7019	-	36,36,36	1.00	1 (2%)	47,47,47	1.43	6 (12%)
20	LMU	A	7020	-	36,36,36	0.40	0	47,47,47	1.82	12 (25%)
20	LMU	A	7021	-	36,36,36	0.75	0	47,47,47	2.11	14 (29%)
20	LMU	A	7022	-	36,36,36	0.69	0	47,47,47	2.23	17 (36%)
20	LMU	A	7023	-	36,36,36	0.67	1 (2%)	47,47,47	2.01	18 (38%)
20	LMU	A	7024	-	36,36,36	0.94	2 (5%)	47,47,47	1.71	11 (23%)
20	LMU	A	7025	-	36,36,36	0.94	1 (2%)	47,47,47	1.61	11 (23%)
20	LMU	A	7026	21	36,36,36	1.20	3 (8%)	47,47,47	3.16	23 (48%)
20	LMU	A	7027	-	36,36,36	1.09	1 (2%)	47,47,47	2.00	15 (31%)
20	LMU	A	7028	-	36,36,36	0.72	2 (5%)	47,47,47	1.92	17 (36%)
20	LMU	A	7030	-	36,36,36	0.90	1 (2%)	47,47,47	2.33	16 (34%)
20	LMU	A	7031	-	36,36,36	1.06	1 (2%)	47,47,47	1.37	6 (12%)
20	LMU	A	7032	-	36,36,36	0.97	3 (8%)	47,47,47	2.83	18 (38%)
20	LMU	A	7033	-	36,36,36	1.00	2 (5%)	47,47,47	2.29	14 (29%)
20	LMU	A	7034	19	36,36,36	0.83	1 (2%)	47,47,47	1.35	4 (8%)
20	LMU	A	7035	-	36,36,36	0.81	1 (2%)	47,47,47	1.63	8 (17%)
20	LMU	A	7036	-	35,35,36	1.20	4 (11%)	46,46,47	2.34	15 (32%)
20	LMU	A	7037	-	36,36,36	0.88	2 (5%)	47,47,47	3.15	22 (46%)
20	LMU	A	7038	-	36,36,36	0.65	0	47,47,47	2.43	17 (36%)
20	LMU	A	7039	-	36,36,36	0.96	2 (5%)	47,47,47	2.64	13 (27%)
20	LMU	A	7040	-	36,36,36	0.95	3 (8%)	47,47,47	2.52	14 (29%)
20	LMU	A	7041	-	36,36,36	0.61	0	47,47,47	1.90	13 (27%)
20	LMU	A	7042	-	36,36,36	0.47	0	47,47,47	2.13	16 (34%)
20	LMU	A	7043	21	36,36,36	0.74	0	47,47,47	2.29	18 (38%)
20	LMU	A	7047	-	36,36,36	1.09	1 (2%)	47,47,47	1.46	4 (8%)
19	CLA	B	1735	-	55,73,73	1.95	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	B	1736	-	32,53,73	2.41	8 (25%)	37,89,113	4.51	15 (40%)
19	CLA	B	1737	-	55,73,73	1.96	10 (18%)	61,113,113	4.42	23 (37%)
19	CLA	B	1738	-	55,73,73	2.04	12 (21%)	61,113,113	4.35	29 (47%)
19	CLA	B	1739	-	55,73,73	2.11	11 (20%)	61,113,113	4.41	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1740	6	55,73,73	1.89	11 (20%)	61,113,113	4.47	17 (27%)
19	CLA	B	1741	6	44,62,73	2.49	10 (22%)	49,100,113	3.25	20 (40%)
19	CLA	B	1742	6	45,63,73	2.11	11 (24%)	49,101,113	4.28	20 (40%)
19	CLA	B	1743	-	55,73,73	2.05	10 (18%)	61,113,113	4.10	19 (31%)
19	CLA	B	1744	-	55,73,73	2.11	10 (18%)	61,113,113	3.54	19 (31%)
19	CLA	B	1745	6	50,68,73	2.06	10 (20%)	55,107,113	4.16	19 (34%)
19	CLA	B	1746	-	36,54,73	2.47	10 (27%)	41,90,113	4.74	16 (39%)
19	CLA	B	1747	-	49,67,73	2.14	10 (20%)	53,105,113	3.75	17 (32%)
19	CLA	B	1748	-	50,68,73	1.99	11 (22%)	55,107,113	4.56	18 (32%)
19	CLA	B	1749	-	51,69,73	1.97	10 (19%)	56,108,113	4.50	19 (33%)
19	CLA	B	1750	-	40,58,73	2.29	11 (27%)	44,95,113	4.47	16 (36%)
19	CLA	B	1751	-	36,54,73	2.43	10 (27%)	41,90,113	5.00	16 (39%)
19	CLA	B	1752	6	45,63,73	2.31	9 (20%)	49,101,113	4.81	18 (36%)
19	CLA	B	1753	-	55,73,73	2.44	18 (32%)	61,113,113	4.63	19 (31%)
19	CLA	B	1754	-	44,62,73	2.30	12 (27%)	47,99,113	4.42	21 (44%)
19	CLA	B	1755	-	48,66,73	2.08	11 (22%)	52,104,113	4.77	17 (32%)
19	CLA	B	1756	-	55,73,73	1.96	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	B	1757	-	55,73,73	2.09	12 (21%)	61,113,113	4.41	20 (32%)
19	CLA	B	1758	-	55,73,73	2.02	12 (21%)	61,113,113	4.03	20 (32%)
19	CLA	B	1759	-	55,73,73	1.97	11 (20%)	61,113,113	4.22	20 (32%)
19	CLA	B	1760	-	40,58,73	2.41	8 (20%)	44,95,113	4.18	19 (43%)
19	CLA	B	1761	6	40,58,73	2.30	9 (22%)	44,95,113	4.92	19 (43%)
19	CLA	B	1762	6	55,73,73	2.10	13 (23%)	61,113,113	4.38	20 (32%)
19	CLA	B	1763	6	40,58,73	2.43	12 (30%)	44,95,113	4.76	19 (43%)
19	CLA	B	1764	19	32,53,73	2.68	9 (28%)	37,89,113	5.07	14 (37%)
19	CLA	B	1765	19	32,53,73	2.51	10 (31%)	37,89,113	5.46	14 (37%)
19	CLA	B	1766	-	41,59,73	2.40	9 (21%)	44,96,113	4.83	17 (38%)
19	CLA	B	1767	-	50,68,73	2.06	11 (22%)	55,107,113	4.48	15 (27%)
19	CLA	B	1768	6	55,73,73	1.93	10 (18%)	61,113,113	3.92	18 (29%)
19	CLA	B	1769	-	37,55,73	2.30	10 (27%)	42,91,113	4.44	17 (40%)
19	CLA	B	1770	-	55,73,73	1.96	10 (18%)	61,113,113	4.10	22 (36%)
19	CLA	B	1771	-	55,73,73	1.92	9 (16%)	61,113,113	3.95	25 (40%)
19	CLA	B	1772	-	24,44,73	2.83	8 (33%)	28,78,113	4.86	16 (57%)
23	PQN	B	1773	-	34,34,34	1.46	2 (5%)	44,45,45	1.50	6 (13%)
22	BCR	B	1774	-	41,41,41	1.94	4 (9%)	56,56,56	5.90	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	B	1775	-	41,41,41	1.93	4 (9%)	56,56,56	5.89	19 (33%)
22	BCR	B	1776	-	41,41,41	1.85	5 (12%)	56,56,56	5.03	24 (42%)
22	BCR	B	1777	-	41,41,41	1.94	3 (7%)	56,56,56	5.90	22 (39%)
22	BCR	B	1778	-	41,41,41	1.93	3 (7%)	56,56,56	5.90	19 (33%)
22	BCR	B	1779	-	41,41,41	2.75	13 (31%)	56,56,56	6.07	31 (55%)
22	BCR	B	1780	-	41,41,41	1.92	3 (7%)	56,56,56	5.91	19 (33%)
22	BCR	B	1781	-	41,41,41	2.66	16 (39%)	56,56,56	5.39	30 (53%)
20	LMU	B	1782	-	26,26,36	1.01	1 (3%)	37,37,47	1.53	7 (18%)
24	LMG	B	1783	-	49,49,55	0.92	2 (4%)	57,57,63	1.02	3 (5%)
25	SF4	B	1784	5,6	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	B	1785	-	55,73,73	1.97	11 (20%)	61,113,113	4.24	23 (37%)
19	CLA	B	1786	-	55,73,73	2.01	11 (20%)	61,113,113	4.11	23 (37%)
19	CLA	B	1787	-	55,73,73	2.08	10 (18%)	61,113,113	3.92	19 (31%)
21	SUC	B	8051	-	24,24,24	0.71	0	36,36,36	1.40	3 (8%)
21	SUC	B	8052	-	24,24,24	0.82	0	36,36,36	1.70	9 (25%)
21	SUC	B	8053	20	24,24,24	0.43	0	36,36,36	0.90	1 (2%)
21	SUC	B	8054	-	24,24,24	1.15	2 (8%)	36,36,36	1.78	10 (27%)
21	SUC	B	8055	-	24,24,24	0.81	1 (4%)	36,36,36	1.79	8 (22%)
21	SUC	B	8056	-	24,24,24	0.98	1 (4%)	36,36,36	1.86	13 (36%)
21	SUC	B	8059	-	24,24,24	0.96	1 (4%)	36,36,36	2.12	12 (33%)
21	SUC	B	8060	-	24,24,24	0.99	0	36,36,36	1.88	7 (19%)
21	SUC	B	8061	-	24,24,24	0.88	0	36,36,36	2.36	17 (47%)
21	SUC	B	8062	20	24,24,24	0.99	1 (4%)	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	3.64	14 (50%)
19	CLA	F	1156	19	30,49,73	2.49	10 (33%)	34,84,113	5.82	15 (44%)
19	CLA	F	1157	19	43,61,73	2.57	15 (34%)	46,98,113	4.72	18 (39%)
19	CLA	G	1099	-	41,59,73	2.37	9 (21%)	44,96,113	4.61	20 (45%)
19	CLA	H	1079	-	55,73,73	2.02	12 (21%)	61,113,113	4.27	19 (31%)
21	SUC	H	1080	12	24,24,24	0.85	0	36,36,36	1.56	8 (22%)
19	CLA	I	1031	-	50,68,73	2.08	11 (22%)	55,107,113	4.88	16 (29%)
22	BCR	I	1032	-	41,41,41	2.65	8 (19%)	56,56,56	6.50	29 (51%)
19	CLA	I	1033	-	45,63,73	2.27	9 (20%)	49,101,113	4.82	19 (38%)
19	CLA	J	1043	-	51,69,73	2.01	11 (21%)	56,108,113	4.59	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	J	1044	19	51,69,73	2.05	13 (25%)	56,108,113	4.69	25 (44%)
19	CLA	J	1045	19	45,63,73	2.27	13 (28%)	49,101,113	4.77	21 (42%)
19	CLA	J	1046	-	16,32,73	1.73	6 (37%)	21,54,113	2.96	11 (52%)
19	CLA	K	1085	20	40,58,73	2.28	11 (27%)	44,95,113	5.18	18 (40%)
20	LMU	K	1086	19	36,36,36	0.74	0	47,47,47	2.41	12 (25%)
19	CLA	K	1142	19	32,53,73	2.41	9 (28%)	37,89,113	5.57	15 (40%)
19	CLA	K	1146	-	40,58,73	2.45	13 (32%)	44,95,113	5.40	22 (50%)
19	CLA	K	3009	-	55,73,73	2.02	10 (18%)	61,113,113	4.20	19 (31%)
19	CLA	L	1166	16	40,58,73	2.35	9 (22%)	44,95,113	5.08	16 (36%)
19	CLA	L	1167	22,16	37,55,73	2.38	10 (27%)	42,91,113	5.18	21 (50%)
19	CLA	L	1168	-	40,58,73	2.52	13 (32%)	44,95,113	5.64	17 (38%)
22	BCR	L	1169	-	41,41,41	2.45	8 (19%)	56,56,56	5.73	20 (35%)
22	BCR	L	1170	19	41,41,41	3.26	19 (46%)	56,56,56	6.41	27 (48%)
20	LMU	L	1171	-	36,36,36	0.97	3 (8%)	47,47,47	1.52	9 (19%)
19	CLA	L	1505	-	45,63,73	2.23	10 (22%)	49,101,113	4.67	19 (38%)
19	CLA	R	1054	-	47,65,73	2.20	12 (25%)	50,103,113	4.89	18 (36%)
19	CLA	R	1055	-	55,73,73	2.17	11 (20%)	61,113,113	3.96	21 (34%)
20	LMU	R	1056	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
20	LMU	R	1057	-	36,36,36	1.14	2 (5%)	47,47,47	2.53	15 (31%)

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	1187	1	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1188	-	3/3/16/25	0/16/114/135	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	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1192	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1193	19	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	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1196	1	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	1	1197	19	4/4/17/25	1/21/119/135	0/0/9/9
19	CLA	1	1198	19	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1199	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1200	-	5/5/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1201	-	3/3/7/25	0/0/66/135	0/0/8/9
20	LMU	1	1202	-	-	0/21/61/61	0/2/2/2
20	LMU	1	7004	-	-	0/21/61/61	0/2/2/2
19	CLA	2	1212	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	2	1213	-	4/4/18/25	0/27/125/135	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	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	1218	19	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	19	4/4/18/25	0/27/125/135	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
19	CLA	2	1224	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	2	1225	-	-	0/21/61/61	0/2/2/2
21	SUC	2	1226	-	1/1/9/9	0/10/49/51	0/2/2/2
19	CLA	2	1227	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2010	-	3/3/7/25	0/0/66/135	0/0/8/9
20	LMU	2	7003	-	-	0/21/61/61	0/2/2/2
20	LMU	2	7006	-	-	0/21/61/61	0/2/2/2
19	CLA	3	1212	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	1213	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1214	-	3/3/7/25	0/0/66/135	0/0/8/9
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	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1219	-	4/4/20/25	0/37/135/135	0/0/9/9
22	BCR	3	1220	-	-	1/29/63/63	0/2/2/2
21	SUC	3	1221	-	1/1/9/9	0/12/51/51	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	3001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3002	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3007	-	3/3/15/25	0/10/108/135	0/0/9/9
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	3014	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3015	-	3/3/7/25	0/0/66/135	0/0/8/9
20	LMU	3	7005	-	-	0/21/61/61	0/2/2/2
19	CLA	4	1196	-	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	-	4/4/17/25	0/22/120/135	0/0/9/9
19	CLA	4	1202	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1203	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1204	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1205	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1206	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1207	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1208	4	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1209	-	3/3/16/25	0/15/113/135	0/0/9/9
20	LMU	4	1210	-	-	0/21/61/61	0/2/2/2
19	CLA	4	4003	-	3/3/7/25	0/0/66/135	0/0/8/9
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	-	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	0/28/126/135	0/0/9/9
19	CLA	A	1763	-	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	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1766	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1767	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
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	4/4/20/25	0/37/135/135	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	-	3/3/14/25	0/0/96/135	0/0/9/9
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	-	4/4/20/25	0/37/135/135	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	5	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1792	-	3/3/17/25	0/21/119/135	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	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1796	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1797	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1798	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	A	1799	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1800	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1801	-	4/4/18/25	0/25/123/135	0/0/9/9
23	PQN	A	1802	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	A	1803	5	-	3/29/63/63	0/2/2/2
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	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1807	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1808	-	-	1/29/63/63	0/2/2/2
20	LMU	A	1809	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1810	-	-	1/21/61/61	0/2/2/2
19	CLA	A	1811	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1812	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1813	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1815	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1816	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1817	-	5/5/16/25	0/16/112/135	0/0/9/9
20	LMU	A	7009	-	-	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	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	-	-	0/21/61/61	0/2/2/2

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1763	6	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1764	19	3/3/16/25	0/11/111/135	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	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	B	1767	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1768	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1769	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	B	1770	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1771	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1772	-	3/3/14/25	0/0/96/135	0/0/9/9
23	PQN	B	1773	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	B	1774	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1775	-	-	1/29/63/63	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	-	-	1/29/63/63	0/2/2/2
22	BCR	B	1779	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1780	-	-	1/29/63/63	0/2/2/2
22	BCR	B	1781	-	-	0/29/63/63	0/2/2/2
20	LMU	B	1782	-	-	0/11/51/61	0/2/2/2
24	LMG	B	1783	-	-	0/44/64/70	0/1/1/1
25	SF4	B	1784	5,6	-	0/0/48/48	0/6/5/5
19	CLA	B	1785	-	4/4/20/25	0/37/135/135	0/0/9/9
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
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	20	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	0/6/5/5
19	CLA	F	1155	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	F	1156	19	3/3/15/25	0/8/106/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	F	1157	19	6/6/17/25	1/23/121/135	0/0/9/9
19	CLA	G	1099	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	H	1079	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	H	1080	12	1/1/9/9	0/12/51/51	0/2/2/2
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	I	1033	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	J	1043	-	4/4/19/25	1/33/131/135	0/0/9/9
19	CLA	J	1044	19	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	J	1045	19	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	J	1046	-	3/3/7/25	0/0/66/135	0/0/8/9
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	K	1142	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	K	1146	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	K	3009	-	4/4/20/25	0/37/135/135	0/0/9/9
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
19	CLA	L	1505	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	R	1054	-	4/4/18/25	1/28/126/135	0/0/9/9
19	CLA	R	1055	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	R	1056	-	-	0/21/61/61	0/2/2/2
20	LMU	R	1057	-	1/1/10/10	0/21/61/61	0/2/2/2

All (1854) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1170	BCR	C21-C22	-11.05	1.21	1.35
19	1	1195	CLA	CAB-C3B	-10.42	1.30	1.51
22	B	1781	BCR	C21-C22	-10.01	1.22	1.35
22	L	1170	BCR	C20-C21	-9.97	1.12	1.43
22	B	1779	BCR	C21-C22	-9.41	1.23	1.35
22	I	1032	BCR	C21-C22	-9.09	1.23	1.35
19	1	1191	CLA	CAB-C3B	-9.01	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1169	BCR	C20-C21	-8.89	1.16	1.43
19	1	1197	CLA	C3B-CAB	-8.73	1.29	1.47
19	4	1197	CLA	CAB-C3B	-8.68	1.33	1.51
19	F	1157	CLA	C3B-CAB	-8.67	1.29	1.47
22	L	1169	BCR	C21-C22	-8.54	1.24	1.35
22	B	1779	BCR	C20-C21	-8.49	1.17	1.43
19	B	1753	CLA	C3B-CAB	-8.44	1.29	1.47
19	B	1741	CLA	CAB-C3B	-8.37	1.34	1.51
22	3	1220	BCR	C20-C21	-8.29	1.18	1.43
19	1	1196	CLA	CAB-C3B	-8.23	1.34	1.51
22	A	1806	BCR	C20-C21	-8.21	1.18	1.43
22	B	1775	BCR	C20-C21	-8.19	1.18	1.43
19	B	1772	CLA	CAB-C3B	-8.18	1.34	1.51
22	B	1781	BCR	C20-C21	-8.18	1.18	1.43
22	B	1778	BCR	C20-C21	-8.17	1.18	1.43
22	B	1777	BCR	C20-C21	-8.16	1.18	1.43
22	A	1803	BCR	C20-C21	-8.15	1.18	1.43
22	A	1807	BCR	C20-C21	-8.14	1.18	1.43
22	A	1808	BCR	C20-C21	-8.12	1.18	1.43
19	4	1207	CLA	CAB-C3B	-8.11	1.35	1.51
22	A	1805	BCR	C20-C21	-8.11	1.18	1.43
22	B	1780	BCR	C20-C21	-8.11	1.18	1.43
22	B	1774	BCR	C20-C21	-8.09	1.18	1.43
22	A	1804	BCR	C20-C21	-8.09	1.18	1.43
19	4	1198	CLA	C3B-CAB	-8.02	1.30	1.47
19	A	1775	CLA	CAB-C3B	-8.01	1.35	1.51
19	A	1817	CLA	CAB-C3B	-7.84	1.35	1.51
22	3	1220	BCR	C21-C22	-7.83	1.25	1.35
19	2	1222	CLA	C3B-CAB	-7.80	1.31	1.47
22	I	1032	BCR	C20-C21	-7.77	1.19	1.43
22	L	1170	BCR	C17-C18	-7.73	1.25	1.35
19	B	1739	CLA	C3B-CAB	-7.70	1.31	1.47
19	B	1738	CLA	C3B-CAB	-7.70	1.31	1.47
22	B	1776	BCR	C20-C21	-7.67	1.19	1.43
19	3	1212	CLA	CAB-C3B	-7.59	1.36	1.51
22	B	1777	BCR	C21-C22	-7.55	1.25	1.35
22	B	1774	BCR	C21-C22	-7.50	1.25	1.35
19	B	1743	CLA	C3B-CAB	-7.49	1.31	1.47
22	A	1807	BCR	C21-C22	-7.49	1.25	1.35
19	B	1753	CLA	C4C-C3C	-7.49	1.31	1.45
19	F	1155	CLA	CAB-C3B	-7.48	1.36	1.51
22	A	1805	BCR	C21-C22	-7.47	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1804	BCR	C21-C22	-7.45	1.25	1.35
22	B	1778	BCR	C21-C22	-7.44	1.25	1.35
19	A	1813	CLA	C3B-CAB	-7.40	1.32	1.47
22	A	1803	BCR	C21-C22	-7.40	1.26	1.35
22	B	1775	BCR	C21-C22	-7.39	1.26	1.35
22	A	1808	BCR	C21-C22	-7.39	1.26	1.35
22	A	1806	BCR	C21-C22	-7.36	1.26	1.35
22	B	1780	BCR	C21-C22	-7.36	1.26	1.35
19	A	1764	CLA	C3B-CAB	-7.33	1.32	1.47
19	4	1209	CLA	C3B-CAB	-7.29	1.32	1.47
19	B	1787	CLA	C3B-CAB	-7.29	1.32	1.47
19	B	1764	CLA	C3B-CAB	-7.19	1.32	1.47
19	J	1045	CLA	C3B-CAB	-7.17	1.32	1.47
19	4	1201	CLA	C4C-C3C	-7.04	1.32	1.45
19	A	1784	CLA	C3B-CAB	-6.96	1.33	1.47
19	A	1783	CLA	C3B-CAB	-6.94	1.33	1.47
19	A	1772	CLA	C3B-CAB	-6.93	1.33	1.47
19	2	1220	CLA	C3B-CAB	-6.93	1.33	1.47
19	B	1768	CLA	C3B-CAB	-6.92	1.33	1.47
19	K	1146	CLA	C3B-CAB	-6.91	1.33	1.47
19	A	1816	CLA	C3B-CAB	-6.89	1.33	1.47
19	B	1754	CLA	C3B-CAB	-6.82	1.33	1.47
19	B	1771	CLA	C3B-CAB	-6.80	1.33	1.47
19	B	1752	CLA	C3B-CAB	-6.76	1.33	1.47
19	1	1198	CLA	C3B-CAB	-6.75	1.33	1.47
19	R	1055	CLA	C3B-CAB	-6.74	1.33	1.47
19	B	1762	CLA	C3B-CAB	-6.72	1.33	1.47
19	A	1767	CLA	C3B-CAB	-6.72	1.33	1.47
19	A	1789	CLA	C3B-CAB	-6.69	1.33	1.47
22	I	1032	BCR	C30-C25	-6.68	1.44	1.53
19	3	3008	CLA	C3B-CAB	-6.67	1.33	1.47
19	B	1767	CLA	C3B-CAB	-6.66	1.33	1.47
19	A	1761	CLA	C3B-CAB	-6.63	1.33	1.47
19	B	1786	CLA	C3B-CAB	-6.60	1.33	1.47
19	B	1760	CLA	C3B-CAB	-6.57	1.33	1.47
19	J	1044	CLA	C3B-CAB	-6.57	1.33	1.47
19	3	1218	CLA	C3B-CAB	-6.56	1.33	1.47
19	A	1792	CLA	C3B-CAB	-6.55	1.33	1.47
19	A	1795	CLA	C3B-CAB	-6.54	1.33	1.47
19	A	1791	CLA	C3B-CAB	-6.54	1.33	1.47
19	3	1219	CLA	C3B-CAB	-6.54	1.33	1.47
19	B	1744	CLA	C3B-CAB	-6.54	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1200	CLA	C3B-CAB	-6.53	1.34	1.47
19	A	1812	CLA	C3B-CAB	-6.53	1.34	1.47
19	A	1796	CLA	C3B-CAB	-6.52	1.34	1.47
19	I	1031	CLA	C3B-CAB	-6.52	1.34	1.47
19	F	1156	CLA	C3B-CAB	-6.52	1.34	1.47
19	A	1794	CLA	C3B-CAB	-6.52	1.34	1.47
19	A	1788	CLA	C3B-CAB	-6.51	1.34	1.47
19	4	4014	CLA	C3B-CAB	-6.51	1.34	1.47
19	A	1781	CLA	C3B-CAB	-6.51	1.34	1.47
19	A	1793	CLA	C3B-CAB	-6.51	1.34	1.47
19	4	1196	CLA	C3B-CAB	-6.51	1.34	1.47
19	B	1735	CLA	C3B-CAB	-6.51	1.34	1.47
19	A	1797	CLA	C3B-CAB	-6.50	1.34	1.47
19	B	1756	CLA	C3B-CAB	-6.50	1.34	1.47
19	2	1212	CLA	C3B-CAB	-6.50	1.34	1.47
19	J	1043	CLA	C3B-CAB	-6.49	1.34	1.47
19	K	1142	CLA	C3B-CAB	-6.49	1.34	1.47
19	K	1085	CLA	C3B-CAB	-6.47	1.34	1.47
19	B	1758	CLA	C3B-CAB	-6.46	1.34	1.47
19	3	1218	CLA	C4C-C3C	-6.43	1.33	1.45
19	A	1782	CLA	C3B-CAB	-6.42	1.34	1.47
19	B	1755	CLA	C3B-CAB	-6.42	1.34	1.47
19	A	1800	CLA	C3B-CAB	-6.40	1.34	1.47
19	B	1757	CLA	C3B-CAB	-6.39	1.34	1.47
19	A	1765	CLA	C3B-CAB	-6.39	1.34	1.47
19	B	1765	CLA	C3B-CAB	-6.37	1.34	1.47
19	A	1759	CLA	C3B-CAB	-6.35	1.34	1.47
19	B	1763	CLA	C3B-CAB	-6.31	1.34	1.47
19	4	1199	CLA	C3B-CAB	-6.28	1.34	1.47
19	L	1167	CLA	C3B-CAB	-6.27	1.34	1.47
19	B	1766	CLA	C3B-CAB	-6.25	1.34	1.47
19	B	1785	CLA	C3B-CAB	-6.22	1.34	1.47
19	1	1193	CLA	C3B-CAB	-6.20	1.34	1.47
19	A	1787	CLA	C3B-CAB	-6.16	1.34	1.47
19	1	1187	CLA	C3B-CAB	-6.15	1.34	1.47
19	A	1773	CLA	C3B-CAB	-6.14	1.34	1.47
19	2	1217	CLA	C3B-CAB	-6.13	1.34	1.47
19	1	1192	CLA	C3B-CAB	-6.11	1.34	1.47
19	L	1168	CLA	C3B-CAB	-6.10	1.34	1.47
19	A	1771	CLA	C3B-CAB	-6.08	1.34	1.47
19	4	4007	CLA	C3B-CAB	-6.08	1.34	1.47
19	I	1033	CLA	C3B-CAB	-6.07	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1746	CLA	C3B-CAB	-6.06	1.35	1.47
19	1	1189	CLA	C3B-CAB	-6.05	1.35	1.47
22	B	1776	BCR	C21-C22	-6.05	1.27	1.35
19	B	1740	CLA	C3B-CAB	-6.05	1.35	1.47
19	A	1786	CLA	C3B-CAB	-6.03	1.35	1.47
19	A	1774	CLA	C3B-CAB	-6.01	1.35	1.47
19	1	1190	CLA	C3B-CAB	-6.00	1.35	1.47
19	A	1798	CLA	C3B-CAB	-5.99	1.35	1.47
19	1	1197	CLA	C4C-C3C	-5.95	1.34	1.45
19	A	1780	CLA	C3B-CAB	-5.95	1.35	1.47
19	B	1750	CLA	C3B-CAB	-5.94	1.35	1.47
19	A	1778	CLA	C3B-CAB	-5.91	1.35	1.47
19	A	1770	CLA	C3B-CAB	-5.90	1.35	1.47
19	2	1218	CLA	C3B-CAB	-5.90	1.35	1.47
19	A	1811	CLA	C3B-CAB	-5.87	1.35	1.47
19	B	1761	CLA	C3B-CAB	-5.86	1.35	1.47
19	A	1801	CLA	C3B-CAB	-5.85	1.35	1.47
19	A	1760	CLA	C3B-CAB	-5.85	1.35	1.47
19	B	1770	CLA	C3B-CAB	-5.85	1.35	1.47
19	L	1166	CLA	C3B-CAB	-5.84	1.35	1.47
19	A	1790	CLA	C3B-CAB	-5.80	1.35	1.47
19	B	1759	CLA	C3B-CAB	-5.79	1.35	1.47
19	2	1224	CLA	C3B-CAB	-5.76	1.35	1.47
19	4	1204	CLA	C3B-CAB	-5.76	1.35	1.47
19	F	1157	CLA	C3B-C2B	-5.75	1.32	1.40
19	A	1779	CLA	C3B-CAB	-5.72	1.35	1.47
19	3	3011	CLA	C3B-CAB	-5.69	1.35	1.47
19	B	1749	CLA	C3B-CAB	-5.69	1.35	1.47
19	A	1815	CLA	C3B-CAB	-5.69	1.35	1.47
19	A	1799	CLA	C3B-CAB	-5.68	1.35	1.47
19	2	1223	CLA	C3B-CAB	-5.67	1.35	1.47
19	A	1762	CLA	C3B-CAB	-5.65	1.35	1.47
19	B	1748	CLA	C3B-CAB	-5.64	1.35	1.47
19	1	1188	CLA	C3B-CAB	-5.61	1.35	1.47
19	A	1785	CLA	C3B-CAB	-5.61	1.35	1.47
19	A	1763	CLA	C3B-CAB	-5.60	1.35	1.47
19	B	1747	CLA	C3B-CAB	-5.58	1.36	1.47
19	G	1099	CLA	C3B-CAB	-5.57	1.36	1.47
19	1	1197	CLA	C3B-C2B	-5.56	1.33	1.40
19	K	3009	CLA	C3B-CAB	-5.56	1.36	1.47
19	A	1777	CLA	C3B-CAB	-5.56	1.36	1.47
19	3	3007	CLA	C3B-CAB	-5.55	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1505	CLA	C3B-CAB	-5.55	1.36	1.47
19	B	1745	CLA	C3B-CAB	-5.53	1.36	1.47
19	B	1737	CLA	C3B-CAB	-5.47	1.36	1.47
19	B	1742	CLA	C3B-CAB	-5.47	1.36	1.47
19	B	1736	CLA	C3B-CAB	-5.46	1.36	1.47
19	A	1766	CLA	C3B-CAB	-5.45	1.36	1.47
19	H	1079	CLA	C3B-CAB	-5.43	1.36	1.47
19	2	1215	CLA	C3B-CAB	-5.39	1.36	1.47
22	L	1170	BCR	C20-C19	-5.39	1.20	1.34
19	B	1753	CLA	C3B-C2B	-5.34	1.33	1.40
19	R	1054	CLA	C3B-CAB	-5.33	1.36	1.47
19	4	1201	CLA	C1C-C2C	-5.31	1.33	1.44
22	B	1779	BCR	C30-C25	-5.30	1.46	1.53
19	B	1769	CLA	C3B-CAB	-5.28	1.36	1.47
22	I	1032	BCR	C26-C25	-5.27	1.25	1.34
19	4	1200	CLA	C3B-CAB	-5.23	1.36	1.47
19	A	1769	CLA	C3B-CAB	-5.19	1.36	1.47
19	K	1146	CLA	C1C-C2C	-5.16	1.34	1.44
19	A	1776	CLA	C3B-CAB	-5.04	1.37	1.47
19	2	1213	CLA	C3B-CAB	-4.91	1.37	1.47
19	1	1200	CLA	C1C-C2C	-4.88	1.34	1.44
19	1	1197	CLA	C3D-CAD	-4.83	1.32	1.45
19	A	1768	CLA	C3B-CAB	-4.79	1.37	1.47
19	4	1201	CLA	C3B-CAB	-4.77	1.37	1.47
19	4	1198	CLA	C3B-C2B	-4.74	1.34	1.40
19	1	1200	CLA	C4C-C3C	-4.66	1.36	1.45
19	B	1751	CLA	C3B-CAB	-4.62	1.38	1.47
19	K	1146	CLA	C4C-C3C	-4.59	1.36	1.45
19	J	1045	CLA	C4C-C3C	-4.57	1.36	1.45
22	B	1779	BCR	C1-C6	-4.54	1.47	1.53
19	4	1198	CLA	C1C-C2C	-4.51	1.35	1.44
19	1	1195	CLA	C4C-C3C	-4.50	1.35	1.44
19	1	1195	CLA	C1C-C2C	-4.49	1.35	1.44
19	3	1218	CLA	C1C-C2C	-4.46	1.35	1.44
19	4	1209	CLA	C4C-C3C	-4.35	1.37	1.45
19	1	1198	CLA	C4C-C3C	-4.32	1.37	1.45
22	L	1169	BCR	C20-C19	-4.30	1.23	1.34
19	F	1157	CLA	C4C-C3C	-4.29	1.37	1.45
19	4	1209	CLA	C3B-C2B	-4.28	1.34	1.40
22	L	1170	BCR	C10-C9	-4.23	1.30	1.35
19	1	1197	CLA	C1C-C2C	-4.21	1.36	1.44
19	A	1816	CLA	C3B-C2B	-4.17	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1220	CLA	C4C-C3C	-4.16	1.37	1.45
19	A	1765	CLA	C1C-C2C	-4.15	1.36	1.44
22	L	1169	BCR	C17-C18	-4.10	1.30	1.35
19	A	1816	CLA	C4C-C3C	-4.08	1.37	1.45
19	1	1187	CLA	C4C-C3C	-4.05	1.37	1.45
19	A	1811	CLA	C4C-C3C	-3.98	1.37	1.45
22	I	1032	BCR	C1-C6	-3.98	1.48	1.53
19	4	1198	CLA	C4C-C3C	-3.95	1.37	1.45
19	4	1204	CLA	C4C-C3C	-3.95	1.37	1.45
19	1	1187	CLA	C1C-C2C	-3.91	1.36	1.44
19	3	1218	CLA	C1C-NC	-3.90	1.31	1.37
19	B	1738	CLA	C1C-C2C	-3.88	1.36	1.44
19	A	1801	CLA	C4C-C3C	-3.82	1.38	1.45
19	J	1045	CLA	C1C-C2C	-3.79	1.37	1.44
19	A	1770	CLA	C3B-C2B	-3.78	1.35	1.40
19	A	1772	CLA	C4C-C3C	-3.77	1.38	1.45
19	B	1753	CLA	C1C-C2C	-3.74	1.37	1.44
19	B	1759	CLA	C4C-C3C	-3.73	1.38	1.45
19	B	1763	CLA	C1C-C2C	-3.73	1.37	1.44
19	B	1753	CLA	C4C-NC	-3.71	1.31	1.37
22	B	1779	BCR	C20-C19	-3.70	1.24	1.34
19	B	1743	CLA	C4C-C3C	-3.68	1.38	1.45
19	4	1201	CLA	C2A-C1A	-3.67	1.44	1.52
20	A	7036	LMU	O1B-C4'	-3.65	1.34	1.43
22	B	1779	BCR	C14-C13	-3.64	1.30	1.35
19	A	1774	CLA	C4C-C3C	-3.64	1.38	1.45
22	B	1781	BCR	C5-C6	-3.61	1.28	1.34
22	B	1781	BCR	C20-C19	-3.58	1.25	1.34
19	B	1787	CLA	C4C-C3C	-3.57	1.38	1.45
19	4	1209	CLA	C1C-C2C	-3.56	1.37	1.44
19	1	1197	CLA	C3D-C2D	-3.53	1.31	1.40
19	B	1756	CLA	C4C-C3C	-3.52	1.38	1.45
19	1	1193	CLA	C2A-C1A	-3.51	1.45	1.52
19	3	3008	CLA	C4C-C3C	-3.50	1.38	1.45
19	B	1753	CLA	C1C-NC	-3.49	1.31	1.37
19	F	1156	CLA	C4C-C3C	-3.48	1.38	1.45
19	B	1764	CLA	C4C-C3C	-3.47	1.38	1.45
19	A	1781	CLA	C4C-C3C	-3.46	1.38	1.45
19	A	1782	CLA	C4C-C3C	-3.44	1.38	1.45
19	A	1816	CLA	C3D-CAD	-3.44	1.36	1.45
19	4	4007	CLA	C4C-C3C	-3.44	1.38	1.45
19	A	1792	CLA	C4C-C3C	-3.44	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1212	CLA	C4C-C3C	-3.44	1.38	1.45
22	3	1220	BCR	C20-C19	-3.44	1.25	1.34
19	4	4014	CLA	C4C-C3C	-3.44	1.38	1.45
19	1	1200	CLA	C1C-NC	-3.44	1.32	1.37
19	J	1043	CLA	C4C-C3C	-3.41	1.38	1.45
19	B	1748	CLA	C4C-C3C	-3.41	1.38	1.45
19	A	1796	CLA	C4C-C3C	-3.41	1.38	1.45
19	B	1738	CLA	C3B-C2B	-3.41	1.35	1.40
19	A	1767	CLA	C1C-C2C	-3.40	1.37	1.44
19	A	1788	CLA	C4C-C3C	-3.40	1.38	1.45
19	K	1142	CLA	C4C-C3C	-3.39	1.38	1.45
19	A	1793	CLA	C4C-C3C	-3.39	1.38	1.45
19	B	1769	CLA	C4C-C3C	-3.39	1.38	1.45
19	B	1735	CLA	C4C-C3C	-3.38	1.38	1.45
19	B	1755	CLA	C4C-C3C	-3.38	1.38	1.45
19	A	1795	CLA	C4C-C3C	-3.38	1.38	1.45
22	A	1804	BCR	C20-C19	-3.38	1.25	1.34
22	B	1781	BCR	C26-C25	-3.37	1.28	1.34
19	A	1797	CLA	C4C-C3C	-3.37	1.38	1.45
19	B	1737	CLA	C1C-C2C	-3.37	1.37	1.44
19	J	1044	CLA	C4C-C3C	-3.37	1.38	1.45
19	K	1085	CLA	C4C-C3C	-3.37	1.38	1.45
19	A	1816	CLA	C1C-NC	-3.35	1.32	1.37
19	3	1219	CLA	C4C-C3C	-3.35	1.39	1.45
19	A	1794	CLA	C4C-C3C	-3.35	1.39	1.45
19	A	1772	CLA	C1C-C2C	-3.34	1.37	1.44
19	A	1791	CLA	C4C-C3C	-3.34	1.39	1.45
22	B	1779	BCR	C17-C18	-3.33	1.31	1.35
19	1	1195	CLA	C1C-NC	-3.33	1.32	1.37
22	B	1780	BCR	C20-C19	-3.33	1.25	1.34
19	4	1196	CLA	C4C-C3C	-3.32	1.39	1.45
22	B	1774	BCR	C20-C19	-3.31	1.25	1.34
19	B	1758	CLA	C4C-C3C	-3.30	1.39	1.45
22	B	1778	BCR	C20-C19	-3.30	1.25	1.34
19	1	1187	CLA	C3D-CAD	-3.29	1.36	1.45
19	B	1739	CLA	C1C-C2C	-3.28	1.38	1.44
22	A	1807	BCR	C20-C19	-3.27	1.25	1.34
22	A	1808	BCR	C20-C19	-3.27	1.25	1.34
22	B	1775	BCR	C20-C19	-3.26	1.25	1.34
19	1	1198	CLA	C1C-C2C	-3.26	1.38	1.44
22	B	1777	BCR	C20-C19	-3.26	1.25	1.34
22	A	1805	BCR	C20-C19	-3.26	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1803	BCR	C20-C19	-3.24	1.26	1.34
19	B	1763	CLA	C4C-C3C	-3.24	1.39	1.45
22	A	1806	BCR	C20-C19	-3.23	1.26	1.34
19	A	1813	CLA	C4C-C3C	-3.23	1.39	1.45
19	A	1789	CLA	C1C-C2C	-3.20	1.38	1.44
19	4	1201	CLA	C3A-C2A	-3.20	1.45	1.54
19	I	1031	CLA	C4C-C3C	-3.19	1.39	1.45
19	1	1200	CLA	C3B-C2B	-3.18	1.36	1.40
19	A	1788	CLA	C1C-C2C	-3.16	1.38	1.44
19	B	1787	CLA	C1C-C2C	-3.13	1.38	1.44
19	A	1784	CLA	C3B-C2B	-3.12	1.36	1.40
19	B	1753	CLA	C3D-CAD	-3.10	1.37	1.45
19	2	1220	CLA	C1C-C2C	-3.10	1.38	1.44
22	I	1032	BCR	C20-C19	-3.10	1.26	1.34
19	J	1044	CLA	C1C-C2C	-3.09	1.38	1.44
19	B	1768	CLA	C1C-C2C	-3.09	1.38	1.44
19	B	1751	CLA	C4C-C3C	-3.08	1.39	1.45
19	A	1812	CLA	C4C-C3C	-3.08	1.39	1.45
19	B	1749	CLA	C4C-C3C	-3.08	1.39	1.45
19	4	1201	CLA	C1C-NC	-3.07	1.32	1.37
22	L	1170	BCR	C14-C13	-3.06	1.31	1.35
19	B	1746	CLA	C1C-C2C	-3.06	1.38	1.44
19	L	1168	CLA	C4C-C3C	-3.05	1.39	1.45
19	A	1813	CLA	C1C-C2C	-3.04	1.38	1.44
19	H	1079	CLA	C4C-C3C	-3.04	1.39	1.45
19	1	1193	CLA	C4C-C3C	-3.02	1.39	1.45
19	A	1783	CLA	C1C-C2C	-3.02	1.38	1.44
19	B	1768	CLA	C4C-C3C	-3.01	1.39	1.45
19	A	1772	CLA	C3B-C2B	-3.01	1.36	1.40
19	4	1209	CLA	C3D-CAD	-3.01	1.37	1.45
19	1	1192	CLA	C4C-C3C	-3.01	1.39	1.45
19	A	1774	CLA	C3B-C2B	-2.98	1.36	1.40
19	1	1197	CLA	C1C-NC	-2.98	1.32	1.37
19	4	1201	CLA	C3D-CAD	-2.98	1.37	1.45
19	A	1762	CLA	C1C-C2C	-2.97	1.38	1.44
19	4	1196	CLA	C1C-C2C	-2.96	1.38	1.44
22	B	1779	BCR	C29-C30	-2.96	1.46	1.54
19	4	4014	CLA	C1C-C2C	-2.96	1.38	1.44
19	4	1201	CLA	CAA-C2A	-2.96	1.48	1.54
19	B	1761	CLA	C4C-C3C	-2.94	1.39	1.45
19	B	1756	CLA	C1C-C2C	-2.94	1.38	1.44
19	4	1201	CLA	C4C-NC	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1765	CLA	C4C-C3C	-2.93	1.39	1.45
19	B	1740	CLA	C1C-C2C	-2.93	1.38	1.44
19	G	1099	CLA	C4C-C3C	-2.93	1.39	1.45
19	A	1817	CLA	C1C-C2C	-2.93	1.38	1.44
19	K	3009	CLA	C4C-C3C	-2.93	1.39	1.45
19	B	1785	CLA	C4C-C3C	-2.93	1.39	1.45
19	L	1166	CLA	C4C-C3C	-2.92	1.39	1.45
19	3	1218	CLA	C3D-CAD	-2.92	1.37	1.45
19	B	1759	CLA	C3D-CAD	-2.92	1.37	1.45
19	A	1764	CLA	C4C-C3C	-2.91	1.39	1.45
19	A	1761	CLA	C1C-C2C	-2.91	1.38	1.44
19	K	1085	CLA	C1C-C2C	-2.91	1.38	1.44
19	4	4007	CLA	C1C-C2C	-2.90	1.38	1.44
19	B	1746	CLA	C4C-C3C	-2.90	1.39	1.45
22	L	1170	BCR	C39-C30	-2.89	1.47	1.53
19	B	1738	CLA	C4C-C3C	-2.89	1.39	1.45
19	J	1043	CLA	C1C-C2C	-2.89	1.38	1.44
19	B	1740	CLA	C4C-C3C	-2.88	1.39	1.45
22	B	1781	BCR	C1-C6	-2.88	1.49	1.53
19	2	1212	CLA	C1C-C2C	-2.88	1.38	1.44
19	A	1769	CLA	C1C-C2C	-2.88	1.38	1.44
19	3	3008	CLA	C1C-C2C	-2.87	1.38	1.44
19	3	1218	CLA	C4C-NC	-2.87	1.33	1.37
19	A	1797	CLA	C1C-C2C	-2.87	1.38	1.44
19	A	1792	CLA	C1C-C2C	-2.87	1.38	1.44
19	B	1735	CLA	C1C-C2C	-2.87	1.38	1.44
19	A	1796	CLA	C1C-C2C	-2.87	1.38	1.44
22	L	1170	BCR	C40-C30	-2.87	1.47	1.53
19	B	1755	CLA	C1C-C2C	-2.87	1.38	1.44
19	A	1793	CLA	C1C-C2C	-2.87	1.38	1.44
19	J	1045	CLA	C3B-C2B	-2.86	1.36	1.40
19	A	1768	CLA	C4C-C3C	-2.86	1.39	1.45
19	A	1791	CLA	C1C-C2C	-2.86	1.38	1.44
19	A	1794	CLA	C1C-C2C	-2.86	1.38	1.44
19	A	1795	CLA	C1C-C2C	-2.85	1.38	1.44
19	A	1781	CLA	C1C-C2C	-2.85	1.38	1.44
19	1	1187	CLA	C3D-C2D	-2.85	1.33	1.40
19	A	1759	CLA	C4C-C3C	-2.85	1.39	1.45
19	A	1782	CLA	C1C-C2C	-2.85	1.38	1.44
19	B	1747	CLA	C1C-C2C	-2.85	1.38	1.44
20	A	7036	LMU	C4'-C5'	-2.84	1.45	1.52
19	1	1195	CLA	C3D-CAD	-2.84	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1199	CLA	C1C-C2C	-2.84	1.38	1.44
19	2	1216	CLA	C4C-NC	-2.84	1.33	1.37
19	J	1045	CLA	C3D-CAD	-2.83	1.37	1.45
19	A	1815	CLA	C1C-C2C	-2.83	1.38	1.44
20	A	7040	LMU	C4B-C5B	-2.83	1.47	1.53
19	3	1219	CLA	C1C-C2C	-2.82	1.38	1.44
19	K	1142	CLA	C1C-C2C	-2.82	1.38	1.44
19	B	1752	CLA	C1C-C2C	-2.82	1.38	1.44
19	A	1778	CLA	C1C-C2C	-2.82	1.38	1.44
19	B	1762	CLA	C4C-C3C	-2.81	1.39	1.45
19	2	1224	CLA	C1C-C2C	-2.81	1.38	1.44
19	B	1759	CLA	C1C-C2C	-2.81	1.38	1.44
19	3	1213	CLA	C2C-C1C	-2.81	1.36	1.43
19	A	1775	CLA	C4C-C3C	-2.81	1.38	1.44
19	A	1776	CLA	C1C-C2C	-2.80	1.39	1.44
19	4	1200	CLA	C4C-C3C	-2.80	1.40	1.45
19	B	1757	CLA	C1C-C2C	-2.80	1.39	1.44
19	A	1768	CLA	C1C-C2C	-2.79	1.39	1.44
19	2	1220	CLA	C3D-CAD	-2.79	1.37	1.45
19	B	1753	CLA	C2A-C1A	-2.78	1.46	1.52
22	L	1170	BCR	C29-C30	-2.77	1.47	1.54
19	F	1156	CLA	C1C-C2C	-2.77	1.39	1.44
19	2	1224	CLA	C4C-C3C	-2.77	1.40	1.45
19	A	1777	CLA	C4C-C3C	-2.76	1.40	1.45
19	F	1155	CLA	C1C-C2C	-2.76	1.39	1.44
19	B	1757	CLA	C4C-C3C	-2.76	1.40	1.45
19	B	1737	CLA	C4C-C3C	-2.75	1.40	1.45
19	A	1811	CLA	C3B-C2B	-2.75	1.36	1.40
19	4	1209	CLA	CBD-CGD	-2.74	1.42	1.52
22	L	1170	BCR	C30-C25	-2.74	1.49	1.53
19	A	1817	CLA	C2A-C1A	-2.74	1.46	1.52
19	1	1190	CLA	C1C-C2C	-2.73	1.39	1.44
19	3	1217	CLA	C2C-C1C	-2.72	1.36	1.43
19	A	1785	CLA	C3B-C2B	-2.72	1.36	1.40
19	2	1223	CLA	C4C-C3C	-2.72	1.40	1.45
22	B	1779	BCR	C39-C30	-2.72	1.47	1.53
22	3	1220	BCR	C1-C6	-2.71	1.49	1.53
19	A	1767	CLA	C4C-C3C	-2.71	1.40	1.45
19	A	1775	CLA	C1C-C2C	-2.71	1.39	1.44
19	2	1223	CLA	C3D-CAD	-2.70	1.38	1.45
19	B	1770	CLA	C1C-C2C	-2.70	1.39	1.44
20	A	7039	LMU	O5B-C5B	-2.70	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	7036	LMU	C3'-C4'	-2.70	1.44	1.52
19	2	1215	CLA	C4C-C3C	-2.69	1.40	1.45
19	3	3008	CLA	C3D-CAD	-2.69	1.38	1.45
19	B	1770	CLA	C4C-C3C	-2.69	1.40	1.45
19	F	1157	CLA	C1C-C2C	-2.69	1.39	1.44
22	B	1779	BCR	C40-C30	-2.68	1.48	1.53
19	A	1760	CLA	C4C-C3C	-2.68	1.40	1.45
19	3	1213	CLA	C1C-NC	-2.68	1.33	1.37
19	A	1783	CLA	C4C-C3C	-2.68	1.40	1.45
22	L	1169	BCR	C30-C25	-2.67	1.50	1.53
19	2	1213	CLA	C1C-C2C	-2.66	1.39	1.44
22	I	1032	BCR	C38-C26	-2.66	1.46	1.51
22	B	1781	BCR	C4-C5	-2.65	1.45	1.51
19	2	1218	CLA	C1C-C2C	-2.65	1.39	1.44
19	A	1773	CLA	C4C-C3C	-2.64	1.40	1.45
19	B	1762	CLA	C3D-CAD	-2.64	1.38	1.45
19	B	1754	CLA	C3B-C2B	-2.64	1.36	1.40
19	A	1766	CLA	C1C-C2C	-2.64	1.39	1.44
19	2	1216	CLA	C2C-C1C	-2.64	1.36	1.43
19	A	1816	CLA	C1C-C2C	-2.64	1.39	1.44
19	B	1741	CLA	C4C-C3C	-2.64	1.40	1.45
19	2	1222	CLA	C1C-C2C	-2.63	1.39	1.44
19	R	1055	CLA	C3B-C2B	-2.63	1.36	1.40
19	2	1216	CLA	C3C-C4C	-2.63	1.36	1.43
21	2	1226	SUC	O5-C5	-2.61	1.38	1.44
19	1	1189	CLA	C3D-CAD	-2.60	1.38	1.45
19	B	1741	CLA	C1C-C2C	-2.60	1.39	1.44
19	B	1769	CLA	C1C-C2C	-2.60	1.39	1.44
19	B	1742	CLA	C4C-C3C	-2.60	1.40	1.45
22	3	1220	BCR	C30-C25	-2.59	1.50	1.53
19	A	1800	CLA	C4C-C3C	-2.59	1.40	1.45
22	L	1170	BCR	C2-C1	-2.58	1.47	1.54
19	A	1762	CLA	C4C-C3C	-2.58	1.40	1.45
19	B	1760	CLA	C1C-C2C	-2.57	1.39	1.44
19	A	1759	CLA	C1C-C2C	-2.56	1.39	1.44
19	B	1767	CLA	C3D-CAD	-2.56	1.38	1.45
19	J	1044	CLA	C3B-C2B	-2.56	1.36	1.40
19	1	1196	CLA	C4C-C3C	-2.56	1.39	1.44
22	L	1170	BCR	C37-C22	-2.56	1.45	1.50
19	3	1212	CLA	C4C-C3C	-2.55	1.39	1.44
19	A	1766	CLA	C4C-C3C	-2.55	1.40	1.45
19	A	1761	CLA	C3B-C2B	-2.55	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	1213	CLA	C3C-C4C	-2.54	1.37	1.43
19	2	1227	CLA	C4C-NC	-2.54	1.33	1.37
19	A	1799	CLA	C1C-C2C	-2.54	1.39	1.44
19	B	1763	CLA	C1C-NC	-2.53	1.33	1.37
19	4	1198	CLA	C3D-CAD	-2.53	1.38	1.45
19	4	1198	CLA	C1C-NC	-2.53	1.33	1.37
22	L	1170	BCR	C31-C1	-2.53	1.48	1.53
19	B	1751	CLA	C3D-CAD	-2.52	1.38	1.45
19	H	1079	CLA	C3D-CAD	-2.51	1.38	1.45
19	B	1736	CLA	C3B-C2B	-2.50	1.37	1.40
19	A	1774	CLA	C1C-C2C	-2.50	1.39	1.44
19	B	1750	CLA	C4C-C3C	-2.50	1.40	1.45
19	B	1748	CLA	C1C-C2C	-2.50	1.39	1.44
19	A	1767	CLA	C3B-C2B	-2.49	1.37	1.40
19	4	1198	CLA	CBD-CHA	-2.49	1.39	1.52
21	B	8056	SUC	O5-C5	-2.49	1.38	1.44
19	A	1786	CLA	C1C-C2C	-2.49	1.39	1.44
19	A	1772	CLA	C3D-CAD	-2.49	1.38	1.45
19	2	1217	CLA	C4C-C3C	-2.49	1.40	1.45
19	B	1736	CLA	C4C-C3C	-2.49	1.40	1.45
20	A	7032	LMU	O5'-C5'	-2.48	1.38	1.44
19	4	1198	CLA	C3D-C2D	-2.48	1.34	1.40
19	4	1197	CLA	C4C-C3C	-2.48	1.39	1.44
19	B	1786	CLA	C4C-C3C	-2.48	1.40	1.45
19	B	1739	CLA	C4C-C3C	-2.48	1.40	1.45
19	B	1763	CLA	C3D-CAD	-2.47	1.38	1.45
19	B	1785	CLA	C1C-C2C	-2.47	1.39	1.44
19	B	1766	CLA	C4C-C3C	-2.47	1.40	1.45
19	1	1198	CLA	C3D-CAD	-2.47	1.38	1.45
19	B	1740	CLA	C3D-CAD	-2.46	1.38	1.45
19	A	1812	CLA	C1C-C2C	-2.46	1.39	1.44
19	B	1753	CLA	CAC-C3C	-2.45	1.44	1.51
19	A	1773	CLA	C1C-C2C	-2.45	1.39	1.44
22	L	1170	BCR	C5-C6	-2.44	1.30	1.34
19	A	1770	CLA	C1C-C2C	-2.44	1.39	1.44
22	B	1776	BCR	C20-C19	-2.44	1.28	1.34
19	F	1157	CLA	C1C-NC	-2.43	1.33	1.37
19	A	1816	CLA	C3D-C2D	-2.43	1.34	1.40
20	A	7037	LMU	C4'-C5'	-2.43	1.46	1.52
19	2	1227	CLA	C1C-NC	-2.42	1.33	1.37
19	I	1031	CLA	C3D-CAD	-2.42	1.38	1.45
22	L	1170	BCR	C36-C18	-2.42	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1763	CLA	C4C-C3C	-2.42	1.40	1.45
19	B	1785	CLA	C3B-C2B	-2.41	1.37	1.40
19	1	1190	CLA	C3D-CAD	-2.40	1.39	1.45
19	B	1745	CLA	C4C-C3C	-2.40	1.40	1.45
19	4	1207	CLA	C1C-C2C	-2.40	1.39	1.44
19	R	1054	CLA	C4C-C3C	-2.40	1.40	1.45
22	L	1169	BCR	C1-C6	-2.40	1.50	1.53
19	1	1191	CLA	C4C-C3C	-2.40	1.39	1.44
19	1	1195	CLA	C3B-C2B	-2.39	1.32	1.41
19	B	1754	CLA	C1C-C2C	-2.38	1.39	1.44
19	B	1762	CLA	C1C-C2C	-2.38	1.39	1.44
20	A	7023	LMU	C4B-C5B	-2.38	1.48	1.53
19	A	1785	CLA	C4C-C3C	-2.38	1.40	1.45
19	3	1213	CLA	C4C-NC	-2.37	1.33	1.37
22	B	1779	BCR	C32-C1	-2.37	1.48	1.53
20	A	7030	LMU	C4B-C5B	-2.37	1.48	1.53
19	A	1769	CLA	C4C-C3C	-2.37	1.40	1.45
19	2	1227	CLA	C2C-C1C	-2.37	1.37	1.43
19	B	1753	CLA	C3C-C2C	-2.37	1.31	1.36
19	A	1771	CLA	C1C-C2C	-2.36	1.39	1.44
19	1	1189	CLA	C4C-C3C	-2.36	1.40	1.45
19	R	1054	CLA	C3D-CAD	-2.36	1.39	1.45
19	1	1190	CLA	C4C-C3C	-2.36	1.40	1.45
19	A	1813	CLA	C1C-NC	-2.35	1.33	1.37
19	B	1757	CLA	C3D-CAD	-2.34	1.39	1.45
19	B	1743	CLA	C1C-C2C	-2.34	1.39	1.44
19	A	1798	CLA	C3B-C2B	-2.34	1.37	1.40
20	A	7028	LMU	C4B-C5B	-2.34	1.48	1.53
19	K	1146	CLA	C3D-CAD	-2.34	1.39	1.45
19	B	1786	CLA	C3B-C2B	-2.34	1.37	1.40
20	A	7016	LMU	O5'-C5'	-2.34	1.38	1.44
19	1	1197	CLA	C4C-NC	-2.34	1.34	1.37
19	B	1764	CLA	C1C-C2C	-2.34	1.39	1.44
19	A	1787	CLA	C4C-C3C	-2.33	1.40	1.45
19	A	1780	CLA	C3D-CAD	-2.33	1.39	1.45
19	A	1812	CLA	C3B-C2B	-2.33	1.37	1.40
19	2	1220	CLA	C3B-C2B	-2.32	1.37	1.40
19	A	1815	CLA	C4C-C3C	-2.32	1.40	1.45
20	A	7032	LMU	C1B-C2B	-2.32	1.45	1.52
19	B	1742	CLA	C1C-C2C	-2.32	1.39	1.44
19	F	1155	CLA	C4C-C3C	-2.32	1.39	1.44
19	2	1224	CLA	C3D-CAD	-2.32	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	1168	CLA	C3B-C2B	-2.31	1.37	1.40
22	B	1781	BCR	C29-C30	-2.31	1.48	1.54
19	1	1200	CLA	C3A-C2A	-2.31	1.47	1.54
19	A	1764	CLA	C3B-C2B	-2.31	1.37	1.40
19	B	1758	CLA	C3B-C2B	-2.29	1.37	1.40
19	A	1771	CLA	C4C-C3C	-2.29	1.40	1.45
19	2	1216	CLA	C1C-NC	-2.29	1.33	1.37
19	3	3007	CLA	C1C-C2C	-2.28	1.40	1.44
19	B	1750	CLA	C3D-CAD	-2.27	1.39	1.45
19	J	1044	CLA	C3A-C2A	-2.27	1.47	1.54
19	A	1784	CLA	C1C-C2C	-2.27	1.40	1.44
19	A	1784	CLA	C4C-C3C	-2.26	1.40	1.45
19	4	1197	CLA	C1C-C2C	-2.26	1.40	1.44
19	B	1772	CLA	C1C-C2C	-2.26	1.40	1.44
19	A	1779	CLA	C4C-C3C	-2.26	1.40	1.45
19	A	1760	CLA	C1C-C2C	-2.26	1.40	1.44
19	A	1764	CLA	C2A-C1A	-2.25	1.47	1.52
19	2	1217	CLA	C1C-C2C	-2.25	1.40	1.44
22	I	1032	BCR	C10-C9	-2.25	1.32	1.35
20	A	7040	LMU	O5B-C5B	-2.25	1.38	1.44
19	1	1192	CLA	C1C-C2C	-2.24	1.40	1.44
19	R	1055	CLA	C4C-C3C	-2.24	1.41	1.45
19	3	1212	CLA	C1C-C2C	-2.23	1.40	1.44
19	2	1227	CLA	C3C-C4C	-2.23	1.37	1.43
22	B	1781	BCR	C34-C9	-2.22	1.46	1.50
19	B	1744	CLA	C4C-C3C	-2.22	1.41	1.45
19	A	1777	CLA	C1C-C2C	-2.22	1.40	1.44
19	B	1739	CLA	C3B-C2B	-2.22	1.37	1.40
22	L	1170	BCR	C34-C9	-2.22	1.46	1.50
19	A	1778	CLA	C3B-C2B	-2.21	1.37	1.40
19	4	1198	CLA	C3A-C2A	-2.20	1.48	1.54
19	3	3011	CLA	C4C-C3C	-2.20	1.41	1.45
19	A	1817	CLA	C3D-CAD	-2.20	1.39	1.45
19	4	1201	CLA	CAC-C3C	-2.20	1.45	1.51
19	1	1195	CLA	C3D-C2D	-2.19	1.34	1.40
19	1	1187	CLA	C1C-NC	-2.19	1.34	1.37
19	K	1146	CLA	C3B-C2B	-2.18	1.37	1.40
19	H	1079	CLA	C1C-C2C	-2.18	1.40	1.44
22	B	1781	BCR	C37-C22	-2.18	1.46	1.50
19	B	1767	CLA	C4C-C3C	-2.18	1.41	1.45
19	1	1188	CLA	C1C-C2C	-2.18	1.40	1.44
19	F	1157	CLA	C3D-CAD	-2.18	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1765	CLA	C1C-C2C	-2.17	1.40	1.44
22	B	1779	BCR	C37-C22	-2.17	1.46	1.50
22	B	1781	BCR	C40-C30	-2.17	1.49	1.53
19	1	1193	CLA	C3D-CAD	-2.17	1.39	1.45
20	A	7017	LMU	C4B-C5B	-2.17	1.48	1.53
22	L	1170	BCR	C16-C15	-2.17	1.30	1.35
19	2	1213	CLA	C4C-C3C	-2.17	1.41	1.45
21	B	8054	SUC	O3'-C3'	-2.16	1.38	1.42
19	A	1786	CLA	C3D-CAD	-2.16	1.39	1.45
19	R	1054	CLA	C1C-C2C	-2.16	1.40	1.44
19	A	1800	CLA	C3D-CAD	-2.16	1.39	1.45
19	F	1157	CLA	CAA-C2A	-2.16	1.49	1.54
19	1	1187	CLA	C3B-C2B	-2.16	1.37	1.40
22	B	1781	BCR	C10-C9	-2.16	1.32	1.35
19	K	1146	CLA	C1C-NC	-2.15	1.34	1.37
19	3	3014	CLA	C2C-C1C	-2.15	1.38	1.43
19	A	1778	CLA	C4C-C3C	-2.15	1.41	1.45
19	J	1044	CLA	C3A-C4A	-2.14	1.44	1.51
19	B	1758	CLA	C1C-C2C	-2.14	1.40	1.44
19	A	1785	CLA	C3D-CAD	-2.14	1.39	1.45
20	A	7037	LMU	C4B-C3B	-2.14	1.46	1.52
22	L	1169	BCR	C40-C30	-2.14	1.49	1.53
21	B	8055	SUC	C4-C5	-2.14	1.48	1.53
22	L	1169	BCR	C26-C25	-2.14	1.30	1.34
19	A	1790	CLA	C1C-C2C	-2.14	1.40	1.44
19	A	1781	CLA	C3D-CAD	-2.14	1.39	1.45
19	A	1789	CLA	C3D-CAD	-2.14	1.39	1.45
19	1	1187	CLA	CMD-C2D	-2.13	1.47	1.51
22	B	1779	BCR	C26-C25	-2.13	1.30	1.34
19	1	1196	CLA	C1C-C2C	-2.13	1.40	1.44
19	1	1193	CLA	C3A-C2A	-2.13	1.48	1.54
21	B	8054	SUC	O2'-C2'	-2.13	1.37	1.42
19	L	1168	CLA	C3D-CAD	-2.13	1.39	1.45
19	A	1798	CLA	C4C-C3C	-2.13	1.41	1.45
19	L	1505	CLA	C4C-C3C	-2.12	1.41	1.45
19	B	1753	CLA	CMB-C2B	-2.12	1.47	1.51
21	B	8059	SUC	O2'-C5'	-2.12	1.38	1.43
19	I	1031	CLA	C1C-C2C	-2.12	1.40	1.44
19	B	1750	CLA	C1C-C2C	-2.12	1.40	1.44
21	B	8062	SUC	O5-C5	-2.12	1.39	1.44
19	A	1788	CLA	C3D-CAD	-2.12	1.39	1.45
19	1	1197	CLA	CBD-CGD	-2.11	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1800	CLA	C1C-C2C	-2.11	1.40	1.44
19	3	1217	CLA	C1C-NC	-2.11	1.34	1.37
19	B	1748	CLA	C3D-CAD	-2.10	1.39	1.45
19	B	1756	CLA	C3D-CAD	-2.10	1.39	1.45
19	B	1753	CLA	CBD-CHA	-2.10	1.41	1.52
19	A	1779	CLA	C1C-C2C	-2.10	1.40	1.44
19	B	1762	CLA	C3B-C2B	-2.10	1.37	1.40
20	A	7032	LMU	C3B-C2B	-2.10	1.46	1.52
19	B	1749	CLA	C3D-CAD	-2.10	1.39	1.45
19	B	1747	CLA	C4C-C3C	-2.10	1.41	1.45
22	L	1170	BCR	C32-C1	-2.10	1.49	1.53
22	B	1781	BCR	C32-C1	-2.09	1.49	1.53
19	A	1764	CLA	C3D-CAD	-2.09	1.39	1.45
19	I	1033	CLA	C1C-C2C	-2.08	1.40	1.44
19	B	1755	CLA	C3D-CAD	-2.08	1.39	1.45
19	1	1197	CLA	CMB-C2B	-2.08	1.47	1.51
22	L	1170	BCR	C4-C5	-2.08	1.46	1.51
20	A	7036	LMU	C4B-C5B	-2.08	1.48	1.53
19	J	1046	CLA	C2C-C1C	-2.07	1.38	1.43
19	J	1046	CLA	C3C-C4C	-2.07	1.38	1.43
19	K	1085	CLA	C3D-CAD	-2.07	1.39	1.45
19	J	1045	CLA	C1C-NC	-2.06	1.34	1.37
20	A	7033	LMU	O1B-C4'	-2.06	1.38	1.43
19	A	1779	CLA	C3D-CAD	-2.06	1.40	1.45
22	B	1781	BCR	C33-C5	-2.06	1.47	1.51
19	4	1201	CLA	C3A-C4A	-2.06	1.45	1.51
19	A	1795	CLA	C3D-CAD	-2.06	1.40	1.45
19	L	1167	CLA	C1C-C2C	-2.06	1.40	1.44
22	B	1774	BCR	C30-C25	-2.05	1.50	1.53
19	L	1168	CLA	C3A-C2A	-2.05	1.48	1.54
19	3	1218	CLA	C3B-C2B	-2.05	1.37	1.40
19	L	1167	CLA	C3D-CAD	-2.05	1.40	1.45
19	4	1196	CLA	C3D-CAD	-2.05	1.40	1.45
19	A	1791	CLA	C3D-CAD	-2.05	1.40	1.45
19	A	1789	CLA	C3A-C2A	-2.05	1.48	1.54
19	F	1157	CLA	C4C-NC	-2.05	1.34	1.37
19	A	1796	CLA	C3D-CAD	-2.05	1.40	1.45
19	A	1794	CLA	C3D-CAD	-2.04	1.40	1.45
19	4	1200	CLA	C1C-C2C	-2.04	1.40	1.44
19	B	1765	CLA	C3D-CAD	-2.04	1.40	1.45
19	3	1214	CLA	C3C-C4C	-2.04	1.38	1.43
19	B	1758	CLA	C3D-CAD	-2.04	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1738	CLA	C1C-NC	-2.04	1.34	1.37
19	B	1735	CLA	C3D-CAD	-2.04	1.40	1.45
19	2	1214	CLA	C3C-C4C	-2.03	1.38	1.43
19	1	1201	CLA	C2B-C1B	-2.03	1.36	1.40
19	K	1146	CLA	C4C-NC	-2.03	1.34	1.37
19	4	1201	CLA	C3C-C2C	-2.03	1.32	1.36
19	F	1156	CLA	C3D-CAD	-2.03	1.40	1.45
19	1	1195	CLA	C4C-NC	-2.03	1.34	1.37
19	A	1793	CLA	C3D-CAD	-2.03	1.40	1.45
19	A	1813	CLA	C3B-C2B	-2.03	1.37	1.40
19	A	1797	CLA	C3D-CAD	-2.03	1.40	1.45
22	B	1781	BCR	C30-C25	-2.03	1.50	1.53
22	B	1775	BCR	C1-C6	-2.03	1.50	1.53
19	3	3011	CLA	C1C-C2C	-2.03	1.40	1.44
19	J	1043	CLA	C3D-CAD	-2.02	1.40	1.45
19	B	1772	CLA	C4C-C3C	-2.02	1.40	1.44
19	A	1792	CLA	C3D-CAD	-2.02	1.40	1.45
19	4	1201	CLA	C3B-C2B	-2.02	1.37	1.40
19	1	1200	CLA	C4C-NC	-2.02	1.34	1.37
19	B	1745	CLA	C1C-C2C	-2.02	1.40	1.44
19	B	1771	CLA	C3B-C2B	-2.02	1.37	1.40
19	3	1215	CLA	C3C-C4C	-2.02	1.38	1.43
19	4	4014	CLA	C3D-CAD	-2.01	1.40	1.45
19	3	3008	CLA	C3B-C2B	-2.01	1.37	1.40
19	1	1191	CLA	C3D-CAD	-2.01	1.40	1.45
19	A	1817	CLA	C3A-C2A	-2.01	1.48	1.54
19	2	1215	CLA	C1C-C2C	-2.01	1.40	1.44
19	A	1812	CLA	C3D-CAD	-2.01	1.40	1.45
20	A	7028	LMU	O5'-C5'	-2.01	1.39	1.44
19	3	1219	CLA	C3D-CAD	-2.00	1.40	1.45
19	A	1811	CLA	C1C-C2C	-2.00	1.40	1.44
19	L	1505	CLA	C3D-CAD	-2.00	1.40	1.45
19	3	1213	CLA	CHA-C1A	2.01	1.47	1.41
19	3	3011	CLA	C1B-CHB	2.01	1.45	1.39
19	J	1044	CLA	C1A-CHA	2.01	1.51	1.43
19	2	1215	CLA	C1A-CHA	2.02	1.51	1.43
19	4	4003	CLA	C1B-CHB	2.03	1.47	1.43
19	1	1194	CLA	C1B-CHB	2.03	1.47	1.43
19	4	1205	CLA	C1B-CHB	2.03	1.47	1.43
19	B	1753	CLA	C1B-CHB	2.05	1.45	1.39
19	A	1811	CLA	C2-C3	2.05	1.37	1.33
19	3	1217	CLA	C4B-CHC	2.06	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1216	CLA	CHA-C1A	2.06	1.47	1.41
19	R	1054	CLA	C2-C3	2.06	1.37	1.33
19	B	1767	CLA	C2-C3	2.06	1.37	1.33
19	B	1786	CLA	C1A-CHA	2.06	1.51	1.43
19	B	1754	CLA	C1A-CHA	2.08	1.51	1.43
19	J	1046	CLA	C1B-CHB	2.08	1.48	1.43
20	A	7035	LMU	O1'-C1'	2.09	1.43	1.40
20	A	7017	LMU	O1'-C1'	2.09	1.43	1.40
19	3	3002	CLA	C1B-CHB	2.09	1.48	1.43
19	A	1799	CLA	C1B-CHB	2.10	1.45	1.39
19	A	1812	CLA	C2-C3	2.10	1.37	1.33
19	R	1055	CLA	C2-C3	2.11	1.37	1.33
19	K	3009	CLA	C2-C3	2.11	1.37	1.33
19	A	1761	CLA	C1A-CHA	2.11	1.51	1.43
22	B	1781	BCR	C16-C17	2.11	1.50	1.43
19	B	1762	CLA	C1A-CHA	2.12	1.51	1.43
19	J	1045	CLA	C1B-CHB	2.13	1.45	1.39
23	A	1802	PQN	O1-C1	2.13	1.27	1.23
19	1	1197	CLA	CBA-CGA	2.14	1.57	1.50
19	3	1215	CLA	C1B-CHB	2.15	1.48	1.43
19	3	3001	CLA	C1B-CHB	2.15	1.48	1.43
19	2	1214	CLA	CHA-C1A	2.16	1.47	1.41
20	A	7024	LMU	O5B-C1B	2.16	1.47	1.41
19	4	1202	CLA	C1B-CHB	2.16	1.48	1.43
20	L	1171	LMU	C4B-C5B	2.17	1.57	1.53
19	3	1214	CLA	C1B-CHB	2.17	1.48	1.43
19	B	1757	CLA	C2-C3	2.17	1.37	1.33
19	A	1768	CLA	C2-C3	2.17	1.37	1.33
19	A	1772	CLA	C1B-CHB	2.18	1.45	1.39
19	1	1199	CLA	C1B-CHB	2.19	1.48	1.43
22	B	1776	BCR	C19-C18	2.20	1.50	1.45
19	B	1742	CLA	C2-C3	2.20	1.37	1.33
19	B	1754	CLA	C1B-CHB	2.21	1.45	1.39
19	2	1223	CLA	C1B-CHB	2.21	1.45	1.39
19	A	1813	CLA	C1B-CHB	2.22	1.46	1.39
19	1	1188	CLA	C1B-CHB	2.23	1.46	1.39
19	H	1079	CLA	C2-C3	2.23	1.37	1.33
19	B	1744	CLA	C2-C3	2.23	1.37	1.33
19	J	1046	CLA	CHA-C1A	2.23	1.47	1.41
19	B	1770	CLA	C1B-CHB	2.23	1.46	1.39
19	3	3014	CLA	CHA-C1A	2.24	1.48	1.41
19	B	1751	CLA	C1B-CHB	2.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1764	CLA	C1B-CHB	2.25	1.46	1.39
19	4	1201	CLA	OBD-CAD	2.27	1.25	1.22
19	4	1209	CLA	OBD-CAD	2.27	1.25	1.22
19	B	1740	CLA	C1B-CHB	2.28	1.46	1.39
20	A	7040	LMU	O1'-C1'	2.29	1.44	1.40
19	A	1764	CLA	C2-C3	2.30	1.37	1.33
22	B	1776	BCR	C12-C13	2.30	1.51	1.45
19	2	1227	CLA	CHA-C1A	2.31	1.48	1.41
19	A	1815	CLA	C2-C3	2.31	1.37	1.33
19	A	1780	CLA	C1B-CHB	2.31	1.46	1.39
19	A	1790	CLA	C1B-CHB	2.32	1.46	1.39
19	4	1203	CLA	CHA-C1A	2.33	1.48	1.41
19	4	4003	CLA	CHA-C1A	2.34	1.48	1.41
20	A	7034	LMU	O1'-C1'	2.34	1.44	1.40
19	4	1203	CLA	C1B-CHB	2.36	1.48	1.43
19	F	1155	CLA	C1B-CHB	2.36	1.46	1.39
19	A	1767	CLA	C1B-CHB	2.37	1.46	1.39
19	4	1205	CLA	CHA-C1A	2.37	1.48	1.41
19	2	1213	CLA	C1B-CHB	2.37	1.46	1.39
19	A	1812	CLA	C1B-CHB	2.38	1.46	1.39
19	2	1227	CLA	C4B-CHC	2.39	1.48	1.43
20	A	7033	LMU	C4B-C5B	2.40	1.58	1.53
19	B	1786	CLA	C1B-CHB	2.41	1.46	1.39
20	L	1171	LMU	O5B-C1B	2.42	1.48	1.41
19	1	1193	CLA	C2-C3	2.42	1.37	1.33
19	4	1207	CLA	C1B-CHB	2.43	1.46	1.39
19	A	1815	CLA	C1B-CHB	2.43	1.46	1.39
19	2	1220	CLA	C1B-CHB	2.43	1.46	1.39
20	A	7039	LMU	C4B-C3B	2.44	1.58	1.52
20	A	7015	LMU	O1'-C1'	2.46	1.44	1.40
19	A	1760	CLA	C2-C3	2.46	1.37	1.33
20	L	1171	LMU	O1'-C1'	2.46	1.44	1.40
19	L	1167	CLA	C1B-CHB	2.46	1.46	1.39
19	B	1738	CLA	C1B-CHB	2.48	1.46	1.39
19	A	1788	CLA	C1B-CHB	2.49	1.46	1.39
19	A	1811	CLA	C1B-CHB	2.50	1.46	1.39
19	B	1743	CLA	C1B-CHB	2.52	1.46	1.39
20	4	1210	LMU	O1'-C1'	2.52	1.44	1.40
20	A	7025	LMU	O1'-C1'	2.52	1.44	1.40
19	A	1768	CLA	C1B-CHB	2.53	1.46	1.39
19	I	1031	CLA	C1B-CHB	2.53	1.46	1.39
19	A	1762	CLA	C1B-CHB	2.54	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1197	CLA	C1B-CHB	2.54	1.46	1.39
19	A	1770	CLA	C1B-CHB	2.54	1.46	1.39
19	2	2010	CLA	CHA-C1A	2.55	1.48	1.41
19	B	1737	CLA	C1B-CHB	2.55	1.46	1.39
19	1	1200	CLA	C4B-CHC	2.55	1.46	1.39
19	B	1787	CLA	C1B-CHB	2.56	1.46	1.39
19	4	1208	CLA	C1B-CHB	2.56	1.49	1.43
19	H	1079	CLA	C1B-CHB	2.57	1.46	1.39
19	1	1197	CLA	OBD-CAD	2.58	1.26	1.22
19	A	1779	CLA	C1B-CHB	2.58	1.47	1.39
19	B	1752	CLA	C1B-CHB	2.59	1.47	1.39
20	2	1225	LMU	O1'-C1'	2.59	1.44	1.40
19	3	3008	CLA	C1B-CHB	2.60	1.47	1.39
20	R	1057	LMU	O1'-C1'	2.60	1.44	1.40
19	B	1739	CLA	C1B-CHB	2.62	1.47	1.39
19	A	1769	CLA	C1B-CHB	2.62	1.47	1.39
19	3	3015	CLA	C1B-CHB	2.62	1.49	1.43
19	A	1776	CLA	C1B-CHB	2.64	1.47	1.39
19	3	3002	CLA	CHA-C1A	2.67	1.49	1.41
19	J	1043	CLA	C1B-CHB	2.67	1.47	1.39
19	B	1754	CLA	C2-C3	2.67	1.38	1.33
19	4	1196	CLA	C1B-CHB	2.68	1.47	1.39
19	A	1794	CLA	C1B-CHB	2.68	1.47	1.39
19	B	1757	CLA	C1B-CHB	2.68	1.47	1.39
19	A	1791	CLA	C1B-CHB	2.68	1.47	1.39
19	4	1198	CLA	C4B-CHC	2.68	1.47	1.39
19	B	1755	CLA	C1B-CHB	2.68	1.47	1.39
19	L	1168	CLA	C1B-CHB	2.68	1.47	1.39
19	4	4014	CLA	C1B-CHB	2.68	1.47	1.39
19	I	1033	CLA	C1B-CHB	2.69	1.47	1.39
19	B	1744	CLA	C1B-CHB	2.69	1.47	1.39
19	A	1781	CLA	C1B-CHB	2.69	1.47	1.39
19	4	1202	CLA	CHA-C1A	2.69	1.49	1.41
20	A	7027	LMU	O1'-C1'	2.69	1.45	1.40
19	K	1085	CLA	C1B-CHB	2.70	1.47	1.39
19	3	1219	CLA	C1B-CHB	2.70	1.47	1.39
19	A	1796	CLA	C1B-CHB	2.70	1.47	1.39
19	3	3015	CLA	CHA-C1A	2.70	1.49	1.41
19	1	1199	CLA	CHA-C1A	2.70	1.49	1.41
19	F	1156	CLA	C1B-CHB	2.70	1.47	1.39
20	A	7026	LMU	O1'-C1'	2.70	1.45	1.40
19	B	1761	CLA	C1B-CHB	2.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	1142	CLA	C1B-CHB	2.71	1.47	1.39
19	B	1785	CLA	C1B-CHB	2.71	1.47	1.39
19	A	1795	CLA	C1B-CHB	2.71	1.47	1.39
19	A	1798	CLA	C1B-CHB	2.71	1.47	1.39
19	2	2010	CLA	C1B-CHB	2.71	1.49	1.43
19	A	1797	CLA	C1B-CHB	2.71	1.47	1.39
19	1	1198	CLA	C1B-CHB	2.71	1.47	1.39
19	A	1760	CLA	C1B-CHB	2.72	1.47	1.39
19	B	1756	CLA	C1B-CHB	2.72	1.47	1.39
19	B	1735	CLA	C1B-CHB	2.72	1.47	1.39
19	A	1793	CLA	C1B-CHB	2.72	1.47	1.39
19	3	1216	CLA	CHA-C1A	2.73	1.49	1.41
19	A	1782	CLA	C1B-CHB	2.73	1.47	1.39
19	A	1792	CLA	C1B-CHB	2.73	1.47	1.39
19	A	1817	CLA	CMA-C3A	2.74	1.59	1.53
19	2	1221	CLA	CHA-C1A	2.74	1.49	1.41
19	2	1212	CLA	C1B-CHB	2.75	1.47	1.39
19	1	1201	CLA	C4B-CHC	2.75	1.49	1.43
19	B	1753	CLA	O2D-CGD	2.75	1.40	1.33
19	4	1201	CLA	C4B-CHC	2.76	1.47	1.39
19	B	1745	CLA	C1B-CHB	2.77	1.47	1.39
19	A	1766	CLA	C1B-CHB	2.77	1.47	1.39
19	A	1784	CLA	C1B-CHB	2.77	1.47	1.39
19	A	1789	CLA	C1B-CHB	2.78	1.47	1.39
19	1	1194	CLA	CHA-C1A	2.79	1.49	1.41
19	I	1031	CLA	OBD-CAD	2.79	1.26	1.22
19	A	1783	CLA	C1B-CHB	2.80	1.47	1.39
19	B	1741	CLA	C1B-CHB	2.80	1.47	1.39
19	G	1099	CLA	C1B-CHB	2.81	1.47	1.39
19	B	1747	CLA	C1B-CHB	2.82	1.47	1.39
19	4	1208	CLA	CHA-C1A	2.82	1.49	1.41
19	A	1777	CLA	C1B-CHB	2.82	1.47	1.39
19	B	1763	CLA	C1B-CHB	2.83	1.47	1.39
19	A	1785	CLA	C1B-CHB	2.84	1.47	1.39
19	A	1787	CLA	C1B-CHB	2.84	1.47	1.39
19	2	1218	CLA	C1B-CHB	2.84	1.47	1.39
19	B	1764	CLA	C1B-CHB	2.84	1.47	1.39
19	B	1742	CLA	C1B-CHB	2.84	1.47	1.39
20	A	1810	LMU	O1'-C1'	2.84	1.45	1.40
19	A	1774	CLA	C1B-CHB	2.85	1.47	1.39
19	F	1157	CLA	C1B-CHB	2.85	1.47	1.39
19	B	1762	CLA	C1B-CHB	2.85	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	7026	LMU	O5'-C1'	2.86	1.49	1.41
19	2	1219	CLA	C4B-CHC	2.86	1.49	1.43
19	1	1190	CLA	C1B-CHB	2.86	1.47	1.39
19	4	4003	CLA	C4B-CHC	2.86	1.49	1.43
19	B	1771	CLA	C1B-CHB	2.87	1.47	1.39
19	4	1199	CLA	C1B-CHB	2.87	1.47	1.39
19	B	1759	CLA	C1B-CHB	2.87	1.47	1.39
20	A	7024	LMU	O1'-C1'	2.88	1.45	1.40
19	1	1197	CLA	C4B-CHC	2.88	1.47	1.39
19	B	1765	CLA	C1B-CHB	2.89	1.47	1.39
19	J	1046	CLA	C4B-CHC	2.91	1.49	1.43
19	3	1212	CLA	C1B-CHB	2.92	1.47	1.39
19	3	1216	CLA	C4B-CHC	2.92	1.49	1.43
19	A	1761	CLA	OBD-CAD	2.93	1.26	1.22
19	A	1765	CLA	C4B-CHC	2.93	1.47	1.39
19	1	1193	CLA	C1B-CHB	2.94	1.47	1.39
19	4	1209	CLA	C1B-CHB	2.95	1.48	1.39
20	B	1782	LMU	O1'-C1'	2.95	1.45	1.40
19	A	1771	CLA	C1B-CHB	2.96	1.48	1.39
19	3	3001	CLA	CHA-C1A	2.96	1.50	1.41
19	1	1189	CLA	C1B-CHB	2.97	1.48	1.39
19	4	1198	CLA	O2A-CGA	2.97	1.42	1.33
19	1	1196	CLA	C1B-CHB	2.98	1.48	1.39
19	2	1214	CLA	C4B-CHC	2.98	1.49	1.43
19	B	1772	CLA	C1B-CHB	2.98	1.48	1.39
19	L	1505	CLA	C1B-CHB	2.98	1.48	1.39
19	B	1746	CLA	C1B-CHB	2.98	1.48	1.39
19	A	1786	CLA	C1B-CHB	2.99	1.48	1.39
19	2	1222	CLA	C1B-CHB	2.99	1.48	1.39
19	K	1146	CLA	OBD-CAD	3.00	1.26	1.22
19	2	1215	CLA	C1B-CHB	3.00	1.48	1.39
19	A	1761	CLA	C1B-CHB	3.01	1.48	1.39
19	3	1215	CLA	CHA-C1A	3.01	1.50	1.41
19	B	1748	CLA	C1B-CHB	3.01	1.48	1.39
19	3	1218	CLA	C4B-CHC	3.01	1.48	1.39
19	A	1773	CLA	C1B-CHB	3.01	1.48	1.39
19	A	1775	CLA	C1B-CHB	3.02	1.48	1.39
19	1	1191	CLA	C1B-CHB	3.02	1.48	1.39
19	2	1219	CLA	CHA-C1A	3.03	1.50	1.41
19	2	1216	CLA	C4B-CHC	3.03	1.50	1.43
19	3	1217	CLA	CHA-C1A	3.05	1.50	1.41
19	3	1218	CLA	C1B-CHB	3.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1740	CLA	O2A-CGA	3.06	1.42	1.33
19	3	1214	CLA	CHA-C1A	3.07	1.50	1.41
19	R	1054	CLA	C1B-CHB	3.08	1.48	1.39
19	B	1738	CLA	OBD-CAD	3.08	1.27	1.22
20	R	1057	LMU	O2B-C2B	3.10	1.50	1.43
19	B	1750	CLA	C1B-CHB	3.10	1.48	1.39
19	1	1188	CLA	C4B-CHC	3.11	1.48	1.39
19	A	1763	CLA	C1B-CHB	3.11	1.48	1.39
19	A	1759	CLA	C1B-CHB	3.12	1.48	1.39
19	K	3009	CLA	C1B-CHB	3.13	1.48	1.39
19	B	1766	CLA	C1B-CHB	3.14	1.48	1.39
19	B	1768	CLA	C4B-CHC	3.15	1.48	1.39
19	B	1767	CLA	C4B-CHC	3.15	1.48	1.39
19	2	1224	CLA	C1B-CHB	3.16	1.48	1.39
19	B	1748	CLA	OBD-CAD	3.17	1.27	1.22
19	A	1817	CLA	C1B-CHB	3.17	1.48	1.39
19	3	1218	CLA	OBD-CAD	3.17	1.27	1.22
19	B	1769	CLA	C1B-CHB	3.19	1.48	1.39
19	B	1753	CLA	CHD-C4C	3.19	1.48	1.41
19	B	1749	CLA	C1B-CHB	3.20	1.48	1.39
20	A	7019	LMU	O1'-C1'	3.22	1.45	1.40
19	2	1217	CLA	C1B-CHB	3.23	1.48	1.39
19	3	3008	CLA	OBD-CAD	3.23	1.27	1.22
19	B	1738	CLA	C4B-CHC	3.23	1.48	1.39
19	4	1202	CLA	C4B-CHC	3.24	1.50	1.43
19	A	1765	CLA	C1B-CHB	3.24	1.48	1.39
19	4	1201	CLA	O2A-CGA	3.25	1.43	1.33
19	B	1768	CLA	C1B-CHB	3.26	1.48	1.39
19	1	1199	CLA	C4B-CHC	3.26	1.50	1.43
19	4	1209	CLA	CHD-C4C	3.29	1.48	1.41
19	B	1759	CLA	C4B-CHC	3.30	1.48	1.39
19	3	1214	CLA	C4B-CHC	3.31	1.50	1.43
19	3	3007	CLA	C1B-CHB	3.31	1.49	1.39
19	A	1761	CLA	C4B-CHC	3.31	1.49	1.39
19	K	1146	CLA	O2A-CGA	3.31	1.43	1.33
19	2	2010	CLA	C4B-CHC	3.32	1.50	1.43
19	4	1200	CLA	C1B-CHB	3.33	1.49	1.39
19	4	1199	CLA	C4B-CHC	3.34	1.49	1.39
19	B	1768	CLA	OBD-CAD	3.35	1.27	1.22
19	A	1778	CLA	C1B-CHB	3.35	1.49	1.39
19	3	3015	CLA	C4B-CHC	3.36	1.50	1.43
19	4	1204	CLA	C1B-CHB	3.36	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1743	CLA	OBD-CAD	3.37	1.27	1.22
19	1	1192	CLA	C1B-CHB	3.37	1.49	1.39
19	3	1215	CLA	C4B-CHC	3.37	1.50	1.43
19	F	1157	CLA	O2A-CGA	3.38	1.43	1.33
19	B	1767	CLA	C1B-CHB	3.41	1.49	1.39
19	B	1753	CLA	O2A-CGA	3.41	1.43	1.33
19	4	1209	CLA	O2D-CGD	3.41	1.41	1.33
19	B	1758	CLA	C1B-CHB	3.42	1.49	1.39
19	4	1208	CLA	C4B-CHC	3.42	1.50	1.43
19	B	1737	CLA	C4B-CHC	3.43	1.49	1.39
19	3	3014	CLA	C4B-CHC	3.44	1.50	1.43
19	4	1206	CLA	C4B-CHC	3.44	1.50	1.43
19	A	1801	CLA	C1B-CHB	3.44	1.49	1.39
19	A	1800	CLA	C1B-CHB	3.44	1.49	1.39
19	A	1817	CLA	C4B-CHC	3.44	1.49	1.39
19	A	1816	CLA	OBD-CAD	3.45	1.27	1.22
19	1	1197	CLA	CHD-C4C	3.45	1.49	1.41
19	A	1789	CLA	C4B-CHC	3.46	1.49	1.39
19	4	4007	CLA	C1B-CHB	3.47	1.49	1.39
19	2	1220	CLA	OBD-CAD	3.47	1.27	1.22
19	A	1778	CLA	C4B-CHC	3.47	1.49	1.39
19	1	1187	CLA	O2A-CGA	3.48	1.44	1.32
20	A	7026	LMU	O3B-C3B	3.49	1.51	1.43
19	J	1045	CLA	C4B-CHC	3.49	1.49	1.39
19	2	1216	CLA	CHD-C4C	3.49	1.49	1.41
19	B	1750	CLA	OBD-CAD	3.51	1.27	1.22
19	B	1769	CLA	OBD-CAD	3.51	1.27	1.22
19	L	1166	CLA	C1B-CHB	3.51	1.49	1.39
19	J	1045	CLA	OBD-CAD	3.52	1.27	1.22
19	1	1195	CLA	C4B-CHC	3.53	1.49	1.39
20	A	7047	LMU	O1'-C1'	3.54	1.46	1.40
19	1	1187	CLA	CHC-C1C	3.55	1.46	1.35
19	3	1218	CLA	O2A-CGA	3.55	1.44	1.33
19	3	1218	CLA	CHC-C1C	3.55	1.46	1.35
19	A	1772	CLA	C4B-CHC	3.55	1.49	1.39
19	A	1759	CLA	C4B-CHC	3.55	1.49	1.39
19	4	1209	CLA	C4B-CHC	3.55	1.49	1.39
19	J	1044	CLA	CHD-C4C	3.56	1.49	1.41
19	A	1774	CLA	C4B-CHC	3.56	1.49	1.39
19	A	1790	CLA	C4B-CHC	3.57	1.49	1.39
19	A	1772	CLA	O2A-CGA	3.57	1.44	1.33
19	4	1203	CLA	C4B-CHC	3.57	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1195	CLA	CHD-C4C	3.58	1.49	1.41
19	1	1194	CLA	C4B-CHC	3.58	1.51	1.43
19	3	3008	CLA	C4B-CHC	3.58	1.49	1.39
19	J	1044	CLA	O2A-CGA	3.58	1.44	1.33
19	F	1157	CLA	CHD-C4C	3.58	1.49	1.41
19	1	1197	CLA	C1B-CHB	3.59	1.49	1.39
19	A	1786	CLA	OBD-CAD	3.59	1.27	1.22
19	A	1815	CLA	C4B-CHC	3.59	1.49	1.39
19	A	1772	CLA	OBD-CAD	3.60	1.27	1.22
19	J	1044	CLA	C4B-CHC	3.61	1.49	1.39
19	1	1198	CLA	C4B-CHC	3.61	1.49	1.39
19	B	1739	CLA	C4B-CHC	3.61	1.49	1.39
20	A	7031	LMU	O1'-C1'	3.62	1.46	1.40
19	3	3007	CLA	C4B-CHC	3.63	1.49	1.39
19	A	1788	CLA	C4B-CHC	3.63	1.49	1.39
19	A	1780	CLA	OBD-CAD	3.64	1.27	1.22
19	J	1045	CLA	O2A-CGA	3.65	1.44	1.33
19	A	1769	CLA	OBD-CAD	3.66	1.27	1.22
19	H	1079	CLA	C4B-CHC	3.66	1.49	1.39
19	2	1218	CLA	C4B-CHC	3.66	1.49	1.39
19	B	1754	CLA	C4B-CHC	3.66	1.49	1.39
19	A	1783	CLA	O2A-CGA	3.66	1.44	1.33
19	B	1742	CLA	C4B-CHC	3.67	1.50	1.39
19	A	1769	CLA	C4B-CHC	3.67	1.50	1.39
19	B	1749	CLA	OBD-CAD	3.67	1.28	1.22
19	B	1787	CLA	C4B-CHC	3.67	1.50	1.39
19	B	1748	CLA	C4B-CHC	3.68	1.50	1.39
19	A	1811	CLA	OBD-CAD	3.68	1.28	1.22
19	B	1746	CLA	O2A-CGA	3.68	1.45	1.32
19	4	1198	CLA	O2D-CGD	3.70	1.42	1.33
19	B	1771	CLA	C4B-CHC	3.70	1.50	1.39
19	A	1784	CLA	C4B-CHC	3.70	1.50	1.39
19	2	1220	CLA	C4B-CHC	3.72	1.50	1.39
19	A	1800	CLA	C4B-CHC	3.72	1.50	1.39
19	A	1762	CLA	C4B-CHC	3.72	1.50	1.39
19	2	1224	CLA	C4B-CHC	3.72	1.50	1.39
19	B	1753	CLA	C4B-CHC	3.75	1.50	1.39
19	B	1761	CLA	C4B-CHC	3.75	1.50	1.39
19	4	1205	CLA	C4B-CHC	3.75	1.51	1.43
19	4	1198	CLA	OBD-CAD	3.75	1.28	1.22
19	1	1187	CLA	CHD-C4C	3.75	1.50	1.41
19	4	1201	CLA	CHD-C4C	3.75	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1209	CLA	O2A-CGA	3.75	1.45	1.32
19	B	1748	CLA	O2A-CGA	3.76	1.44	1.33
19	2	1214	CLA	CHD-C4C	3.76	1.50	1.41
19	B	1752	CLA	C4B-CHC	3.76	1.50	1.39
19	4	4007	CLA	C4B-CHC	3.76	1.50	1.39
19	4	1197	CLA	C4B-CHC	3.76	1.50	1.39
19	R	1054	CLA	C4B-CHC	3.77	1.50	1.39
19	2	1222	CLA	C4B-CHC	3.77	1.50	1.39
19	3	1218	CLA	CHD-C4C	3.77	1.50	1.41
19	3	3001	CLA	C4B-CHC	3.77	1.51	1.43
19	3	3002	CLA	C4B-CHC	3.77	1.51	1.43
19	B	1736	CLA	C4B-CHC	3.77	1.50	1.39
19	3	3008	CLA	O2A-CGA	3.79	1.44	1.33
19	K	1146	CLA	C4B-CHC	3.79	1.50	1.39
19	J	1043	CLA	C4B-CHC	3.79	1.50	1.39
19	F	1157	CLA	C4B-CHC	3.79	1.50	1.39
19	A	1813	CLA	O2A-CGA	3.81	1.44	1.33
19	A	1786	CLA	C4B-CHC	3.81	1.50	1.39
19	2	1212	CLA	C4B-CHC	3.82	1.50	1.39
19	A	1764	CLA	C4B-CHC	3.82	1.50	1.39
19	R	1055	CLA	C1B-CHB	3.82	1.50	1.39
19	2	1227	CLA	CHD-C4C	3.83	1.50	1.41
19	A	1785	CLA	C4B-CHC	3.83	1.50	1.39
19	A	1787	CLA	C4B-CHC	3.83	1.50	1.39
19	1	1200	CLA	CHC-C1C	3.83	1.47	1.35
19	A	1798	CLA	C4B-CHC	3.83	1.50	1.39
19	1	1198	CLA	CHD-C4C	3.83	1.50	1.41
19	4	4014	CLA	C4B-CHC	3.84	1.50	1.39
19	K	1085	CLA	C4B-CHC	3.84	1.50	1.39
19	F	1155	CLA	C4B-CHC	3.84	1.50	1.39
19	F	1156	CLA	C4B-CHC	3.85	1.50	1.39
19	3	1219	CLA	C4B-CHC	3.85	1.50	1.39
19	B	1735	CLA	C4B-CHC	3.85	1.50	1.39
19	A	1782	CLA	C4B-CHC	3.85	1.50	1.39
19	K	1142	CLA	C4B-CHC	3.86	1.50	1.39
19	A	1796	CLA	C4B-CHC	3.86	1.50	1.39
19	B	1785	CLA	O2A-CGA	3.86	1.45	1.33
19	A	1799	CLA	C4B-CHC	3.86	1.50	1.39
19	B	1756	CLA	C4B-CHC	3.87	1.50	1.39
19	A	1794	CLA	C4B-CHC	3.87	1.50	1.39
19	B	1755	CLA	C4B-CHC	3.87	1.50	1.39
19	A	1812	CLA	C4B-CHC	3.87	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1795	CLA	C4B-CHC	3.87	1.50	1.39
19	A	1801	CLA	C4B-CHC	3.87	1.50	1.39
19	4	1196	CLA	C4B-CHC	3.87	1.50	1.39
19	J	1045	CLA	CHD-C4C	3.87	1.50	1.41
19	A	1792	CLA	C4B-CHC	3.87	1.50	1.39
19	A	1791	CLA	C4B-CHC	3.88	1.50	1.39
19	A	1780	CLA	C4B-CHC	3.88	1.50	1.39
19	B	1749	CLA	C4B-CHC	3.88	1.50	1.39
19	1	1190	CLA	C4B-CHC	3.88	1.50	1.39
19	A	1797	CLA	C4B-CHC	3.89	1.50	1.39
19	A	1793	CLA	C4B-CHC	3.89	1.50	1.39
19	A	1781	CLA	C4B-CHC	3.90	1.50	1.39
24	B	1783	LMG	O7-C10	3.91	1.46	1.34
19	B	1763	CLA	C4B-CHC	3.91	1.50	1.39
19	A	1763	CLA	C4B-CHC	3.91	1.50	1.39
19	A	1767	CLA	C4B-CHC	3.92	1.50	1.39
19	B	1744	CLA	C4B-CHC	3.92	1.50	1.39
19	B	1771	CLA	OBD-CAD	3.93	1.28	1.22
19	B	1758	CLA	O2A-CGA	3.93	1.45	1.33
19	3	3011	CLA	C4B-CHC	3.94	1.50	1.39
19	B	1747	CLA	C4B-CHC	3.94	1.50	1.39
19	B	1751	CLA	C4B-CHC	3.95	1.50	1.39
19	2	1217	CLA	C4B-CHC	3.95	1.50	1.39
19	B	1767	CLA	OBD-CAD	3.96	1.28	1.22
19	B	1785	CLA	C4B-CHC	3.96	1.50	1.39
19	L	1167	CLA	C4B-CHC	3.96	1.50	1.39
19	A	1775	CLA	C4B-CHC	3.96	1.50	1.39
19	2	1223	CLA	C4B-CHC	3.97	1.50	1.39
19	4	1204	CLA	C4B-CHC	3.97	1.50	1.39
19	B	1757	CLA	O2A-CGA	3.97	1.45	1.33
19	B	1740	CLA	C4B-CHC	3.98	1.50	1.39
19	2	1221	CLA	CHD-C4C	3.98	1.50	1.41
19	3	1212	CLA	C4B-CHC	3.98	1.50	1.39
19	A	1789	CLA	OBD-CAD	3.99	1.28	1.22
19	1	1200	CLA	CHD-C4C	3.99	1.50	1.41
19	A	1765	CLA	CHC-C1C	4.00	1.47	1.35
19	B	1762	CLA	OBD-CAD	4.01	1.28	1.22
19	A	1783	CLA	C4B-CHC	4.01	1.50	1.39
19	A	1813	CLA	C4B-CHC	4.02	1.50	1.39
19	4	1208	CLA	CHD-C4C	4.02	1.50	1.41
19	A	1763	CLA	O2A-CGA	4.03	1.46	1.32
19	1	1198	CLA	O2A-CGA	4.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1219	CLA	CHD-C4C	4.04	1.50	1.41
19	2	1221	CLA	C4B-CHC	4.04	1.52	1.43
19	B	1758	CLA	C4B-CHC	4.04	1.51	1.39
19	A	1816	CLA	CHD-C4C	4.04	1.50	1.41
19	B	1759	CLA	CHD-C4C	4.05	1.50	1.41
19	A	1774	CLA	OBD-CAD	4.05	1.28	1.22
19	B	1787	CLA	OBD-CAD	4.05	1.28	1.22
19	B	1760	CLA	OBD-CAD	4.05	1.28	1.22
19	B	1759	CLA	O2A-CGA	4.05	1.45	1.33
19	F	1157	CLA	O2D-CGD	4.06	1.43	1.33
19	1	1195	CLA	OBD-CAD	4.06	1.28	1.22
19	1	1192	CLA	C4B-CHC	4.06	1.51	1.39
19	A	1816	CLA	O2A-CGA	4.07	1.45	1.33
19	B	1740	CLA	OBD-CAD	4.07	1.28	1.22
19	4	1206	CLA	CHD-C4C	4.07	1.50	1.41
19	3	3014	CLA	CHD-C4C	4.07	1.50	1.41
19	A	1764	CLA	O2D-CGD	4.07	1.43	1.33
19	J	1046	CLA	CHD-C4C	4.07	1.50	1.41
19	A	1772	CLA	CHD-C4C	4.08	1.50	1.41
19	4	1207	CLA	C4B-CHC	4.08	1.51	1.39
19	2	1215	CLA	C4B-CHC	4.09	1.51	1.39
19	K	1085	CLA	O2A-CGA	4.10	1.45	1.33
19	2	1220	CLA	CHD-C4C	4.10	1.50	1.41
19	4	4003	CLA	CHD-C4C	4.11	1.50	1.41
19	A	1773	CLA	C4B-CHC	4.11	1.51	1.39
19	B	1772	CLA	C4B-CHC	4.11	1.51	1.39
19	1	1193	CLA	C4B-CHC	4.12	1.51	1.39
19	1	1200	CLA	O2A-CGA	4.12	1.45	1.33
19	A	1764	CLA	OBD-CAD	4.12	1.28	1.22
19	4	1196	CLA	O2A-CGA	4.12	1.45	1.33
24	B	1783	LMG	O8-C28	4.12	1.45	1.33
19	1	1190	CLA	O2A-CGA	4.13	1.47	1.32
19	1	1195	CLA	CHC-C1C	4.13	1.48	1.35
19	J	1043	CLA	O2A-CGA	4.13	1.45	1.33
19	A	1771	CLA	C4B-CHC	4.14	1.51	1.39
19	A	1811	CLA	O2A-CGA	4.14	1.45	1.33
19	B	1765	CLA	C4B-CHC	4.14	1.51	1.39
19	B	1753	CLA	CHC-C1C	4.14	1.48	1.35
19	B	1738	CLA	O2A-CGA	4.14	1.45	1.33
19	K	1146	CLA	CHD-C4C	4.14	1.50	1.41
19	R	1054	CLA	OBD-CAD	4.14	1.28	1.22
19	A	1817	CLA	OBD-CAD	4.14	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1212	CLA	O2A-CGA	4.14	1.45	1.33
19	B	1769	CLA	CHD-C4C	4.14	1.51	1.41
19	3	1219	CLA	O2A-CGA	4.15	1.45	1.33
19	B	1735	CLA	O2A-CGA	4.15	1.45	1.33
19	A	1793	CLA	O2A-CGA	4.15	1.45	1.33
19	A	1794	CLA	O2A-CGA	4.16	1.45	1.33
19	L	1505	CLA	C4B-CHC	4.16	1.51	1.39
19	2	1215	CLA	OBD-CAD	4.16	1.28	1.22
19	A	1766	CLA	C4B-CHC	4.17	1.51	1.39
19	A	1792	CLA	O2A-CGA	4.17	1.45	1.33
19	A	1795	CLA	O2A-CGA	4.17	1.45	1.33
19	1	1192	CLA	CHD-C4C	4.17	1.51	1.41
19	A	1781	CLA	O2A-CGA	4.17	1.45	1.33
19	A	1796	CLA	O2A-CGA	4.17	1.45	1.33
19	B	1756	CLA	O2A-CGA	4.17	1.45	1.33
19	B	1764	CLA	C4B-CHC	4.17	1.51	1.39
19	A	1780	CLA	O2A-CGA	4.18	1.45	1.33
19	A	1782	CLA	O2A-CGA	4.18	1.45	1.33
19	A	1797	CLA	O2A-CGA	4.18	1.45	1.33
19	A	1760	CLA	C4B-CHC	4.18	1.51	1.39
19	4	4014	CLA	O2A-CGA	4.18	1.45	1.33
19	B	1755	CLA	O2A-CGA	4.19	1.45	1.33
19	1	1197	CLA	O2A-CGA	4.19	1.45	1.33
19	I	1033	CLA	C4B-CHC	4.19	1.51	1.39
19	L	1168	CLA	C4B-CHC	4.19	1.51	1.39
19	B	1759	CLA	OBD-CAD	4.19	1.28	1.22
19	B	1760	CLA	C4B-CHC	4.20	1.51	1.39
19	A	1779	CLA	C4B-CHC	4.20	1.51	1.39
19	A	1765	CLA	O2D-CGD	4.20	1.43	1.33
19	2	1222	CLA	OBD-CAD	4.20	1.28	1.22
19	B	1749	CLA	CHD-C4C	4.20	1.51	1.41
19	2	1212	CLA	OBD-CAD	4.20	1.28	1.22
19	B	1742	CLA	OBD-CAD	4.22	1.28	1.22
19	B	1748	CLA	CHD-C4C	4.23	1.51	1.41
19	B	1786	CLA	C4B-CHC	4.23	1.51	1.39
19	B	1746	CLA	C4B-CHC	4.23	1.51	1.39
19	1	1198	CLA	OBD-CAD	4.23	1.28	1.22
19	B	1771	CLA	CHD-C4C	4.23	1.51	1.41
19	B	1770	CLA	OBD-CAD	4.23	1.28	1.22
19	A	1782	CLA	OBD-CAD	4.23	1.28	1.22
19	B	1758	CLA	CHD-C4C	4.24	1.51	1.41
19	B	1750	CLA	C4B-CHC	4.24	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1759	CLA	O2A-CGA	4.24	1.46	1.33
19	K	1142	CLA	OBD-CAD	4.25	1.28	1.22
19	B	1770	CLA	C4B-CHC	4.25	1.51	1.39
19	B	1769	CLA	C4B-CHC	4.25	1.51	1.39
19	2	1217	CLA	O2A-CGA	4.25	1.46	1.33
19	A	1768	CLA	C4B-CHC	4.25	1.51	1.39
19	A	1776	CLA	C4B-CHC	4.26	1.51	1.39
19	A	1812	CLA	OBD-CAD	4.26	1.28	1.22
19	A	1816	CLA	C4B-CHC	4.26	1.51	1.39
19	A	1764	CLA	O2A-CGA	4.26	1.46	1.33
19	2	1223	CLA	CHD-C4C	4.26	1.51	1.41
19	B	1763	CLA	O2A-CGA	4.26	1.46	1.33
19	J	1044	CLA	OBD-CAD	4.27	1.28	1.22
19	3	1216	CLA	CHD-C4C	4.27	1.51	1.41
19	A	1790	CLA	OBD-CAD	4.27	1.28	1.22
19	3	1213	CLA	CHD-C4C	4.27	1.51	1.41
19	B	1739	CLA	O2A-CGA	4.28	1.46	1.33
19	A	1791	CLA	OBD-CAD	4.28	1.28	1.22
19	B	1741	CLA	C4B-CHC	4.28	1.51	1.39
19	4	1204	CLA	O2A-CGA	4.28	1.46	1.33
19	B	1761	CLA	OBD-CAD	4.28	1.28	1.22
19	4	1207	CLA	CHD-C4C	4.29	1.51	1.41
19	A	1796	CLA	OBD-CAD	4.29	1.28	1.22
19	F	1156	CLA	OBD-CAD	4.29	1.28	1.22
19	B	1745	CLA	OBD-CAD	4.29	1.28	1.22
19	A	1800	CLA	O2A-CGA	4.29	1.46	1.33
19	A	1783	CLA	O2D-CGD	4.29	1.44	1.33
19	3	1219	CLA	OBD-CAD	4.30	1.28	1.22
19	2	1220	CLA	O2A-CGA	4.30	1.46	1.33
19	A	1770	CLA	C4B-CHC	4.31	1.51	1.39
19	1	1197	CLA	CHC-C1C	4.31	1.48	1.35
19	A	1795	CLA	OBD-CAD	4.31	1.28	1.22
19	B	1756	CLA	OBD-CAD	4.31	1.28	1.22
19	L	1166	CLA	C4B-CHC	4.31	1.51	1.39
19	4	4014	CLA	OBD-CAD	4.32	1.28	1.22
19	K	1146	CLA	CHC-C1C	4.32	1.48	1.35
19	B	1755	CLA	OBD-CAD	4.32	1.28	1.22
19	A	1797	CLA	OBD-CAD	4.32	1.28	1.22
19	3	3015	CLA	CHD-C4C	4.32	1.51	1.41
19	A	1799	CLA	O2A-CGA	4.32	1.46	1.33
19	A	1816	CLA	O2D-CGD	4.33	1.44	1.33
19	A	1765	CLA	OBD-CAD	4.33	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1762	CLA	O2A-CGA	4.33	1.46	1.33
19	B	1735	CLA	OBD-CAD	4.34	1.29	1.22
19	A	1785	CLA	O2A-CGA	4.34	1.46	1.33
19	4	1196	CLA	OBD-CAD	4.34	1.29	1.22
19	A	1777	CLA	C4B-CHC	4.34	1.51	1.39
19	K	1085	CLA	OBD-CAD	4.34	1.29	1.22
19	A	1792	CLA	OBD-CAD	4.34	1.29	1.22
19	B	1768	CLA	O2D-CGD	4.35	1.44	1.33
19	J	1043	CLA	OBD-CAD	4.35	1.29	1.22
19	B	1766	CLA	C4B-CHC	4.35	1.51	1.39
19	B	1757	CLA	C4B-CHC	4.35	1.51	1.39
19	B	1757	CLA	OBD-CAD	4.35	1.29	1.22
19	B	1752	CLA	O2A-CGA	4.35	1.46	1.33
19	A	1793	CLA	OBD-CAD	4.36	1.29	1.22
19	1	1197	CLA	O2D-CGD	4.36	1.44	1.33
19	I	1031	CLA	C4B-CHC	4.37	1.51	1.39
19	4	1200	CLA	C4B-CHC	4.37	1.51	1.39
19	A	1794	CLA	OBD-CAD	4.37	1.29	1.22
19	B	1742	CLA	CHD-C4C	4.38	1.51	1.41
19	2	1217	CLA	CHD-C4C	4.38	1.51	1.41
19	4	1197	CLA	CHD-C4C	4.39	1.51	1.41
19	B	1772	CLA	CHD-C4C	4.39	1.51	1.41
19	B	1763	CLA	CHC-C1C	4.39	1.49	1.35
19	A	1788	CLA	O2D-CGD	4.39	1.44	1.33
19	4	1205	CLA	CHD-C4C	4.40	1.51	1.41
19	A	1768	CLA	OBD-CAD	4.40	1.29	1.22
19	B	1762	CLA	CHD-C4C	4.41	1.51	1.41
19	L	1166	CLA	CHD-C4C	4.41	1.51	1.41
19	B	1771	CLA	CHC-C1C	4.41	1.49	1.35
19	A	1781	CLA	OBD-CAD	4.42	1.29	1.22
19	4	1198	CLA	CHC-C1C	4.42	1.49	1.35
19	G	1099	CLA	C4B-CHC	4.42	1.52	1.39
19	3	3002	CLA	CHD-C4C	4.42	1.51	1.41
19	1	1194	CLA	CHD-C4C	4.43	1.51	1.41
19	B	1745	CLA	C4B-CHC	4.43	1.52	1.39
19	1	1191	CLA	C4B-CHC	4.44	1.52	1.39
19	3	3008	CLA	CHD-C4C	4.44	1.51	1.41
19	L	1168	CLA	CMA-C3A	4.45	1.63	1.53
19	R	1055	CLA	CHD-C4C	4.46	1.51	1.41
19	J	1043	CLA	CHD-C4C	4.47	1.51	1.41
19	3	1215	CLA	CHD-C4C	4.47	1.51	1.41
19	3	1214	CLA	CHD-C4C	4.47	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	1055	CLA	C4B-CHC	4.47	1.52	1.39
19	A	1801	CLA	CHD-C4C	4.47	1.51	1.41
19	4	1200	CLA	O2A-CGA	4.47	1.46	1.33
19	2	1224	CLA	CHD-C4C	4.48	1.51	1.41
19	1	1193	CLA	CHD-C4C	4.49	1.51	1.41
19	J	1045	CLA	CHC-C1C	4.50	1.49	1.35
19	1	1189	CLA	O2A-CGA	4.50	1.46	1.33
19	B	1745	CLA	CHD-C4C	4.50	1.51	1.41
19	2	1213	CLA	C4B-CHC	4.50	1.52	1.39
19	B	1755	CLA	CHD-C4C	4.50	1.51	1.41
19	A	1784	CLA	OBD-CAD	4.50	1.29	1.22
19	A	1794	CLA	CHD-C4C	4.50	1.51	1.41
19	B	1737	CLA	OBD-CAD	4.50	1.29	1.22
19	K	1142	CLA	CHD-C4C	4.51	1.51	1.41
19	4	4007	CLA	O2A-CGA	4.51	1.46	1.33
19	A	1767	CLA	OBD-CAD	4.51	1.29	1.22
19	A	1791	CLA	CHD-C4C	4.51	1.51	1.41
19	L	1166	CLA	OBD-CAD	4.52	1.29	1.22
19	A	1811	CLA	CHD-C4C	4.52	1.51	1.41
19	A	1781	CLA	CHD-C4C	4.52	1.51	1.41
19	F	1156	CLA	CHD-C4C	4.52	1.51	1.41
19	A	1782	CLA	CHD-C4C	4.52	1.51	1.41
19	A	1796	CLA	CHD-C4C	4.53	1.51	1.41
19	A	1793	CLA	CHD-C4C	4.53	1.51	1.41
19	I	1031	CLA	CHD-C4C	4.53	1.51	1.41
19	A	1795	CLA	CHD-C4C	4.53	1.51	1.41
19	A	1815	CLA	OBD-CAD	4.54	1.29	1.22
19	1	1192	CLA	O2A-CGA	4.54	1.47	1.33
19	L	1505	CLA	O2A-CGA	4.54	1.47	1.33
19	4	1196	CLA	CHD-C4C	4.54	1.51	1.41
19	1	1196	CLA	C4B-CHC	4.54	1.52	1.39
19	A	1787	CLA	O2A-CGA	4.54	1.47	1.33
19	2	1215	CLA	O2A-CGA	4.54	1.47	1.33
19	B	1735	CLA	CHD-C4C	4.55	1.51	1.41
19	A	1797	CLA	CHD-C4C	4.55	1.51	1.41
19	3	1219	CLA	CHD-C4C	4.55	1.51	1.41
19	K	1085	CLA	CHD-C4C	4.55	1.51	1.41
19	A	1792	CLA	CHD-C4C	4.55	1.51	1.41
19	B	1764	CLA	CHD-C4C	4.56	1.51	1.41
19	F	1157	CLA	CHC-C1C	4.56	1.49	1.35
19	1	1188	CLA	CHD-C4C	4.56	1.51	1.41
19	B	1763	CLA	CHD-C4C	4.56	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1786	CLA	O2D-CGD	4.56	1.44	1.33
19	L	1167	CLA	O2A-CGA	4.57	1.47	1.33
19	B	1761	CLA	CHC-C1C	4.57	1.49	1.35
19	B	1745	CLA	O2A-CGA	4.57	1.47	1.33
19	B	1754	CLA	O2A-CGA	4.57	1.47	1.33
19	1	1198	CLA	CHC-C1C	4.57	1.49	1.35
19	B	1742	CLA	O2A-CGA	4.58	1.47	1.33
19	2	1212	CLA	CHD-C4C	4.58	1.52	1.41
19	A	1776	CLA	OBD-CAD	4.58	1.29	1.22
19	A	1765	CLA	O2A-CGA	4.58	1.47	1.33
19	A	1789	CLA	O2A-CGA	4.58	1.47	1.33
19	A	1813	CLA	CHC-C1C	4.59	1.49	1.35
19	3	3011	CLA	OBD-CAD	4.59	1.29	1.22
19	B	1756	CLA	CHD-C4C	4.59	1.52	1.41
19	2	1218	CLA	O2A-CGA	4.59	1.47	1.33
19	L	1168	CLA	O2A-CGA	4.59	1.47	1.33
19	2	1222	CLA	O2A-CGA	4.60	1.47	1.33
19	A	1780	CLA	O2D-CGD	4.60	1.44	1.33
19	B	1769	CLA	O2A-CGA	4.60	1.47	1.33
19	B	1738	CLA	CHC-C1C	4.60	1.49	1.35
19	B	1754	CLA	CHC-C1C	4.60	1.49	1.35
19	B	1767	CLA	O2D-CGD	4.61	1.45	1.33
19	B	1743	CLA	CHD-C4C	4.61	1.52	1.41
19	B	1761	CLA	CHD-C4C	4.61	1.52	1.41
19	A	1777	CLA	O2A-CGA	4.61	1.47	1.33
19	B	1785	CLA	OBD-CAD	4.61	1.29	1.22
19	A	1773	CLA	OBD-CAD	4.61	1.29	1.22
19	I	1033	CLA	O2A-CGA	4.62	1.47	1.33
19	4	4007	CLA	CHD-C4C	4.62	1.52	1.41
19	1	1188	CLA	OBD-CAD	4.62	1.29	1.22
19	K	3009	CLA	C4B-CHC	4.62	1.52	1.39
19	4	4014	CLA	CHD-C4C	4.62	1.52	1.41
19	A	1812	CLA	CHD-C4C	4.63	1.52	1.41
19	G	1099	CLA	O2A-CGA	4.63	1.47	1.33
19	1	1190	CLA	CHD-C4C	4.64	1.52	1.41
19	K	3009	CLA	CHD-C4C	4.64	1.52	1.41
19	A	1775	CLA	CHD-C4C	4.64	1.52	1.41
19	L	1167	CLA	OBD-CAD	4.64	1.29	1.22
19	A	1784	CLA	CHD-C4C	4.64	1.52	1.41
19	B	1762	CLA	O2D-CGD	4.64	1.45	1.33
19	A	1788	CLA	OBD-CAD	4.64	1.29	1.22
19	B	1737	CLA	CHC-C1C	4.65	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1202	CLA	CHD-C4C	4.65	1.52	1.41
19	B	1762	CLA	C4B-CHC	4.65	1.52	1.39
19	B	1743	CLA	O2A-CGA	4.66	1.47	1.33
19	1	1188	CLA	CHC-C1C	4.66	1.49	1.35
19	B	1771	CLA	O2A-CGA	4.67	1.47	1.33
19	A	1769	CLA	O2A-CGA	4.67	1.47	1.33
19	3	3007	CLA	CHD-C4C	4.67	1.52	1.41
19	B	1785	CLA	O2D-CGD	4.67	1.45	1.33
19	B	1768	CLA	CHC-C1C	4.68	1.50	1.35
19	A	1761	CLA	CHC-C1C	4.68	1.50	1.35
19	4	1204	CLA	CHD-C4C	4.68	1.52	1.41
19	B	1736	CLA	O2D-CGD	4.68	1.45	1.33
19	B	1738	CLA	CHD-C4C	4.69	1.52	1.41
19	B	1743	CLA	C4B-CHC	4.69	1.52	1.39
19	A	1789	CLA	CHC-C1C	4.70	1.50	1.35
19	A	1772	CLA	CHC-C1C	4.70	1.50	1.35
19	1	1199	CLA	CHD-C4C	4.70	1.52	1.41
19	B	1770	CLA	O2A-CGA	4.70	1.47	1.33
19	B	1751	CLA	CHD-C4C	4.70	1.52	1.41
19	3	3011	CLA	O2A-CGA	4.70	1.47	1.33
19	B	1787	CLA	CHD-C4C	4.70	1.52	1.41
19	A	1773	CLA	CHD-C4C	4.71	1.52	1.41
19	A	1788	CLA	O2A-CGA	4.71	1.47	1.33
19	L	1505	CLA	OBD-CAD	4.71	1.29	1.22
19	1	1201	CLA	CHD-C4C	4.71	1.52	1.41
19	A	1798	CLA	O2A-CGA	4.71	1.47	1.33
19	A	1774	CLA	CHD-C4C	4.72	1.52	1.41
19	A	1800	CLA	CHD-C4C	4.72	1.52	1.41
19	A	1811	CLA	C4B-CHC	4.72	1.52	1.39
19	1	1189	CLA	CHD-C4C	4.72	1.52	1.41
19	3	3011	CLA	CHD-C4C	4.73	1.52	1.41
19	A	1769	CLA	CHD-C4C	4.73	1.52	1.41
19	A	1759	CLA	OBD-CAD	4.73	1.29	1.22
19	2	1222	CLA	O2D-CGD	4.73	1.45	1.33
19	1	1189	CLA	C4B-CHC	4.73	1.52	1.39
19	J	1044	CLA	CHC-C1C	4.74	1.50	1.35
19	A	1772	CLA	O2D-CGD	4.74	1.45	1.33
19	A	1783	CLA	OBD-CAD	4.74	1.29	1.22
19	B	1786	CLA	OBD-CAD	4.75	1.29	1.22
19	A	1769	CLA	O2D-CGD	4.75	1.45	1.33
19	A	1774	CLA	O2A-CGA	4.75	1.47	1.33
19	1	1196	CLA	OBD-CAD	4.76	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	4007	CLA	CHC-C1C	4.76	1.50	1.35
19	1	1193	CLA	O2A-CGA	4.76	1.47	1.33
19	B	1750	CLA	CHD-C4C	4.77	1.52	1.41
19	2	1220	CLA	CHC-C1C	4.77	1.50	1.35
19	4	1199	CLA	CHD-C4C	4.77	1.52	1.41
19	2	2010	CLA	CHD-C4C	4.77	1.52	1.41
19	A	1778	CLA	CHC-C1C	4.77	1.50	1.35
19	A	1779	CLA	CHD-C4C	4.77	1.52	1.41
19	A	1799	CLA	CHC-C1C	4.77	1.50	1.35
19	1	1190	CLA	CHC-C1C	4.77	1.50	1.35
19	4	1201	CLA	CHC-C1C	4.77	1.50	1.35
19	I	1031	CLA	O2D-CGD	4.78	1.45	1.33
19	A	1760	CLA	O2D-CGD	4.79	1.45	1.33
19	A	1759	CLA	CHC-C1C	4.79	1.50	1.35
19	B	1761	CLA	O2A-CGA	4.80	1.47	1.33
19	B	1770	CLA	O2D-CGD	4.80	1.45	1.33
19	B	1765	CLA	CHD-C4C	4.80	1.52	1.41
19	A	1790	CLA	O2A-CGA	4.80	1.47	1.33
19	B	1768	CLA	O2A-CGA	4.80	1.47	1.33
19	B	1739	CLA	OBD-CAD	4.80	1.29	1.22
19	L	1168	CLA	CHD-C4C	4.81	1.52	1.41
19	J	1045	CLA	O2D-CGD	4.81	1.45	1.33
19	B	1743	CLA	O2D-CGD	4.81	1.45	1.33
19	A	1776	CLA	O2A-CGA	4.82	1.47	1.33
19	A	1776	CLA	CHD-C4C	4.83	1.52	1.41
19	B	1754	CLA	CHD-C4C	4.83	1.52	1.41
19	4	1199	CLA	CHC-C1C	4.83	1.50	1.35
19	B	1758	CLA	CHC-C1C	4.83	1.50	1.35
19	2	1217	CLA	CHC-C1C	4.83	1.50	1.35
19	3	1217	CLA	CHD-C4C	4.83	1.52	1.41
19	4	1199	CLA	O2A-CGA	4.84	1.47	1.33
19	A	1788	CLA	CHD-C4C	4.84	1.52	1.41
19	F	1155	CLA	OBD-CAD	4.84	1.29	1.22
19	A	1759	CLA	CHD-C4C	4.84	1.52	1.41
19	A	1801	CLA	O2A-CGA	4.84	1.47	1.33
19	A	1771	CLA	O2A-CGA	4.84	1.47	1.33
19	A	1800	CLA	CHC-C1C	4.84	1.50	1.35
19	3	3008	CLA	CHC-C1C	4.85	1.50	1.35
19	B	1767	CLA	CHC-C1C	4.85	1.50	1.35
19	B	1747	CLA	OBD-CAD	4.85	1.29	1.22
19	B	1785	CLA	CHD-C4C	4.86	1.52	1.41
19	B	1766	CLA	CHD-C4C	4.86	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1746	CLA	CHD-C4C	4.86	1.52	1.41
19	B	1767	CLA	O2A-CGA	4.86	1.48	1.33
19	A	1788	CLA	CHC-C1C	4.86	1.50	1.35
19	B	1749	CLA	O2D-CGD	4.86	1.45	1.33
19	2	1224	CLA	CHC-C1C	4.86	1.50	1.35
19	1	1200	CLA	O2D-CGD	4.86	1.45	1.33
19	1	1191	CLA	CHD-C4C	4.87	1.52	1.41
19	2	1215	CLA	CHD-C4C	4.87	1.52	1.41
19	4	1200	CLA	CHD-C4C	4.87	1.52	1.41
19	A	1763	CLA	CHC-C1C	4.88	1.50	1.35
19	A	1800	CLA	OBD-CAD	4.88	1.29	1.22
19	B	1746	CLA	CHC-C1C	4.88	1.50	1.35
19	B	1740	CLA	CHD-C4C	4.88	1.52	1.41
19	A	1815	CLA	CHC-C1C	4.88	1.50	1.35
19	3	3001	CLA	CHD-C4C	4.89	1.52	1.41
19	B	1755	CLA	O2D-CGD	4.89	1.45	1.33
19	K	1142	CLA	O2D-CGD	4.89	1.45	1.33
19	A	1813	CLA	O2D-CGD	4.89	1.45	1.33
19	H	1079	CLA	CHD-C4C	4.89	1.52	1.41
19	B	1758	CLA	O2D-CGD	4.89	1.45	1.33
19	A	1781	CLA	O2D-CGD	4.89	1.45	1.33
19	A	1779	CLA	OBD-CAD	4.90	1.29	1.22
19	A	1780	CLA	CHD-C4C	4.90	1.52	1.41
19	B	1786	CLA	O2A-CGA	4.90	1.48	1.33
19	A	1786	CLA	CHD-C4C	4.90	1.52	1.41
19	B	1771	CLA	O2D-CGD	4.90	1.45	1.33
23	B	1773	PQN	C10-C5	4.91	1.48	1.40
19	3	1219	CLA	CHC-C1C	4.91	1.50	1.35
19	B	1766	CLA	O2A-CGA	4.91	1.48	1.33
19	2	1212	CLA	O2D-CGD	4.91	1.45	1.33
19	A	1781	CLA	CHC-C1C	4.92	1.50	1.35
19	K	3009	CLA	O2A-CGA	4.92	1.48	1.33
19	B	1752	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1812	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1793	CLA	CHC-C1C	4.92	1.50	1.35
19	1	1192	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1790	CLA	CHD-C4C	4.92	1.52	1.41
19	B	1751	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1797	CLA	CHC-C1C	4.92	1.50	1.35
19	4	1209	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1785	CLA	CHD-C4C	4.92	1.52	1.41
19	A	1763	CLA	CHD-C4C	4.92	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	1156	CLA	CHC-C1C	4.92	1.50	1.35
19	A	1767	CLA	CHD-C4C	4.93	1.52	1.41
19	1	1196	CLA	CHD-C4C	4.93	1.52	1.41
19	3	3011	CLA	CHC-C1C	4.93	1.50	1.35
19	B	1763	CLA	OBD-CAD	4.93	1.29	1.22
19	A	1796	CLA	CHC-C1C	4.93	1.50	1.35
19	3	1219	CLA	O2D-CGD	4.93	1.45	1.33
19	3	3008	CLA	O2D-CGD	4.93	1.45	1.33
19	A	1782	CLA	CHC-C1C	4.93	1.50	1.35
19	K	1142	CLA	CHC-C1C	4.93	1.50	1.35
19	J	1043	CLA	CHC-C1C	4.93	1.50	1.35
19	A	1766	CLA	OBD-CAD	4.93	1.29	1.22
19	A	1794	CLA	CHC-C1C	4.94	1.50	1.35
19	A	1795	CLA	CHC-C1C	4.94	1.50	1.35
19	B	1756	CLA	CHC-C1C	4.94	1.50	1.35
19	B	1786	CLA	O2D-CGD	4.94	1.45	1.33
19	A	1768	CLA	CHC-C1C	4.94	1.50	1.35
19	A	1791	CLA	O2D-CGD	4.94	1.45	1.33
19	B	1735	CLA	CHC-C1C	4.94	1.50	1.35
19	A	1791	CLA	CHC-C1C	4.94	1.50	1.35
19	B	1765	CLA	OBD-CAD	4.94	1.29	1.22
19	A	1762	CLA	CHC-C1C	4.94	1.50	1.35
19	A	1793	CLA	O2D-CGD	4.95	1.45	1.33
19	H	1079	CLA	CHC-C1C	4.95	1.50	1.35
19	A	1760	CLA	CHD-C4C	4.95	1.52	1.41
19	F	1156	CLA	O2D-CGD	4.95	1.45	1.33
19	B	1740	CLA	O2D-CGD	4.95	1.45	1.33
19	B	1756	CLA	O2D-CGD	4.95	1.45	1.33
19	L	1166	CLA	O2A-CGA	4.95	1.48	1.33
19	B	1755	CLA	CHC-C1C	4.95	1.50	1.35
19	B	1735	CLA	O2D-CGD	4.95	1.45	1.33
19	B	1772	CLA	CHC-C1C	4.95	1.50	1.35
19	A	1792	CLA	CHC-C1C	4.96	1.50	1.35
19	K	1085	CLA	O2D-CGD	4.96	1.45	1.33
19	A	1759	CLA	O2D-CGD	4.96	1.45	1.33
19	4	4014	CLA	CHC-C1C	4.96	1.50	1.35
19	J	1043	CLA	O2D-CGD	4.96	1.45	1.33
19	A	1792	CLA	O2D-CGD	4.96	1.45	1.33
19	A	1795	CLA	O2D-CGD	4.96	1.45	1.33
19	A	1797	CLA	O2D-CGD	4.97	1.45	1.33
19	A	1767	CLA	O2D-CGD	4.97	1.45	1.33
19	3	3007	CLA	CHC-C1C	4.97	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1764	CLA	CHD-C4C	4.97	1.52	1.41
19	2	1212	CLA	CHC-C1C	4.97	1.50	1.35
19	A	1796	CLA	O2D-CGD	4.98	1.45	1.33
19	A	1794	CLA	O2D-CGD	4.98	1.45	1.33
19	B	1741	CLA	O2D-CGD	4.98	1.45	1.33
19	H	1079	CLA	O2A-CGA	4.98	1.48	1.33
19	A	1775	CLA	CHC-C1C	4.98	1.50	1.35
19	R	1054	CLA	CHD-C4C	4.98	1.53	1.41
19	G	1099	CLA	CHD-C4C	4.98	1.53	1.41
19	A	1785	CLA	OBD-CAD	4.99	1.30	1.22
19	2	1224	CLA	OBD-CAD	4.99	1.30	1.22
19	K	1085	CLA	CHC-C1C	4.99	1.51	1.35
19	4	1196	CLA	CHC-C1C	4.99	1.51	1.35
19	2	1220	CLA	O2D-CGD	4.99	1.45	1.33
19	4	4014	CLA	O2D-CGD	4.99	1.45	1.33
19	B	1742	CLA	CHC-C1C	5.00	1.51	1.35
19	4	1196	CLA	O2D-CGD	5.00	1.46	1.33
19	A	1767	CLA	CHC-C1C	5.00	1.51	1.35
19	A	1790	CLA	CHC-C1C	5.00	1.51	1.35
19	L	1168	CLA	CHC-C1C	5.00	1.51	1.35
19	4	1198	CLA	CHD-C4C	5.00	1.53	1.41
19	B	1786	CLA	CHC-C1C	5.00	1.51	1.35
19	L	1505	CLA	CHD-C4C	5.00	1.53	1.41
19	4	1201	CLA	O2D-CGD	5.00	1.46	1.33
19	2	1213	CLA	OBD-CAD	5.01	1.30	1.22
19	A	1782	CLA	O2D-CGD	5.01	1.46	1.33
19	3	1212	CLA	CHC-C1C	5.02	1.51	1.35
19	2	1218	CLA	CHC-C1C	5.02	1.51	1.35
19	A	1771	CLA	OBD-CAD	5.02	1.30	1.22
19	A	1774	CLA	CHC-C1C	5.02	1.51	1.35
19	B	1736	CLA	CHD-C4C	5.03	1.53	1.41
19	1	1189	CLA	O2D-CGD	5.03	1.46	1.33
19	B	1740	CLA	CHC-C1C	5.03	1.51	1.35
19	A	1774	CLA	O2D-CGD	5.03	1.46	1.33
19	2	1224	CLA	O2A-CGA	5.03	1.48	1.33
19	K	1146	CLA	O2D-CGD	5.03	1.46	1.33
19	B	1750	CLA	O2A-CGA	5.03	1.48	1.33
19	B	1759	CLA	O2D-CGD	5.03	1.46	1.33
19	A	1787	CLA	CHC-C1C	5.03	1.51	1.35
19	B	1786	CLA	CHD-C4C	5.03	1.53	1.41
19	B	1759	CLA	CHC-C1C	5.04	1.51	1.35
19	A	1777	CLA	OBD-CAD	5.05	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1751	CLA	O2A-CGA	5.05	1.50	1.32
19	A	1783	CLA	CHC-C1C	5.06	1.51	1.35
19	B	1737	CLA	O2A-CGA	5.06	1.48	1.33
19	A	1779	CLA	CHC-C1C	5.06	1.51	1.35
19	A	1817	CLA	O2A-CGA	5.06	1.48	1.33
19	A	1762	CLA	CHD-C4C	5.06	1.53	1.41
19	3	1212	CLA	OBD-CAD	5.06	1.30	1.22
19	B	1749	CLA	CHC-C1C	5.06	1.51	1.35
19	B	1750	CLA	O2D-CGD	5.06	1.46	1.33
19	B	1738	CLA	O2D-CGD	5.07	1.46	1.33
19	A	1773	CLA	CHC-C1C	5.07	1.51	1.35
19	A	1767	CLA	O2A-CGA	5.07	1.48	1.33
19	L	1167	CLA	CHC-C1C	5.07	1.51	1.35
19	A	1798	CLA	OBD-CAD	5.08	1.30	1.22
19	B	1739	CLA	CHC-C1C	5.08	1.51	1.35
19	3	1212	CLA	CHD-C4C	5.08	1.53	1.41
19	A	1768	CLA	CHD-C4C	5.08	1.53	1.41
19	B	1741	CLA	OBD-CAD	5.08	1.30	1.22
19	A	1812	CLA	O2A-CGA	5.09	1.48	1.33
19	4	1207	CLA	OBD-CAD	5.09	1.30	1.22
19	R	1054	CLA	CHC-C1C	5.09	1.51	1.35
19	F	1155	CLA	CHC-C1C	5.09	1.51	1.35
19	A	1817	CLA	CHC-C1C	5.10	1.51	1.35
19	B	1769	CLA	O2D-CGD	5.10	1.46	1.33
19	4	1203	CLA	CHD-C4C	5.10	1.53	1.41
19	B	1742	CLA	O2D-CGD	5.10	1.46	1.33
19	H	1079	CLA	OBD-CAD	5.10	1.30	1.22
19	B	1787	CLA	O2A-CGA	5.10	1.48	1.33
19	B	1749	CLA	O2A-CGA	5.11	1.48	1.33
19	L	1167	CLA	CHD-C4C	5.12	1.53	1.41
19	R	1055	CLA	O2A-CGA	5.12	1.48	1.33
19	B	1744	CLA	CHD-C4C	5.12	1.53	1.41
19	K	3009	CLA	O2D-CGD	5.12	1.46	1.33
19	L	1505	CLA	CHC-C1C	5.12	1.51	1.35
19	A	1780	CLA	CHC-C1C	5.12	1.51	1.35
19	B	1741	CLA	CHC-C1C	5.13	1.51	1.35
19	A	1778	CLA	CHD-C4C	5.13	1.53	1.41
19	1	1193	CLA	OBD-CAD	5.13	1.30	1.22
19	A	1784	CLA	CHC-C1C	5.13	1.51	1.35
19	A	1789	CLA	CHD-C4C	5.13	1.53	1.41
19	A	1770	CLA	CHD-C4C	5.13	1.53	1.41
19	4	1199	CLA	OBD-CAD	5.14	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1200	CLA	OBD-CAD	5.14	1.30	1.22
19	A	1761	CLA	CHD-C4C	5.14	1.53	1.41
19	B	1747	CLA	O2A-CGA	5.15	1.48	1.33
19	B	1787	CLA	O2D-CGD	5.16	1.46	1.33
19	2	1222	CLA	CHC-C1C	5.16	1.51	1.35
19	2	1213	CLA	CHD-C4C	5.16	1.53	1.41
19	2	1213	CLA	CHC-C1C	5.16	1.51	1.35
19	A	1769	CLA	CHC-C1C	5.16	1.51	1.35
19	L	1168	CLA	OBD-CAD	5.17	1.30	1.22
19	B	1785	CLA	CHC-C1C	5.17	1.51	1.35
19	A	1811	CLA	CHC-C1C	5.17	1.51	1.35
19	A	1773	CLA	O2A-CGA	5.17	1.48	1.33
19	A	1800	CLA	O2D-CGD	5.17	1.46	1.33
19	I	1033	CLA	CHC-C1C	5.17	1.51	1.35
19	A	1798	CLA	CHC-C1C	5.17	1.51	1.35
23	A	1802	PQN	C10-C5	5.17	1.48	1.40
19	1	1198	CLA	O2D-CGD	5.18	1.46	1.33
19	B	1741	CLA	CHD-C4C	5.18	1.53	1.41
19	B	1767	CLA	CHD-C4C	5.18	1.53	1.41
19	A	1777	CLA	CHD-C4C	5.18	1.53	1.41
19	1	1193	CLA	O2D-CGD	5.18	1.46	1.33
19	3	3007	CLA	OBD-CAD	5.18	1.30	1.22
19	A	1798	CLA	CHD-C4C	5.19	1.53	1.41
19	B	1747	CLA	CHD-C4C	5.19	1.53	1.41
19	4	1199	CLA	O2D-CGD	5.19	1.46	1.33
19	2	1223	CLA	OBD-CAD	5.19	1.30	1.22
19	B	1744	CLA	CHC-C1C	5.20	1.51	1.35
19	I	1033	CLA	OBD-CAD	5.20	1.30	1.22
19	B	1760	CLA	O2A-CGA	5.20	1.49	1.33
19	F	1155	CLA	CHD-C4C	5.20	1.53	1.41
19	A	1812	CLA	O2D-CGD	5.21	1.46	1.33
19	B	1747	CLA	CHC-C1C	5.21	1.51	1.35
19	K	3009	CLA	CHC-C1C	5.21	1.51	1.35
19	B	1768	CLA	CHD-C4C	5.22	1.53	1.41
19	A	1784	CLA	O2A-CGA	5.22	1.49	1.33
19	A	1760	CLA	CHC-C1C	5.22	1.51	1.35
19	4	1207	CLA	CHC-C1C	5.22	1.51	1.35
19	B	1736	CLA	CHC-C1C	5.23	1.51	1.35
19	B	1770	CLA	CHD-C4C	5.23	1.53	1.41
19	B	1758	CLA	OBD-CAD	5.23	1.30	1.22
19	A	1765	CLA	CHD-C4C	5.24	1.53	1.41
19	B	1750	CLA	CHC-C1C	5.24	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1762	CLA	O2A-CGA	5.24	1.49	1.33
19	A	1763	CLA	OBD-CAD	5.25	1.30	1.22
19	B	1770	CLA	CHC-C1C	5.26	1.51	1.35
19	A	1771	CLA	CHC-C1C	5.26	1.51	1.35
19	B	1748	CLA	CHC-C1C	5.26	1.51	1.35
19	A	1786	CLA	O2A-CGA	5.26	1.49	1.33
19	B	1748	CLA	O2D-CGD	5.27	1.46	1.33
19	2	1223	CLA	CHC-C1C	5.28	1.51	1.35
19	A	1787	CLA	CHD-C4C	5.28	1.53	1.41
19	A	1785	CLA	CHC-C1C	5.28	1.51	1.35
19	A	1768	CLA	O2A-CGA	5.28	1.49	1.33
19	A	1760	CLA	OBD-CAD	5.28	1.30	1.22
19	F	1157	CLA	OBD-CAD	5.28	1.30	1.22
19	A	1770	CLA	CHC-C1C	5.28	1.51	1.35
19	2	1222	CLA	CHD-C4C	5.28	1.53	1.41
19	B	1762	CLA	CHC-C1C	5.28	1.51	1.35
19	A	1764	CLA	CHC-C1C	5.29	1.51	1.35
19	R	1055	CLA	CHC-C1C	5.29	1.51	1.35
19	A	1799	CLA	O2D-CGD	5.29	1.46	1.33
19	2	1218	CLA	CHD-C4C	5.29	1.53	1.41
19	I	1033	CLA	CHD-C4C	5.29	1.53	1.41
19	A	1815	CLA	O2A-CGA	5.29	1.49	1.33
19	2	1215	CLA	O2D-CGD	5.29	1.46	1.33
19	A	1784	CLA	O2D-CGD	5.29	1.46	1.33
19	B	1739	CLA	CHD-C4C	5.29	1.53	1.41
19	G	1099	CLA	CHC-C1C	5.30	1.51	1.35
19	2	1213	CLA	O2A-CGA	5.30	1.49	1.33
19	A	1817	CLA	CHD-C4C	5.30	1.53	1.41
19	B	1757	CLA	O2D-CGD	5.30	1.46	1.33
19	A	1777	CLA	CHC-C1C	5.30	1.52	1.35
19	L	1166	CLA	CHC-C1C	5.31	1.52	1.35
19	B	1751	CLA	OBD-CAD	5.31	1.30	1.22
19	3	3011	CLA	O2D-CGD	5.31	1.46	1.33
19	1	1189	CLA	CHC-C1C	5.31	1.52	1.35
19	4	1197	CLA	CHC-C1C	5.32	1.52	1.35
19	1	1189	CLA	OBD-CAD	5.32	1.30	1.22
19	B	1745	CLA	O2D-CGD	5.32	1.46	1.33
19	A	1768	CLA	O2D-CGD	5.32	1.46	1.33
19	B	1737	CLA	O2D-CGD	5.33	1.46	1.33
19	B	1752	CLA	CHD-C4C	5.33	1.53	1.41
19	B	1787	CLA	CHC-C1C	5.33	1.52	1.35
19	B	1737	CLA	CHD-C4C	5.34	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1204	CLA	CHC-C1C	5.35	1.52	1.35
19	1	1191	CLA	CHC-C1C	5.35	1.52	1.35
19	4	4007	CLA	OBD-CAD	5.35	1.30	1.22
19	B	1736	CLA	OBD-CAD	5.35	1.30	1.22
19	A	1763	CLA	O2D-CGD	5.35	1.46	1.33
19	A	1777	CLA	O2D-CGD	5.37	1.46	1.33
19	B	1757	CLA	CHC-C1C	5.37	1.52	1.35
19	B	1760	CLA	CHD-C4C	5.38	1.53	1.41
19	G	1099	CLA	OBD-CAD	5.38	1.30	1.22
19	A	1799	CLA	CHD-C4C	5.39	1.53	1.41
19	1	1193	CLA	CHC-C1C	5.39	1.52	1.35
19	B	1765	CLA	CHC-C1C	5.39	1.52	1.35
19	I	1031	CLA	O2A-CGA	5.39	1.49	1.33
19	B	1764	CLA	CHC-C1C	5.39	1.52	1.35
19	1	1196	CLA	CHC-C1C	5.40	1.52	1.35
19	J	1044	CLA	O2D-CGD	5.41	1.47	1.33
19	2	1213	CLA	O2D-CGD	5.41	1.47	1.33
19	L	1167	CLA	O2D-CGD	5.42	1.47	1.33
19	R	1054	CLA	O2A-CGA	5.42	1.49	1.33
19	A	1771	CLA	CHD-C4C	5.44	1.54	1.41
19	I	1031	CLA	CHC-C1C	5.45	1.52	1.35
19	1	1191	CLA	OBD-CAD	5.45	1.30	1.22
19	B	1766	CLA	OBD-CAD	5.45	1.30	1.22
19	1	1187	CLA	O2D-CGD	5.46	1.47	1.33
19	A	1801	CLA	CHC-C1C	5.46	1.52	1.35
19	A	1786	CLA	CHC-C1C	5.46	1.52	1.35
19	A	1816	CLA	CHC-C1C	5.47	1.52	1.35
19	A	1785	CLA	O2D-CGD	5.47	1.47	1.33
19	B	1744	CLA	OBD-CAD	5.48	1.30	1.22
19	B	1766	CLA	CHC-C1C	5.48	1.52	1.35
19	A	1760	CLA	O2A-CGA	5.48	1.49	1.33
19	A	1787	CLA	OBD-CAD	5.49	1.30	1.22
19	B	1754	CLA	OBD-CAD	5.50	1.30	1.22
19	B	1765	CLA	O2D-CGD	5.50	1.47	1.33
19	A	1776	CLA	CHC-C1C	5.51	1.52	1.35
19	2	1224	CLA	O2D-CGD	5.51	1.47	1.33
19	B	1769	CLA	CHC-C1C	5.51	1.52	1.35
19	B	1760	CLA	CHC-C1C	5.52	1.52	1.35
19	B	1744	CLA	O2A-CGA	5.52	1.49	1.33
19	A	1815	CLA	CHD-C4C	5.55	1.54	1.41
19	A	1779	CLA	O2A-CGA	5.56	1.50	1.33
19	B	1745	CLA	CHC-C1C	5.57	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1223	CLA	O2A-CGA	5.58	1.50	1.33
19	A	1787	CLA	O2D-CGD	5.58	1.47	1.33
19	B	1739	CLA	O2D-CGD	5.59	1.47	1.33
19	B	1746	CLA	OBD-CAD	5.59	1.30	1.22
19	4	1200	CLA	OBD-CAD	5.59	1.30	1.22
19	B	1764	CLA	O2D-CGD	5.59	1.47	1.33
19	B	1746	CLA	O2D-CGD	5.60	1.47	1.33
19	A	1762	CLA	O2D-CGD	5.60	1.47	1.33
19	A	1783	CLA	CHD-C4C	5.60	1.54	1.41
19	H	1079	CLA	O2D-CGD	5.60	1.47	1.33
19	1	1187	CLA	OBD-CAD	5.60	1.30	1.22
19	2	1218	CLA	O2D-CGD	5.61	1.47	1.33
19	A	1799	CLA	OBD-CAD	5.62	1.30	1.22
19	A	1789	CLA	O2D-CGD	5.62	1.47	1.33
19	A	1775	CLA	OBD-CAD	5.63	1.30	1.22
19	A	1766	CLA	CHC-C1C	5.63	1.53	1.35
19	B	1754	CLA	O2D-CGD	5.63	1.47	1.33
19	B	1744	CLA	O2D-CGD	5.64	1.47	1.33
19	A	1779	CLA	O2D-CGD	5.64	1.47	1.33
19	2	1215	CLA	CHC-C1C	5.64	1.53	1.35
19	A	1776	CLA	O2D-CGD	5.64	1.47	1.33
19	L	1168	CLA	O2D-CGD	5.64	1.47	1.33
19	B	1757	CLA	CHD-C4C	5.65	1.54	1.41
19	B	1743	CLA	CHC-C1C	5.65	1.53	1.35
19	1	1188	CLA	O2A-CGA	5.66	1.50	1.33
19	A	1813	CLA	CHD-C4C	5.66	1.54	1.41
19	B	1752	CLA	OBD-CAD	5.66	1.31	1.22
19	A	1790	CLA	O2D-CGD	5.68	1.47	1.33
19	R	1055	CLA	OBD-CAD	5.69	1.31	1.22
19	A	1761	CLA	O2A-CGA	5.70	1.50	1.33
19	A	1770	CLA	O2D-CGD	5.70	1.47	1.33
19	K	3009	CLA	OBD-CAD	5.73	1.31	1.22
19	A	1766	CLA	O2D-CGD	5.73	1.47	1.33
19	B	1766	CLA	O2D-CGD	5.73	1.47	1.33
19	A	1766	CLA	CHD-C4C	5.73	1.54	1.41
19	A	1761	CLA	O2D-CGD	5.73	1.47	1.33
19	B	1741	CLA	O2A-CGA	5.74	1.50	1.33
19	1	1190	CLA	O2D-CGD	5.74	1.47	1.33
19	A	1798	CLA	O2D-CGD	5.75	1.47	1.33
19	A	1770	CLA	OBD-CAD	5.78	1.31	1.22
23	B	1773	PQN	C3-C2	5.79	1.48	1.35
19	R	1054	CLA	O2D-CGD	5.79	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1747	CLA	O2D-CGD	5.80	1.48	1.33
19	2	1223	CLA	O2D-CGD	5.81	1.48	1.33
19	A	1773	CLA	O2D-CGD	5.82	1.48	1.33
19	B	1772	CLA	OBD-CAD	5.82	1.31	1.22
19	A	1811	CLA	O2D-CGD	5.82	1.48	1.33
19	3	3007	CLA	O2D-CGD	5.82	1.48	1.33
19	A	1801	CLA	O2D-CGD	5.82	1.48	1.33
19	4	1200	CLA	CHC-C1C	5.82	1.53	1.35
19	A	1813	CLA	OBD-CAD	5.83	1.31	1.22
19	R	1055	CLA	O2D-CGD	5.83	1.48	1.33
19	B	1761	CLA	O2D-CGD	5.85	1.48	1.33
19	B	1760	CLA	O2D-CGD	5.86	1.48	1.33
19	4	1204	CLA	O2D-CGD	5.88	1.48	1.33
19	I	1033	CLA	O2D-CGD	5.89	1.48	1.33
19	2	1218	CLA	OBD-CAD	5.89	1.31	1.22
19	A	1778	CLA	OBD-CAD	5.89	1.31	1.22
19	B	1763	CLA	O2D-CGD	5.90	1.48	1.33
19	A	1771	CLA	O2D-CGD	5.92	1.48	1.33
19	4	1204	CLA	OBD-CAD	5.93	1.31	1.22
19	B	1752	CLA	O2D-CGD	5.94	1.48	1.33
19	L	1166	CLA	O2D-CGD	5.96	1.48	1.33
19	A	1815	CLA	O2D-CGD	5.97	1.48	1.33
19	A	1778	CLA	O2D-CGD	5.98	1.48	1.33
19	G	1099	CLA	O2D-CGD	5.99	1.48	1.33
19	4	4007	CLA	O2D-CGD	6.01	1.48	1.33
19	1	1192	CLA	O2D-CGD	6.01	1.48	1.33
19	1	1192	CLA	OBD-CAD	6.02	1.31	1.22
23	A	1802	PQN	C3-C2	6.04	1.49	1.35
19	4	1200	CLA	O2D-CGD	6.08	1.48	1.33
19	2	1217	CLA	O2D-CGD	6.09	1.48	1.33
19	3	1218	CLA	O2D-CGD	6.10	1.48	1.33
19	B	1751	CLA	O2D-CGD	6.13	1.48	1.33
19	1	1188	CLA	O2D-CGD	6.13	1.48	1.33
19	A	1762	CLA	OBD-CAD	6.14	1.31	1.22
19	L	1505	CLA	O2D-CGD	6.15	1.48	1.33
19	B	1764	CLA	OBD-CAD	6.19	1.31	1.22
19	2	1217	CLA	OBD-CAD	6.34	1.32	1.22
19	A	1817	CLA	O2D-CGD	6.36	1.49	1.33
19	4	1197	CLA	OBD-CAD	6.46	1.32	1.22
19	A	1801	CLA	OBD-CAD	6.74	1.32	1.22
19	1	1190	CLA	OBD-CAD	6.96	1.33	1.22

All (4035) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1200	CLA	OBD-CAD-CBD	-24.06	89.63	125.94
19	A	1763	CLA	OBD-CAD-CBD	-18.56	97.94	125.94
19	B	1748	CLA	OBD-CAD-CBD	-17.07	100.19	125.94
19	4	1201	CLA	OBD-CAD-CBD	-16.53	100.99	125.94
19	2	1224	CLA	OBD-CAD-CBD	-16.52	101.01	125.94
19	A	1799	CLA	OBD-CAD-CBD	-16.34	101.29	125.94
19	A	1815	CLA	OBD-CAD-CBD	-16.22	101.46	125.94
19	2	1223	CLA	OBD-CAD-CBD	-15.95	101.87	125.94
19	3	1218	CLA	OBD-CAD-CBD	-15.86	102.01	125.94
19	A	1811	CLA	OBD-CAD-CBD	-15.78	102.13	125.94
19	A	1783	CLA	OBD-CAD-CBD	-15.58	102.43	125.94
19	B	1757	CLA	OBD-CAD-CBD	-15.53	102.50	125.94
19	2	1224	CLA	OBD-CAD-C3D	-15.50	96.73	128.35
19	1	1197	CLA	OBD-CAD-C3D	-15.50	96.73	128.35
19	I	1033	CLA	OBD-CAD-CBD	-15.48	102.58	125.94
19	B	1737	CLA	OBD-CAD-CBD	-15.43	102.65	125.94
19	A	1800	CLA	OBD-CAD-CBD	-15.36	102.76	125.94
19	2	1220	CLA	OBD-CAD-CBD	-15.33	102.81	125.94
19	B	1743	CLA	OBD-CAD-CBD	-15.24	102.94	125.94
19	I	1031	CLA	OBD-CAD-CBD	-15.23	102.95	125.94
19	2	1215	CLA	OBD-CAD-CBD	-15.20	103.00	125.94
19	1	1195	CLA	CAB-C3B-C4B	-14.87	103.76	128.36
19	B	1753	CLA	OBD-CAD-CBD	-14.73	103.71	125.94
19	4	1200	CLA	OBD-CAD-CBD	-14.52	104.02	125.94
19	R	1054	CLA	OBD-CAD-CBD	-14.22	104.49	125.94
19	3	1218	CLA	OBD-CAD-C3D	-14.21	99.36	128.35
19	A	1766	CLA	OBD-CAD-CBD	-13.83	105.08	125.94
19	4	1197	CLA	CAB-C3B-C4B	-13.72	105.67	128.36
19	3	3007	CLA	OBD-CAD-CBD	-13.69	105.28	125.94
19	2	1217	CLA	OBD-CAD-C3D	-13.66	100.48	128.35
22	B	1781	BCR	C24-C23-C22	-13.65	105.41	126.22
19	A	1785	CLA	OBD-CAD-CBD	-13.51	105.55	125.94
19	B	1766	CLA	OBD-CAD-CBD	-13.48	105.59	125.94
19	1	1200	CLA	OBD-CAD-C3D	-13.46	100.88	128.35
19	B	1749	CLA	OBD-CAD-CBD	-13.45	105.65	125.94
19	B	1767	CLA	OBD-CAD-C3D	-13.41	100.99	128.35
19	A	1817	CLA	OBD-CAD-C3D	-13.39	101.03	128.35
19	3	3008	CLA	OBD-CAD-CBD	-13.38	105.75	125.94
19	B	1740	CLA	OBD-CAD-C3D	-13.24	101.33	128.35
19	B	1757	CLA	OBD-CAD-C3D	-13.09	101.63	128.35
19	L	1168	CLA	OBD-CAD-CBD	-13.09	106.19	125.94
19	K	1146	CLA	OBD-CAD-CBD	-13.02	106.29	125.94
19	A	1784	CLA	OBD-CAD-CBD	-13.00	106.32	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1166	CLA	OBD-CAD-CBD	-12.99	106.33	125.94
22	L	1170	BCR	C7-C8-C9	-12.94	106.49	126.22
19	H	1079	CLA	OBD-CAD-C3D	-12.88	102.06	128.35
19	A	1770	CLA	OBD-CAD-CBD	-12.74	106.71	125.94
19	B	1772	CLA	CAB-C3B-C4B	-12.74	107.28	128.36
19	A	1764	CLA	OBD-CAD-C3D	-12.71	102.42	128.35
19	B	1752	CLA	OBD-CAD-CBD	-12.69	106.79	125.94
19	I	1031	CLA	OBD-CAD-C3D	-12.65	102.53	128.35
19	1	1195	CLA	CAB-C3B-C2B	-12.59	99.40	125.14
19	B	1751	CLA	OBD-CAD-C3D	-12.57	102.69	128.35
19	L	1168	CLA	OBD-CAD-C3D	-12.56	102.72	128.35
19	A	1768	CLA	OBD-CAD-CBD	-12.55	107.01	125.94
19	A	1816	CLA	OBD-CAD-C3D	-12.55	102.75	128.35
19	B	1785	CLA	OBD-CAD-CBD	-12.53	107.03	125.94
19	2	1223	CLA	OBD-CAD-C3D	-12.44	102.96	128.35
19	A	1817	CLA	CAB-C3B-C4B	-12.34	107.94	128.36
22	I	1032	BCR	C30-C25-C26	-12.31	104.59	122.66
19	A	1800	CLA	OBD-CAD-C3D	-12.29	103.27	128.35
19	4	1207	CLA	CAB-C3B-C4B	-12.28	108.05	128.36
19	4	1201	CLA	OBD-CAD-C3D	-12.27	103.31	128.35
19	A	1762	CLA	OBD-CAD-CBD	-12.21	107.51	125.94
19	A	1774	CLA	OBD-CAD-CBD	-12.18	107.56	125.94
19	F	1157	CLA	OBD-CAD-CBD	-12.08	107.70	125.94
19	A	1815	CLA	OBD-CAD-C3D	-12.07	103.72	128.35
19	1	1191	CLA	OBD-CAD-C3D	-12.05	103.76	128.35
19	A	1816	CLA	OBD-CAD-CBD	-12.04	107.78	125.94
19	B	1769	CLA	OBD-CAD-CBD	-12.03	107.78	125.94
19	B	1766	CLA	OBD-CAD-C3D	-12.02	103.82	128.35
19	A	1786	CLA	OBD-CAD-CBD	-12.00	107.84	125.94
19	B	1755	CLA	OBD-CAD-CBD	-11.99	107.85	125.94
19	1	1187	CLA	OBD-CAD-C3D	-11.99	103.89	128.35
19	A	1773	CLA	OBD-CAD-CBD	-11.98	107.87	125.94
19	A	1781	CLA	OBD-CAD-CBD	-11.94	107.92	125.94
19	4	1196	CLA	OBD-CAD-CBD	-11.94	107.92	125.94
19	B	1756	CLA	OBD-CAD-CBD	-11.92	107.95	125.94
19	A	1794	CLA	OBD-CAD-CBD	-11.92	107.95	125.94
19	F	1156	CLA	OBD-CAD-CBD	-11.91	107.96	125.94
19	A	1786	CLA	OBD-CAD-C3D	-11.91	104.04	128.35
19	B	1753	CLA	OBD-CAD-C3D	-11.91	104.05	128.35
19	A	1795	CLA	OBD-CAD-CBD	-11.91	107.97	125.94
19	B	1735	CLA	OBD-CAD-CBD	-11.91	107.97	125.94
19	J	1043	CLA	OBD-CAD-CBD	-11.90	107.98	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1797	CLA	OBD-CAD-CBD	-11.88	108.01	125.94
19	K	1085	CLA	OBD-CAD-CBD	-11.88	108.01	125.94
19	B	1786	CLA	OBD-CAD-CBD	-11.88	108.02	125.94
19	A	1792	CLA	OBD-CAD-CBD	-11.87	108.02	125.94
19	A	1796	CLA	OBD-CAD-CBD	-11.87	108.03	125.94
19	A	1793	CLA	OBD-CAD-CBD	-11.87	108.03	125.94
19	2	1212	CLA	OBD-CAD-CBD	-11.87	108.03	125.94
19	A	1783	CLA	OBD-CAD-C3D	-11.87	104.13	128.35
19	B	1760	CLA	OBD-CAD-CBD	-11.86	108.04	125.94
19	A	1791	CLA	OBD-CAD-CBD	-11.85	108.05	125.94
19	A	1779	CLA	OBD-CAD-C3D	-11.84	104.18	128.35
19	4	4014	CLA	OBD-CAD-CBD	-11.83	108.08	125.94
19	3	1219	CLA	OBD-CAD-CBD	-11.83	108.08	125.94
19	1	1189	CLA	OBD-CAD-CBD	-11.83	108.09	125.94
19	A	1782	CLA	OBD-CAD-CBD	-11.82	108.09	125.94
19	K	1142	CLA	OBD-CAD-CBD	-11.81	108.12	125.94
19	H	1079	CLA	OBD-CAD-CBD	-11.78	108.17	125.94
19	A	1813	CLA	OBD-CAD-C3D	-11.71	104.46	128.35
19	A	1775	CLA	OBD-CAD-C3D	-11.70	104.47	128.35
19	A	1778	CLA	OBD-CAD-CBD	-11.67	108.33	125.94
19	A	1776	CLA	OBD-CAD-CBD	-11.65	108.36	125.94
19	A	1788	CLA	OBD-CAD-CBD	-11.60	108.43	125.94
19	B	1740	CLA	OBD-CAD-CBD	-11.60	108.44	125.94
19	B	1742	CLA	OBD-CAD-CBD	-11.53	108.55	125.94
19	2	1217	CLA	OBD-CAD-CBD	-11.49	108.61	125.94
19	B	1785	CLA	OBD-CAD-C3D	-11.49	104.91	128.35
19	1	1196	CLA	CAB-C3B-C4B	-11.46	109.39	128.36
19	A	1776	CLA	OBD-CAD-C3D	-11.46	104.96	128.35
19	G	1099	CLA	OBD-CAD-CBD	-11.46	108.64	125.94
19	4	1198	CLA	OBD-CAD-C3D	-11.45	105.00	128.35
19	A	1769	CLA	OBD-CAD-CBD	-11.43	108.69	125.94
19	B	1763	CLA	OBD-CAD-C3D	-11.35	105.19	128.35
19	1	1198	CLA	OBD-CAD-CBD	-11.33	108.84	125.94
19	A	1785	CLA	OBD-CAD-C3D	-11.33	105.23	128.35
19	L	1505	CLA	OBD-CAD-CBD	-11.30	108.89	125.94
19	B	1764	CLA	OBD-CAD-C3D	-11.29	105.32	128.35
19	B	1765	CLA	OBD-CAD-C3D	-11.28	105.34	128.35
19	1	1195	CLA	C3D-CAD-CBD	-11.25	100.23	107.75
19	1	1189	CLA	OBD-CAD-C3D	-11.24	105.41	128.35
19	A	1788	CLA	OBD-CAD-C3D	-11.14	105.62	128.35
19	4	1200	CLA	OBD-CAD-C3D	-11.13	105.64	128.35
19	A	1812	CLA	OBD-CAD-CBD	-11.10	109.19	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1762	CLA	OBD-CAD-C3D	-11.08	105.73	128.35
19	A	1771	CLA	OBD-CAD-CBD	-11.08	109.22	125.94
19	A	1766	CLA	OBD-CAD-C3D	-11.03	105.83	128.35
19	A	1817	CLA	OBD-CAD-CBD	-11.00	109.34	125.94
19	4	1197	CLA	C3D-CAD-CBD	-10.99	100.41	107.75
19	A	1773	CLA	OBD-CAD-C3D	-10.97	105.97	128.35
19	A	1772	CLA	OBD-CAD-C3D	-10.92	106.06	128.35
19	A	1813	CLA	OBD-CAD-CBD	-10.90	109.49	125.94
19	I	1033	CLA	OBD-CAD-C3D	-10.89	106.14	128.35
19	A	1790	CLA	OBD-CAD-CBD	-10.87	109.54	125.94
22	L	1170	BCR	C15-C16-C17	-10.86	99.38	123.39
19	2	1220	CLA	OBD-CAD-C3D	-10.85	106.22	128.35
19	4	4007	CLA	OBD-CAD-CBD	-10.83	109.59	125.94
19	A	1761	CLA	OBD-CAD-C3D	-10.82	106.26	128.35
19	L	1167	CLA	OBD-CAD-CBD	-10.75	109.71	125.94
22	B	1781	BCR	C7-C8-C9	-10.68	109.94	126.22
19	B	1742	CLA	OBD-CAD-C3D	-10.64	106.63	128.35
19	A	1775	CLA	CAB-C3B-C4B	-10.63	110.78	128.36
19	3	3008	CLA	OBD-CAD-C3D	-10.57	106.78	128.35
19	4	1207	CLA	C3D-CAD-CBD	-10.57	100.69	107.75
19	A	1777	CLA	OBD-CAD-C3D	-10.55	106.83	128.35
19	2	1222	CLA	OBD-CAD-C3D	-10.53	106.85	128.35
19	A	1759	CLA	OBD-CAD-C3D	-10.51	106.91	128.35
19	B	1746	CLA	OBD-CAD-CBD	-10.51	110.08	125.94
19	B	1763	CLA	OBD-CAD-CBD	-10.49	110.11	125.94
19	B	1749	CLA	OBD-CAD-C3D	-10.48	106.96	128.35
19	R	1054	CLA	OBD-CAD-C3D	-10.46	107.01	128.35
19	A	1772	CLA	OBD-CAD-CBD	-10.42	110.21	125.94
22	I	1032	BCR	C24-C23-C22	-10.34	110.45	126.22
19	1	1198	CLA	OBD-CAD-C3D	-10.33	107.27	128.35
19	L	1167	CLA	OBD-CAD-C3D	-10.30	107.34	128.35
19	4	1207	CLA	OBD-CAD-C3D	-10.23	107.47	128.35
19	A	1777	CLA	OBD-CAD-CBD	-10.22	110.52	125.94
19	J	1044	CLA	OBD-CAD-CBD	-10.22	110.52	125.94
19	K	1146	CLA	OBD-CAD-C3D	-10.17	107.59	128.35
19	1	1195	CLA	OBD-CAD-C3D	-10.12	107.71	128.35
19	K	3009	CLA	OBD-CAD-CBD	-10.04	110.78	125.94
19	4	4014	CLA	OBD-CAD-C3D	-10.01	107.93	128.35
19	3	1219	CLA	OBD-CAD-C3D	-10.00	107.95	128.35
19	B	1762	CLA	OBD-CAD-C3D	-10.00	107.95	128.35
19	2	1212	CLA	OBD-CAD-C3D	-10.00	107.95	128.35
19	J	1043	CLA	OBD-CAD-C3D	-9.99	107.96	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1793	CLA	OBD-CAD-C3D	-9.99	107.96	128.35
19	A	1792	CLA	OBD-CAD-C3D	-9.99	107.96	128.35
19	B	1755	CLA	OBD-CAD-C3D	-9.98	107.98	128.35
19	A	1797	CLA	OBD-CAD-C3D	-9.98	107.98	128.35
19	B	1756	CLA	OBD-CAD-C3D	-9.98	107.99	128.35
19	B	1772	CLA	C3D-CAD-CBD	-9.98	101.08	107.75
19	K	1142	CLA	OBD-CAD-C3D	-9.98	107.99	128.35
19	A	1794	CLA	OBD-CAD-C3D	-9.98	107.99	128.35
19	A	1791	CLA	OBD-CAD-C3D	-9.97	108.00	128.35
19	A	1796	CLA	OBD-CAD-C3D	-9.96	108.02	128.35
19	A	1781	CLA	OBD-CAD-C3D	-9.96	108.03	128.35
19	B	1735	CLA	OBD-CAD-C3D	-9.96	108.03	128.35
19	A	1789	CLA	OBD-CAD-CBD	-9.96	110.91	125.94
19	4	1196	CLA	OBD-CAD-C3D	-9.96	108.03	128.35
19	A	1782	CLA	OBD-CAD-C3D	-9.96	108.04	128.35
19	A	1795	CLA	OBD-CAD-C3D	-9.95	108.04	128.35
19	B	1739	CLA	OBD-CAD-CBD	-9.95	110.93	125.94
19	K	1085	CLA	OBD-CAD-C3D	-9.94	108.07	128.35
19	F	1156	CLA	OBD-CAD-C3D	-9.93	108.08	128.35
19	R	1055	CLA	OBD-CAD-CBD	-9.91	110.99	125.94
19	3	1212	CLA	OBD-CAD-C3D	-9.90	108.15	128.35
19	4	1197	CLA	OBD-CAD-C3D	-9.87	108.21	128.35
19	B	1748	CLA	OBD-CAD-C3D	-9.84	108.27	128.35
19	F	1155	CLA	C3D-CAD-CBD	-9.83	101.19	107.75
19	A	1817	CLA	C3D-CAD-CBD	-9.82	93.72	107.60
19	B	1737	CLA	OBD-CAD-C3D	-9.81	108.34	128.35
19	B	1786	CLA	OBD-CAD-C3D	-9.77	108.42	128.35
19	F	1157	CLA	OBD-CAD-C3D	-9.72	108.53	128.35
19	B	1750	CLA	OBD-CAD-C3D	-9.68	108.60	128.35
19	B	1741	CLA	CAB-C3B-C4B	-9.67	112.37	128.36
19	A	1779	CLA	OBD-CAD-CBD	-9.63	111.40	125.94
19	4	4007	CLA	OBD-CAD-C3D	-9.63	108.70	128.35
19	B	1751	CLA	OBD-CAD-CBD	-9.63	111.41	125.94
19	1	1196	CLA	C3D-CAD-CBD	-9.59	101.35	107.75
19	2	1218	CLA	OBD-CAD-CBD	-9.58	111.48	125.94
19	B	1761	CLA	OBD-CAD-CBD	-9.58	111.48	125.94
19	B	1761	CLA	OBD-CAD-C3D	-9.52	108.92	128.35
19	L	1505	CLA	OBD-CAD-C3D	-9.51	108.94	128.35
19	1	1191	CLA	C3D-CAD-CBD	-9.46	101.43	107.75
19	A	1771	CLA	OBD-CAD-C3D	-9.45	109.06	128.35
19	B	1745	CLA	OBD-CAD-C3D	-9.45	109.08	128.35
19	B	1738	CLA	OBD-CAD-CBD	-9.44	111.69	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1193	CLA	OBD-CAD-CBD	-9.44	111.69	125.94
19	B	1738	CLA	OBD-CAD-C3D	-9.37	109.22	128.35
19	3	3007	CLA	OBD-CAD-C3D	-9.37	109.22	128.35
19	A	1812	CLA	OBD-CAD-C3D	-9.35	109.27	128.35
19	1	1196	CLA	CAB-C3B-C2B	-9.33	106.06	125.14
22	B	1779	BCR	C15-C14-C13	-9.32	113.74	127.20
19	J	1044	CLA	OBD-CAD-C3D	-9.31	109.35	128.35
19	J	1045	CLA	OBD-CAD-C3D	-9.31	109.35	128.35
19	B	1739	CLA	O1D-CGD-CBD	-9.31	111.28	124.62
19	A	1816	CLA	C1D-CHD-C4C	-9.21	108.66	122.60
19	1	1191	CLA	CAB-C3B-C4B	-9.20	113.14	128.36
19	B	1752	CLA	OBD-CAD-C3D	-9.17	109.63	128.35
19	A	1790	CLA	OBD-CAD-C3D	-9.11	109.77	128.35
19	2	1218	CLA	OBD-CAD-C3D	-9.09	109.81	128.35
22	I	1032	BCR	C1-C6-C5	-9.06	109.35	122.66
19	B	1745	CLA	OBD-CAD-CBD	-9.05	112.29	125.94
19	B	1765	CLA	OBD-CAD-CBD	-9.00	112.36	125.94
19	3	1218	CLA	O1D-CGD-CBD	-8.96	111.79	124.62
19	B	1750	CLA	OBD-CAD-CBD	-8.95	112.44	125.94
19	A	1763	CLA	OBD-CAD-C3D	-8.93	110.13	128.35
19	2	1222	CLA	OBD-CAD-CBD	-8.93	112.47	125.94
22	B	1781	BCR	C3-C4-C5	-8.91	99.73	113.87
22	3	1220	BCR	C16-C17-C18	-8.90	114.35	127.20
19	B	1758	CLA	OBD-CAD-CBD	-8.89	112.52	125.94
19	B	1762	CLA	CAA-C2A-C3A	-8.89	87.67	113.22
19	A	1817	CLA	CAB-C3B-C2B	-8.85	107.05	125.14
21	B	8062	SUC	C1-O5-C5	-8.80	96.66	113.75
19	4	1198	CLA	C3D-CAD-CBD	-8.79	95.17	107.60
19	A	1798	CLA	OBD-CAD-C3D	-8.72	110.56	128.35
19	A	1768	CLA	OBD-CAD-C3D	-8.71	110.58	128.35
19	B	1746	CLA	OBD-CAD-C3D	-8.71	110.58	128.35
19	3	1212	CLA	CAB-C3B-C4B	-8.71	113.96	128.36
19	1	1200	CLA	C1D-CHD-C4C	-8.68	109.46	122.60
20	A	7032	LMU	C1B-C2B-C3B	-8.67	92.88	109.97
19	A	1761	CLA	OBD-CAD-CBD	-8.67	112.85	125.94
20	A	7030	LMU	C3B-C4B-C5B	-8.67	95.09	110.20
19	A	1784	CLA	OBD-CAD-C3D	-8.65	110.69	128.35
19	4	1198	CLA	OBD-CAD-CBD	-8.63	112.92	125.94
19	B	1759	CLA	OBD-CAD-C3D	-8.62	110.77	128.35
19	B	1769	CLA	OBD-CAD-C3D	-8.62	110.77	128.35
19	B	1762	CLA	OBD-CAD-CBD	-8.61	112.94	125.94
19	G	1099	CLA	OBD-CAD-C3D	-8.59	110.82	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1789	CLA	OBD-CAD-C3D	-8.59	110.83	128.35
19	L	1166	CLA	OBD-CAD-C3D	-8.55	110.91	128.35
19	2	1215	CLA	OBD-CAD-C3D	-8.54	110.92	128.35
19	B	1758	CLA	OBD-CAD-C3D	-8.54	110.93	128.35
19	B	1760	CLA	OBD-CAD-C3D	-8.49	111.03	128.35
19	A	1778	CLA	OBD-CAD-C3D	-8.48	111.05	128.35
19	4	1199	CLA	OBD-CAD-C3D	-8.48	111.05	128.35
19	A	1765	CLA	OBD-CAD-CBD	-8.47	113.16	125.94
19	B	1787	CLA	OBD-CAD-C3D	-8.42	111.16	128.35
19	J	1045	CLA	OBD-CAD-CBD	-8.41	113.24	125.94
19	A	1799	CLA	OBD-CAD-C3D	-8.39	111.22	128.35
19	1	1192	CLA	OBD-CAD-CBD	-8.37	113.31	125.94
19	4	1209	CLA	O1D-CGD-CBD	-8.32	112.70	124.62
19	B	1768	CLA	OBD-CAD-CBD	-8.30	113.41	125.94
19	A	1775	CLA	C3D-CAD-CBD	-8.29	102.21	107.75
19	2	1213	CLA	OBD-CAD-C3D	-8.27	111.48	128.35
19	B	1772	CLA	OBD-CAD-C3D	-8.18	111.65	128.35
20	A	7017	LMU	C1B-O1B-C4'	-8.17	96.66	118.01
19	A	1811	CLA	OBD-CAD-C3D	-8.13	111.76	128.35
19	1	1193	CLA	OBD-CAD-C3D	-8.12	111.78	128.35
19	B	1764	CLA	OBD-CAD-CBD	-8.12	113.69	125.94
19	B	1772	CLA	CAB-C3B-C2B	-8.11	108.55	125.14
19	4	1198	CLA	C1D-CHD-C4C	-8.09	110.36	122.60
19	A	1765	CLA	OBD-CAD-C3D	-8.08	111.86	128.35
22	L	1170	BCR	C3-C4-C5	-8.07	101.06	113.87
19	3	1212	CLA	C3D-CAD-CBD	-8.06	102.36	107.75
19	B	1767	CLA	OBD-CAD-CBD	-8.04	113.81	125.94
19	A	1798	CLA	OBD-CAD-CBD	-8.03	113.82	125.94
19	4	1204	CLA	OBD-CAD-C3D	-8.02	111.98	128.35
19	4	1197	CLA	C1D-CHD-C4C	-8.00	110.49	122.60
19	4	1201	CLA	C1D-CHD-C4C	-7.98	110.53	122.60
20	A	7033	LMU	C1B-O1B-C4'	-7.98	97.17	118.01
19	3	3011	CLA	OBD-CAD-C3D	-7.96	112.10	128.35
20	A	7037	LMU	C1B-O5B-C5B	-7.89	98.43	113.75
19	B	1736	CLA	OBD-CAD-C3D	-7.87	112.30	128.35
19	1	1192	CLA	OBD-CAD-C3D	-7.86	112.31	128.35
22	B	1779	BCR	C30-C25-C26	-7.84	111.15	122.66
19	A	1787	CLA	OBD-CAD-C3D	-7.79	112.46	128.35
19	1	1187	CLA	C4B-CHC-C1C	-7.78	112.54	129.26
19	A	1764	CLA	OBD-CAD-CBD	-7.77	114.22	125.94
19	1	1188	CLA	OBD-CAD-CBD	-7.73	114.27	125.94
20	A	7026	LMU	C3B-C4B-C5B	-7.73	96.72	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1187	CLA	OBD-CAD-CBD	-7.72	114.30	125.94
19	A	1759	CLA	OBD-CAD-CBD	-7.71	114.30	125.94
22	L	1170	BCR	C4-C5-C6	-7.61	113.09	122.78
19	B	1770	CLA	OBD-CAD-C3D	-7.60	112.84	128.35
20	A	7037	LMU	O2'-C2'-C1'	-7.60	93.37	110.02
19	B	1771	CLA	OBD-CAD-C3D	-7.55	112.94	128.35
19	A	1769	CLA	OBD-CAD-C3D	-7.55	112.94	128.35
19	B	1743	CLA	OBD-CAD-C3D	-7.53	112.99	128.35
19	A	1775	CLA	CAB-C3B-C2B	-7.53	109.75	125.14
19	B	1770	CLA	OBD-CAD-CBD	-7.52	114.59	125.94
19	A	1780	CLA	OBD-CAD-C3D	-7.52	113.01	128.35
19	A	1778	CLA	O1D-CGD-CBD	-7.50	113.87	124.62
19	4	1202	CLA	C3A-C4A-CHB	-7.48	116.51	124.06
19	3	1218	CLA	C1D-CHD-C4C	-7.48	111.28	122.60
19	1	1197	CLA	C1D-CHD-C4C	-7.47	111.29	122.60
19	1	1199	CLA	C3A-C4A-CHB	-7.47	116.52	124.06
20	A	7039	LMU	C1B-O5B-C5B	-7.46	99.26	113.75
19	B	1787	CLA	OBD-CAD-CBD	-7.46	114.69	125.94
19	A	1774	CLA	OBD-CAD-C3D	-7.43	113.18	128.35
19	B	1768	CLA	OBD-CAD-C3D	-7.42	113.20	128.35
22	L	1170	BCR	C15-C14-C13	-7.38	116.54	127.20
20	A	7026	LMU	C1B-C2B-C3B	-7.36	95.47	109.97
19	A	1801	CLA	OBD-CAD-C3D	-7.35	113.36	128.35
19	B	1770	CLA	C4B-CHC-C1C	-7.33	113.51	129.26
19	3	3014	CLA	C3A-C4A-CHB	-7.29	116.70	124.06
19	A	1770	CLA	OBD-CAD-C3D	-7.29	113.48	128.35
19	K	3009	CLA	OBD-CAD-C3D	-7.28	113.50	128.35
19	A	1760	CLA	OBD-CAD-CBD	-7.26	114.98	125.94
19	J	1044	CLA	C1D-CHD-C4C	-7.24	111.64	122.60
20	A	7036	LMU	C2'-C3'-C4'	-7.24	93.70	109.60
19	A	1761	CLA	C4B-CHC-C1C	-7.24	113.70	129.26
22	I	1032	BCR	C16-C15-C14	-7.22	107.42	123.39
19	3	1214	CLA	C3A-C4A-CHB	-7.21	116.78	124.06
20	A	7037	LMU	C4B-C3B-C2B	-7.21	97.34	110.79
19	L	1167	CLA	CAA-C2A-C3A	-7.19	92.53	113.22
19	3	1215	CLA	C3A-C4A-CHB	-7.18	116.81	124.06
22	B	1779	BCR	C3-C4-C5	-7.17	102.49	113.87
19	A	1811	CLA	C3D-CAD-CBD	-7.17	97.46	107.60
19	4	1199	CLA	C4B-CHC-C1C	-7.12	113.96	129.26
19	L	1168	CLA	C1D-CHD-C4C	-7.11	111.84	122.60
19	4	1198	CLA	C4B-CHC-C1C	-7.10	114.00	129.26
19	A	1815	CLA	C3D-CAD-CBD	-7.08	97.59	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1198	CLA	C1D-CHD-C4C	-7.07	111.90	122.60
20	A	7040	LMU	O5B-C5B-C4B	-7.06	96.43	109.68
19	B	1785	CLA	C4B-CHC-C1C	-7.06	114.09	129.26
22	I	1032	BCR	C34-C9-C10	-7.05	112.49	122.90
19	3	1218	CLA	CHD-C4C-C3C	-7.03	114.08	124.94
19	A	1789	CLA	O1D-CGD-CBD	-7.03	114.55	124.62
20	A	7038	LMU	C3'-C4'-C5'	-7.02	94.96	110.84
19	B	1771	CLA	OBD-CAD-CBD	-6.98	115.40	125.94
19	4	1209	CLA	OBD-CAD-C3D	-6.96	114.14	128.35
19	4	1204	CLA	OBD-CAD-CBD	-6.96	115.43	125.94
20	K	1086	LMU	C3B-C4B-C5B	-6.96	98.07	110.20
19	3	3001	CLA	C3A-C4A-CHB	-6.95	117.05	124.06
19	K	1146	CLA	C4B-CHC-C1C	-6.92	114.39	129.26
19	A	1760	CLA	C4B-CHC-C1C	-6.89	114.45	129.26
19	J	1045	CLA	C1D-CHD-C4C	-6.88	112.19	122.60
19	4	1209	CLA	C1D-CHD-C4C	-6.87	112.21	122.60
19	B	1741	CLA	CAB-C3B-C2B	-6.86	111.11	125.14
19	A	1767	CLA	OBD-CAD-CBD	-6.86	115.59	125.94
19	B	1747	CLA	OBD-CAD-CBD	-6.85	115.59	125.94
22	I	1032	BCR	C38-C26-C25	-6.85	117.88	124.61
19	B	1751	CLA	C1D-CHD-C4C	-6.85	112.24	122.60
19	4	1209	CLA	OBD-CAD-CBD	-6.83	115.63	125.94
19	A	1765	CLA	C4B-CHC-C1C	-6.83	114.58	129.26
19	B	1737	CLA	C4B-CHC-C1C	-6.82	114.61	129.26
19	A	1811	CLA	C4B-CHC-C1C	-6.80	114.66	129.26
19	B	1771	CLA	C4B-CHC-C1C	-6.79	114.67	129.26
19	B	1737	CLA	CAA-C2A-C3A	-6.79	93.69	113.22
19	1	1197	CLA	CHD-C4C-C3C	-6.79	114.45	124.94
19	A	1767	CLA	OBD-CAD-C3D	-6.78	114.51	128.35
19	1	1200	CLA	C4B-CHC-C1C	-6.76	114.73	129.26
19	B	1753	CLA	C4B-CHC-C1C	-6.75	114.75	129.26
22	L	1169	BCR	C27-C26-C25	-6.74	114.19	122.78
20	A	7026	LMU	C3'-C4'-C5'	-6.73	95.61	110.84
19	3	1218	CLA	C4B-CHC-C1C	-6.73	114.80	129.26
19	1	1188	CLA	C4B-CHC-C1C	-6.73	114.81	129.26
19	4	1197	CLA	CAB-C3B-C2B	-6.72	111.39	125.14
22	3	1220	BCR	C11-C10-C9	-6.72	117.50	127.20
19	B	1743	CLA	C1D-CHD-C4C	-6.70	112.46	122.60
19	A	1787	CLA	OBD-CAD-CBD	-6.70	115.83	125.94
19	1	1197	CLA	O2A-CGA-O1A	-6.69	106.22	123.49
19	B	1741	CLA	OBD-CAD-C3D	-6.69	114.71	128.35
19	I	1031	CLA	C1D-CHD-C4C	-6.63	112.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1768	CLA	C4B-CHC-C1C	-6.62	115.04	129.26
19	1	1197	CLA	C4B-CHC-C1C	-6.60	115.09	129.26
19	1	1201	CLA	C3A-C4A-CHB	-6.59	117.41	124.06
19	B	1741	CLA	OBD-CAD-CBD	-6.58	116.00	125.94
19	1	1195	CLA	C1D-CHD-C4C	-6.55	112.69	122.60
19	2	1218	CLA	C4B-CHC-C1C	-6.55	115.20	129.26
19	B	1759	CLA	C4B-CHC-C1C	-6.53	115.23	129.26
19	A	1766	CLA	C4B-CHC-C1C	-6.52	115.25	129.26
19	4	1205	CLA	C3A-C4A-CHB	-6.52	117.48	124.06
19	B	1740	CLA	C1D-CHD-C4C	-6.52	112.74	122.60
19	4	1199	CLA	OBD-CAD-CBD	-6.51	116.11	125.94
19	B	1759	CLA	C1D-CHD-C4C	-6.49	112.78	122.60
19	4	1204	CLA	C1D-CHD-C4C	-6.49	112.79	122.60
19	4	4007	CLA	C4B-CHC-C1C	-6.48	115.34	129.26
19	B	1763	CLA	O1D-CGD-CBD	-6.47	115.35	124.62
19	A	1788	CLA	C4B-CHC-C1C	-6.47	115.36	129.26
19	B	1736	CLA	OBD-CAD-CBD	-6.44	116.23	125.94
19	A	1816	CLA	C4-C3-C2	-6.42	110.89	123.50
19	A	1774	CLA	C4B-CHC-C1C	-6.42	115.47	129.26
19	B	1764	CLA	C1D-CHD-C4C	-6.40	112.91	122.60
19	2	1221	CLA	C3A-C4A-CHB	-6.39	117.61	124.06
20	A	7026	LMU	C1'-C2'-C3'	-6.38	97.40	109.97
19	1	1192	CLA	C1D-CHD-C4C	-6.38	112.95	122.60
19	2	1217	CLA	C1D-CHD-C4C	-6.37	112.96	122.60
19	A	1767	CLA	C1D-CHD-C4C	-6.37	112.96	122.60
19	B	1757	CLA	O1D-CGD-CBD	-6.37	115.50	124.62
19	A	1767	CLA	C4B-CHC-C1C	-6.36	115.60	129.26
19	4	1201	CLA	C4B-CHC-C1C	-6.34	115.64	129.26
19	3	1216	CLA	C3A-C4A-CHB	-6.31	117.69	124.06
19	B	1765	CLA	C4B-CHC-C1C	-6.30	115.72	129.26
20	R	1057	LMU	C4B-C3B-C2B	-6.29	99.05	110.79
19	A	1759	CLA	C4B-CHC-C1C	-6.29	115.75	129.26
19	A	1784	CLA	C4B-CHC-C1C	-6.29	115.75	129.26
19	4	1201	CLA	CMB-C2B-C1B	-6.29	117.96	128.36
19	L	1168	CLA	C3D-CAD-CBD	-6.29	98.71	107.60
19	2	1223	CLA	C1D-CHD-C4C	-6.28	113.09	122.60
19	2	1220	CLA	C1D-CHD-C4C	-6.28	113.10	122.60
19	B	1747	CLA	OBD-CAD-C3D	-6.28	115.55	128.35
19	A	1812	CLA	C1D-CHD-C4C	-6.27	113.12	122.60
19	2	1220	CLA	C4B-CHC-C1C	-6.27	115.80	129.26
19	A	1778	CLA	C4B-CHC-C1C	-6.26	115.81	129.26
19	B	1747	CLA	C4B-CHC-C1C	-6.25	115.83	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1187	CLA	C1D-CHD-C4C	-6.25	113.14	122.60
22	B	1781	BCR	C4-C5-C6	-6.25	114.82	122.78
19	B	1752	CLA	C4B-CHC-C1C	-6.24	115.85	129.26
19	B	1740	CLA	C4B-CHC-C1C	-6.24	115.86	129.26
19	A	1779	CLA	C4B-CHC-C1C	-6.23	115.88	129.26
19	R	1055	CLA	C4B-CHC-C1C	-6.23	115.88	129.26
19	F	1157	CLA	C1D-CHD-C4C	-6.23	113.18	122.60
19	A	1772	CLA	C1D-CHD-C4C	-6.23	113.18	122.60
19	1	1193	CLA	CBA-CAA-C2A	-6.22	96.19	113.73
19	1	1198	CLA	C4B-CHC-C1C	-6.22	115.90	129.26
19	2	1217	CLA	C4B-CHC-C1C	-6.21	115.91	129.26
19	J	1044	CLA	CAA-C2A-C3A	-6.21	95.37	113.22
19	B	1763	CLA	C4B-CHC-C1C	-6.20	115.94	129.26
19	2	1223	CLA	C4B-CHC-C1C	-6.20	115.94	129.26
22	B	1779	BCR	C24-C23-C22	-6.20	116.77	126.22
19	1	1194	CLA	C3A-C4A-CHB	-6.20	117.81	124.06
19	A	1762	CLA	C4B-CHC-C1C	-6.19	115.95	129.26
19	4	1198	CLA	CAA-C2A-C3A	-6.19	95.41	113.22
19	B	1763	CLA	C1D-CHD-C4C	-6.19	113.23	122.60
19	B	1754	CLA	C1D-CHD-C4C	-6.18	113.25	122.60
19	A	1789	CLA	C4B-CHC-C1C	-6.17	116.00	129.26
19	2	1213	CLA	OBD-CAD-CBD	-6.17	116.62	125.94
19	B	1739	CLA	C4B-CHC-C1C	-6.15	116.04	129.26
19	1	1188	CLA	OBD-CAD-C3D	-6.14	115.82	128.35
19	1	1195	CLA	C4B-CHC-C1C	-6.14	116.07	129.26
19	H	1079	CLA	C4B-CHC-C1C	-6.13	116.09	129.26
19	B	1751	CLA	C4B-CHC-C1C	-6.13	116.09	129.26
19	B	1742	CLA	C4B-CHC-C1C	-6.12	116.10	129.26
19	A	1764	CLA	C4B-CHC-C1C	-6.12	116.12	129.26
19	B	1744	CLA	C4B-CHC-C1C	-6.12	116.12	129.26
19	3	1212	CLA	CAB-C3B-C2B	-6.12	112.63	125.14
19	A	1817	CLA	C4B-CHC-C1C	-6.11	116.12	129.26
19	B	1750	CLA	C4B-CHC-C1C	-6.11	116.12	129.26
19	3	3011	CLA	OBD-CAD-CBD	-6.11	116.71	125.94
19	L	1167	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	L	1505	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	B	1751	CLA	CHD-C4C-C3C	-6.10	115.52	124.94
19	A	1763	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	A	1812	CLA	C4B-CHC-C1C	-6.09	116.17	129.26
19	1	1196	CLA	OBD-CAD-C3D	-6.09	115.92	128.35
19	B	1753	CLA	CHD-C4C-C3C	-6.09	115.53	124.94
19	F	1156	CLA	C4B-CHC-C1C	-6.09	116.18	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1738	CLA	C1D-CHD-C4C	-6.08	113.39	122.60
19	3	3007	CLA	C4B-CHC-C1C	-6.08	116.19	129.26
19	B	1755	CLA	C4B-CHC-C1C	-6.08	116.19	129.26
19	A	1775	CLA	C1D-CHD-C4C	-6.07	113.41	122.60
19	B	1769	CLA	C1D-CHD-C4C	-6.07	113.41	122.60
19	F	1155	CLA	OBD-CAD-C3D	-6.07	115.97	128.35
19	B	1753	CLA	C6-C5-C3	-6.07	99.16	112.48
19	K	1085	CLA	C4B-CHC-C1C	-6.07	116.22	129.26
19	4	1207	CLA	CAB-C3B-C2B	-6.07	112.73	125.14
19	B	1744	CLA	OBD-CAD-CBD	-6.06	116.79	125.94
19	4	4014	CLA	C4B-CHC-C1C	-6.06	116.23	129.26
19	A	1782	CLA	C4B-CHC-C1C	-6.06	116.24	129.26
19	2	1212	CLA	C4B-CHC-C1C	-6.06	116.25	129.26
19	A	1791	CLA	C4B-CHC-C1C	-6.05	116.26	129.26
19	B	1769	CLA	C4B-CHC-C1C	-6.05	116.26	129.26
19	K	1142	CLA	C4B-CHC-C1C	-6.05	116.26	129.26
19	A	1793	CLA	C4B-CHC-C1C	-6.05	116.27	129.26
19	B	1756	CLA	C4B-CHC-C1C	-6.05	116.27	129.26
19	A	1794	CLA	C4B-CHC-C1C	-6.05	116.27	129.26
19	4	1196	CLA	C4B-CHC-C1C	-6.05	116.27	129.26
19	A	1795	CLA	C4B-CHC-C1C	-6.05	116.27	129.26
19	A	1796	CLA	C4B-CHC-C1C	-6.04	116.28	129.26
19	B	1735	CLA	C4B-CHC-C1C	-6.04	116.28	129.26
19	A	1786	CLA	C4B-CHC-C1C	-6.04	116.29	129.26
19	A	1797	CLA	C4B-CHC-C1C	-6.04	116.29	129.26
19	3	1219	CLA	C4B-CHC-C1C	-6.04	116.29	129.26
19	A	1792	CLA	C4B-CHC-C1C	-6.03	116.30	129.26
19	1	1197	CLA	CMD-C2D-C3D	-6.03	113.29	125.09
19	A	1781	CLA	C4B-CHC-C1C	-6.03	116.31	129.26
19	2	1216	CLA	C2D-C3D-C4D	-6.03	101.00	106.30
19	B	1749	CLA	C4B-CHC-C1C	-6.03	116.31	129.26
19	B	1748	CLA	C1D-CHD-C4C	-6.02	113.49	122.60
19	K	1085	CLA	C1D-CHD-C4C	-6.01	113.50	122.60
19	K	1142	CLA	C1D-CHD-C4C	-6.01	113.50	122.60
19	3	3008	CLA	C4B-CHC-C1C	-6.01	116.34	129.26
19	J	1045	CLA	C4B-CHC-C1C	-6.01	116.36	129.26
19	B	1748	CLA	C4B-CHC-C1C	-6.01	116.36	129.26
19	4	1196	CLA	C1D-CHD-C4C	-5.99	113.53	122.60
19	2	1212	CLA	C1D-CHD-C4C	-5.99	113.54	122.60
19	3	1212	CLA	C1D-CHD-C4C	-5.99	113.54	122.60
19	A	1797	CLA	C1D-CHD-C4C	-5.98	113.55	122.60
19	2	1224	CLA	C4B-CHC-C1C	-5.98	116.41	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3008	CLA	C1D-CHD-C4C	-5.98	113.55	122.60
19	4	4014	CLA	C1D-CHD-C4C	-5.98	113.55	122.60
19	J	1043	CLA	C1D-CHD-C4C	-5.98	113.55	122.60
19	B	1735	CLA	C1D-CHD-C4C	-5.98	113.56	122.60
19	A	1791	CLA	C1D-CHD-C4C	-5.98	113.56	122.60
19	J	1043	CLA	C4B-CHC-C1C	-5.97	116.42	129.26
19	B	1761	CLA	C4B-CHC-C1C	-5.97	116.42	129.26
19	F	1156	CLA	C1D-CHD-C4C	-5.97	113.56	122.60
19	B	1755	CLA	C1D-CHD-C4C	-5.97	113.56	122.60
19	3	1219	CLA	C1D-CHD-C4C	-5.97	113.57	122.60
19	A	1795	CLA	C1D-CHD-C4C	-5.96	113.58	122.60
19	A	1800	CLA	C4B-CHC-C1C	-5.96	116.45	129.26
19	A	1794	CLA	C1D-CHD-C4C	-5.96	113.58	122.60
19	1	1193	CLA	C4B-CHC-C1C	-5.96	116.46	129.26
19	A	1780	CLA	C4B-CHC-C1C	-5.96	116.47	129.26
19	B	1756	CLA	C1D-CHD-C4C	-5.95	113.60	122.60
19	A	1792	CLA	C1D-CHD-C4C	-5.95	113.60	122.60
19	A	1793	CLA	C1D-CHD-C4C	-5.95	113.60	122.60
19	A	1811	CLA	CHD-C4C-C3C	-5.94	115.75	124.94
19	F	1155	CLA	C4B-CHC-C1C	-5.94	116.49	129.26
19	A	1782	CLA	C1D-CHD-C4C	-5.94	113.61	122.60
19	A	1781	CLA	C1D-CHD-C4C	-5.94	113.61	122.60
19	1	1191	CLA	C4B-CHC-C1C	-5.94	116.50	129.26
19	2	1222	CLA	C4B-CHC-C1C	-5.93	116.51	129.26
19	A	1796	CLA	C1D-CHD-C4C	-5.93	113.62	122.60
19	4	1201	CLA	CBA-CAA-C2A	-5.93	97.00	113.73
19	A	1775	CLA	C4B-CHC-C1C	-5.93	116.52	129.26
20	A	7040	LMU	C3B-C4B-C5B	-5.92	99.88	110.20
20	A	7039	LMU	O5B-C5B-C6B	-5.91	91.41	106.36
19	B	1758	CLA	C1D-CHD-C4C	-5.91	113.66	122.60
19	B	1762	CLA	C4B-CHC-C1C	-5.89	116.61	129.26
22	I	1032	BCR	C11-C10-C9	-5.88	118.70	127.20
19	A	1772	CLA	C4B-CHC-C1C	-5.88	116.63	129.26
19	R	1054	CLA	C4B-CHC-C1C	-5.87	116.65	129.26
19	A	1787	CLA	C4B-CHC-C1C	-5.86	116.66	129.26
19	4	1200	CLA	C1D-CHD-C4C	-5.85	113.74	122.60
19	1	1190	CLA	C4B-CHC-C1C	-5.85	116.69	129.26
19	1	1196	CLA	C1D-CHD-C4C	-5.85	113.75	122.60
19	4	1207	CLA	C1D-CHD-C4C	-5.84	113.76	122.60
19	B	1760	CLA	C4B-CHC-C1C	-5.84	116.71	129.26
19	2	1215	CLA	C4B-CHC-C1C	-5.84	116.72	129.26
19	F	1155	CLA	C1D-CHD-C4C	-5.84	113.77	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1798	CLA	C1D-CHD-C4C	-5.83	113.78	122.60
19	L	1168	CLA	O1D-CGD-CBD	-5.83	116.27	124.62
19	A	1761	CLA	C1D-CHD-C4C	-5.82	113.80	122.60
19	I	1033	CLA	C4B-CHC-C1C	-5.81	116.77	129.26
19	2	1214	CLA	C3A-C4A-CHB	-5.81	118.19	124.06
19	L	1166	CLA	C1D-CHD-C4C	-5.81	113.81	122.60
19	1	1191	CLA	CAB-C3B-C2B	-5.81	113.26	125.14
19	B	1758	CLA	C4B-CHC-C1C	-5.80	116.80	129.26
19	B	1767	CLA	C1D-CHD-C4C	-5.80	113.83	122.60
19	1	1192	CLA	C4B-CHC-C1C	-5.79	116.82	129.26
19	A	1769	CLA	C1D-CHD-C4C	-5.79	113.84	122.60
19	A	1768	CLA	C1D-CHD-C4C	-5.79	113.84	122.60
19	B	1744	CLA	OBD-CAD-C3D	-5.78	116.55	128.35
20	A	7032	LMU	C3B-C4B-C5B	-5.78	100.12	110.20
19	B	1736	CLA	C1D-CHD-C4C	-5.78	113.86	122.60
19	4	1204	CLA	CHD-C4C-C3C	-5.77	116.02	124.94
19	A	1789	CLA	C1D-CHD-C4C	-5.77	113.87	122.60
19	B	1750	CLA	C1D-CHD-C4C	-5.75	113.90	122.60
19	B	1743	CLA	C4B-CHC-C1C	-5.75	116.91	129.26
19	A	1778	CLA	C3D-CAD-CBD	-5.75	99.47	107.60
19	B	1743	CLA	CHD-C4C-C3C	-5.74	116.06	124.94
20	A	7016	LMU	C1'-O5'-C5'	-5.74	102.60	113.75
19	A	1785	CLA	C4B-CHC-C1C	-5.74	116.94	129.26
19	A	1783	CLA	C1D-CHD-C4C	-5.73	113.93	122.60
19	L	1505	CLA	C1D-CHD-C4C	-5.73	113.93	122.60
19	B	1762	CLA	C1D-CHD-C4C	-5.73	113.93	122.60
19	G	1099	CLA	C1D-CHD-C4C	-5.73	113.93	122.60
19	2	1227	CLA	C3A-C4A-CHB	-5.73	118.28	124.06
19	A	1777	CLA	C4B-CHC-C1C	-5.73	116.96	129.26
19	1	1191	CLA	C1D-CHD-C4C	-5.72	113.94	122.60
19	A	1770	CLA	C4B-CHC-C1C	-5.72	116.97	129.26
19	A	1769	CLA	C4B-CHC-C1C	-5.72	116.98	129.26
21	3	1221	SUC	C3-C4-C5	-5.71	100.24	110.20
19	B	1746	CLA	C4B-CHC-C1C	-5.71	117.00	129.26
19	A	1801	CLA	C1D-CHD-C4C	-5.70	113.97	122.60
19	A	1773	CLA	C4B-CHC-C1C	-5.70	117.02	129.26
19	4	1207	CLA	C4B-CHC-C1C	-5.70	117.02	129.26
19	A	1813	CLA	C4B-CHC-C1C	-5.69	117.03	129.26
20	A	7040	LMU	O3B-C3B-C2B	-5.67	97.57	110.34
19	A	1773	CLA	C1D-CHD-C4C	-5.67	114.02	122.60
19	I	1033	CLA	C1D-CHD-C4C	-5.67	114.02	122.60
19	3	1212	CLA	C4B-CHC-C1C	-5.67	117.09	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1752	CLA	C1D-CHD-C4C	-5.66	114.03	122.60
22	3	1220	BCR	C33-C5-C6	-5.66	119.05	124.61
19	B	1750	CLA	C3D-CAD-CBD	-5.66	99.59	107.60
19	3	3015	CLA	C3A-C4A-CHB	-5.65	118.36	124.06
19	A	1815	CLA	C4B-CHC-C1C	-5.64	117.14	129.26
19	3	1213	CLA	C3A-C4A-CHB	-5.64	118.36	124.06
22	B	1779	BCR	C10-C11-C12	-5.64	105.93	123.13
19	J	1044	CLA	C4B-CHC-C1C	-5.64	117.15	129.26
19	A	1785	CLA	C1D-CHD-C4C	-5.63	114.08	122.60
19	A	1774	CLA	C1D-CHD-C4C	-5.62	114.10	122.60
19	2	1219	CLA	C3A-C4A-CHB	-5.62	118.39	124.06
19	A	1771	CLA	C4B-CHC-C1C	-5.62	117.20	129.26
19	B	1757	CLA	C1D-CHD-C4C	-5.61	114.10	122.60
19	B	1766	CLA	C4B-CHC-C1C	-5.61	117.21	129.26
22	L	1170	BCR	C34-C9-C10	-5.61	114.62	122.90
19	A	1790	CLA	C4B-CHC-C1C	-5.60	117.23	129.26
19	B	1787	CLA	C1D-CHD-C4C	-5.60	114.13	122.60
19	A	1768	CLA	C4B-CHC-C1C	-5.60	117.23	129.26
19	A	1780	CLA	C1D-CHD-C4C	-5.60	114.13	122.60
19	A	1799	CLA	C4B-CHC-C1C	-5.59	117.24	129.26
19	3	3011	CLA	C4B-CHC-C1C	-5.57	117.28	129.26
19	A	1817	CLA	CMD-C2D-C3D	-5.57	114.19	125.09
22	L	1169	BCR	C33-C5-C6	-5.57	119.14	124.61
19	B	1757	CLA	C4B-CHC-C1C	-5.57	117.30	129.26
19	A	1788	CLA	C1D-CHD-C4C	-5.56	114.18	122.60
19	B	1761	CLA	CHD-C4C-C3C	-5.55	116.36	124.94
19	1	1196	CLA	C4B-CHC-C1C	-5.55	117.33	129.26
22	B	1776	BCR	C27-C26-C25	-5.55	115.71	122.78
19	3	1217	CLA	C3A-C4A-CHB	-5.54	118.46	124.06
19	1	1201	CLA	C2A-C1A-CHA	-5.54	112.76	122.58
20	A	7040	LMU	C1B-O1B-C4'	-5.54	103.52	118.01
19	B	1749	CLA	C1D-CHD-C4C	-5.54	114.22	122.60
19	B	1741	CLA	C1D-CHD-C4C	-5.54	114.22	122.60
19	2	1213	CLA	C4B-CHC-C1C	-5.54	117.37	129.26
19	4	1209	CLA	C4B-CHC-C1C	-5.54	117.37	129.26
19	4	1200	CLA	C4B-CHC-C1C	-5.53	117.37	129.26
20	A	7039	LMU	C1B-C2B-C3B	-5.53	99.08	109.97
19	B	1767	CLA	O2D-CGD-O1D	-5.52	112.39	123.79
19	2	1227	CLA	C2D-C3D-C4D	-5.52	101.45	106.30
19	2	1224	CLA	C1D-CHD-C4C	-5.51	114.26	122.60
20	A	7021	LMU	O3B-C3B-C4B	-5.51	97.93	110.34
19	B	1741	CLA	C4B-CHC-C1C	-5.51	117.42	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1738	CLA	C4B-CHC-C1C	-5.51	117.43	129.26
19	B	1746	CLA	O1D-CGD-CBD	-5.49	116.75	124.62
19	B	1767	CLA	C4B-CHC-C1C	-5.49	117.47	129.26
19	1	1189	CLA	C4B-CHC-C1C	-5.49	117.47	129.26
19	1	1197	CLA	CGD-CBD-CAD	-5.49	92.03	110.62
19	B	1787	CLA	C3D-CAD-CBD	-5.48	99.84	107.60
19	A	1798	CLA	C4B-CHC-C1C	-5.47	117.51	129.26
22	I	1032	BCR	C16-C17-C18	-5.46	119.31	127.20
19	B	1772	CLA	C4B-CHC-C1C	-5.46	117.53	129.26
19	B	1754	CLA	C4B-CHC-C1C	-5.45	117.55	129.26
19	B	1786	CLA	C4B-CHC-C1C	-5.45	117.56	129.26
19	K	3009	CLA	C1D-CHD-C4C	-5.44	114.37	122.60
19	2	2010	CLA	C3A-C4A-CHB	-5.44	118.57	124.06
19	A	1776	CLA	C1D-CHD-C4C	-5.44	114.37	122.60
20	A	7022	LMU	O3B-C3B-C4B	-5.44	98.09	110.34
19	B	1737	CLA	C1D-CHD-C4C	-5.43	114.38	122.60
19	K	3009	CLA	C4B-CHC-C1C	-5.43	117.59	129.26
19	1	1190	CLA	C1D-CHD-C4C	-5.43	114.38	122.60
19	B	1787	CLA	C4B-CHC-C1C	-5.43	117.59	129.26
19	B	1736	CLA	C4B-CHC-C1C	-5.43	117.59	129.26
19	1	1192	CLA	CHD-C4C-C3C	-5.43	116.55	124.94
19	B	1745	CLA	C1D-CHD-C4C	-5.43	114.39	122.60
19	B	1764	CLA	C4B-CHC-C1C	-5.42	117.62	129.26
19	1	1193	CLA	CGD-CBD-CAD	-5.40	92.32	110.62
19	A	1759	CLA	C1D-CHD-C4C	-5.40	114.43	122.60
22	I	1032	BCR	C29-C30-C25	-5.40	101.82	110.36
22	B	1779	BCR	C35-C13-C14	-5.39	114.93	122.90
19	B	1739	CLA	C3D-CAD-CBD	-5.39	99.98	107.60
19	L	1166	CLA	C4B-CHC-C1C	-5.38	117.70	129.26
19	1	1201	CLA	C3B-C2B-C1B	-5.38	101.58	106.29
19	4	1204	CLA	C4B-CHC-C1C	-5.37	117.71	129.26
21	B	8062	SUC	C3-C4-C5	-5.37	100.84	110.20
20	R	1057	LMU	C1'-C2'-C3'	-5.35	99.42	109.97
19	A	1760	CLA	C1D-CHD-C4C	-5.35	114.50	122.60
19	B	1786	CLA	C1D-CHD-C4C	-5.35	114.50	122.60
19	B	1745	CLA	C4B-CHC-C1C	-5.35	117.77	129.26
19	H	1079	CLA	C1D-CHD-C4C	-5.34	114.52	122.60
19	B	1746	CLA	C1D-CHD-C4C	-5.34	114.52	122.60
20	A	7039	LMU	O5B-C1B-C2B	-5.33	99.34	110.28
20	A	7043	LMU	O3'-C3'-C4'	-5.33	97.27	109.87
20	A	7037	LMU	C3B-C4B-C5B	-5.32	100.92	110.20
19	4	1209	CLA	CHD-C4C-C3C	-5.32	116.72	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1168	CLA	CHD-C4C-C3C	-5.31	116.73	124.94
19	A	1779	CLA	C1D-CHD-C4C	-5.30	114.59	122.60
19	J	1046	CLA	C3A-C4A-CHB	-5.29	118.72	124.06
19	A	1816	CLA	CMD-C2D-C3D	-5.29	114.75	125.09
19	L	1167	CLA	C1D-CHD-C4C	-5.28	114.61	122.60
19	4	1205	CLA	C1D-CHD-C4C	-5.28	112.75	126.32
19	B	1739	CLA	OBD-CAD-C3D	-5.27	117.59	128.35
21	B	8061	SUC	C3-C4-C5	-5.27	101.02	110.20
19	A	1816	CLA	CHD-C4C-C3C	-5.25	116.82	124.94
20	A	7037	LMU	O1'-C1'-C2'	-5.25	101.41	108.04
19	3	3002	CLA	C3A-C4A-CHB	-5.25	118.76	124.06
19	3	1215	CLA	C1D-CHD-C4C	-5.25	112.82	126.32
19	3	1214	CLA	C1D-CHD-C4C	-5.24	112.83	126.32
19	A	1784	CLA	C1D-CHD-C4C	-5.24	114.67	122.60
21	B	8062	SUC	O5-C1-C2	-5.24	99.52	110.28
22	B	1781	BCR	C28-C27-C26	-5.24	105.55	113.87
19	A	1799	CLA	C1D-CHD-C4C	-5.24	114.67	122.60
19	A	1765	CLA	C1D-CHD-C4C	-5.23	114.68	122.60
19	4	1206	CLA	C3A-C4A-CHB	-5.23	118.78	124.06
19	A	1790	CLA	C1D-CHD-C4C	-5.23	114.69	122.60
21	B	8055	SUC	C6-C5-C4	-5.22	100.13	113.02
19	B	1753	CLA	CBC-CAC-C3C	-5.22	96.47	112.39
19	B	1771	CLA	C3D-CAD-CBD	-5.21	100.23	107.60
19	2	1216	CLA	C2A-C1A-CHA	-5.21	113.35	122.58
19	A	1777	CLA	C1D-CHD-C4C	-5.20	114.74	122.60
19	A	1801	CLA	C4B-CHC-C1C	-5.19	118.10	129.26
19	A	1776	CLA	C4B-CHC-C1C	-5.19	118.11	129.26
19	1	1198	CLA	CHD-C4C-C3C	-5.18	116.93	124.94
22	L	1170	BCR	C10-C11-C12	-5.18	107.34	123.13
20	A	7041	LMU	C6B-C5B-C4B	-5.18	100.24	113.02
19	3	1213	CLA	C2A-C1A-CHA	-5.17	113.42	122.58
19	1	1201	CLA	C2D-C3D-C4D	-5.17	101.75	106.30
19	I	1031	CLA	C4B-CHC-C1C	-5.16	118.18	129.26
19	B	1738	CLA	C6-C5-C3	-5.15	101.17	112.48
19	A	1779	CLA	C3D-CAD-CBD	-5.15	100.31	107.60
21	2	1226	SUC	O5-C5-C4	-5.15	100.60	109.53
19	2	1213	CLA	C1D-CHD-C4C	-5.15	114.81	122.60
19	4	4003	CLA	C3A-C4A-CHB	-5.15	118.86	124.06
19	A	1815	CLA	C1D-CHD-C4C	-5.14	114.83	122.60
22	L	1169	BCR	C30-C25-C26	-5.13	115.12	122.66
19	1	1188	CLA	C1D-CHD-C4C	-5.13	114.84	122.60
19	B	1749	CLA	CHD-C4C-C3C	-5.13	117.01	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	8060	SUC	C6'-C5'-C4'	-5.13	102.95	115.08
19	1	1200	CLA	CAA-C2A-C3A	-5.13	98.47	113.22
19	B	1764	CLA	C3D-CAD-CBD	-5.12	100.35	107.60
20	A	7017	LMU	O4'-C4B-C5B	-5.12	95.68	109.24
19	3	3014	CLA	C3B-C2B-C1B	-5.12	101.81	106.29
19	3	3011	CLA	C1D-CHD-C4C	-5.11	114.87	122.60
19	1	1189	CLA	C1D-CHD-C4C	-5.10	114.88	122.60
19	3	1217	CLA	C3B-C2B-C1B	-5.10	101.83	106.29
19	B	1765	CLA	C1D-CHD-C4C	-5.10	114.88	122.60
19	4	1203	CLA	C3A-C4A-CHB	-5.09	118.92	124.06
19	R	1055	CLA	C1D-CHD-C4C	-5.09	114.90	122.60
19	1	1187	CLA	CMD-C2D-C3D	-5.08	115.15	125.09
22	B	1778	BCR	C11-C10-C9	-5.08	119.86	127.20
21	3	1221	SUC	C4-C3-C2	-5.08	101.32	110.79
20	A	7036	LMU	C1B-O1B-C4'	-5.07	104.76	118.01
19	1	1193	CLA	C3D-CAD-CBD	-5.07	100.43	107.60
22	B	1778	BCR	C15-C14-C13	-5.07	119.88	127.20
19	R	1054	CLA	C1D-CHD-C4C	-5.07	114.93	122.60
19	A	1767	CLA	CMD-C2D-C3D	-5.06	115.18	125.09
19	4	1198	CLA	CMD-C2D-C3D	-5.06	115.19	125.09
19	4	1208	CLA	C3A-C4A-CHB	-5.06	118.95	124.06
22	B	1776	BCR	C24-C23-C22	-5.06	118.51	126.22
22	B	1775	BCR	C11-C10-C9	-5.05	119.90	127.20
19	2	1221	CLA	C3B-C2B-C1B	-5.05	101.87	106.29
22	A	1807	BCR	C16-C17-C18	-5.05	119.91	127.20
19	1	1193	CLA	C1D-CHD-C4C	-5.05	114.97	122.60
19	A	1801	CLA	CHD-C4C-C3C	-5.04	117.15	124.94
19	R	1054	CLA	C3D-CAD-CBD	-5.03	100.48	107.60
22	A	1806	BCR	C15-C14-C13	-5.03	119.93	127.20
19	A	1816	CLA	O2D-CGD-O1D	-5.03	113.40	123.79
20	A	7041	LMU	C4B-C3B-C2B	-5.03	101.41	110.79
22	L	1169	BCR	C3-C4-C5	-5.02	105.91	113.87
19	B	1763	CLA	C3D-CAD-CBD	-5.02	100.51	107.60
22	A	1808	BCR	C15-C14-C13	-5.02	119.95	127.20
22	B	1780	BCR	C16-C17-C18	-5.01	119.95	127.20
19	A	1812	CLA	O1D-CGD-CBD	-5.01	117.44	124.62
22	A	1806	BCR	C11-C10-C9	-5.01	119.96	127.20
19	B	1761	CLA	C1D-CHD-C4C	-5.01	115.03	122.60
19	4	1203	CLA	C1D-CHD-C4C	-5.00	113.45	126.32
19	4	1197	CLA	C4B-CHC-C1C	-5.00	118.52	129.26
22	A	1803	BCR	C16-C17-C18	-4.99	119.98	127.20
22	B	1775	BCR	C15-C14-C13	-4.99	119.98	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1803	BCR	C15-C14-C13	-4.99	119.98	127.20
22	B	1778	BCR	C16-C17-C18	-4.99	119.99	127.20
22	A	1805	BCR	C11-C10-C9	-4.99	119.99	127.20
19	A	1786	CLA	C1D-CHD-C4C	-4.99	115.05	122.60
23	B	1773	PQN	C11-C12-C13	-4.99	118.25	126.70
19	4	1204	CLA	C3D-CAD-CBD	-4.99	100.55	107.60
22	A	1808	BCR	C16-C17-C18	-4.98	120.00	127.20
22	B	1777	BCR	C15-C14-C13	-4.98	120.00	127.20
19	B	1758	CLA	CHD-C4C-C3C	-4.98	117.24	124.94
22	B	1777	BCR	C11-C10-C9	-4.98	120.01	127.20
22	A	1804	BCR	C11-C10-C9	-4.98	120.01	127.20
22	A	1807	BCR	C11-C10-C9	-4.98	120.01	127.20
19	A	1778	CLA	C1D-CHD-C4C	-4.98	115.07	122.60
22	A	1804	BCR	C15-C14-C13	-4.98	120.01	127.20
19	3	3014	CLA	C2D-C3D-C4D	-4.98	101.92	106.30
22	A	1806	BCR	C16-C17-C18	-4.97	120.01	127.20
19	A	1759	CLA	O1D-CGD-CBD	-4.97	117.49	124.62
22	A	1805	BCR	C16-C17-C18	-4.97	120.02	127.20
22	A	1804	BCR	C16-C17-C18	-4.97	120.02	127.20
19	A	1771	CLA	C1D-CHD-C4C	-4.96	115.09	122.60
22	B	1780	BCR	C15-C14-C13	-4.96	120.03	127.20
19	B	1772	CLA	C1D-CHD-C4C	-4.96	115.09	122.60
22	B	1780	BCR	C11-C10-C9	-4.96	120.03	127.20
19	A	1787	CLA	C1D-CHD-C4C	-4.96	115.10	122.60
22	B	1777	BCR	C16-C17-C18	-4.95	120.05	127.20
21	B	8060	SUC	C2'-O1-C1	-4.95	104.49	117.53
19	B	1748	CLA	CHD-C4C-C3C	-4.95	117.29	124.94
22	B	1775	BCR	C16-C17-C18	-4.95	120.05	127.20
19	B	1739	CLA	C1D-CHD-C4C	-4.94	115.12	122.60
22	A	1808	BCR	C11-C10-C9	-4.94	120.06	127.20
22	A	1805	BCR	C15-C14-C13	-4.94	120.06	127.20
22	A	1807	BCR	C15-C14-C13	-4.94	120.07	127.20
19	L	1168	CLA	C4B-CHC-C1C	-4.94	118.66	129.26
22	3	1220	BCR	C38-C26-C25	-4.93	119.76	124.61
19	2	1227	CLA	C3B-C2B-C1B	-4.93	101.97	106.29
19	F	1157	CLA	CHD-C4C-C3C	-4.93	117.32	124.94
19	1	1189	CLA	C3D-CAD-CBD	-4.93	100.63	107.60
22	B	1774	BCR	C16-C17-C18	-4.93	120.08	127.20
22	B	1774	BCR	C15-C14-C13	-4.93	120.08	127.20
19	B	1740	CLA	C3D-CAD-CBD	-4.93	100.63	107.60
22	B	1774	BCR	C11-C10-C9	-4.92	120.09	127.20
19	1	1195	CLA	CHD-C4C-C3C	-4.92	116.59	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1146	CLA	C1D-CHD-C4C	-4.92	115.16	122.60
19	A	1764	CLA	C1D-CHD-C4C	-4.91	115.17	122.60
22	A	1803	BCR	C11-C10-C9	-4.91	120.11	127.20
19	4	1198	CLA	O2A-CGA-O1A	-4.91	110.83	123.49
19	3	3002	CLA	C1D-CHD-C4C	-4.91	113.70	126.32
19	1	1189	CLA	CMD-C2D-C3D	-4.90	115.50	125.09
19	1	1187	CLA	CAC-C3C-C2C	-4.90	118.92	127.51
22	B	1781	BCR	C37-C22-C21	-4.90	115.67	122.90
19	B	1766	CLA	C1D-CHD-C4C	-4.90	115.19	122.60
19	F	1157	CLA	C4B-CHC-C1C	-4.89	118.76	129.26
19	1	1195	CLA	CMD-C2D-C3D	-4.89	115.53	125.09
19	B	1751	CLA	C3D-CAD-CBD	-4.87	100.71	107.60
22	I	1032	BCR	C27-C26-C25	-4.87	116.58	122.78
19	4	1202	CLA	C3B-C2B-C1B	-4.87	102.03	106.29
19	A	1817	CLA	C1D-CHD-C4C	-4.87	115.24	122.60
19	4	1201	CLA	CHD-C4C-C3C	-4.86	117.42	124.94
19	1	1199	CLA	C3B-C2B-C1B	-4.86	102.03	106.29
19	B	1765	CLA	C3D-CAD-CBD	-4.86	100.73	107.60
19	A	1788	CLA	C3D-CAD-CBD	-4.86	100.73	107.60
19	B	1736	CLA	O2D-CGD-O1D	-4.85	113.78	123.79
19	3	1217	CLA	C2D-C3D-C4D	-4.85	102.03	106.30
19	4	1206	CLA	C2A-C1A-CHA	-4.84	114.00	122.58
22	B	1780	BCR	C38-C26-C25	-4.84	119.86	124.61
19	2	1220	CLA	CHD-C4C-C3C	-4.83	117.47	124.94
19	B	1769	CLA	O1D-CGD-CBD	-4.83	117.70	124.62
19	G	1099	CLA	C4B-CHC-C1C	-4.83	118.89	129.26
19	3	3008	CLA	CMD-C2D-C3D	-4.83	115.65	125.09
20	A	7017	LMU	O5B-C5B-C4B	-4.82	100.63	109.68
19	J	1045	CLA	CHD-C4C-C3C	-4.82	117.49	124.94
19	2	1220	CLA	C3D-CAD-CBD	-4.82	100.79	107.60
19	B	1763	CLA	CHD-C4C-C3C	-4.82	117.50	124.94
19	B	1746	CLA	C3D-CAD-CBD	-4.81	100.79	107.60
19	A	1812	CLA	CHD-C4C-C3C	-4.81	117.50	124.94
19	4	1206	CLA	C3B-C2B-C1B	-4.81	102.08	106.29
19	4	4007	CLA	C1D-CHD-C4C	-4.81	115.33	122.60
22	B	1779	BCR	C16-C17-C18	-4.80	120.26	127.20
19	B	1751	CLA	O1D-CGD-CBD	-4.80	117.75	124.62
19	A	1762	CLA	C1D-CHD-C4C	-4.80	115.34	122.60
19	1	1199	CLA	C1D-CHD-C4C	-4.79	114.01	126.32
22	A	1807	BCR	C33-C5-C6	-4.78	119.91	124.61
19	B	1742	CLA	C1D-CHD-C4C	-4.78	115.36	122.60
19	1	1198	CLA	O1D-CGD-CBD	-4.78	117.77	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1803	BCR	C38-C26-C25	-4.78	119.91	124.61
19	1	1194	CLA	C3B-C2B-C1B	-4.78	102.11	106.29
19	B	1753	CLA	C2A-C1A-CHA	-4.78	115.09	123.89
19	2	1214	CLA	C1D-CHD-C4C	-4.77	114.05	126.32
19	B	1771	CLA	C1D-CHD-C4C	-4.77	115.38	122.60
20	A	7026	LMU	O5B-C5B-C4B	-4.77	100.73	109.68
22	3	1220	BCR	C7-C8-C9	-4.77	118.95	126.22
19	4	1202	CLA	C1D-CHD-C4C	-4.77	114.06	126.32
22	A	1804	BCR	C38-C26-C25	-4.77	119.92	124.61
22	L	1169	BCR	C7-C8-C9	-4.77	118.95	126.22
20	A	7030	LMU	O5'-C1'-C2'	-4.77	100.50	110.28
19	A	1786	CLA	O2D-CGD-O1D	-4.76	113.95	123.79
20	A	7032	LMU	O1'-C1'-C2'	-4.76	102.03	108.04
19	2	1219	CLA	C1D-CHD-C4C	-4.76	114.08	126.32
19	B	1758	CLA	C3D-CAD-CBD	-4.75	100.88	107.60
19	A	1783	CLA	C4B-CHC-C1C	-4.75	119.05	129.26
19	2	1222	CLA	C1D-CHD-C4C	-4.75	115.42	122.60
19	A	1770	CLA	C1D-CHD-C4C	-4.75	115.42	122.60
19	A	1800	CLA	C1D-CHD-C4C	-4.74	115.42	122.60
19	1	1194	CLA	C1D-CHD-C4C	-4.74	114.12	126.32
22	A	1805	BCR	C33-C5-C6	-4.74	119.95	124.61
22	A	1806	BCR	C38-C26-C25	-4.74	119.95	124.61
19	1	1192	CLA	C3D-CAD-CBD	-4.74	100.89	107.60
19	3	3001	CLA	C1D-CHD-C4C	-4.74	114.13	126.32
22	A	1808	BCR	C38-C26-C25	-4.74	119.95	124.61
19	4	1198	CLA	CHD-C4C-C3C	-4.74	117.62	124.94
22	A	1806	BCR	C33-C5-C6	-4.73	119.96	124.61
20	K	1086	LMU	O5B-C5B-C4B	-4.73	100.81	109.68
21	B	8054	SUC	O1'-C1'-C2'	-4.73	96.79	111.91
19	A	1811	CLA	C1D-CHD-C4C	-4.72	115.46	122.60
19	B	1785	CLA	C3D-CAD-CBD	-4.72	100.93	107.60
19	2	1221	CLA	C1D-CHD-C4C	-4.72	114.19	126.32
22	B	1774	BCR	C33-C5-C6	-4.72	119.97	124.61
19	4	1203	CLA	C2A-C1A-CHA	-4.71	114.24	122.58
20	A	7030	LMU	C4B-C3B-C2B	-4.71	102.01	110.79
19	B	1765	CLA	O1D-CGD-CBD	-4.71	117.88	124.62
19	A	1783	CLA	C3D-CAD-CBD	-4.70	100.95	107.60
19	B	1768	CLA	C1D-CHD-C4C	-4.70	115.49	122.60
19	4	1204	CLA	C4-C3-C2	-4.69	114.29	123.50
19	2	1215	CLA	C1D-CHD-C4C	-4.69	115.50	122.60
19	B	1765	CLA	CHD-C4C-C3C	-4.69	117.69	124.94
22	A	1804	BCR	C33-C5-C6	-4.69	120.00	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1774	BCR	C38-C26-C25	-4.68	120.01	124.61
22	B	1778	BCR	C33-C5-C6	-4.68	120.01	124.61
19	A	1773	CLA	C3D-CAD-CBD	-4.68	100.98	107.60
22	B	1780	BCR	C33-C5-C6	-4.68	120.01	124.61
22	B	1777	BCR	C33-C5-C6	-4.67	120.02	124.61
22	B	1778	BCR	C38-C26-C25	-4.67	120.02	124.61
22	B	1775	BCR	C33-C5-C6	-4.67	120.02	124.61
19	A	1789	CLA	CMD-C2D-C3D	-4.66	115.96	125.09
19	2	1227	CLA	C2A-C1A-CHA	-4.66	114.32	122.58
19	2	2010	CLA	C1D-CHD-C4C	-4.66	114.34	126.32
19	A	1767	CLA	C3D-CAD-CBD	-4.66	101.01	107.60
19	4	4007	CLA	C3D-CAD-CBD	-4.66	101.02	107.60
20	A	7043	LMU	C4B-C3B-C2B	-4.65	102.11	110.79
19	L	1166	CLA	CHD-C4C-C3C	-4.65	117.76	124.94
19	B	1762	CLA	C3D-CAD-CBD	-4.64	101.03	107.60
21	B	8052	SUC	C3-C4-C5	-4.64	102.10	110.20
22	A	1805	BCR	C38-C26-C25	-4.64	120.05	124.61
22	B	1777	BCR	C38-C26-C25	-4.64	120.05	124.61
19	1	1188	CLA	C3D-CAD-CBD	-4.64	101.04	107.60
22	A	1807	BCR	C38-C26-C25	-4.64	120.05	124.61
19	B	1770	CLA	CMD-C2D-C3D	-4.64	116.02	125.09
19	R	1055	CLA	CMD-C2D-C3D	-4.63	116.03	125.09
19	A	1799	CLA	C3D-CAD-CBD	-4.62	101.06	107.60
19	A	1813	CLA	C1D-CHD-C4C	-4.62	115.61	122.60
19	A	1784	CLA	O1D-CGD-CBD	-4.62	118.01	124.62
19	3	3007	CLA	C1D-CHD-C4C	-4.62	115.62	122.60
19	B	1744	CLA	C3D-CAD-CBD	-4.61	101.08	107.60
19	B	1764	CLA	CHD-C4C-C3C	-4.61	117.82	124.94
19	B	1754	CLA	OBD-CAD-CBD	-4.60	118.99	125.94
19	B	1753	CLA	O2D-CGD-O1D	-4.60	114.29	123.79
19	4	1201	CLA	C3D-CAD-CBD	-4.60	101.09	107.60
22	A	1803	BCR	C33-C5-C6	-4.60	120.09	124.61
22	A	1808	BCR	C33-C5-C6	-4.60	120.09	124.61
19	3	3015	CLA	C1D-CHD-C4C	-4.60	114.50	126.32
22	B	1776	BCR	C16-C17-C18	-4.60	120.56	127.20
19	B	1767	CLA	CMD-C2D-C3D	-4.59	116.10	125.09
19	A	1799	CLA	CMD-C2D-C3D	-4.59	116.11	125.09
19	2	1219	CLA	C3C-C4C-CHD	-4.59	117.77	125.32
19	A	1798	CLA	C3D-CAD-CBD	-4.59	101.11	107.60
19	F	1157	CLA	C4-C3-C2	-4.59	114.50	123.50
19	4	1201	CLA	CBC-CAC-C3C	-4.57	98.43	112.39
19	L	1505	CLA	C3D-CAD-CBD	-4.57	101.14	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1218	CLA	C1D-CHD-C4C	-4.57	115.69	122.60
19	A	1765	CLA	CHC-C1C-C2C	-4.56	114.36	126.35
20	A	7040	LMU	O3'-C3'-C2'	-4.56	100.08	110.34
20	A	7038	LMU	C6B-C5B-C4B	-4.55	101.79	113.02
19	B	1750	CLA	CHD-C4C-C3C	-4.55	117.91	124.94
19	3	1213	CLA	C2C-C1C-CHC	-4.55	117.07	125.15
19	K	3009	CLA	CHD-C4C-C3C	-4.54	117.92	124.94
22	B	1775	BCR	C38-C26-C25	-4.54	120.15	124.61
19	2	1213	CLA	C3D-CAD-CBD	-4.54	101.18	107.60
19	B	1744	CLA	C1D-CHD-C4C	-4.54	115.73	122.60
19	K	1146	CLA	C1-C2-C3	-4.54	119.28	126.71
19	A	1759	CLA	CHD-C4C-C3C	-4.53	117.93	124.94
19	3	3014	CLA	C2A-C1A-CHA	-4.53	114.56	122.58
19	B	1747	CLA	C1D-CHD-C4C	-4.52	115.76	122.60
19	3	3002	CLA	C2A-C1A-CHA	-4.52	114.57	122.58
19	J	1046	CLA	C2A-C1A-CHA	-4.52	114.58	122.58
19	1	1197	CLA	C3D-CAD-CBD	-4.50	101.23	107.60
19	3	1217	CLA	C2A-C1A-CHA	-4.50	114.61	122.58
19	3	1214	CLA	C3C-C4C-CHD	-4.50	117.92	125.32
19	B	1768	CLA	O2D-CGD-O1D	-4.49	114.51	123.79
20	A	7033	LMU	O1B-C4'-C5'	-4.49	97.52	109.32
19	2	1222	CLA	C3D-CAD-CBD	-4.48	101.26	107.60
19	R	1055	CLA	C3D-CAD-CBD	-4.48	101.26	107.60
19	A	1763	CLA	C1D-CHD-C4C	-4.48	115.82	122.60
19	4	1201	CLA	O2A-CGA-O1A	-4.48	111.94	123.49
19	2	1218	CLA	C6-C5-C3	-4.48	102.66	112.48
22	B	1781	BCR	C30-C25-C26	-4.47	116.09	122.66
19	3	1215	CLA	C3C-C4C-CHD	-4.47	117.97	125.32
19	1	1201	CLA	C1D-CHD-C4C	-4.47	114.82	126.32
19	B	1759	CLA	CMD-C2D-C3D	-4.47	116.35	125.09
19	A	1773	CLA	O1D-CGD-CBD	-4.47	118.22	124.62
19	R	1054	CLA	CMD-C2D-C3D	-4.46	116.36	125.09
19	B	1744	CLA	CMD-C2D-C3D	-4.46	116.36	125.09
19	A	1798	CLA	CHD-C4C-C3C	-4.46	118.05	124.94
19	2	1216	CLA	C3A-C4A-CHB	-4.46	119.56	124.06
20	A	7036	LMU	C6B-C5B-C4B	-4.45	102.03	113.02
19	4	4007	CLA	CHD-C4C-C3C	-4.45	118.06	124.94
20	A	7027	LMU	C1B-O1B-C4'	-4.45	106.39	118.01
19	G	1099	CLA	CHD-C4C-C3C	-4.44	118.07	124.94
19	3	3007	CLA	C3D-CAD-CBD	-4.44	101.32	107.60
19	B	1741	CLA	CMD-C2D-C3D	-4.44	116.41	125.09
19	L	1505	CLA	CMD-C2D-C3D	-4.43	116.42	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1205	CLA	C3B-C2B-C1B	-4.43	102.41	106.29
19	B	1762	CLA	CHD-C4C-C3C	-4.43	118.09	124.94
20	A	1810	LMU	C3B-C4B-C5B	-4.43	102.47	110.20
19	1	1200	CLA	CHD-C4C-C3C	-4.43	118.09	124.94
19	A	1800	CLA	CHD-C4C-C3C	-4.43	118.09	124.94
20	A	7022	LMU	O2'-C2'-C1'	-4.42	100.33	110.02
20	A	7042	LMU	C1'-O5'-C5'	-4.41	105.19	113.75
19	B	1767	CLA	C3D-CAD-CBD	-4.40	101.37	107.60
22	B	1781	BCR	C37-C22-C23	-4.40	110.77	118.10
19	3	1217	CLA	C2C-C1C-CHC	-4.40	117.33	125.15
19	B	1769	CLA	CHD-C4C-C3C	-4.40	118.14	124.94
19	4	1208	CLA	C1D-CHD-C4C	-4.40	115.01	126.32
22	L	1170	BCR	C16-C17-C18	-4.39	120.86	127.20
19	2	1223	CLA	CHD-C4C-C3C	-4.39	118.16	124.94
20	A	7038	LMU	C2'-C3'-C4'	-4.39	99.96	109.60
19	B	1772	CLA	CAA-C2A-C3A	-4.39	105.69	116.20
19	I	1031	CLA	CHD-C4C-C3C	-4.39	118.16	124.94
19	A	1773	CLA	CHD-C4C-C3C	-4.38	118.16	124.94
19	4	1206	CLA	C1D-CHD-C4C	-4.38	115.04	126.32
19	3	1212	CLA	CHD-C4C-C3C	-4.38	117.50	124.83
19	2	1213	CLA	CMD-C2D-C3D	-4.38	116.52	125.09
19	2	1218	CLA	O2D-CGD-O1D	-4.37	114.76	123.79
19	B	1736	CLA	CMD-C2D-C3D	-4.36	116.56	125.09
19	B	1770	CLA	C1D-CHD-C4C	-4.36	116.00	122.60
19	B	1742	CLA	C3D-CAD-CBD	-4.36	101.43	107.60
20	A	7032	LMU	O5B-C5B-C4B	-4.36	101.50	109.68
19	2	1213	CLA	C4-C3-C2	-4.35	114.96	123.50
19	3	1216	CLA	C1D-CHD-C4C	-4.35	115.13	126.32
19	R	1055	CLA	CHD-C4C-C3C	-4.35	118.22	124.94
19	B	1759	CLA	C3D-CAD-CBD	-4.35	101.45	107.60
22	B	1779	BCR	C27-C26-C25	-4.34	117.25	122.78
19	B	1737	CLA	CMD-C2D-C3D	-4.34	116.61	125.09
20	A	7035	LMU	C3'-C4'-C5'	-4.34	101.03	110.84
19	B	1755	CLA	CHD-C4C-C3C	-4.34	118.24	124.94
19	F	1156	CLA	CHD-C4C-C3C	-4.33	118.25	124.94
19	4	1196	CLA	CHD-C4C-C3C	-4.33	118.25	124.94
19	A	1759	CLA	C3D-CAD-CBD	-4.33	101.47	107.60
19	B	1753	CLA	CAA-C2A-C1A	-4.32	97.22	112.47
19	4	1201	CLA	O1D-CGD-CBD	-4.32	118.42	124.62
19	4	1199	CLA	C3D-CAD-CBD	-4.32	101.49	107.60
19	B	1756	CLA	CHD-C4C-C3C	-4.31	118.27	124.94
19	K	1085	CLA	CHD-C4C-C3C	-4.31	118.28	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1193	CLA	CHD-C4C-C3C	-4.31	118.28	124.94
19	B	1743	CLA	C3D-CAD-CBD	-4.31	101.50	107.60
19	A	1791	CLA	CHD-C4C-C3C	-4.31	118.29	124.94
19	A	1797	CLA	CHD-C4C-C3C	-4.30	118.29	124.94
19	1	1189	CLA	O2D-CGD-O1D	-4.30	114.91	123.79
22	B	1779	BCR	C8-C7-C6	-4.30	114.40	127.32
19	A	1793	CLA	CHD-C4C-C3C	-4.30	118.30	124.94
19	2	1214	CLA	C3C-C4C-CHD	-4.29	118.26	125.32
19	3	1219	CLA	CHD-C4C-C3C	-4.29	118.31	124.94
19	A	1766	CLA	C1D-CHD-C4C	-4.29	116.11	122.60
19	B	1762	CLA	O2D-CGD-O1D	-4.29	114.93	123.79
21	B	8061	SUC	C4-C3-C2	-4.29	102.79	110.79
19	A	1794	CLA	CHD-C4C-C3C	-4.29	118.32	124.94
19	J	1043	CLA	CHD-C4C-C3C	-4.28	118.32	124.94
19	4	4014	CLA	CHD-C4C-C3C	-4.28	118.32	124.94
19	B	1736	CLA	C3D-CAD-CBD	-4.28	101.54	107.60
19	B	1735	CLA	CHD-C4C-C3C	-4.28	118.32	124.94
19	3	1215	CLA	C3B-C2B-C1B	-4.28	102.54	106.29
19	2	2010	CLA	C3C-C4C-CHD	-4.28	118.28	125.32
19	A	1795	CLA	CHD-C4C-C3C	-4.28	118.33	124.94
19	B	1741	CLA	C3D-CAD-CBD	-4.28	101.55	107.60
21	B	8052	SUC	C6-C5-C4	-4.28	102.47	113.02
19	B	1760	CLA	C1D-CHD-C4C	-4.28	116.13	122.60
19	K	1142	CLA	CHD-C4C-C3C	-4.27	118.34	124.94
19	B	1736	CLA	CHD-C4C-C3C	-4.27	118.34	124.94
21	B	8062	SUC	O2-C2-C3	-4.27	100.73	110.34
19	2	1216	CLA	C3C-C4C-CHD	-4.27	118.30	125.32
19	A	1781	CLA	CHD-C4C-C3C	-4.27	118.35	124.94
19	A	1796	CLA	CHD-C4C-C3C	-4.26	118.35	124.94
19	A	1766	CLA	CMD-C2D-C3D	-4.26	116.75	125.09
19	J	1046	CLA	C1D-CHD-C4C	-4.26	115.36	126.32
19	A	1760	CLA	CHD-C4C-C3C	-4.26	118.35	124.94
19	B	1759	CLA	CHD-C4C-C3C	-4.26	118.35	124.94
19	A	1792	CLA	CHD-C4C-C3C	-4.26	118.35	124.94
19	A	1782	CLA	CHD-C4C-C3C	-4.26	118.36	124.94
20	A	7032	LMU	C1'-C2'-C3'	-4.26	101.58	109.97
19	3	3002	CLA	C3C-C4C-CHD	-4.26	118.31	125.32
19	2	1220	CLA	O1D-CGD-CBD	-4.26	118.52	124.62
19	3	3008	CLA	CHD-C4C-C3C	-4.25	118.37	124.94
19	2	1212	CLA	CHD-C4C-C3C	-4.25	118.37	124.94
19	A	1817	CLA	O2D-CGD-O1D	-4.25	115.01	123.79
19	4	1206	CLA	C2D-C3D-C4D	-4.25	102.56	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1200	CLA	O2A-CGA-O1A	-4.24	112.54	123.49
19	4	1197	CLA	CHD-C4C-C3C	-4.24	117.73	124.83
20	A	7023	LMU	O3'-C3'-C2'	-4.24	100.79	110.34
19	2	1217	CLA	CHD-C4C-C3C	-4.24	118.39	124.94
19	B	1770	CLA	CHD-C4C-C3C	-4.24	118.39	124.94
19	I	1031	CLA	O1D-CGD-CBD	-4.24	118.55	124.62
19	A	1774	CLA	CHD-C4C-C3C	-4.23	118.40	124.94
20	A	7036	LMU	O3B-C3B-C4B	-4.23	100.82	110.34
19	A	1764	CLA	C6-C5-C3	-4.23	103.20	112.48
22	3	1220	BCR	C16-C15-C14	-4.23	114.05	123.39
19	3	3015	CLA	C2A-C1A-CHA	-4.22	115.10	122.58
19	1	1189	CLA	CGD-CBD-CAD	-4.22	96.31	110.62
19	A	1764	CLA	CHD-C4C-C3C	-4.22	118.42	124.94
19	F	1155	CLA	CAB-C3B-C4B	-4.22	121.39	128.36
22	B	1781	BCR	C38-C26-C25	-4.21	120.47	124.61
19	B	1746	CLA	CHD-C4C-C3C	-4.21	118.43	124.94
19	1	1189	CLA	CHD-C4C-C3C	-4.21	118.43	124.94
19	A	1784	CLA	C3D-CAD-CBD	-4.21	101.65	107.60
19	2	1214	CLA	C2A-C1A-CHA	-4.20	115.14	122.58
22	L	1170	BCR	C37-C22-C21	-4.20	116.70	122.90
19	3	3001	CLA	C2A-C1A-CHA	-4.19	115.15	122.58
19	L	1166	CLA	O1D-CGD-CBD	-4.19	118.61	124.62
19	1	1194	CLA	C3C-C4C-CHD	-4.19	118.42	125.32
19	B	1752	CLA	C3D-CAD-CBD	-4.19	101.67	107.60
19	1	1193	CLA	CMD-C2D-C3D	-4.19	116.90	125.09
19	A	1790	CLA	C3D-CAD-CBD	-4.19	101.68	107.60
19	A	1775	CLA	CHD-C4C-C3C	-4.18	117.82	124.83
19	A	1766	CLA	O1D-CGD-CBD	-4.18	118.63	124.62
19	A	1769	CLA	C3D-CAD-CBD	-4.18	101.69	107.60
19	4	1205	CLA	C3C-C4C-CHD	-4.17	118.46	125.32
19	A	1765	CLA	CMD-C2D-C3D	-4.17	116.93	125.09
22	B	1776	BCR	C30-C25-C26	-4.17	116.54	122.66
19	3	3008	CLA	C3D-CAD-CBD	-4.17	101.71	107.60
19	A	1770	CLA	O1D-CGD-CBD	-4.17	118.65	124.62
19	2	1219	CLA	C2A-C1A-CHA	-4.17	115.20	122.58
19	B	1785	CLA	C1D-CHD-C4C	-4.16	116.30	122.60
22	B	1781	BCR	C24-C25-C26	-4.16	111.83	121.37
19	A	1776	CLA	C3D-CAD-CBD	-4.16	101.71	107.60
19	1	1187	CLA	CBC-CAC-C3C	-4.16	99.68	112.39
19	F	1155	CLA	CMD-C2D-C3D	-4.16	116.95	125.09
19	3	3014	CLA	C1D-CHD-C4C	-4.16	115.63	126.32
20	A	7042	LMU	C4B-C3B-C2B	-4.15	103.04	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1214	CLA	C2D-C3D-C4D	-4.15	102.65	106.30
19	J	1044	CLA	C3D-CAD-CBD	-4.15	101.73	107.60
19	K	3009	CLA	C3D-CAD-CBD	-4.15	101.73	107.60
19	3	3015	CLA	C3C-C4C-CHD	-4.15	118.50	125.32
19	A	1765	CLA	C3D-CAD-CBD	-4.15	101.74	107.60
22	A	1805	BCR	C7-C8-C9	-4.14	119.90	126.22
22	A	1803	BCR	C24-C23-C22	-4.14	119.90	126.22
19	A	1764	CLA	O2D-CGD-O1D	-4.14	115.24	123.79
22	A	1808	BCR	C7-C8-C9	-4.14	119.91	126.22
19	3	1213	CLA	C3C-C4C-CHD	-4.14	118.51	125.32
20	A	7032	LMU	O2B-C2B-C3B	-4.14	101.02	110.34
19	B	1740	CLA	CHD-C4C-C3C	-4.14	118.55	124.94
22	A	1804	BCR	C7-C8-C9	-4.14	119.91	126.22
19	B	1786	CLA	C5-C3-C2	-4.13	113.21	121.05
19	2	1216	CLA	C2C-C1C-CHC	-4.13	117.81	125.15
19	B	1753	CLA	C3D-CAD-CBD	-4.13	101.76	107.60
19	3	3008	CLA	C1-C2-C3	-4.13	119.94	126.71
19	2	1222	CLA	O2D-CGD-O1D	-4.13	115.27	123.79
19	A	1774	CLA	C3D-CAD-CBD	-4.12	101.77	107.60
19	A	1813	CLA	C3D-CAD-CBD	-4.12	101.77	107.60
19	L	1505	CLA	CHD-C4C-C3C	-4.12	118.58	124.94
19	B	1768	CLA	C3D-CAD-CBD	-4.11	101.78	107.60
19	2	1221	CLA	C3C-C4C-CHD	-4.11	118.56	125.32
19	4	1209	CLA	CGD-CBD-CAD	-4.11	96.69	110.62
19	A	1812	CLA	C3D-CAD-CBD	-4.11	101.79	107.60
19	B	1771	CLA	CHD-C4C-C3C	-4.11	118.60	124.94
19	A	1800	CLA	C6-C5-C3	-4.11	103.47	112.48
22	B	1774	BCR	C7-C8-C9	-4.10	119.96	126.22
19	A	1801	CLA	C3D-CAD-CBD	-4.10	101.80	107.60
19	A	1815	CLA	CAA-C2A-C3A	-4.10	101.42	113.22
19	3	1213	CLA	C1D-CHD-C4C	-4.10	115.77	126.32
22	B	1780	BCR	C24-C23-C22	-4.10	119.96	126.22
22	B	1778	BCR	C24-C23-C22	-4.10	119.97	126.22
19	1	1190	CLA	CHD-C4C-C3C	-4.10	118.61	124.94
22	B	1775	BCR	C24-C23-C22	-4.10	119.97	126.22
22	B	1777	BCR	C7-C8-C9	-4.10	119.97	126.22
19	A	1816	CLA	C3D-CAD-CBD	-4.10	101.81	107.60
22	A	1806	BCR	C24-C23-C22	-4.10	119.97	126.22
22	A	1803	BCR	C7-C8-C9	-4.09	119.97	126.22
19	B	1754	CLA	O2D-CGD-O1D	-4.09	115.34	123.79
22	A	1805	BCR	C24-C23-C22	-4.09	119.98	126.22
22	B	1780	BCR	C7-C8-C9	-4.09	119.98	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	8054	SUC	C2'-O1-C1	-4.09	106.76	117.53
19	4	1200	CLA	C3D-CAD-CBD	-4.08	101.83	107.60
20	A	7017	LMU	C1B-O5B-C5B	-4.08	105.83	113.75
22	A	1807	BCR	C24-C23-C22	-4.07	120.00	126.22
19	4	1208	CLA	C3C-C4C-CHD	-4.07	118.62	125.32
19	A	1767	CLA	CAA-C2A-C3A	-4.07	101.51	113.22
22	B	1778	BCR	C7-C8-C9	-4.07	120.01	126.22
19	2	1212	CLA	C3D-CAD-CBD	-4.07	101.84	107.60
19	A	1759	CLA	O2D-CGD-O1D	-4.07	115.39	123.79
19	1	1200	CLA	O1D-CGD-CBD	-4.07	118.79	124.62
19	B	1745	CLA	CHD-C4C-C3C	-4.07	118.65	124.94
20	A	7040	LMU	O2'-C2'-C3'	-4.07	101.18	110.34
19	A	1782	CLA	C3D-CAD-CBD	-4.07	101.85	107.60
22	B	1776	BCR	C37-C22-C21	-4.07	116.89	122.90
22	B	1775	BCR	C7-C8-C9	-4.07	120.02	126.22
19	3	3001	CLA	C3B-C2B-C1B	-4.06	102.73	106.29
20	A	7033	LMU	O2B-C2B-C1B	-4.06	101.12	110.02
19	A	1764	CLA	CAA-C2A-C1A	-4.06	98.15	112.47
19	K	1085	CLA	C3D-CAD-CBD	-4.06	101.86	107.60
19	B	1744	CLA	O1D-CGD-CBD	-4.05	118.81	124.62
19	B	1735	CLA	C3D-CAD-CBD	-4.05	101.87	107.60
22	A	1807	BCR	C7-C8-C9	-4.05	120.04	126.22
19	3	1219	CLA	C3D-CAD-CBD	-4.05	101.87	107.60
19	2	1223	CLA	O1D-CGD-CBD	-4.05	118.82	124.62
19	A	1790	CLA	CMD-C2D-C3D	-4.05	117.17	125.09
19	A	1797	CLA	C3D-CAD-CBD	-4.05	101.88	107.60
20	A	7016	LMU	C1-O1'-C1'	-4.04	106.88	113.94
19	4	1205	CLA	C2A-C1A-CHA	-4.04	115.42	122.58
19	A	1791	CLA	C3D-CAD-CBD	-4.04	101.88	107.60
19	F	1156	CLA	C3D-CAD-CBD	-4.04	101.88	107.60
19	A	1777	CLA	C3D-CAD-CBD	-4.04	101.88	107.60
19	1	1198	CLA	C3D-CAD-CBD	-4.04	101.88	107.60
22	B	1777	BCR	C24-C23-C22	-4.04	120.06	126.22
22	A	1806	BCR	C7-C8-C9	-4.04	120.06	126.22
19	B	1759	CLA	O1D-CGD-CBD	-4.04	118.84	124.62
19	A	1792	CLA	C3D-CAD-CBD	-4.04	101.89	107.60
19	A	1794	CLA	C3D-CAD-CBD	-4.04	101.89	107.60
19	4	4003	CLA	C1D-CHD-C4C	-4.03	115.94	126.32
19	4	4003	CLA	C2A-C1A-CHA	-4.03	115.44	122.58
19	3	1214	CLA	C3B-C2B-C1B	-4.03	102.76	106.29
19	A	1796	CLA	C3D-CAD-CBD	-4.03	101.90	107.60
19	2	1214	CLA	C3B-C2B-C1B	-4.03	102.76	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1808	BCR	C24-C23-C22	-4.03	120.07	126.22
19	A	1793	CLA	C3D-CAD-CBD	-4.03	101.90	107.60
21	2	1226	SUC	O4'-C4'-C3'	-4.03	99.21	112.01
19	A	1795	CLA	C3D-CAD-CBD	-4.02	101.91	107.60
19	B	1758	CLA	O1D-CGD-CBD	-4.02	118.86	124.62
20	A	7013	LMU	C4B-C3B-C2B	-4.02	103.29	110.79
19	A	1816	CLA	C4B-CHC-C1C	-4.02	120.63	129.26
19	B	1755	CLA	C3D-CAD-CBD	-4.02	101.92	107.60
20	A	7028	LMU	O5'-C1'-C2'	-4.02	102.03	110.28
19	J	1043	CLA	C3D-CAD-CBD	-4.02	101.92	107.60
19	A	1768	CLA	CHD-C4C-C3C	-4.01	118.74	124.94
19	L	1168	CLA	O2D-CGD-O1D	-4.01	115.50	123.79
19	1	1200	CLA	CGD-CBD-CAD	-4.01	97.03	110.62
19	A	1813	CLA	CMD-C2D-C3D	-4.01	117.25	125.09
19	2	2010	CLA	C2A-C1A-CHA	-4.01	115.48	122.58
20	A	7041	LMU	O6B-C6B-C5B	-4.00	98.10	111.33
19	4	1197	CLA	CAA-C2A-C3A	-4.00	106.61	116.20
19	2	1216	CLA	C1D-CHD-C4C	-4.00	116.03	126.32
19	J	1046	CLA	C3C-C4C-CHD	-4.00	118.74	125.32
19	B	1749	CLA	O1D-CGD-CBD	-4.00	118.89	124.62
19	F	1157	CLA	O2D-CGD-O1D	-4.00	115.53	123.79
19	4	1196	CLA	C3D-CAD-CBD	-4.00	101.94	107.60
22	A	1804	BCR	C24-C23-C22	-4.00	120.12	126.22
19	1	1187	CLA	CGD-CBD-CAD	-4.00	97.08	110.62
19	2	1222	CLA	CMD-C2D-C3D	-4.00	117.27	125.09
22	B	1774	BCR	C24-C23-C22	-3.99	120.13	126.22
20	A	7022	LMU	O2'-C2'-C3'	-3.99	101.35	110.34
19	A	1781	CLA	C3D-CAD-CBD	-3.99	101.95	107.60
19	A	1770	CLA	C3D-CAD-CBD	-3.99	101.95	107.60
19	1	1187	CLA	C3D-CAD-CBD	-3.99	101.95	107.60
19	2	1219	CLA	C2D-C3D-C4D	-3.99	102.79	106.30
19	K	1142	CLA	C3D-CAD-CBD	-3.98	101.97	107.60
20	A	7043	LMU	C6'-C5'-C4'	-3.98	101.66	113.25
20	K	1086	LMU	O3'-C3'-C2'	-3.98	101.38	110.34
19	1	1187	CLA	CAA-C2A-C3A	-3.98	101.78	113.22
19	B	1768	CLA	CMD-C2D-C3D	-3.98	117.31	125.09
19	K	1146	CLA	CMD-C2D-C3D	-3.98	117.31	125.09
19	B	1742	CLA	C4-C3-C2	-3.98	115.69	123.50
20	A	7037	LMU	O5'-C1'-C2'	-3.97	102.12	110.28
19	B	1753	CLA	C1D-CHD-C4C	-3.97	116.59	122.60
19	B	1786	CLA	CHD-C4C-C3C	-3.97	118.80	124.94
19	A	1785	CLA	CHD-C4C-C3C	-3.97	118.81	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1756	CLA	C3D-CAD-CBD	-3.97	101.98	107.60
19	B	1749	CLA	C3D-CAD-CBD	-3.97	101.99	107.60
19	A	1780	CLA	OBD-CAD-CBD	-3.97	119.95	125.94
19	A	1799	CLA	O1D-CGD-CBD	-3.97	118.94	124.62
19	3	3001	CLA	C2D-C3D-C4D	-3.96	102.81	106.30
19	1	1190	CLA	O2D-CGD-O1D	-3.96	115.61	123.79
19	2	1224	CLA	CHD-C4C-C3C	-3.96	118.82	124.94
19	G	1099	CLA	C3D-CAD-CBD	-3.96	102.00	107.60
19	B	1752	CLA	CMD-C2D-C3D	-3.96	117.35	125.09
19	A	1790	CLA	C1-C2-C3	-3.95	120.23	126.71
19	A	1771	CLA	C3D-CAD-CBD	-3.95	102.02	107.60
19	B	1772	CLA	CMA-C3A-C2A	-3.95	106.75	116.20
19	A	1760	CLA	CMD-C2D-C3D	-3.95	117.37	125.09
19	K	1146	CLA	O2D-CGD-O1D	-3.95	115.64	123.79
19	A	1760	CLA	OBD-CAD-C3D	-3.95	120.30	128.35
19	A	1765	CLA	O2D-CGD-O1D	-3.94	115.66	123.79
19	A	1783	CLA	CMD-C2D-C3D	-3.94	117.38	125.09
19	1	1196	CLA	CHD-C4C-C3C	-3.94	118.23	124.83
19	B	1761	CLA	O1D-CGD-CBD	-3.94	118.98	124.62
19	R	1055	CLA	OBD-CAD-C3D	-3.94	120.32	128.35
19	A	1762	CLA	C3D-CAD-CBD	-3.93	102.03	107.60
19	A	1777	CLA	CHD-C4C-C3C	-3.93	118.86	124.94
19	1	1197	CLA	CAA-C2A-C1A	-3.93	98.60	112.47
19	L	1167	CLA	C3D-CAD-CBD	-3.93	102.04	107.60
19	A	1772	CLA	CHD-C4C-C3C	-3.93	118.87	124.94
20	A	7037	LMU	C1B-O1B-C4'	-3.93	107.74	118.01
19	4	4014	CLA	C3D-CAD-CBD	-3.92	102.05	107.60
19	B	1743	CLA	O1D-CGD-CBD	-3.92	119.00	124.62
19	B	1766	CLA	CHD-C4C-C3C	-3.92	118.88	124.94
19	A	1762	CLA	CHD-C4C-C3C	-3.92	118.88	124.94
20	A	7022	LMU	C6B-C5B-C4B	-3.92	103.36	113.02
19	B	1787	CLA	CHD-C4C-C3C	-3.91	118.89	124.94
19	B	1745	CLA	C3D-CAD-CBD	-3.91	102.06	107.60
22	3	1220	BCR	C11-C12-C13	-3.91	114.80	126.32
19	B	1770	CLA	C3D-CAD-CBD	-3.91	102.06	107.60
19	2	1227	CLA	C1D-CHD-C4C	-3.91	116.27	126.32
19	4	1200	CLA	CHD-C4C-C3C	-3.91	118.90	124.94
19	2	1213	CLA	CHD-C4C-C3C	-3.91	118.90	124.94
21	2	1226	SUC	C1-O5-C5	-3.90	106.99	113.64
22	B	1776	BCR	C34-C9-C10	-3.90	117.14	122.90
19	3	1216	CLA	C2A-C1A-CHA	-3.90	115.67	122.58
20	A	7042	LMU	C1B-O1B-C4'	-3.89	107.83	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	1033	CLA	O1D-CGD-CBD	-3.89	119.05	124.62
22	B	1779	BCR	C40-C30-C25	-3.88	104.22	110.30
19	A	1761	CLA	CHD-C4C-C3C	-3.88	118.95	124.94
19	1	1191	CLA	CHD-C4C-C3C	-3.87	118.34	124.83
19	B	1767	CLA	CHD-C4C-C3C	-3.87	118.95	124.94
19	L	1166	CLA	C3D-CAD-CBD	-3.87	102.12	107.60
19	3	1216	CLA	C3B-C2B-C1B	-3.86	102.91	106.29
19	B	1758	CLA	O2D-CGD-O1D	-3.86	115.81	123.79
19	B	1760	CLA	C3D-CAD-CBD	-3.86	102.14	107.60
19	A	1769	CLA	CHD-C4C-C3C	-3.86	118.98	124.94
19	4	1203	CLA	C3B-C2B-C1B	-3.85	102.92	106.29
19	B	1785	CLA	CBA-CAA-C2A	-3.84	102.90	113.73
21	B	8056	SUC	O5-C5-C4	-3.84	102.48	109.68
19	3	3015	CLA	C2C-C1C-CHC	-3.84	118.33	125.15
19	A	1789	CLA	CHC-C1C-C2C	-3.84	116.26	126.35
19	A	1777	CLA	CMD-C2D-C3D	-3.84	117.58	125.09
19	4	1198	CLA	C11-C10-C8	-3.83	102.78	115.49
19	A	1801	CLA	O2D-CGD-O1D	-3.82	115.89	123.79
19	A	1815	CLA	O1D-CGD-CBD	-3.82	119.14	124.62
19	H	1079	CLA	CHD-C4C-C3C	-3.82	119.04	124.94
19	A	1767	CLA	C11-C12-C13	-3.82	102.83	115.49
19	1	1199	CLA	C2A-C1A-CHA	-3.81	115.82	122.58
19	1	1196	CLA	CMD-C2D-C3D	-3.81	117.63	125.09
19	K	3009	CLA	O2D-CGD-O1D	-3.81	115.92	123.79
19	B	1741	CLA	O1D-CGD-CBD	-3.81	119.16	124.62
19	A	1772	CLA	C3D-CAD-CBD	-3.80	102.22	107.60
19	B	1757	CLA	CHD-C4C-C3C	-3.80	119.07	124.94
21	2	1226	SUC	O2-C2-C1	-3.80	101.69	110.02
19	A	1761	CLA	C3D-CAD-CBD	-3.80	102.23	107.60
22	B	1781	BCR	C27-C26-C25	-3.80	117.94	122.78
19	3	3015	CLA	C3B-C2B-C1B	-3.80	102.97	106.29
19	2	1224	CLA	O1D-CGD-CBD	-3.79	119.18	124.62
19	B	1750	CLA	CMD-C2D-C3D	-3.79	117.67	125.09
19	2	1220	CLA	CMD-C2D-C3D	-3.79	117.67	125.09
19	1	1188	CLA	CHD-C4C-C3C	-3.79	119.09	124.94
20	A	7021	LMU	C6B-C5B-C4B	-3.78	103.68	113.02
20	A	7036	LMU	C3'-C4'-C5'	-3.78	102.28	110.84
19	4	1202	CLA	C2A-C1A-CHA	-3.78	115.89	122.58
19	A	1776	CLA	CHD-C4C-C3C	-3.78	119.11	124.94
19	B	1754	CLA	CAA-CBA-CGA	-3.77	102.28	113.32
19	3	1216	CLA	C3C-C4C-CHD	-3.77	119.12	125.32
19	B	1757	CLA	CMD-C2D-C3D	-3.76	117.72	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1054	CLA	CHD-C4C-C3C	-3.76	119.12	124.94
19	A	1788	CLA	CHD-C4C-C3C	-3.76	119.13	124.94
20	A	7025	LMU	C1B-O1B-C4'	-3.76	108.19	118.01
19	K	1085	CLA	C1-C2-C3	-3.75	120.56	126.71
19	A	1801	CLA	OBD-CAD-CBD	-3.75	120.28	125.94
19	K	1146	CLA	CMB-C2B-C1B	-3.75	122.17	128.36
19	4	1199	CLA	CMD-C2D-C3D	-3.74	117.77	125.09
21	B	8059	SUC	O1'-C1'-C2'	-3.73	99.97	111.91
19	B	1785	CLA	CAA-C2A-C3A	-3.73	102.48	113.22
19	B	1748	CLA	C3D-CAD-CBD	-3.73	102.32	107.60
20	A	7023	LMU	O2'-C2'-C3'	-3.73	101.94	110.34
19	1	1193	CLA	O2D-CGD-O1D	-3.73	116.08	123.79
19	B	1754	CLA	C3D-CAD-CBD	-3.73	102.32	107.60
19	A	1763	CLA	C3D-CAD-CBD	-3.73	102.33	107.60
19	B	1745	CLA	C4-C3-C2	-3.73	116.19	123.50
19	A	1789	CLA	C3D-CAD-CBD	-3.73	102.33	107.60
19	3	1214	CLA	C2C-C1C-CHC	-3.72	118.53	125.15
19	2	1213	CLA	O2D-CGD-O1D	-3.72	116.10	123.79
19	A	1763	CLA	O1D-CGD-CBD	-3.72	119.29	124.62
21	B	8059	SUC	C4-C3-C2	-3.72	103.85	110.79
19	B	1786	CLA	O2D-CGD-O1D	-3.72	116.11	123.79
19	A	1768	CLA	C3D-CAD-CBD	-3.72	102.34	107.60
19	J	1045	CLA	C3D-CAD-CBD	-3.71	102.34	107.60
19	4	1201	CLA	CMD-C2D-C3D	-3.71	117.83	125.09
19	2	1216	CLA	C3B-C2B-C1B	-3.71	103.04	106.29
20	A	7024	LMU	C3B-C4B-C5B	-3.71	103.73	110.20
20	A	7032	LMU	C4B-C3B-C2B	-3.70	103.88	110.79
19	B	1737	CLA	C3D-CAD-CBD	-3.70	102.36	107.60
20	R	1057	LMU	C1B-O1B-C4'	-3.70	108.35	118.01
19	3	1215	CLA	C2C-C1C-CHC	-3.69	118.58	125.15
19	A	1762	CLA	O2D-CGD-O1D	-3.69	116.17	123.79
20	A	7033	LMU	C3'-C4'-C5'	-3.69	102.50	110.84
19	B	1738	CLA	O2D-CGD-O1D	-3.69	116.18	123.79
19	B	1772	CLA	CHD-C4C-C3C	-3.69	118.66	124.83
22	B	1779	BCR	C4-C5-C6	-3.69	118.08	122.78
21	H	1080	SUC	C1'-C2'-C3'	-3.68	102.06	114.49
20	A	7023	LMU	C3B-C4B-C5B	-3.68	103.78	110.20
20	A	7020	LMU	C3'-C4'-C5'	-3.68	102.52	110.84
19	4	1199	CLA	O2D-CGD-O1D	-3.68	116.19	123.79
19	1	1187	CLA	CBA-CAA-C2A	-3.68	103.36	113.73
19	3	3001	CLA	C3C-C4C-CHD	-3.68	119.27	125.32
19	2	1218	CLA	C3D-CAD-CBD	-3.68	102.40	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	1086	LMU	O2B-C2B-C1B	-3.67	101.98	110.02
19	A	1813	CLA	CHD-C4C-C3C	-3.67	119.27	124.94
19	1	1201	CLA	C3C-C4C-CHD	-3.67	119.28	125.32
19	4	1204	CLA	O1D-CGD-CBD	-3.67	119.37	124.62
20	A	7026	LMU	C1B-O5B-C5B	-3.66	106.64	113.75
19	A	1787	CLA	CHD-C4C-C3C	-3.66	119.28	124.94
19	1	1190	CLA	CMD-C2D-C3D	-3.66	117.93	125.09
19	B	1761	CLA	C1-C2-C3	-3.66	120.71	126.71
19	B	1755	CLA	CMD-C2D-C3D	-3.66	117.93	125.09
19	4	1199	CLA	CHC-C1C-C2C	-3.66	116.73	126.35
22	L	1169	BCR	C11-C10-C9	-3.65	121.92	127.20
19	A	1781	CLA	CMD-C2D-C3D	-3.65	117.94	125.09
19	A	1766	CLA	C2A-C1A-CHA	-3.65	117.17	123.89
19	A	1775	CLA	CMD-C2D-C3D	-3.65	117.95	125.09
19	B	1756	CLA	CMD-C2D-C3D	-3.65	117.96	125.09
19	A	1797	CLA	CMD-C2D-C3D	-3.64	117.96	125.09
19	B	1738	CLA	C3D-CAD-CBD	-3.64	102.45	107.60
19	K	1142	CLA	CMD-C2D-C3D	-3.64	117.97	125.09
19	A	1791	CLA	CMD-C2D-C3D	-3.64	117.97	125.09
19	B	1766	CLA	CMD-C2D-C3D	-3.64	117.97	125.09
19	4	1206	CLA	C3C-C4C-CHD	-3.64	119.33	125.32
19	A	1796	CLA	CMD-C2D-C3D	-3.63	117.98	125.09
19	4	1198	CLA	O2D-CGD-O1D	-3.63	116.29	123.79
19	A	1817	CLA	CHC-C1C-C2C	-3.63	116.81	126.35
19	A	1793	CLA	CMD-C2D-C3D	-3.63	117.99	125.09
19	B	1735	CLA	CMD-C2D-C3D	-3.63	118.00	125.09
19	A	1794	CLA	CMD-C2D-C3D	-3.63	118.00	125.09
19	A	1792	CLA	CMD-C2D-C3D	-3.63	118.00	125.09
22	B	1776	BCR	C33-C5-C6	-3.62	121.05	124.61
19	3	1214	CLA	C2A-C1A-CHA	-3.62	116.16	122.58
21	B	8060	SUC	O6'-C6'-C5'	-3.62	99.36	111.33
19	A	1795	CLA	CMD-C2D-C3D	-3.62	118.00	125.09
19	4	1196	CLA	CMD-C2D-C3D	-3.62	118.00	125.09
19	H	1079	CLA	C3D-CAD-CBD	-3.62	102.48	107.60
19	2	1212	CLA	CMD-C2D-C3D	-3.62	118.01	125.09
21	B	8056	SUC	O1-C1-C2	-3.61	96.30	108.36
19	2	1218	CLA	CHC-C1C-C2C	-3.61	116.85	126.35
19	2	1223	CLA	CGD-CBD-CAD	-3.61	98.39	110.62
19	A	1780	CLA	CHD-C4C-C3C	-3.61	119.36	124.94
19	4	4014	CLA	CMD-C2D-C3D	-3.61	118.03	125.09
22	L	1170	BCR	C7-C6-C5	-3.61	113.11	121.37
20	A	7022	LMU	O1B-C1B-O5B	-3.61	101.55	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7036	LMU	C4B-C3B-C2B	-3.61	104.06	110.79
19	J	1044	CLA	CHD-C4C-C3C	-3.61	119.37	124.94
19	3	3007	CLA	CMD-C2D-C3D	-3.60	118.04	125.09
19	3	1215	CLA	C2A-C1A-CHA	-3.60	116.20	122.58
19	B	1759	CLA	O2D-CGD-O1D	-3.60	116.36	123.79
19	J	1043	CLA	CMD-C2D-C3D	-3.60	118.05	125.09
19	A	1782	CLA	CMD-C2D-C3D	-3.60	118.05	125.09
19	A	1761	CLA	CHC-C1C-C2C	-3.60	116.89	126.35
19	3	1219	CLA	CMD-C2D-C3D	-3.60	118.05	125.09
20	A	7022	LMU	C3B-C4B-C5B	-3.60	103.93	110.20
19	B	1740	CLA	O2A-CGA-O1A	-3.60	114.21	123.49
19	A	1770	CLA	CHD-C4C-C3C	-3.59	119.39	124.94
19	A	1771	CLA	O2D-CGD-O1D	-3.59	116.38	123.79
19	J	1044	CLA	O1D-CGD-CBD	-3.59	119.48	124.62
19	4	1199	CLA	C1D-CHD-C4C	-3.59	117.17	122.60
19	K	1085	CLA	CMD-C2D-C3D	-3.59	118.07	125.09
19	L	1167	CLA	CGD-CBD-CAD	-3.59	98.47	110.62
19	B	1742	CLA	CHD-C4C-C3C	-3.59	119.40	124.94
19	1	1195	CLA	CAA-C2A-C3A	-3.59	107.61	116.20
19	4	1203	CLA	C3C-C4C-CHD	-3.58	119.42	125.32
19	F	1156	CLA	CMD-C2D-C3D	-3.58	118.08	125.09
19	2	1219	CLA	C2C-C1C-CHC	-3.58	118.79	125.15
21	B	8062	SUC	O5-C5-C4	-3.58	102.96	109.68
19	4	1201	CLA	C2C-C1C-NC	-3.58	107.58	110.24
19	A	1813	CLA	O2D-CGD-O1D	-3.57	116.42	123.79
19	L	1167	CLA	CHD-C4C-C3C	-3.57	119.42	124.94
22	B	1776	BCR	C35-C13-C14	-3.57	117.63	122.90
19	4	1197	CLA	CMD-C2D-C3D	-3.57	118.10	125.09
19	B	1738	CLA	CHC-C1C-C2C	-3.57	116.96	126.35
19	1	1188	CLA	CMD-C2D-C3D	-3.57	118.11	125.09
19	L	1167	CLA	O2D-CGD-O1D	-3.57	116.42	123.79
19	J	1046	CLA	C2C-C1C-CHC	-3.57	118.81	125.15
20	A	7020	LMU	C1-O1'-C1'	-3.56	107.71	113.94
19	4	1208	CLA	C2A-C1A-CHA	-3.56	116.27	122.58
20	A	7028	LMU	O3'-C3'-C4'	-3.56	101.45	109.87
19	B	1754	CLA	CGD-CBD-CAD	-3.56	98.56	110.62
19	B	1766	CLA	C3D-CAD-CBD	-3.56	102.56	107.60
19	B	1742	CLA	CMD-C2D-C3D	-3.56	118.13	125.09
19	1	1200	CLA	CHC-C1C-C2C	-3.56	117.00	126.35
19	A	1783	CLA	CHD-C4C-C3C	-3.55	119.45	124.94
19	3	3011	CLA	CHD-C4C-C3C	-3.55	119.46	124.94
19	B	1744	CLA	CHD-C4C-C3C	-3.55	119.46	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1194	CLA	C2D-C3D-C4D	-3.54	103.18	106.30
19	3	1216	CLA	C2C-C1C-CHC	-3.54	118.86	125.15
19	2	1223	CLA	C3D-CAD-CBD	-3.53	102.60	107.60
19	2	1215	CLA	CMD-C2D-C3D	-3.53	118.18	125.09
19	A	1767	CLA	CHC-C1C-C2C	-3.53	117.06	126.35
19	1	1201	CLA	C2C-C1C-CHC	-3.53	118.87	125.15
19	A	1773	CLA	CMD-C2D-C3D	-3.53	118.19	125.09
19	2	1217	CLA	C3D-CAD-CBD	-3.53	102.61	107.60
19	F	1155	CLA	CHD-C4C-C3C	-3.53	118.92	124.83
19	1	1187	CLA	CHC-C1C-C2C	-3.52	117.08	126.35
21	B	8059	SUC	O6-C6-C5	-3.52	99.69	111.33
19	A	1815	CLA	CMA-C3A-C2A	-3.52	98.77	114.35
19	4	1203	CLA	C2D-C3D-C4D	-3.52	103.20	106.30
20	A	7032	LMU	O1B-C1B-C2B	-3.52	99.54	108.10
19	4	4003	CLA	C2D-C3D-C4D	-3.52	103.21	106.30
20	A	7020	LMU	C3B-C4B-C5B	-3.52	104.07	110.20
19	B	1747	CLA	O2D-CGD-O1D	-3.51	116.53	123.79
19	I	1033	CLA	C3D-CAD-CBD	-3.51	102.63	107.60
23	B	1773	PQN	C2M-C2-C3	-3.51	116.59	124.10
20	A	7020	LMU	C1'-O5'-C5'	-3.51	106.93	113.75
19	4	4003	CLA	C2C-C1C-CHC	-3.51	118.91	125.15
19	4	1204	CLA	CMD-C2D-C3D	-3.51	118.23	125.09
19	4	1202	CLA	C3C-C4C-CHD	-3.51	119.55	125.32
19	A	1778	CLA	CMD-C2D-C3D	-3.51	118.23	125.09
19	B	1787	CLA	CMD-C2D-C3D	-3.50	118.23	125.09
22	B	1779	BCR	C28-C29-C30	-3.50	101.86	114.83
19	2	1214	CLA	C2C-C1C-CHC	-3.50	118.93	125.15
19	A	1764	CLA	CMD-C2D-C3D	-3.50	118.24	125.09
19	4	1203	CLA	C2C-C1C-CHC	-3.50	118.94	125.15
19	J	1046	CLA	C3B-C2B-C1B	-3.50	103.23	106.29
21	B	8059	SUC	C3-C4-C5	-3.49	104.11	110.20
20	A	7039	LMU	O3'-C3'-C4'	-3.49	101.61	109.87
19	2	1215	CLA	CHD-C4C-C3C	-3.49	119.55	124.94
19	1	1199	CLA	C3C-C4C-CHD	-3.49	119.58	125.32
19	4	1205	CLA	C2C-C1C-CHC	-3.49	118.95	125.15
19	A	1780	CLA	CMD-C2D-C3D	-3.49	118.27	125.09
19	A	1785	CLA	O2D-CGD-O1D	-3.49	116.59	123.79
19	L	1167	CLA	CMD-C2D-C3D	-3.48	118.27	125.09
19	A	1789	CLA	CMA-C3A-C2A	-3.48	98.95	114.35
19	A	1800	CLA	C3D-CAD-CBD	-3.48	102.68	107.60
19	1	1187	CLA	CHD-C4C-C3C	-3.48	119.57	124.94
19	2	1221	CLA	C2A-C1A-CHA	-3.47	116.43	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1764	CLA	O1D-CGD-CBD	-3.47	119.65	124.62
19	3	3014	CLA	C2C-C1C-CHC	-3.47	118.98	125.15
22	B	1779	BCR	C1-C6-C5	-3.47	117.56	122.66
19	A	1763	CLA	CHD-C4C-C3C	-3.47	119.58	124.94
19	A	1780	CLA	C3D-CAD-CBD	-3.46	102.70	107.60
19	1	1188	CLA	CHC-C1C-C2C	-3.45	117.27	126.35
19	A	1771	CLA	CHD-C4C-C3C	-3.45	119.61	124.94
19	J	1045	CLA	CMD-C2D-C3D	-3.45	118.34	125.09
19	1	1192	CLA	O1D-CGD-CBD	-3.45	119.68	124.62
19	1	1199	CLA	C2C-C1C-CHC	-3.44	119.04	125.15
19	2	2010	CLA	C2C-C1C-CHC	-3.44	119.04	125.15
19	A	1784	CLA	CHD-C4C-C3C	-3.44	119.63	124.94
19	4	1202	CLA	C2C-C1C-CHC	-3.44	119.05	125.15
19	B	1785	CLA	CHD-C4C-C3C	-3.43	119.63	124.94
21	B	8062	SUC	C4-C3-C2	-3.43	104.38	110.79
19	4	1202	CLA	C2D-C3D-C4D	-3.43	103.28	106.30
20	A	7032	LMU	C1-O1'-C1'	-3.43	107.95	113.94
19	A	1759	CLA	C1-C2-C3	-3.43	121.09	126.71
19	1	1199	CLA	C2D-C3D-C4D	-3.41	103.30	106.30
19	B	1754	CLA	OBD-CAD-C3D	-3.41	121.40	128.35
19	B	1750	CLA	O1D-CGD-CBD	-3.41	119.74	124.62
19	3	3011	CLA	C3D-CAD-CBD	-3.40	102.79	107.60
21	B	8061	SUC	O3'-C3'-C4'	-3.40	101.09	113.29
21	B	8054	SUC	O3'-C3'-C4'	-3.39	101.12	113.29
19	A	1801	CLA	C4-C3-C2	-3.38	116.87	123.50
19	2	1215	CLA	C3D-CAD-CBD	-3.38	102.82	107.60
20	A	7041	LMU	O5'-C1'-C2'	-3.38	103.35	110.28
20	A	7032	LMU	C1'-O5'-C5'	-3.38	107.19	113.75
20	A	7016	LMU	O3'-C3'-C4'	-3.37	101.89	109.87
19	G	1099	CLA	O2D-CGD-O1D	-3.37	116.82	123.79
19	B	1749	CLA	O2D-CGD-O1D	-3.37	116.83	123.79
19	4	1207	CLA	CAA-C2A-C3A	-3.37	108.14	116.20
19	B	1764	CLA	CMD-C2D-C3D	-3.36	118.51	125.09
19	1	1194	CLA	C2A-C1A-CHA	-3.36	116.63	122.58
20	A	7042	LMU	C1'-C2'-C3'	-3.36	103.35	109.97
19	4	1209	CLA	C3D-CAD-CBD	-3.36	102.85	107.60
19	A	1786	CLA	C3D-CAD-CBD	-3.36	102.85	107.60
19	I	1033	CLA	C4-C3-C2	-3.36	116.91	123.50
19	1	1197	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
19	3	3014	CLA	C3C-C4C-CHD	-3.35	119.80	125.32
19	K	1146	CLA	O2A-CGA-O1A	-3.35	114.85	123.49
23	A	1802	PQN	C21-C20-C18	-3.35	104.38	115.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1218	CLA	C2A-C1A-CHA	-3.35	117.72	123.89
19	A	1760	CLA	C3D-CAD-CBD	-3.35	102.86	107.60
21	B	8061	SUC	C1'-C2'-C3'	-3.35	103.19	114.49
19	A	1776	CLA	CMD-C2D-C3D	-3.35	118.54	125.09
19	B	1751	CLA	CMD-C2D-C3D	-3.34	118.55	125.09
19	2	1221	CLA	C2D-C3D-C4D	-3.34	103.36	106.30
19	2	1227	CLA	C3C-C4C-CHD	-3.34	119.83	125.32
19	B	1761	CLA	C3D-CAD-CBD	-3.34	102.88	107.60
19	3	3001	CLA	C2C-C1C-CHC	-3.34	119.22	125.15
19	A	1784	CLA	O2D-CGD-O1D	-3.34	116.90	123.79
19	3	3008	CLA	O1D-CGD-CBD	-3.33	119.85	124.62
19	B	1757	CLA	O2A-CGA-O1A	-3.33	114.90	123.49
19	F	1157	CLA	CAA-C2A-C3A	-3.33	103.65	113.22
19	B	1770	CLA	O1D-CGD-CBD	-3.32	119.86	124.62
20	A	7028	LMU	C1B-O1B-C4'	-3.32	109.32	118.01
19	A	1765	CLA	CAC-C3C-C2C	-3.32	121.68	127.51
19	1	1191	CLA	CMD-C2D-C3D	-3.32	118.59	125.09
19	4	4003	CLA	C3C-C4C-CHD	-3.31	119.87	125.32
19	4	1199	CLA	CAC-C3C-C2C	-3.31	121.70	127.51
19	1	1194	CLA	C2C-C1C-CHC	-3.31	119.27	125.15
20	A	7030	LMU	C1'-O5'-C5'	-3.31	107.33	113.75
22	B	1779	BCR	C37-C22-C21	-3.30	118.03	122.90
19	A	1778	CLA	CHC-C1C-C2C	-3.30	117.67	126.35
19	J	1045	CLA	CAA-CBA-CGA	-3.30	103.66	113.32
22	I	1032	BCR	C8-C7-C6	-3.30	117.41	127.32
20	A	7033	LMU	O1B-C1B-O5B	-3.30	102.34	110.68
20	A	7036	LMU	O5'-C1'-C2'	-3.29	103.52	110.28
19	A	1764	CLA	C3D-CAD-CBD	-3.29	102.94	107.60
19	3	3002	CLA	C2C-C1C-CHC	-3.29	119.31	125.15
19	2	1224	CLA	C3D-CAD-CBD	-3.29	102.95	107.60
20	A	7030	LMU	O3'-C3'-C2'	-3.29	102.94	110.34
19	3	3002	CLA	C3B-C2B-C1B	-3.28	103.41	106.29
19	A	1779	CLA	CHD-C4C-C3C	-3.28	119.87	124.94
19	A	1790	CLA	CHD-C4C-C3C	-3.28	119.87	124.94
19	B	1758	CLA	C16-C15-C13	-3.28	104.61	115.49
19	A	1812	CLA	O2A-CGA-O1A	-3.28	115.03	123.49
19	B	1768	CLA	CHD-C4C-C3C	-3.27	119.89	124.94
19	A	1787	CLA	C3D-CAD-CBD	-3.27	102.97	107.60
19	3	1213	CLA	C3B-C2B-C1B	-3.27	103.43	106.29
20	A	7028	LMU	O5B-C5B-C4B	-3.27	103.55	109.68
19	B	1762	CLA	CMD-C2D-C3D	-3.27	118.70	125.09
19	4	4003	CLA	C3B-C2B-C1B	-3.27	103.43	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1752	CLA	C5-C3-C2	-3.27	114.86	121.05
19	A	1815	CLA	CHD-C4C-C3C	-3.26	119.90	124.94
22	3	1220	BCR	C23-C24-C25	-3.26	117.51	127.32
19	4	1198	CLA	CHC-C1C-C2C	-3.26	117.77	126.35
19	A	1779	CLA	CMD-C2D-C3D	-3.26	118.71	125.09
21	B	8055	SUC	O3'-C3'-C2'	-3.25	103.53	113.96
19	A	1766	CLA	C3D-CAD-CBD	-3.25	103.00	107.60
21	B	8062	SUC	O1'-C1'-C2'	-3.25	101.53	111.91
22	I	1032	BCR	C32-C1-C6	-3.25	105.21	110.30
19	A	1767	CLA	CHD-C4C-C3C	-3.25	119.92	124.94
20	A	7013	LMU	O5B-C1B-C2B	-3.24	103.63	110.28
19	3	1212	CLA	CMD-C2D-C3D	-3.24	118.75	125.09
19	A	1811	CLA	CAA-C2A-C3A	-3.24	103.90	113.22
19	A	1785	CLA	C3D-CAD-CBD	-3.24	103.02	107.60
20	A	7037	LMU	C6'-C5'-C4'	-3.23	103.84	113.25
22	B	1781	BCR	C36-C18-C19	-3.23	112.72	118.10
19	A	1785	CLA	O1D-CGD-CBD	-3.23	119.99	124.62
19	A	1798	CLA	O2D-CGD-O1D	-3.23	117.12	123.79
19	2	1227	CLA	C2C-C1C-CHC	-3.23	119.41	125.15
21	B	8060	SUC	C4-C3-C2	-3.23	104.77	110.79
19	A	1786	CLA	CHC-C1C-C2C	-3.23	117.86	126.35
19	A	1769	CLA	CHC-C1C-C2C	-3.23	117.86	126.35
19	B	1757	CLA	C3D-CAD-CBD	-3.22	103.04	107.60
19	A	1778	CLA	CHD-C4C-C3C	-3.22	119.96	124.94
19	A	1767	CLA	CAA-C2A-C1A	-3.22	101.11	112.47
20	A	7016	LMU	O5'-C1'-O1'	-3.22	102.30	110.05
19	A	1780	CLA	C4-C3-C2	-3.22	117.18	123.50
19	F	1157	CLA	CBA-CAA-C2A	-3.22	104.65	113.73
19	K	3009	CLA	C4-C3-C2	-3.22	117.19	123.50
20	A	7022	LMU	O5B-C1B-C2B	-3.22	103.68	110.28
19	A	1770	CLA	CMD-C2D-C3D	-3.22	118.80	125.09
19	B	1739	CLA	O2A-CGA-O1A	-3.21	115.22	123.49
22	3	1220	BCR	C15-C14-C13	-3.20	122.57	127.20
19	4	1199	CLA	O1D-CGD-CBD	-3.20	120.03	124.62
19	B	1769	CLA	CAA-C2A-C3A	-3.20	104.02	113.22
19	B	1747	CLA	CHD-C4C-C3C	-3.20	120.00	124.94
19	A	1800	CLA	O1D-CGD-CBD	-3.20	120.04	124.62
19	B	1738	CLA	CMD-C2D-C3D	-3.20	118.83	125.09
19	B	1737	CLA	CHC-C1C-C2C	-3.19	117.95	126.35
19	B	1747	CLA	C3D-CAD-CBD	-3.19	103.08	107.60
19	4	1201	CLA	C6-C5-C3	-3.19	109.10	114.43
19	B	1769	CLA	C3D-CAD-CBD	-3.19	103.09	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1737	CLA	CHD-C4C-C3C	-3.19	120.02	124.94
19	R	1054	CLA	C4-C3-C2	-3.18	117.25	123.50
19	A	1761	CLA	O1D-CGD-CBD	-3.18	120.07	124.62
19	A	1762	CLA	CMD-C2D-C3D	-3.17	118.88	125.09
19	A	1772	CLA	CMD-C2D-C3D	-3.17	118.88	125.09
22	L	1170	BCR	C24-C23-C22	-3.17	121.38	126.22
19	1	1193	CLA	O1D-CGD-CBD	-3.17	120.08	124.62
19	A	1788	CLA	CMD-C2D-C3D	-3.17	118.89	125.09
20	A	7028	LMU	O2'-C2'-C1'	-3.16	103.09	110.02
19	2	1221	CLA	C2C-C1C-CHC	-3.16	119.54	125.15
20	A	1810	LMU	O2B-C2B-C1B	-3.16	103.10	110.02
19	A	1766	CLA	CMA-C3A-C2A	-3.16	100.38	114.35
19	J	1046	CLA	C2D-C3D-C4D	-3.15	103.53	106.30
20	A	7028	LMU	O5B-C1B-C2B	-3.15	103.81	110.28
19	H	1079	CLA	CMD-C2D-C3D	-3.15	118.93	125.09
20	A	7013	LMU	C3B-C4B-C5B	-3.14	104.72	110.20
19	B	1754	CLA	CHD-C4C-C3C	-3.14	120.09	124.94
19	B	1759	CLA	CMA-C3A-C2A	-3.14	100.47	114.35
22	L	1169	BCR	C15-C16-C17	-3.14	116.46	123.39
19	B	1786	CLA	C3D-CAD-CBD	-3.13	103.17	107.60
19	A	1816	CLA	C2A-C1A-CHA	-3.13	118.12	123.89
19	3	3007	CLA	CHC-C1C-C2C	-3.13	118.13	126.35
19	4	1207	CLA	CHD-C4C-C3C	-3.12	119.60	124.83
19	L	1167	CLA	CHC-C1C-C2C	-3.12	118.14	126.35
19	A	1815	CLA	CMD-C2D-C3D	-3.12	118.98	125.09
19	B	1760	CLA	O2D-CGD-O1D	-3.12	117.35	123.79
19	3	1213	CLA	C2D-C3D-C4D	-3.12	103.56	106.30
20	A	7021	LMU	C1'-O5'-C5'	-3.12	107.69	113.75
19	B	1768	CLA	CHC-C1C-C2C	-3.11	118.16	126.35
21	B	8059	SUC	C6-C5-C4	-3.11	105.33	113.02
19	A	1783	CLA	C4-C3-C2	-3.11	117.39	123.50
19	3	1214	CLA	C2D-C3D-C4D	-3.10	103.57	106.30
19	K	1146	CLA	CHD-C4C-C3C	-3.10	120.15	124.94
20	A	7028	LMU	O5'-C1'-O1'	-3.10	102.60	110.05
19	B	1746	CLA	CMD-C2D-C3D	-3.09	119.03	125.09
19	4	1200	CLA	CMD-C2D-C3D	-3.09	119.04	125.09
19	B	1763	CLA	O2A-CGA-O1A	-3.09	115.51	123.49
19	B	1741	CLA	CAA-C2A-C3A	-3.09	104.32	113.22
19	B	1741	CLA	CHD-C4C-C3C	-3.09	120.17	124.94
19	A	1815	CLA	CHC-C1C-C2C	-3.09	118.22	126.35
19	1	1197	CLA	CHC-C1C-C2C	-3.09	118.23	126.35
19	1	1187	CLA	O1D-CGD-CBD	-3.09	120.20	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	1031	CLA	C3D-CAD-CBD	-3.09	103.23	107.60
19	2	2010	CLA	C3B-C2B-C1B	-3.09	103.59	106.29
19	B	1737	CLA	O2D-CGD-O1D	-3.09	117.42	123.79
19	B	1771	CLA	O2A-CGA-O1A	-3.08	115.54	123.49
20	A	7030	LMU	O5'-C5'-C4'	-3.08	103.24	109.75
21	B	8061	SUC	O3-C3-C4	-3.08	103.40	110.34
19	R	1055	CLA	C4-C3-C2	-3.08	117.46	123.50
19	B	1763	CLA	CMD-C2D-C3D	-3.08	119.07	125.09
22	I	1032	BCR	C40-C30-C25	-3.08	105.48	110.30
19	B	1739	CLA	CHC-C1C-C2C	-3.08	118.26	126.35
19	B	1747	CLA	CMD-C2D-C3D	-3.07	119.08	125.09
19	2	1224	CLA	CHC-C1C-C2C	-3.07	118.27	126.35
23	B	1773	PQN	C16-C15-C13	-3.07	105.74	112.48
22	3	1220	BCR	C36-C18-C17	-3.07	118.37	122.90
19	1	1190	CLA	OBD-CAD-C3D	-3.07	122.09	128.35
19	B	1753	CLA	C3A-C2A-C1A	-3.07	96.30	101.50
19	A	1817	CLA	CAC-C3C-C2C	-3.07	122.13	127.51
19	R	1055	CLA	O1D-CGD-CBD	-3.07	120.23	124.62
19	F	1155	CLA	CAA-C2A-C1A	-3.07	103.68	112.17
19	4	4007	CLA	CMD-C2D-C3D	-3.06	119.09	125.09
19	1	1198	CLA	C6-C5-C3	-3.06	105.76	112.48
19	A	1787	CLA	O2D-CGD-O1D	-3.06	117.46	123.79
19	R	1054	CLA	O2A-CGA-O1A	-3.06	115.59	123.49
19	A	1761	CLA	CMD-C2D-C3D	-3.06	119.10	125.09
19	4	1198	CLA	C2C-C1C-NC	-3.06	107.97	110.24
19	B	1785	CLA	CHC-C1C-C2C	-3.06	118.31	126.35
21	H	1080	SUC	O4'-C4'-C3'	-3.06	102.30	112.01
19	4	1201	CLA	CHC-C1C-C2C	-3.05	118.32	126.35
19	4	1198	CLA	C16-C15-C13	-3.05	105.36	115.49
19	4	1198	CLA	C7-C6-C5	-3.05	104.04	113.06
19	A	1776	CLA	O1D-CGD-CBD	-3.05	120.25	124.62
21	B	8052	SUC	C4-C3-C2	-3.05	105.10	110.79
19	A	1771	CLA	CMD-C2D-C3D	-3.05	119.12	125.09
19	J	1044	CLA	O2D-CGD-O1D	-3.05	117.50	123.79
19	B	1770	CLA	CAA-C2A-C3A	-3.05	104.45	113.22
20	K	1086	LMU	C1B-O5B-C5B	-3.05	107.83	113.75
19	A	1801	CLA	CMD-C2D-C3D	-3.05	119.13	125.09
19	B	1752	CLA	CHC-C1C-C2C	-3.04	118.34	126.35
19	A	1766	CLA	CHD-C4C-C3C	-3.04	120.25	124.94
19	A	1780	CLA	O2A-CGA-O1A	-3.04	115.66	123.49
19	B	1759	CLA	CHC-C1C-C2C	-3.04	118.37	126.35
19	3	1216	CLA	C2D-C3D-C4D	-3.04	103.63	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	1170	BCR	C36-C18-C17	-3.04	118.42	122.90
19	B	1759	CLA	C2A-C1A-CHA	-3.04	118.30	123.89
20	A	7013	LMU	O3'-C3'-C4'	-3.03	102.70	109.87
19	I	1033	CLA	O2D-CGD-O1D	-3.03	117.53	123.79
20	A	7037	LMU	C3'-C4'-C5'	-3.03	104.00	110.84
19	3	3007	CLA	CHD-C4C-C3C	-3.02	120.27	124.94
22	B	1776	BCR	C15-C14-C13	-3.02	122.83	127.20
19	4	4007	CLA	CHC-C1C-C2C	-3.02	118.40	126.35
20	A	7043	LMU	O2'-C2'-C1'	-3.02	103.39	110.02
21	B	8056	SUC	C1-O5-C5	-3.02	107.88	113.75
20	A	7030	LMU	C3'-C4'-C5'	-3.02	104.02	110.84
19	B	1738	CLA	CMA-C3A-C2A	-3.01	101.01	114.35
22	L	1169	BCR	C19-C18-C17	-3.01	114.13	118.98
19	A	1785	CLA	CAA-C2A-C1A	-3.01	101.84	112.47
19	B	1739	CLA	CAA-C2A-C3A	-3.01	104.55	113.22
20	A	7037	LMU	O3B-C3B-C4B	-3.01	103.56	110.34
19	B	1763	CLA	CAA-CBA-CGA	-3.01	104.50	113.32
19	3	1218	CLA	C3D-CAD-CBD	-3.01	103.34	107.60
20	A	7041	LMU	O2B-C2B-C1B	-3.01	103.43	110.02
19	3	1215	CLA	C2D-C3D-C4D	-3.00	103.66	106.30
19	A	1774	CLA	O2D-CGD-O1D	-3.00	117.61	123.79
19	3	1217	CLA	C1D-CHD-C4C	-2.99	118.62	126.32
21	B	8059	SUC	C2'-O1-C1	-2.98	109.67	117.53
19	F	1157	CLA	C2A-C1A-CHA	-2.98	118.40	123.89
19	2	1218	CLA	CMD-C2D-C3D	-2.98	119.26	125.09
19	A	1763	CLA	CAA-C2A-C1A	-2.98	101.96	112.47
19	3	1218	CLA	CAC-C3C-C4C	-2.98	120.51	124.83
20	A	7041	LMU	O2'-C2'-C1'	-2.97	103.50	110.02
19	A	1768	CLA	CMD-C2D-C3D	-2.97	119.27	125.09
19	B	1787	CLA	CHC-C1C-C2C	-2.97	118.53	126.35
19	2	1223	CLA	CHC-C1C-C2C	-2.96	118.56	126.35
20	A	7023	LMU	C1'-O5'-C5'	-2.96	108.01	113.75
22	B	1776	BCR	C16-C15-C14	-2.95	116.86	123.39
19	B	1742	CLA	CHC-C1C-C2C	-2.95	118.58	126.35
19	K	3009	CLA	CAA-CBA-CGA	-2.95	104.68	113.32
19	B	1771	CLA	CHC-C1C-C2C	-2.95	118.60	126.35
20	A	7025	LMU	O3B-C3B-C2B	-2.94	103.72	110.34
19	A	1789	CLA	O2A-CGA-O1A	-2.94	115.91	123.49
19	A	1762	CLA	C2A-C1A-CHA	-2.94	118.47	123.89
19	4	1198	CLA	CBC-CAC-C3C	-2.93	103.44	112.39
19	B	1747	CLA	CHC-C1C-C2C	-2.93	118.64	126.35
19	B	1763	CLA	CHC-C1C-C2C	-2.93	118.65	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7032	LMU	O1B-C4'-C3'	-2.93	99.62	107.17
19	A	1811	CLA	C6-C7-C8	-2.92	105.79	115.49
19	K	1146	CLA	C3D-CAD-CBD	-2.92	103.46	107.60
19	A	1787	CLA	CMD-C2D-C3D	-2.92	119.37	125.09
19	2	1217	CLA	CMD-C2D-C3D	-2.92	119.37	125.09
19	1	1190	CLA	O1D-CGD-CBD	-2.92	120.44	124.62
19	4	1208	CLA	C3B-C2B-C1B	-2.92	103.73	106.29
19	B	1752	CLA	CHD-C4C-C3C	-2.92	120.43	124.94
19	B	1738	CLA	CAA-C2A-C3A	-2.91	104.83	113.22
20	A	7027	LMU	O3'-C3'-C4'	-2.91	102.98	109.87
20	A	7023	LMU	C6B-C5B-C4B	-2.91	105.83	113.02
19	4	1209	CLA	CBA-CAA-C2A	-2.91	105.53	113.73
19	B	1754	CLA	CMD-C2D-C3D	-2.91	119.40	125.09
20	L	1171	LMU	O5'-C5'-C4'	-2.91	103.60	109.75
19	I	1033	CLA	CHC-C1C-C2C	-2.91	118.71	126.35
19	B	1754	CLA	CHC-C1C-C2C	-2.90	118.71	126.35
19	A	1762	CLA	CHC-C1C-C2C	-2.90	118.72	126.35
20	A	7024	LMU	C4B-C3B-C2B	-2.90	105.38	110.79
19	B	1743	CLA	CMD-C2D-C3D	-2.90	119.42	125.09
19	A	1788	CLA	CHC-C1C-C2C	-2.90	118.73	126.35
19	A	1798	CLA	CMD-C2D-C3D	-2.89	119.43	125.09
19	J	1044	CLA	CBC-CAC-C3C	-2.89	103.56	112.39
19	3	3011	CLA	CMD-C2D-C3D	-2.89	119.43	125.09
19	A	1789	CLA	CAC-C3C-C2C	-2.89	122.44	127.51
19	B	1749	CLA	C4-C3-C2	-2.89	117.82	123.50
19	2	1219	CLA	C3B-C2B-C1B	-2.89	103.76	106.29
19	A	1765	CLA	O2A-CGA-O1A	-2.89	116.03	123.49
19	A	1786	CLA	CMD-C2D-C3D	-2.89	119.44	125.09
19	1	1198	CLA	CMD-C2D-C3D	-2.88	119.45	125.09
21	B	8056	SUC	O1-C2'-C1'	-2.88	100.45	109.69
19	4	1208	CLA	C2C-C1C-CHC	-2.88	120.03	125.15
19	2	1222	CLA	CHC-C1C-C2C	-2.88	118.78	126.35
19	A	1769	CLA	CAA-C2A-C1A	-2.88	102.32	112.47
19	A	1813	CLA	C2A-C1A-CHA	-2.88	118.58	123.89
19	R	1054	CLA	O2D-CGD-O1D	-2.88	117.85	123.79
21	2	1226	SUC	O1-C2'-O2'	-2.88	101.38	110.52
21	B	8056	SUC	C1-C2-C3	-2.88	104.31	109.97
19	2	1224	CLA	CMD-C2D-C3D	-2.87	119.47	125.09
19	K	1146	CLA	CHC-C1C-C2C	-2.87	118.79	126.35
19	A	1798	CLA	C7-C6-C5	-2.87	104.58	113.06
19	3	3011	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
19	A	1769	CLA	CMD-C2D-C3D	-2.87	119.48	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1777	BCR	C3-C4-C5	-2.87	109.32	113.87
19	A	1763	CLA	C2A-C1A-CHA	-2.86	118.61	123.89
19	B	1755	CLA	O1D-CGD-CBD	-2.86	120.52	124.62
19	3	3007	CLA	O1D-CGD-CBD	-2.86	120.52	124.62
19	B	1765	CLA	CMD-C2D-C3D	-2.86	119.49	125.09
20	A	7037	LMU	O6B-C6B-C5B	-2.86	101.89	111.33
19	A	1773	CLA	CHC-C1C-C2C	-2.86	118.84	126.35
19	3	1218	CLA	CHC-C1C-C2C	-2.86	118.84	126.35
19	4	1205	CLA	C2D-C3D-C4D	-2.85	103.79	106.30
19	L	1505	CLA	O1D-CGD-CBD	-2.85	120.53	124.62
19	A	1790	CLA	O1D-CGD-CBD	-2.85	120.53	124.62
21	B	8062	SUC	O1-C2'-C1'	-2.85	100.55	109.69
19	B	1785	CLA	CBC-CAC-C3C	-2.85	103.69	112.39
19	A	1811	CLA	C3B-C4B-NB	-2.85	105.53	109.21
19	A	1771	CLA	CHC-C1C-C2C	-2.85	118.86	126.35
19	L	1166	CLA	O2D-CGD-O1D	-2.85	117.91	123.79
19	A	1759	CLA	CMD-C2D-C3D	-2.84	119.53	125.09
20	A	7033	LMU	O5'-C5'-C4'	-2.84	103.74	109.75
19	4	1207	CLA	CHC-C1C-C2C	-2.84	118.88	126.35
19	4	1208	CLA	C2D-C3D-C4D	-2.84	103.80	106.30
20	A	7028	LMU	C1B-C2B-C3B	-2.84	104.38	109.97
19	J	1044	CLA	CHC-C1C-C2C	-2.84	118.89	126.35
22	B	1774	BCR	C3-C4-C5	-2.84	109.37	113.87
19	B	1738	CLA	O2A-CGA-O1A	-2.83	116.18	123.49
19	A	1770	CLA	CHC-C1C-C2C	-2.83	118.90	126.35
19	A	1781	CLA	O1D-CGD-CBD	-2.83	120.57	124.62
19	A	1764	CLA	O2A-CGA-O1A	-2.83	116.19	123.49
22	3	1220	BCR	C24-C23-C22	-2.83	121.91	126.22
19	A	1787	CLA	C4-C3-C2	-2.83	117.95	123.50
19	B	1748	CLA	CGD-CBD-CAD	-2.82	101.05	110.62
19	A	1787	CLA	O1D-CGD-CBD	-2.82	120.58	124.62
19	4	1201	CLA	C4-C3-C2	-2.82	117.97	123.50
21	B	8059	SUC	C1-C2-C3	-2.82	104.42	109.97
19	A	1790	CLA	CHC-C1C-C2C	-2.81	118.95	126.35
21	B	8055	SUC	O4-C4-C5	-2.81	101.78	109.24
20	A	7043	LMU	O2B-C2B-C3B	-2.81	104.00	110.34
20	A	7037	LMU	O5'-C5'-C4'	-2.81	103.81	109.75
22	B	1778	BCR	C28-C27-C26	-2.81	109.41	113.87
19	B	1756	CLA	O1D-CGD-CBD	-2.80	120.60	124.62
19	A	1776	CLA	CHC-C1C-C2C	-2.80	118.98	126.35
22	B	1778	BCR	C3-C4-C5	-2.80	109.42	113.87
19	B	1754	CLA	CAC-C3C-C2C	-2.79	122.61	127.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7041	LMU	C1B-O5B-C5B	-2.79	108.32	113.75
19	4	4007	CLA	CAA-C2A-C1A	-2.79	102.63	112.47
19	B	1760	CLA	CHC-C1C-C2C	-2.79	119.02	126.35
22	A	1803	BCR	C28-C27-C26	-2.79	109.44	113.87
22	A	1806	BCR	C3-C4-C5	-2.79	109.45	113.87
19	A	1784	CLA	CHC-C1C-C2C	-2.79	119.02	126.35
19	A	1782	CLA	O1D-CGD-CBD	-2.79	120.63	124.62
19	2	1212	CLA	O1D-CGD-CBD	-2.78	120.63	124.62
22	B	1774	BCR	C28-C27-C26	-2.78	109.46	113.87
19	B	1739	CLA	CMD-C2D-C3D	-2.78	119.65	125.09
19	B	1769	CLA	CMD-C2D-C3D	-2.78	119.66	125.09
19	A	1791	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
19	3	1219	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
19	4	1200	CLA	O2D-CGD-O1D	-2.78	118.06	123.79
19	B	1746	CLA	CHC-C1C-C2C	-2.77	119.05	126.35
20	L	1171	LMU	O3'-C3'-C4'	-2.77	103.31	109.87
19	A	1777	CLA	O1D-CGD-CBD	-2.77	120.65	124.62
19	A	1779	CLA	CAA-C2A-C3A	-2.77	105.24	113.22
22	A	1808	BCR	C28-C27-C26	-2.77	109.47	113.87
19	B	1770	CLA	O2D-CGD-O1D	-2.77	118.06	123.79
19	G	1099	CLA	CAA-CBA-CGA	-2.77	105.20	113.32
19	4	1206	CLA	C2C-C1C-CHC	-2.77	120.22	125.15
21	2	1226	SUC	C2'-O1-C1	-2.77	110.22	117.53
19	B	1738	CLA	CHD-C4C-C3C	-2.77	120.66	124.94
19	1	1187	CLA	O2D-CGD-O1D	-2.77	118.07	123.79
19	A	1759	CLA	CHC-C1C-C2C	-2.77	119.06	126.35
19	I	1033	CLA	CHD-C4C-C3C	-2.77	120.66	124.94
19	2	1218	CLA	O1D-CGD-CBD	-2.77	120.65	124.62
19	B	1735	CLA	O1D-CGD-CBD	-2.77	120.66	124.62
19	J	1045	CLA	CHC-C1C-C2C	-2.76	119.08	126.35
19	A	1795	CLA	O1D-CGD-CBD	-2.76	120.66	124.62
22	B	1775	BCR	C28-C27-C26	-2.76	109.48	113.87
22	A	1804	BCR	C3-C4-C5	-2.76	109.48	113.87
19	4	1196	CLA	O1D-CGD-CBD	-2.76	120.66	124.62
19	A	1768	CLA	CHC-C1C-C2C	-2.76	119.09	126.35
19	A	1792	CLA	O1D-CGD-CBD	-2.76	120.67	124.62
22	B	1775	BCR	C3-C4-C5	-2.76	109.49	113.87
20	A	7017	LMU	C6'-C5'-C4'	-2.76	105.22	113.25
19	A	1798	CLA	O1D-CGD-CBD	-2.76	120.67	124.62
19	B	1738	CLA	C16-C15-C13	-2.75	106.35	115.49
19	B	1758	CLA	CMA-C3A-C2A	-2.75	102.16	114.35
22	B	1780	BCR	C3-C4-C5	-2.75	109.50	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7027	LMU	O5B-C5B-C4B	-2.75	104.51	109.68
19	B	1741	CLA	O2D-CGD-O1D	-2.75	118.11	123.79
19	2	1218	CLA	CHD-C4C-C3C	-2.75	120.69	124.94
19	A	1793	CLA	O1D-CGD-CBD	-2.75	120.68	124.62
19	B	1762	CLA	CAA-CBA-CGA	-2.75	105.27	113.32
19	4	1201	CLA	CMA-C3A-C2A	-2.75	102.19	114.35
19	3	3008	CLA	C2A-C1A-CHA	-2.75	118.83	123.89
19	R	1055	CLA	CHC-C1C-C2C	-2.75	119.13	126.35
19	B	1758	CLA	CHC-C1C-C2C	-2.75	119.13	126.35
19	A	1796	CLA	O1D-CGD-CBD	-2.74	120.69	124.62
19	J	1043	CLA	O1D-CGD-CBD	-2.74	120.69	124.62
19	3	1217	CLA	C3C-C4C-CHD	-2.74	120.81	125.32
19	A	1797	CLA	O1D-CGD-CBD	-2.74	120.69	124.62
19	K	1142	CLA	O1D-CGD-CBD	-2.74	120.69	124.62
19	1	1198	CLA	CHC-C1C-C2C	-2.74	119.14	126.35
20	L	1171	LMU	O3B-C3B-C2B	-2.74	104.17	110.34
20	A	7030	LMU	O3'-C3'-C4'	-2.74	103.39	109.87
19	A	1794	CLA	O1D-CGD-CBD	-2.74	120.70	124.62
22	B	1777	BCR	C28-C27-C26	-2.74	109.52	113.87
22	A	1807	BCR	C3-C4-C5	-2.74	109.52	113.87
22	A	1807	BCR	C28-C27-C26	-2.74	109.52	113.87
19	B	1768	CLA	CBC-CAC-C3C	-2.74	104.04	112.39
21	B	8062	SUC	O3'-C3'-C2'	-2.74	105.19	113.96
19	K	1085	CLA	O1D-CGD-CBD	-2.73	120.70	124.62
19	B	1758	CLA	C11-C12-C13	-2.73	106.42	115.49
19	B	1770	CLA	O2A-CGA-O1A	-2.73	116.44	123.49
19	F	1156	CLA	O1D-CGD-CBD	-2.73	120.71	124.62
19	B	1748	CLA	CHC-C1C-C2C	-2.73	119.17	126.35
19	A	1799	CLA	CHC-C1C-C2C	-2.73	119.17	126.35
19	2	1224	CLA	C4-C3-C2	-2.73	118.14	123.50
20	A	7028	LMU	C3B-C4B-C5B	-2.73	105.44	110.20
20	A	7042	LMU	C3B-C4B-C5B	-2.73	105.45	110.20
22	A	1805	BCR	C3-C4-C5	-2.72	109.54	113.87
19	2	1217	CLA	CHC-C1C-C2C	-2.72	119.19	126.35
19	2	1215	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
23	B	1773	PQN	C14-C13-C12	-2.72	118.16	123.50
22	A	1806	BCR	C28-C27-C26	-2.72	109.55	113.87
19	4	4014	CLA	O1D-CGD-CBD	-2.72	120.73	124.62
19	B	1752	CLA	O1D-CGD-CBD	-2.71	120.73	124.62
19	A	1799	CLA	CHD-C4C-C3C	-2.71	120.75	124.94
19	A	1801	CLA	C2A-C1A-CHA	-2.71	118.89	123.89
21	B	8059	SUC	O3'-C3'-C2'	-2.71	105.27	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1816	CLA	O2A-CGA-O1A	-2.71	116.50	123.49
22	A	1804	BCR	C28-C27-C26	-2.71	109.57	113.87
22	A	1805	BCR	C28-C27-C26	-2.70	109.58	113.87
22	A	1803	BCR	C3-C4-C5	-2.70	109.58	113.87
22	B	1779	BCR	C32-C1-C6	-2.70	106.07	110.30
19	2	1222	CLA	CHD-C4C-C3C	-2.70	120.77	124.94
22	B	1780	BCR	C28-C27-C26	-2.70	109.59	113.87
19	R	1054	CLA	CHC-C1C-C2C	-2.70	119.26	126.35
20	A	7032	LMU	O6'-C6'-C5'	-2.70	102.42	111.33
19	A	1799	CLA	O2A-CGA-O1A	-2.69	116.54	123.49
22	B	1776	BCR	C39-C30-C25	-2.69	106.08	110.30
23	A	1802	PQN	C2M-C2-C3	-2.69	118.34	124.10
19	3	3008	CLA	O2A-CGA-O1A	-2.69	116.55	123.49
21	B	8055	SUC	O4'-C4'-C5'	-2.69	102.99	111.05
19	2	1224	CLA	O2A-CGA-O1A	-2.69	116.55	123.49
19	B	1757	CLA	CAA-C2A-C3A	-2.69	105.49	113.22
19	A	1759	CLA	CAA-C2A-C3A	-2.69	105.49	113.22
19	B	1748	CLA	O2A-CGA-O1A	-2.69	116.56	123.49
19	1	1190	CLA	CHC-C1C-C2C	-2.69	119.28	126.35
19	F	1155	CLA	CHC-C1C-C2C	-2.69	119.29	126.35
19	L	1505	CLA	CHC-C1C-C2C	-2.69	119.29	126.35
20	A	7037	LMU	O2B-C2B-C3B	-2.68	104.30	110.34
19	A	1798	CLA	C4-C3-C2	-2.68	118.25	123.50
22	A	1808	BCR	C3-C4-C5	-2.68	109.62	113.87
19	3	1219	CLA	CHC-C1C-C2C	-2.67	119.32	126.35
19	A	1763	CLA	O2D-CGD-O1D	-2.67	118.27	123.79
19	B	1766	CLA	O1D-CGD-CBD	-2.67	120.79	124.62
19	A	1774	CLA	C4-C3-C2	-2.67	118.25	123.50
19	B	1740	CLA	CMB-C2B-C1B	-2.67	123.94	128.36
20	A	7026	LMU	C1B-O1B-C4'	-2.67	111.02	118.01
19	A	1772	CLA	O2D-CGD-O1D	-2.67	118.27	123.79
19	A	1769	CLA	CAA-CBA-CGA	-2.67	105.50	113.32
20	A	7025	LMU	C4B-C3B-C2B	-2.67	105.81	110.79
19	4	1207	CLA	CAC-C3C-C2C	-2.67	121.33	126.81
19	B	1750	CLA	CHC-C1C-C2C	-2.67	119.34	126.35
19	3	3008	CLA	CHC-C1C-C2C	-2.66	119.34	126.35
22	B	1781	BCR	C32-C1-C31	-2.66	99.83	108.37
19	F	1156	CLA	CHC-C1C-C2C	-2.66	119.35	126.35
19	B	1741	CLA	CHC-C1C-C2C	-2.66	119.35	126.35
19	A	1798	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
19	A	1771	CLA	C1-C2-C3	-2.66	122.35	126.71
19	A	1811	CLA	CMD-C2D-C3D	-2.66	119.89	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1099	CLA	CMD-C2D-C3D	-2.66	119.89	125.09
19	K	1085	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
20	A	7039	LMU	O3B-C3B-C2B	-2.66	104.35	110.34
19	A	1775	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
19	H	1079	CLA	O2D-CGD-O1D	-2.66	118.31	123.79
19	B	1755	CLA	CHC-C1C-C2C	-2.65	119.37	126.35
19	B	1756	CLA	CHC-C1C-C2C	-2.65	119.38	126.35
19	2	1213	CLA	CHC-C1C-C2C	-2.65	119.38	126.35
19	A	1782	CLA	CHC-C1C-C2C	-2.65	119.38	126.35
22	3	1220	BCR	C34-C9-C10	-2.65	118.99	122.90
20	A	7016	LMU	O5B-C5B-C4B	-2.64	104.72	109.68
19	A	1760	CLA	CHC-C1C-C2C	-2.64	119.40	126.35
20	A	7023	LMU	C1-O1'-C1'	-2.64	109.32	113.94
19	A	1793	CLA	CHC-C1C-C2C	-2.64	119.40	126.35
19	B	1743	CLA	CBA-CAA-C2A	-2.64	106.28	113.73
19	B	1735	CLA	CHC-C1C-C2C	-2.64	119.41	126.35
21	H	1080	SUC	C4-C3-C2	-2.64	105.87	110.79
19	A	1794	CLA	CHC-C1C-C2C	-2.64	119.41	126.35
19	3	1218	CLA	C4-C3-C2	-2.63	118.33	123.50
19	A	1800	CLA	C6-C7-C8	-2.63	106.75	115.49
19	K	1142	CLA	CHC-C1C-C2C	-2.63	119.42	126.35
19	A	1791	CLA	CHC-C1C-C2C	-2.63	119.43	126.35
20	A	7035	LMU	C2'-C3'-C4'	-2.63	103.82	109.60
19	A	1792	CLA	CHC-C1C-C2C	-2.63	119.44	126.35
19	B	1742	CLA	O2D-CGD-O1D	-2.63	118.36	123.79
20	A	7035	LMU	O5'-C5'-C4'	-2.63	104.19	109.75
19	A	1797	CLA	CHC-C1C-C2C	-2.63	119.44	126.35
19	A	1795	CLA	CHC-C1C-C2C	-2.63	119.44	126.35
19	2	1212	CLA	CHC-C1C-C2C	-2.62	119.45	126.35
19	A	1796	CLA	CHC-C1C-C2C	-2.62	119.45	126.35
19	A	1781	CLA	CHC-C1C-C2C	-2.62	119.45	126.35
19	3	3007	CLA	CAC-C3C-C2C	-2.62	122.91	127.51
19	4	1196	CLA	CHC-C1C-C2C	-2.62	119.45	126.35
20	A	7034	LMU	O2B-C2B-C3B	-2.62	104.43	110.34
19	J	1044	CLA	CAC-C3C-C2C	-2.62	122.91	127.51
19	3	1218	CLA	CAA-C2A-C1A	-2.62	103.23	112.47
19	A	1762	CLA	CAA-C2A-C1A	-2.62	103.23	112.47
21	B	8052	SUC	C2'-O1-C1	-2.62	110.63	117.53
19	A	1776	CLA	CAA-C2A-C3A	-2.62	105.69	113.22
19	R	1055	CLA	CGD-CBD-CAD	-2.62	101.76	110.62
19	B	1738	CLA	C11-C12-C13	-2.61	106.81	115.49
19	A	1817	CLA	O2A-CGA-O1A	-2.61	116.75	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1192	CLA	O2A-CGA-O1A	-2.61	116.75	123.49
19	B	1737	CLA	O1D-CGD-CBD	-2.61	120.89	124.62
19	B	1760	CLA	C1-C2-C3	-2.61	122.44	126.71
19	A	1774	CLA	CMD-C2D-C3D	-2.61	119.99	125.09
19	3	3002	CLA	C2D-C3D-C4D	-2.60	104.01	106.30
19	A	1772	CLA	CHC-C1C-C2C	-2.60	119.50	126.35
19	B	1744	CLA	CHC-C1C-C2C	-2.60	119.51	126.35
20	A	7042	LMU	C1-O1'-C1'	-2.60	109.39	113.94
19	4	4014	CLA	CHC-C1C-C2C	-2.60	119.51	126.35
20	A	7023	LMU	C8-C7-C6	-2.60	101.09	114.53
19	B	1785	CLA	C7-C6-C5	-2.60	105.38	113.06
19	A	1817	CLA	O1D-CGD-CBD	-2.60	120.89	124.62
19	A	1780	CLA	CHC-C1C-C2C	-2.60	119.52	126.35
20	A	7027	LMU	C4B-C3B-C2B	-2.60	105.94	110.79
20	A	7041	LMU	C6'-C5'-C4'	-2.60	105.69	113.25
22	L	1169	BCR	C28-C27-C26	-2.60	109.75	113.87
20	A	7032	LMU	C1B-O1B-C4'	-2.60	111.22	118.01
19	B	1738	CLA	O1D-CGD-CBD	-2.59	120.91	124.62
19	B	1767	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
19	J	1043	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
19	A	1766	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
19	B	1740	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
19	B	1759	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
19	A	1774	CLA	CHC-C1C-C2C	-2.58	119.56	126.35
20	K	1086	LMU	O2'-C2'-C3'	-2.58	104.53	110.34
19	B	1786	CLA	CMD-C2D-C3D	-2.57	120.05	125.09
20	A	7043	LMU	C3'-C4'-C5'	-2.57	105.02	110.84
22	B	1779	BCR	C34-C9-C10	-2.57	119.10	122.90
19	J	1044	CLA	O2A-CGA-O1A	-2.57	116.86	123.49
19	K	3009	CLA	CMD-C2D-C3D	-2.57	120.06	125.09
24	B	1783	LMG	C8-O7-C10	-2.57	111.73	117.89
19	A	1772	CLA	O1D-CGD-CBD	-2.56	120.95	124.62
20	A	7040	LMU	C4B-C3B-C2B	-2.56	106.01	110.79
19	F	1157	CLA	C3D-CAD-CBD	-2.56	103.97	107.60
19	I	1033	CLA	CMD-C2D-C3D	-2.56	120.08	125.09
19	1	1200	CLA	O2D-CGD-O1D	-2.56	118.51	123.79
19	A	1768	CLA	O2D-CGD-O1D	-2.55	118.52	123.79
19	1	1190	CLA	C2A-C1A-CHA	-2.55	119.18	123.89
19	2	1215	CLA	CHC-C1C-C2C	-2.55	119.65	126.35
19	H	1079	CLA	CHC-C1C-C2C	-2.55	119.65	126.35
19	A	1783	CLA	C6-C7-C8	-2.55	107.04	115.49
19	A	1769	CLA	O2D-CGD-O1D	-2.54	118.55	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	1170	BCR	C19-C18-C17	-2.54	114.89	118.98
19	K	1146	CLA	O1D-CGD-CBD	-2.54	120.99	124.62
19	B	1785	CLA	C16-C17-C18	-2.54	103.09	115.87
19	B	1770	CLA	CHC-C1C-C2C	-2.53	119.69	126.35
19	4	4007	CLA	O1D-CGD-CBD	-2.53	120.99	124.62
19	J	1044	CLA	C11-C12-C13	-2.53	107.09	115.49
19	2	1220	CLA	C2A-C1A-CHA	-2.53	119.22	123.89
22	B	1779	BCR	C2-C3-C4	-2.53	105.15	111.53
19	I	1031	CLA	CHC-C1C-C2C	-2.53	119.70	126.35
19	A	1785	CLA	CHC-C1C-C2C	-2.52	119.71	126.35
19	G	1099	CLA	C2A-C1A-CHA	-2.52	119.24	123.89
20	A	7023	LMU	O5'-C5'-C6'	-2.52	99.98	106.36
19	K	3009	CLA	C6-C7-C8	-2.52	107.12	115.49
22	3	1220	BCR	C28-C27-C26	-2.52	109.87	113.87
19	A	1812	CLA	CHC-C1C-C2C	-2.52	119.73	126.35
19	A	1783	CLA	O2A-CGA-O1A	-2.52	117.00	123.49
19	A	1763	CLA	CMD-C2D-C3D	-2.51	120.17	125.09
19	A	1811	CLA	CMA-C3A-C2A	-2.51	103.23	114.35
19	J	1045	CLA	O2D-CGD-O1D	-2.51	118.60	123.79
22	L	1169	BCR	C37-C22-C21	-2.51	119.19	122.90
19	3	1212	CLA	CHC-C1C-C2C	-2.51	119.75	126.35
19	B	1769	CLA	CHC-C1C-C2C	-2.51	119.75	126.35
19	J	1045	CLA	CGD-CBD-CAD	-2.51	102.12	110.62
22	L	1169	BCR	C8-C7-C6	-2.51	119.79	127.32
21	B	8062	SUC	O4-C4-C3	-2.50	104.70	110.34
20	A	7036	LMU	O3'-C3'-C4'	-2.50	103.95	109.87
22	I	1032	BCR	C4-C5-C6	-2.50	119.59	122.78
20	A	7030	LMU	O2'-C2'-C1'	-2.50	104.54	110.02
19	A	1787	CLA	CHC-C1C-C2C	-2.50	119.78	126.35
19	A	1785	CLA	CMD-C2D-C3D	-2.50	120.21	125.09
19	A	1771	CLA	CAA-C2A-C3A	-2.49	106.04	113.22
19	A	1800	CLA	O2D-CGD-O1D	-2.49	118.65	123.79
19	B	1764	CLA	CHC-C1C-C2C	-2.49	119.81	126.35
19	L	1168	CLA	C1-C2-C3	-2.49	122.63	126.71
20	A	7028	LMU	O5'-C5'-C6'	-2.49	100.07	106.36
19	B	1761	CLA	O2D-CGD-O1D	-2.48	118.66	123.79
19	A	1788	CLA	O2D-CGD-O1D	-2.48	118.67	123.79
22	3	1220	BCR	C37-C22-C21	-2.48	119.24	122.90
19	B	1765	CLA	CHC-C1C-C2C	-2.48	119.83	126.35
19	I	1033	CLA	O2A-CGA-O1A	-2.48	117.10	123.49
20	R	1057	LMU	C1'-O5'-C5'	-2.48	108.94	113.75
22	B	1780	BCR	C23-C24-C25	-2.48	119.88	127.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1754	CLA	O1D-CGD-CBD	-2.47	121.08	124.62
21	H	1080	SUC	O1'-C1'-C2'	-2.47	104.02	111.91
19	A	1766	CLA	O2D-CGD-O1D	-2.47	118.70	123.79
19	A	1764	CLA	CHC-C1C-C2C	-2.46	119.87	126.35
22	B	1775	BCR	C23-C24-C25	-2.46	119.92	127.32
19	A	1777	CLA	O2D-CGD-O1D	-2.46	118.71	123.79
19	B	1760	CLA	CHD-C4C-C3C	-2.46	121.14	124.94
19	A	1789	CLA	CAA-C2A-C3A	-2.46	106.15	113.22
19	2	1213	CLA	CAA-C2A-C1A	-2.45	103.81	112.47
20	A	7030	LMU	O5B-C5B-C4B	-2.45	105.08	109.68
21	B	8052	SUC	O3-C3-C4	-2.45	104.81	110.34
22	B	1774	BCR	C8-C7-C6	-2.45	119.95	127.32
22	A	1805	BCR	C23-C24-C25	-2.45	119.96	127.32
19	1	1197	CLA	C3A-C2A-C1A	-2.45	97.35	101.50
19	L	1168	CLA	CAA-CBA-CGA	-2.45	106.15	113.32
19	B	1751	CLA	CHC-C1C-C2C	-2.45	119.91	126.35
19	1	1195	CLA	CHC-C1C-C2C	-2.45	119.92	126.35
22	A	1805	BCR	C8-C7-C6	-2.45	119.97	127.32
19	B	1757	CLA	CHC-C1C-C2C	-2.45	119.92	126.35
19	2	1212	CLA	C2A-C1A-CHA	-2.45	119.38	123.89
19	B	1771	CLA	CMA-C3A-C2A	-2.45	103.53	114.35
19	B	1772	CLA	CHC-C1C-C2C	-2.45	119.92	126.35
22	B	1780	BCR	C8-C7-C6	-2.44	119.98	127.32
20	A	7023	LMU	C4B-C3B-C2B	-2.44	106.23	110.79
21	B	8052	SUC	O4'-C4'-C5'	-2.44	103.72	111.05
19	B	1756	CLA	C2A-C1A-CHA	-2.44	119.39	123.89
19	L	1505	CLA	CGD-CBD-CAD	-2.44	102.35	110.62
19	1	1193	CLA	CHC-C1C-C2C	-2.44	119.93	126.35
19	A	1787	CLA	O2A-CGA-O1A	-2.44	117.19	123.49
22	A	1804	BCR	C8-C7-C6	-2.44	119.99	127.32
19	A	1813	CLA	CHC-C1C-C2C	-2.44	119.94	126.35
22	A	1803	BCR	C23-C24-C25	-2.44	120.00	127.32
22	A	1806	BCR	C23-C24-C25	-2.44	120.00	127.32
19	I	1031	CLA	CMD-C2D-C3D	-2.44	120.32	125.09
19	A	1774	CLA	CAA-CBA-CGA	-2.44	106.19	113.32
22	B	1777	BCR	C23-C24-C25	-2.43	120.00	127.32
20	A	7028	LMU	O4'-C4B-C5B	-2.43	102.79	109.24
19	A	1782	CLA	C2A-C1A-CHA	-2.43	119.40	123.89
22	B	1778	BCR	C23-C24-C25	-2.43	120.01	127.32
19	A	1772	CLA	CAC-C3C-C2C	-2.43	123.25	127.51
22	A	1808	BCR	C8-C7-C6	-2.43	120.01	127.32
22	B	1777	BCR	C8-C7-C6	-2.43	120.02	127.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1803	BCR	C8-C7-C6	-2.43	120.02	127.32
20	1	1202	LMU	C1B-O1B-C4'	-2.43	111.66	118.01
20	A	7021	LMU	C3B-C4B-C5B	-2.43	105.96	110.20
22	A	1807	BCR	C23-C24-C25	-2.43	120.02	127.32
19	A	1791	CLA	C2A-C1A-CHA	-2.43	119.41	123.89
20	A	7026	LMU	C4B-C3B-C2B	-2.43	106.26	110.79
22	A	1806	BCR	C8-C7-C6	-2.43	120.03	127.32
19	A	1764	CLA	CAA-C2A-C3A	-2.43	106.24	113.22
19	J	1043	CLA	C2A-C1A-CHA	-2.43	119.42	123.89
20	A	7015	LMU	O5B-C5B-C4B	-2.42	105.13	109.68
19	A	1793	CLA	C2A-C1A-CHA	-2.42	119.42	123.89
19	B	1736	CLA	CHC-C1C-C2C	-2.42	119.98	126.35
19	A	1765	CLA	C5-C3-C2	-2.42	116.46	121.05
19	B	1763	CLA	CAA-C2A-C1A	-2.42	103.93	112.47
19	B	1757	CLA	CAA-C2A-C1A	-2.42	103.94	112.47
22	A	1807	BCR	C8-C7-C6	-2.42	120.05	127.32
20	2	7006	LMU	C1B-O1B-C4'	-2.42	111.69	118.01
19	2	1220	CLA	CHC-C1C-C2C	-2.42	119.99	126.35
20	A	7039	LMU	O5'-C1'-C2'	-2.42	105.31	110.28
19	B	1737	CLA	CAA-C2A-C1A	-2.42	103.95	112.47
20	A	1809	LMU	O6'-C6'-C5'	-2.42	103.35	111.33
19	G	1099	CLA	C4-C3-C2	-2.42	118.76	123.50
19	A	1796	CLA	C2A-C1A-CHA	-2.41	119.44	123.89
19	K	1085	CLA	C2A-C1A-CHA	-2.41	119.44	123.89
22	A	1808	BCR	C23-C24-C25	-2.41	120.07	127.32
19	3	1219	CLA	C2A-C1A-CHA	-2.41	119.44	123.89
19	F	1156	CLA	C2A-C1A-CHA	-2.41	119.44	123.89
19	1	1197	CLA	CMB-C2B-C3B	-2.41	120.37	125.09
19	K	1142	CLA	C2A-C1A-CHA	-2.41	119.44	123.89
20	A	7028	LMU	O2B-C2B-C1B	-2.41	104.73	110.02
19	B	1755	CLA	C2A-C1A-CHA	-2.41	119.45	123.89
20	A	7009	LMU	C1B-O1B-C4'	-2.41	111.72	118.01
19	A	1797	CLA	C2A-C1A-CHA	-2.41	119.45	123.89
19	4	1206	CLA	C2D-C1D-ND	-2.41	107.99	110.13
22	B	1778	BCR	C8-C7-C6	-2.41	120.09	127.32
19	A	1781	CLA	C2A-C1A-CHA	-2.40	119.46	123.89
19	A	1795	CLA	C2A-C1A-CHA	-2.40	119.46	123.89
19	B	1762	CLA	CHC-C1C-C2C	-2.40	120.03	126.35
19	B	1735	CLA	C2A-C1A-CHA	-2.40	119.46	123.89
19	B	1760	CLA	CMD-C2D-C3D	-2.40	120.39	125.09
22	B	1775	BCR	C8-C7-C6	-2.40	120.11	127.32
19	3	3011	CLA	CHC-C1C-C2C	-2.40	120.04	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1787	CLA	CAA-C2A-C3A	-2.40	106.32	113.22
22	B	1774	BCR	C23-C24-C25	-2.40	120.11	127.32
19	4	1204	CLA	C2A-C1A-CHA	-2.40	119.47	123.89
19	2	1217	CLA	C4-C3-C2	-2.40	118.80	123.50
19	A	1772	CLA	C2A-C1A-CHA	-2.40	119.47	123.89
19	A	1794	CLA	C2A-C1A-CHA	-2.40	119.47	123.89
19	A	1792	CLA	C2A-C1A-CHA	-2.39	119.47	123.89
21	H	1080	SUC	O2-C2-C3	-2.39	104.95	110.34
20	A	7010	LMU	C1B-O1B-C4'	-2.39	111.75	118.01
19	A	1785	CLA	O2A-CGA-O1A	-2.39	117.32	123.49
22	A	1804	BCR	C23-C24-C25	-2.39	120.14	127.32
19	A	1816	CLA	CMC-C2C-C1C	-2.39	121.33	125.02
19	A	1786	CLA	O1D-CGD-CBD	-2.39	121.20	124.62
19	B	1737	CLA	CBC-CAC-C3C	-2.38	105.12	112.39
19	B	1739	CLA	CHD-C4C-C3C	-2.38	121.26	124.94
19	1	1191	CLA	CMA-C3A-C2A	-2.38	110.50	116.20
19	A	1788	CLA	C4-C3-C2	-2.38	118.83	123.50
20	1	7004	LMU	C1B-O1B-C4'	-2.38	111.79	118.01
19	A	1761	CLA	C6-C7-C8	-2.38	107.61	115.49
20	A	7038	LMU	C4B-C3B-C2B	-2.37	106.36	110.79
22	B	1781	BCR	C34-C9-C8	-2.37	114.15	118.10
20	R	1056	LMU	C1B-O1B-C4'	-2.37	111.81	118.01
19	A	1760	CLA	O2A-CGA-O1A	-2.37	117.37	123.49
19	4	4014	CLA	C2A-C1A-CHA	-2.37	119.52	123.89
20	L	1171	LMU	C1B-O1B-C4'	-2.37	111.82	118.01
19	A	1761	CLA	O1A-CGA-CBA	-2.37	114.25	123.72
19	4	1196	CLA	C2A-C1A-CHA	-2.37	119.53	123.89
19	B	1745	CLA	O2D-CGD-O1D	-2.36	118.91	123.79
19	A	1785	CLA	C5-C3-C2	-2.36	116.57	121.05
19	A	1779	CLA	CAC-C3C-C2C	-2.36	123.37	127.51
19	4	1200	CLA	CHC-C1C-C2C	-2.36	120.14	126.35
19	3	3015	CLA	C2D-C3D-C4D	-2.36	104.23	106.30
19	B	1743	CLA	C11-C10-C8	-2.36	107.67	115.49
19	1	1198	CLA	C6-C7-C8	-2.36	107.68	115.49
22	3	1220	BCR	C8-C7-C6	-2.35	120.25	127.32
19	B	1766	CLA	O2D-CGD-O1D	-2.35	118.93	123.79
19	B	1750	CLA	CMA-C3A-C2A	-2.35	103.93	114.35
19	A	1783	CLA	C11-C10-C8	-2.35	107.68	115.49
21	B	8062	SUC	O5-C1-O1	-2.35	102.06	109.96
20	3	7005	LMU	C1B-O1B-C4'	-2.35	111.86	118.01
19	B	1768	CLA	O1D-CGD-CBD	-2.35	121.25	124.62
20	A	7032	LMU	O3'-C3'-C4'	-2.35	104.31	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1811	CLA	C2A-C1A-CHA	-2.35	119.56	123.89
19	1	1200	CLA	CHA-C1A-NA	-2.35	120.29	126.06
19	B	1759	CLA	C7-C6-C5	-2.34	106.15	113.06
19	B	1785	CLA	C11-C10-C8	-2.34	107.73	115.49
19	B	1738	CLA	CBC-CAC-C3C	-2.34	105.25	112.39
19	B	1749	CLA	CHC-C1C-C2C	-2.34	120.21	126.35
19	4	4007	CLA	C4-C3-C2	-2.34	118.92	123.50
19	1	1198	CLA	C2A-C1A-CHA	-2.33	119.59	123.89
19	3	3007	CLA	O2D-CGD-O1D	-2.33	118.97	123.79
21	B	8056	SUC	O3'-C3'-C4'	-2.33	104.91	113.29
19	B	1771	CLA	CMD-C2D-C3D	-2.33	120.53	125.09
19	4	1200	CLA	O2A-CGA-O1A	-2.33	117.48	123.49
21	B	8054	SUC	O4'-C4'-C3'	-2.33	104.61	112.01
19	B	1770	CLA	C2C-C1C-NC	-2.33	108.51	110.24
22	L	1170	BCR	C27-C26-C25	-2.33	119.81	122.78
19	B	1743	CLA	C16-C15-C13	-2.32	107.78	115.49
19	2	1218	CLA	CAA-CBA-CGA	-2.32	106.52	113.32
20	2	7003	LMU	C1B-O1B-C4'	-2.32	111.94	118.01
19	1	1192	CLA	CHC-C1C-C2C	-2.32	120.24	126.35
19	B	1758	CLA	O2A-CGA-O1A	-2.32	117.50	123.49
19	B	1737	CLA	C6-C7-C8	-2.32	107.81	115.49
19	2	1222	CLA	CAC-C3C-C2C	-2.32	123.45	127.51
19	B	1761	CLA	CHC-C1C-C2C	-2.31	120.27	126.35
19	L	1166	CLA	CHC-C1C-C2C	-2.31	120.28	126.35
19	4	1198	CLA	CHA-C1A-NA	-2.31	120.38	126.06
19	B	1786	CLA	CAC-C3C-C2C	-2.31	123.47	127.51
20	A	7019	LMU	O2'-C2'-C3'	-2.30	105.15	110.34
19	B	1762	CLA	CAA-C2A-C1A	-2.30	104.35	112.47
19	B	1771	CLA	C4-C3-C2	-2.30	118.99	123.50
19	B	1743	CLA	CHC-C1C-C2C	-2.30	120.31	126.35
19	A	1763	CLA	CHC-C1C-C2C	-2.30	120.31	126.35
19	B	1745	CLA	O2A-CGA-O1A	-2.30	117.56	123.49
19	A	1779	CLA	CHC-C1C-C2C	-2.30	120.31	126.35
19	B	1786	CLA	CBA-CAA-C2A	-2.30	107.26	113.73
21	B	8055	SUC	O2'-C2'-C3'	-2.29	100.36	105.58
19	1	1188	CLA	CMB-C2B-C1B	-2.29	124.58	128.36
20	L	1171	LMU	C1'-C2'-C3'	-2.29	105.46	109.97
19	B	1761	CLA	C2A-C1A-CHA	-2.29	119.67	123.89
19	3	3011	CLA	C5-C3-C2	-2.29	116.71	121.05
20	A	7021	LMU	C1-O1'-C1'	-2.29	109.95	113.94
19	A	1776	CLA	O2D-CGD-O1D	-2.28	119.09	123.79
22	A	1805	BCR	C27-C26-C25	-2.27	119.88	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1786	CLA	CHD-C4C-C3C	-2.27	121.43	124.94
20	4	1210	LMU	C4B-C3B-C2B	-2.27	106.55	110.79
19	4	4014	CLA	O2D-CGD-O1D	-2.27	119.10	123.79
19	B	1768	CLA	C4-C3-C2	-2.27	119.05	123.50
19	B	1748	CLA	CAA-C2A-C3A	-2.27	106.69	113.22
20	A	7042	LMU	O1B-C1B-C2B	-2.27	102.58	108.10
19	A	1800	CLA	CHC-C1C-C2C	-2.27	120.39	126.35
19	A	1788	CLA	O2A-CGA-O1A	-2.26	117.65	123.49
19	K	1085	CLA	O2D-CGD-O1D	-2.26	119.11	123.79
19	A	1782	CLA	O2D-CGD-O1D	-2.26	119.11	123.79
19	2	1215	CLA	CAA-C2A-C3A	-2.26	106.71	113.22
22	B	1777	BCR	C27-C26-C25	-2.26	119.90	122.78
20	A	7036	LMU	O5'-C5'-C4'	-2.26	104.97	109.75
19	B	1769	CLA	O2D-CGD-O1D	-2.26	119.12	123.79
21	2	1226	SUC	O4-C4-C5	-2.26	104.53	109.84
19	B	1745	CLA	CHC-C1C-C2C	-2.26	120.41	126.35
19	B	1785	CLA	C12-C11-C10	-2.26	101.78	112.99
19	K	1142	CLA	O2D-CGD-O1D	-2.26	119.13	123.79
22	B	1775	BCR	C27-C26-C25	-2.26	119.91	122.78
19	J	1043	CLA	O2D-CGD-O1D	-2.26	119.13	123.79
20	A	7013	LMU	O5'-C1'-C2'	-2.25	105.65	110.28
19	A	1793	CLA	O2D-CGD-O1D	-2.25	119.14	123.79
21	3	1221	SUC	C1'-C2'-C3'	-2.25	106.89	114.49
19	A	1792	CLA	O2D-CGD-O1D	-2.25	119.15	123.79
19	A	1795	CLA	O2D-CGD-O1D	-2.25	119.15	123.79
19	A	1794	CLA	O2D-CGD-O1D	-2.24	119.16	123.79
22	A	1803	BCR	C4-C5-C6	-2.24	119.92	122.78
19	A	1801	CLA	O1D-CGD-CBD	-2.24	121.41	124.62
20	A	7036	LMU	C6'-C5'-C4'	-2.24	106.72	113.25
19	A	1797	CLA	O2D-CGD-O1D	-2.24	119.17	123.79
19	A	1796	CLA	O2D-CGD-O1D	-2.24	119.17	123.79
22	B	1778	BCR	C27-C26-C25	-2.24	119.93	122.78
21	B	8056	SUC	C2'-O1-C1	-2.24	111.64	117.53
19	F	1156	CLA	O2D-CGD-O1D	-2.23	119.17	123.79
19	1	1198	CLA	C11-C12-C13	-2.23	108.08	115.49
19	A	1791	CLA	O2D-CGD-O1D	-2.23	119.18	123.79
19	L	1166	CLA	CMD-C2D-C3D	-2.23	120.72	125.09
20	A	7023	LMU	O4'-C4B-C5B	-2.23	103.33	109.24
19	B	1735	CLA	O2D-CGD-O1D	-2.23	119.18	123.79
19	A	1777	CLA	CHC-C1C-C2C	-2.23	120.49	126.35
19	2	1212	CLA	O2D-CGD-O1D	-2.23	119.19	123.79
19	A	1760	CLA	C3B-C4B-NB	-2.23	106.33	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1774	BCR	C27-C26-C25	-2.22	119.95	122.78
20	A	7016	LMU	C4-C3-C2	-2.22	103.05	114.53
19	B	1752	CLA	C2A-C1A-CHA	-2.22	119.79	123.89
19	4	4007	CLA	CAA-CBA-CGA	-2.22	106.81	113.32
19	3	1219	CLA	O2D-CGD-O1D	-2.22	119.21	123.79
19	A	1772	CLA	O2A-CGA-O1A	-2.22	117.77	123.49
19	A	1786	CLA	O2A-CGA-O1A	-2.22	117.77	123.49
20	A	7042	LMU	C5-C4-C3	-2.22	103.08	114.53
19	4	1196	CLA	O2D-CGD-O1D	-2.22	119.21	123.79
19	1	1196	CLA	CHC-C1C-C2C	-2.22	120.52	126.35
19	A	1790	CLA	O2A-CGA-O1A	-2.21	117.78	123.49
22	A	1808	BCR	C4-C5-C6	-2.21	119.97	122.78
19	B	1760	CLA	CAA-CBA-CGA	-2.21	106.85	113.32
19	B	1738	CLA	C2A-C1A-CHA	-2.21	119.82	123.89
22	B	1777	BCR	C4-C5-C6	-2.21	119.97	122.78
19	A	1763	CLA	CBC-CAC-C3C	-2.21	105.66	112.39
19	1	1198	CLA	CBA-CAA-C2A	-2.21	107.51	113.73
20	A	7041	LMU	O1'-C1-C2	-2.20	101.11	109.88
19	A	1781	CLA	O2D-CGD-O1D	-2.20	119.24	123.79
19	A	1767	CLA	O2D-CGD-O1D	-2.20	119.24	123.79
22	B	1775	BCR	C4-C5-C6	-2.20	119.97	122.78
19	B	1787	CLA	CMA-C3A-C2A	-2.20	104.60	114.35
19	B	1756	CLA	O2D-CGD-O1D	-2.20	119.24	123.79
19	B	1741	CLA	CAC-C3C-C2C	-2.20	123.65	127.51
21	B	8059	SUC	C1'-C2'-C3'	-2.20	107.06	114.49
19	K	3009	CLA	C2A-C1A-CHA	-2.20	119.83	123.89
22	B	1781	BCR	C16-C15-C14	-2.20	118.52	123.39
20	A	7020	LMU	O2B-C2B-C3B	-2.20	105.38	110.34
19	B	1739	CLA	C11-C12-C13	-2.20	108.19	115.49
21	B	8054	SUC	O1-C2'-C1'	-2.20	102.64	109.69
20	A	7041	LMU	O5B-C1B-C2B	-2.20	105.77	110.28
19	A	1789	CLA	C5-C3-C2	-2.20	116.88	121.05
19	L	1505	CLA	C4-C3-C2	-2.20	119.19	123.50
19	B	1744	CLA	CAC-C3C-C2C	-2.20	123.66	127.51
22	A	1803	BCR	C11-C12-C13	-2.20	119.85	126.32
20	A	7020	LMU	C8-C7-C6	-2.19	103.20	114.53
20	A	7030	LMU	O2B-C2B-C3B	-2.19	105.40	110.34
19	A	1772	CLA	CBC-CAC-C3C	-2.19	105.70	112.39
21	H	1080	SUC	O1-C2'-C1'	-2.19	102.67	109.69
19	1	1191	CLA	CHC-C1C-C2C	-2.19	120.59	126.35
22	B	1774	BCR	C4-C5-C6	-2.19	119.99	122.78
22	B	1780	BCR	C11-C12-C13	-2.19	119.88	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1044	CLA	CMD-C2D-C3D	-2.19	120.81	125.09
22	A	1807	BCR	C27-C26-C25	-2.18	120.00	122.78
19	A	1786	CLA	CAA-C2A-C3A	-2.18	106.94	113.22
19	A	1785	CLA	C2A-C1A-CHA	-2.18	119.86	123.89
22	I	1032	BCR	C3-C2-C1	-2.18	106.75	114.83
19	J	1044	CLA	C6-C5-C3	-2.18	107.70	112.48
19	B	1766	CLA	CHC-C1C-C2C	-2.18	120.61	126.35
19	I	1031	CLA	O2D-CGD-O1D	-2.18	119.29	123.79
21	B	8052	SUC	O1-C2'-O2'	-2.18	103.59	110.52
22	A	1804	BCR	C11-C12-C13	-2.18	119.90	126.32
22	A	1805	BCR	C4-C5-C6	-2.18	120.00	122.78
22	B	1780	BCR	C4-C5-C6	-2.18	120.01	122.78
22	B	1779	BCR	C8-C9-C10	-2.18	115.48	118.98
19	B	1745	CLA	CMD-C2D-C3D	-2.18	120.83	125.09
19	B	1787	CLA	C6-C7-C8	-2.18	108.27	115.49
19	4	1197	CLA	CHC-C1C-C2C	-2.17	120.63	126.35
22	B	1777	BCR	C11-C12-C13	-2.17	119.92	126.32
22	A	1807	BCR	C20-C19-C18	-2.17	119.92	126.32
19	B	1787	CLA	O1D-CGD-CBD	-2.17	121.51	124.62
22	A	1808	BCR	C27-C26-C25	-2.17	120.02	122.78
19	A	1812	CLA	CMD-C2D-C3D	-2.17	120.84	125.09
19	B	1743	CLA	C5-C3-C2	-2.17	116.94	121.05
19	2	1224	CLA	O2D-CGD-O1D	-2.17	119.31	123.79
19	B	1748	CLA	O2D-CGD-O1D	-2.17	119.31	123.79
22	L	1170	BCR	C32-C1-C31	-2.17	101.42	108.37
22	B	1781	BCR	C10-C11-C12	-2.17	116.52	123.13
20	A	7020	LMU	O6B-C6B-C5B	-2.17	104.17	111.33
19	R	1055	CLA	O2A-CGA-O1A	-2.17	117.90	123.49
19	A	1763	CLA	CGD-CBD-CAD	-2.17	103.28	110.62
22	A	1803	BCR	C27-C26-C25	-2.16	120.02	122.78
19	A	1764	CLA	C2A-C1A-CHA	-2.16	119.90	123.89
22	A	1805	BCR	C20-C19-C18	-2.16	119.95	126.32
19	1	1192	CLA	CMD-C2D-C3D	-2.16	120.86	125.09
19	A	1813	CLA	O2A-CGA-O1A	-2.16	117.91	123.49
19	1	1189	CLA	C2A-C1A-CHA	-2.16	119.90	123.89
21	B	8052	SUC	C6'-C5'-C4'	-2.16	109.98	115.08
22	A	1804	BCR	C4-C5-C6	-2.16	120.03	122.78
19	B	1741	CLA	C5-C3-C2	-2.16	116.96	121.05
20	A	7037	LMU	C6-C5-C4	-2.16	103.39	114.53
22	B	1774	BCR	C11-C12-C13	-2.16	119.97	126.32
22	A	1808	BCR	C20-C19-C18	-2.16	119.97	126.32
22	A	1807	BCR	C4-C5-C6	-2.16	120.03	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1742	CLA	C2A-C1A-CHA	-2.16	119.91	123.89
22	B	1778	BCR	C11-C12-C13	-2.15	119.97	126.32
19	2	1213	CLA	C2A-C1A-CHA	-2.15	119.92	123.89
19	A	1769	CLA	O1D-CGD-CBD	-2.15	121.54	124.62
19	4	1207	CLA	CMD-C2D-C3D	-2.15	120.88	125.09
22	A	1807	BCR	C11-C12-C13	-2.15	119.98	126.32
22	A	1806	BCR	C27-C26-C25	-2.15	120.04	122.78
19	A	1783	CLA	CHC-C1C-C2C	-2.15	120.70	126.35
22	B	1774	BCR	C20-C19-C18	-2.15	120.00	126.32
19	B	1755	CLA	O2D-CGD-O1D	-2.15	119.36	123.79
20	A	7040	LMU	O5'-C5'-C4'	-2.15	105.21	109.75
19	B	1753	CLA	C7-C6-C5	-2.15	106.72	113.06
22	3	1220	BCR	C39-C30-C25	-2.15	106.94	110.30
20	A	7024	LMU	C1'-O5'-C5'	-2.14	109.58	113.75
22	A	1806	BCR	C4-C5-C6	-2.14	120.05	122.78
22	A	1804	BCR	C27-C26-C25	-2.14	120.05	122.78
19	1	1197	CLA	C6-C5-C3	-2.14	101.72	112.89
19	B	1772	CLA	CMD-C2D-C3D	-2.14	120.90	125.09
19	J	1045	CLA	CAA-C2A-C1A	-2.14	104.91	112.47
20	A	7021	LMU	O5'-C5'-C6'	-2.14	100.94	106.36
22	A	1808	BCR	C11-C12-C13	-2.14	120.02	126.32
22	A	1806	BCR	C11-C12-C13	-2.14	120.03	126.32
19	1	1190	CLA	CAA-C2A-C3A	-2.14	107.07	113.22
19	2	1218	CLA	C11-C10-C8	-2.14	108.41	115.49
22	B	1780	BCR	C20-C19-C18	-2.14	120.03	126.32
19	B	1739	CLA	C4-C3-C2	-2.13	119.31	123.50
19	1	1189	CLA	CHC-C1C-C2C	-2.13	120.75	126.35
20	A	7022	LMU	C6'-C5'-C4'	-2.13	107.05	113.25
22	A	1806	BCR	C20-C19-C18	-2.13	120.05	126.32
22	A	1804	BCR	C20-C19-C18	-2.13	120.06	126.32
19	F	1157	CLA	CHC-C1C-C2C	-2.13	120.76	126.35
22	A	1803	BCR	C20-C19-C18	-2.12	120.06	126.32
22	B	1775	BCR	C11-C12-C13	-2.12	120.06	126.32
22	B	1778	BCR	C20-C19-C18	-2.12	120.07	126.32
22	B	1777	BCR	C20-C19-C18	-2.12	120.07	126.32
19	2	1222	CLA	CAA-C2A-C3A	-2.12	107.11	113.22
20	A	7028	LMU	C1-O1'-C1'	-2.12	110.23	113.94
19	B	1737	CLA	C11-C12-C13	-2.12	108.46	115.49
22	B	1775	BCR	C20-C19-C18	-2.12	120.08	126.32
19	A	1779	CLA	C4-C3-C2	-2.11	119.35	123.50
20	A	7042	LMU	O3'-C3'-C2'	-2.11	105.58	110.34
19	1	1200	CLA	CMA-C3A-C2A	-2.11	105.02	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1155	CLA	CAA-C2A-C3A	-2.11	111.15	116.20
21	B	8056	SUC	O4'-C4'-C3'	-2.11	105.31	112.01
20	A	7016	LMU	C6B-C5B-C4B	-2.11	107.81	113.02
20	A	7042	LMU	C6B-C5B-C4B	-2.11	107.81	113.02
22	B	1778	BCR	C4-C5-C6	-2.11	120.10	122.78
22	L	1169	BCR	C24-C23-C22	-2.11	123.01	126.22
19	B	1785	CLA	O2D-CGD-O1D	-2.10	119.45	123.79
19	2	1220	CLA	O2A-CGA-O1A	-2.10	118.06	123.49
19	B	1742	CLA	O2A-CGA-O1A	-2.10	118.06	123.49
21	B	8062	SUC	C6'-C5'-C4'	-2.10	110.11	115.08
19	B	1770	CLA	C2A-C1A-CHA	-2.10	120.02	123.89
19	2	1218	CLA	C6-C7-C8	-2.10	108.52	115.49
19	B	1757	CLA	C2A-C1A-CHA	-2.10	120.02	123.89
19	B	1786	CLA	CHC-C1C-C2C	-2.10	120.83	126.35
22	A	1805	BCR	C11-C12-C13	-2.10	120.14	126.32
19	A	1817	CLA	CHD-C4C-C3C	-2.10	121.70	124.94
19	B	1749	CLA	CAA-C2A-C3A	-2.10	107.18	113.22
20	A	1810	LMU	C4B-C3B-C2B	-2.10	106.88	110.79
19	R	1054	CLA	CGD-CBD-CAD	-2.10	103.52	110.62
22	B	1780	BCR	C27-C26-C25	-2.09	120.11	122.78
19	A	1774	CLA	CAA-C2A-C1A	-2.09	105.10	112.47
22	L	1169	BCR	C23-C24-C25	-2.09	121.04	127.32
19	A	1766	CLA	C3B-C4B-NB	-2.09	106.51	109.21
19	A	1786	CLA	C2A-C1A-CHA	-2.08	120.05	123.89
20	A	7023	LMU	O5B-C5B-C4B	-2.08	105.77	109.68
22	B	1776	BCR	C8-C7-C6	-2.08	121.06	127.32
19	A	1811	CLA	CBC-CAC-C3C	-2.08	106.04	112.39
20	A	1809	LMU	C1-O1'-C1'	-2.08	110.31	113.94
22	B	1779	BCR	C20-C19-C18	-2.08	120.20	126.32
21	B	8054	SUC	O1-C2'-O2'	-2.08	103.92	110.52
19	4	1200	CLA	C2A-C1A-CHA	-2.07	120.07	123.89
19	B	1768	CLA	C2A-C1A-CHA	-2.07	120.07	123.89
20	A	7043	LMU	O3B-C3B-C4B	-2.07	105.68	110.34
19	B	1744	CLA	CAA-C2A-C3A	-2.07	107.27	113.22
19	4	1209	CLA	CHC-C1C-C2C	-2.07	120.92	126.35
20	A	7036	LMU	O5'-C1'-O1'	-2.07	105.08	110.05
19	H	1079	CLA	CAC-C3C-C2C	-2.06	123.89	127.51
22	I	1032	BCR	C31-C1-C6	-2.06	107.07	110.30
19	A	1769	CLA	CBC-CAC-C3C	-2.06	106.10	112.39
19	A	1813	CLA	C16-C15-C13	-2.06	108.66	115.49
19	A	1767	CLA	C4-C3-C2	-2.06	119.46	123.50
22	I	1032	BCR	C28-C27-C26	-2.06	110.60	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	1167	CLA	O1D-CGD-CBD	-2.05	121.68	124.62
19	A	1775	CLA	C2A-C1A-CHA	-2.05	120.11	123.89
22	B	1779	BCR	C15-C16-C17	-2.05	118.86	123.39
20	A	7016	LMU	O6'-C6'-C5'	-2.05	104.56	111.33
19	B	1738	CLA	CBA-CAA-C2A	-2.05	107.95	113.73
19	4	1200	CLA	O1D-CGD-CBD	-2.05	121.69	124.62
19	A	1800	CLA	CMD-C2D-C3D	-2.04	121.09	125.09
19	G	1099	CLA	CHC-C1C-C2C	-2.04	120.98	126.35
19	B	1758	CLA	C12-C11-C10	-2.04	102.85	112.99
19	A	1759	CLA	O2A-CGA-O1A	-2.04	118.22	123.49
20	R	1057	LMU	O5'-C1'-C2'	-2.04	106.09	110.28
20	A	7022	LMU	O2B-C2B-C3B	-2.04	105.75	110.34
19	1	1200	CLA	C5-C3-C2	-2.04	116.20	120.74
19	K	1146	CLA	C2A-C1A-CHA	-2.04	120.13	123.89
21	B	8061	SUC	O1'-C1'-C2'	-2.04	105.40	111.91
20	A	7038	LMU	C1'-C2'-C3'	-2.04	105.96	109.97
19	B	1771	CLA	C2A-C1A-CHA	-2.03	120.14	123.89
20	A	7036	LMU	O1B-C4'-C3'	-2.03	101.92	107.17
19	3	1212	CLA	CAA-C2A-C3A	-2.03	111.33	116.20
19	A	1813	CLA	C5-C3-C2	-2.03	117.20	121.05
21	B	8061	SUC	C6-C5-C4	-2.03	108.00	113.02
19	A	1762	CLA	O2A-CGA-O1A	-2.03	118.26	123.49
19	A	1768	CLA	C2A-C1A-CHA	-2.03	120.15	123.89
19	J	1045	CLA	CAA-C2A-C3A	-2.03	107.39	113.22
19	J	1045	CLA	CBA-CAA-C2A	-2.03	108.02	113.73
22	B	1777	BCR	C34-C9-C10	-2.03	119.91	122.90
19	A	1786	CLA	CAC-C3C-C2C	-2.02	123.96	127.51
20	A	1810	LMU	O3'-C3'-C2'	-2.02	105.78	110.34
22	B	1777	BCR	C37-C22-C21	-2.02	119.91	122.90
22	B	1774	BCR	C34-C9-C10	-2.02	119.92	122.90
19	B	1760	CLA	CAA-C2A-C3A	-2.02	107.40	113.22
22	B	1776	BCR	C36-C18-C17	-2.02	119.92	122.90
19	L	1166	CLA	CAA-CBA-CGA	-2.01	107.42	113.32
19	1	1200	CLA	C2A-C1A-CHA	-2.01	120.19	123.89
21	B	8060	SUC	O2-C2-C3	-2.01	105.82	110.34
19	B	1737	CLA	C2A-C1A-CHA	-2.01	120.19	123.89
22	B	1777	BCR	C36-C18-C17	-2.01	119.94	122.90
19	B	1738	CLA	CAC-C3C-C2C	-2.01	123.99	127.51
22	B	1781	BCR	C29-C30-C25	-2.00	107.19	110.36
19	B	1786	CLA	O1D-CGD-CBD	-2.00	121.75	124.62
19	A	1783	CLA	O2D-CGD-O1D	-2.00	119.66	123.79
19	B	1736	CLA	O1D-CGD-CBD	-2.00	121.75	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1215	CLA	CMB-C2B-C3B	2.00	129.00	125.09
19	A	1812	CLA	C4-C3-C5	2.00	118.47	115.41
20	A	7047	LMU	O5B-C5B-C6B	2.00	111.42	106.36
20	A	7020	LMU	O5B-C5B-C4B	2.00	113.44	109.68
19	2	1224	CLA	C2C-C1C-NC	2.00	111.73	110.24
19	2	1213	CLA	C3A-C2A-C1A	2.00	104.90	101.50
20	A	7039	LMU	O2B-C2B-C1B	2.00	114.42	110.02
19	B	1751	CLA	CGD-CBD-CAD	2.01	117.42	110.62
21	B	8053	SUC	O5-C5-C6	2.01	111.43	106.36
20	A	7043	LMU	O5'-C1'-C2'	2.01	114.39	110.28
21	B	8061	SUC	C2'-O1-C1	2.01	122.82	117.53
19	1	1198	CLA	CED-O2D-CGD	2.01	120.70	115.99
19	1	1193	CLA	CMC-C2C-C1C	2.01	128.13	125.02
19	B	1761	CLA	C4A-NA-C1A	2.01	108.96	106.36
19	A	1774	CLA	CHB-C4A-NA	2.01	127.30	124.51
19	B	1769	CLA	CHB-C4A-NA	2.01	127.30	124.51
20	A	1809	LMU	O1'-C1'-C2'	2.01	110.58	108.04
21	B	8051	SUC	O3-C3-C2	2.02	114.88	110.34
19	1	1188	CLA	C1-O2A-CGA	2.02	123.10	116.73
19	2	1213	CLA	CED-O2D-CGD	2.02	120.72	115.99
21	2	1226	SUC	O1-C2'-C1'	2.02	116.16	109.69
19	1	1187	CLA	CAA-C2A-C1A	2.02	119.60	112.47
20	A	7040	LMU	C1B-C2B-C3B	2.02	113.96	109.97
19	B	1742	CLA	O2A-CGA-CBA	2.02	118.06	111.90
23	B	1773	PQN	C15-C13-C12	2.02	124.89	121.05
20	A	7027	LMU	O6B-C6B-C5B	2.03	118.03	111.33
21	3	1221	SUC	C6-C5-C4	2.03	118.03	113.02
19	A	1776	CLA	O2A-CGA-CBA	2.03	118.10	111.90
22	L	1170	BCR	C38-C26-C27	2.04	117.29	113.43
19	B	1749	CLA	CMB-C2B-C3B	2.04	129.07	125.09
19	2	1222	CLA	C4A-NA-C1A	2.04	109.00	106.36
20	A	7047	LMU	C1B-C2B-C3B	2.04	114.00	109.97
20	A	7033	LMU	C1'-C2'-C3'	2.04	114.00	109.97
19	A	1771	CLA	CHB-C4A-NA	2.04	127.34	124.51
19	B	1737	CLA	CMB-C2B-C1B	2.04	131.75	128.36
19	A	1779	CLA	CGD-CBD-CAD	2.05	117.56	110.62
19	B	1746	CLA	C4A-NA-C1A	2.05	109.01	106.36
19	R	1055	CLA	C5-C3-C2	2.05	124.94	121.05
20	A	7024	LMU	C3'-C4'-C5'	2.05	115.48	110.84
19	4	1201	CLA	C4C-C3C-C2C	2.05	110.28	106.94
19	2	1219	CLA	C3B-C4B-NB	2.06	111.94	110.09
19	L	1166	CLA	CMB-C2B-C3B	2.06	129.11	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7030	LMU	C2'-C3'-C4'	2.06	114.12	109.60
20	A	7015	LMU	O4'-C4B-C5B	2.06	114.69	109.24
20	R	1057	LMU	O4'-C4B-C3B	2.06	114.97	110.34
20	A	7026	LMU	O2'-C2'-C1'	2.06	114.54	110.02
21	3	1221	SUC	C1-O5-C5	2.06	117.75	113.75
19	A	1817	CLA	C4A-NA-C1A	2.06	109.03	106.36
19	A	1771	CLA	CED-O2D-CGD	2.06	120.83	115.99
19	B	1767	CLA	CAC-C3C-C4C	2.07	127.83	124.83
19	B	1738	CLA	C4-C3-C5	2.07	118.57	115.41
19	4	1198	CLA	C1C-NC-C4C	2.07	108.78	106.27
19	4	1207	CLA	C4A-NA-C1A	2.07	109.04	106.36
19	1	1187	CLA	C2C-C1C-NC	2.08	111.79	110.24
19	3	3011	CLA	CED-O2D-CGD	2.08	120.87	115.99
19	3	1217	CLA	C2B-C3B-C4B	2.08	108.11	106.29
19	4	1198	CLA	CAC-C3C-C4C	2.08	127.85	124.83
19	B	1753	CLA	CHC-C1C-NC	2.08	127.59	123.67
19	B	1748	CLA	CED-O2D-CGD	2.08	120.87	115.99
19	4	1208	CLA	C3D-C4D-ND	2.08	111.98	110.13
20	A	7013	LMU	O2B-C2B-C1B	2.09	114.59	110.02
19	A	1801	CLA	CHB-C4A-NA	2.09	127.40	124.51
19	A	1769	CLA	CAC-C3C-C4C	2.09	127.86	124.83
20	B	1782	LMU	C1'-C2'-C3'	2.09	114.09	109.97
21	B	8056	SUC	O5-C5-C6	2.09	111.63	106.36
19	B	1762	CLA	CBA-CAA-C2A	2.09	119.63	113.73
19	A	1778	CLA	C4A-NA-C1A	2.09	109.06	106.36
19	A	1767	CLA	C4-C3-C5	2.09	118.60	115.41
19	1	1190	CLA	CHB-C4A-NA	2.09	127.41	124.51
19	B	1747	CLA	CHB-C4A-NA	2.10	127.41	124.51
21	B	8061	SUC	C2'-C3'-C4'	2.10	107.27	102.00
19	B	1771	CLA	CAC-C3C-C4C	2.10	127.88	124.83
19	A	1783	CLA	CMB-C2B-C3B	2.10	129.19	125.09
20	A	7025	LMU	C3'-C4'-C5'	2.10	115.59	110.84
19	1	1197	CLA	C3B-C4B-NB	2.10	111.92	109.21
19	L	1167	CLA	CMC-C2C-C1C	2.10	128.27	125.02
19	A	1816	CLA	CAC-C3C-C2C	2.11	131.20	127.51
19	L	1168	CLA	CHB-C4A-NA	2.11	127.43	124.51
19	A	1767	CLA	O2A-CGA-CBA	2.11	118.33	111.90
19	B	1751	CLA	O2A-CGA-CBA	2.11	121.15	112.36
19	4	1198	CLA	C1C-C2C-C3C	2.11	109.43	106.91
19	B	1753	CLA	O1D-CGD-CBD	2.11	127.65	124.62
19	L	1167	CLA	CMB-C2B-C3B	2.11	129.22	125.09
20	4	1210	LMU	C1B-C2B-C3B	2.11	114.14	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1217	CLA	O2A-CGA-CBA	2.11	118.34	111.90
19	1	1195	CLA	CHB-C4A-NA	2.12	127.44	124.51
19	A	1776	CLA	CMB-C2B-C3B	2.12	129.24	125.09
19	A	1772	CLA	CMB-C2B-C3B	2.12	129.24	125.09
20	A	7023	LMU	O3'-C3'-C4'	2.12	114.90	109.87
19	4	4007	CLA	C4A-NA-C1A	2.12	109.10	106.36
19	A	1770	CLA	CHB-C4A-NA	2.12	127.45	124.51
20	R	1057	LMU	O1B-C4'-C3'	2.12	112.65	107.17
19	B	1759	CLA	O2A-CGA-CBA	2.13	118.38	111.90
19	B	1750	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	B	1762	CLA	C3A-C2A-C1A	2.13	105.11	101.50
19	A	1769	CLA	CMB-C2B-C3B	2.13	129.25	125.09
19	A	1778	CLA	CED-O2D-CGD	2.13	120.98	115.99
19	A	1785	CLA	CHB-C4A-NA	2.13	127.46	124.51
19	B	1769	CLA	CED-O2D-CGD	2.13	120.99	115.99
19	2	1215	CLA	O2A-CGA-CBA	2.13	118.40	111.90
19	B	1771	CLA	C6-C5-C3	2.14	117.17	112.48
19	R	1055	CLA	CBA-CAA-C2A	2.14	119.77	113.73
19	2	1222	CLA	O2A-CGA-CBA	2.14	118.42	111.90
20	A	7021	LMU	O5B-C5B-C6B	2.14	111.77	106.36
19	4	1197	CLA	CBD-CHA-C1A	2.14	129.57	128.59
19	1	1198	CLA	CHB-C4A-NA	2.15	127.48	124.51
19	A	1777	CLA	CED-O2D-CGD	2.15	121.02	115.99
19	L	1505	CLA	CAC-C3C-C4C	2.15	127.95	124.83
19	K	1085	CLA	C5-C3-C4	2.15	119.92	114.64
19	B	1765	CLA	CED-O2D-CGD	2.15	121.03	115.99
19	B	1771	CLA	CED-O2D-CGD	2.15	121.04	115.99
19	2	1218	CLA	C2C-C1C-NC	2.15	111.85	110.24
19	2	1216	CLA	C2A-C1A-NA	2.15	115.39	110.36
19	B	1771	CLA	C2C-C1C-NC	2.15	111.85	110.24
19	B	1771	CLA	C4A-NA-C1A	2.16	109.14	106.36
19	B	1759	CLA	C4A-NA-C1A	2.16	109.15	106.36
20	R	1057	LMU	O5B-C5B-C4B	2.16	113.74	109.68
19	B	1736	CLA	CMB-C2B-C3B	2.17	129.33	125.09
19	A	1762	CLA	CED-O2D-CGD	2.17	121.08	115.99
20	A	7041	LMU	C1'-O5'-C5'	2.17	117.96	113.75
21	B	8062	SUC	O1-C2'-C3'	2.17	115.62	108.04
19	A	1765	CLA	C3B-C4B-NB	2.17	112.02	109.21
19	A	1812	CLA	CMB-C2B-C3B	2.17	129.34	125.09
19	B	1770	CLA	CBA-CAA-C2A	2.18	119.87	113.73
19	4	1197	CLA	CAC-C3C-C4C	2.18	128.39	125.02
19	F	1157	CLA	CMC-C2C-C1C	2.18	128.39	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7042	LMU	O4'-C4B-C5B	2.18	115.02	109.24
19	1	1192	CLA	CMB-C2B-C3B	2.18	129.35	125.09
19	B	1752	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	A	1786	CLA	CGD-CBD-CAD	2.18	118.02	110.62
19	1	1190	CLA	OBD-CAD-CBD	2.19	129.24	125.94
20	A	7038	LMU	O1'-C1'-C2'	2.19	110.80	108.04
19	B	1751	CLA	CMB-C2B-C3B	2.19	129.37	125.09
19	B	1747	CLA	C4-C3-C5	2.19	118.75	115.41
19	B	1765	CLA	CHB-C4A-NA	2.19	127.55	124.51
20	L	1171	LMU	O1B-C1B-O5B	2.19	116.23	110.68
19	B	1785	CLA	CMB-C2B-C3B	2.20	129.38	125.09
22	B	1776	BCR	C35-C13-C12	2.20	121.75	118.10
19	A	1760	CLA	CHB-C4A-NA	2.20	127.55	124.51
20	A	7043	LMU	O3'-C3'-C2'	2.20	115.28	110.34
22	B	1781	BCR	C15-C14-C13	2.20	130.37	127.20
19	A	1769	CLA	C4-C3-C5	2.20	118.77	115.41
19	2	1220	CLA	CED-O2D-CGD	2.20	121.15	115.99
19	A	1800	CLA	O2A-CGA-CBA	2.20	118.60	111.90
19	B	1757	CLA	C4-C3-C5	2.21	118.78	115.41
19	2	1217	CLA	CHB-C4A-NA	2.21	127.56	124.51
19	1	1187	CLA	CMA-C3A-C2A	2.21	124.12	114.35
19	4	1204	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	4	1200	CLA	CAC-C3C-C4C	2.21	128.04	124.83
19	B	1739	CLA	CAC-C3C-C4C	2.21	128.04	124.83
19	B	1785	CLA	CAC-C3C-C4C	2.21	128.04	124.83
19	1	1188	CLA	C4A-NA-C1A	2.22	109.22	106.36
19	A	1800	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	A	1759	CLA	CHB-C4A-NA	2.22	127.58	124.51
20	A	7026	LMU	O1B-C1B-O5B	2.22	116.31	110.68
20	A	7040	LMU	O4'-C4B-C3B	2.22	115.35	110.34
19	4	1205	CLA	C2B-C3B-C4B	2.23	108.23	106.29
19	A	1760	CLA	C6-C5-C3	2.23	117.37	112.48
20	A	7017	LMU	C3B-C4B-C5B	2.23	114.08	110.20
20	A	7022	LMU	C1B-O1B-C4'	2.23	123.83	118.01
19	B	1769	CLA	O2A-CGA-CBA	2.23	118.69	111.90
19	A	1766	CLA	CED-O2D-CGD	2.23	121.22	115.99
19	1	1199	CLA	C2B-C3B-C4B	2.23	108.24	106.29
21	B	8061	SUC	O1-C2'-C3'	2.23	115.83	108.04
19	B	1746	CLA	CAC-C3C-C4C	2.24	128.08	124.83
20	A	7027	LMU	C3B-C4B-C5B	2.24	114.10	110.20
19	B	1741	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	A	1799	CLA	O2A-CGA-CBA	2.24	118.73	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1787	CLA	CED-O2D-CGD	2.25	121.26	115.99
20	A	7038	LMU	O5'-C1'-C2'	2.25	114.89	110.28
22	B	1776	BCR	C2-C1-C6	2.25	113.92	110.36
19	A	1801	CLA	CED-O2D-CGD	2.25	121.27	115.99
20	A	7041	LMU	O4'-C4B-C3B	2.25	115.41	110.34
19	B	1762	CLA	C9-C8-C10	2.25	119.73	111.08
19	B	1772	CLA	CAC-C3C-C4C	2.25	128.50	125.02
20	A	7016	LMU	C4B-C3B-C2B	2.25	115.00	110.79
19	B	1739	CLA	C4A-NA-C1A	2.25	109.27	106.36
19	I	1031	CLA	C4-C3-C5	2.26	118.86	115.41
20	A	7015	LMU	C6B-C5B-C4B	2.26	118.59	113.02
20	A	7031	LMU	C1-O1'-C1'	2.26	117.90	113.94
19	A	1787	CLA	CHB-C4A-NA	2.26	127.64	124.51
19	K	1146	CLA	CED-O2D-CGD	2.26	121.30	115.99
19	2	1222	CLA	C5-C3-C4	2.27	120.21	114.64
19	A	1799	CLA	C5-C3-C4	2.27	120.21	114.64
19	B	1763	CLA	C3A-C2A-C1A	2.27	105.34	101.50
21	B	8055	SUC	C1-O5-C5	2.27	118.15	113.75
20	A	7015	LMU	O1B-C1B-C2B	2.27	113.63	108.10
19	B	1759	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	A	1764	CLA	O2A-CGA-CBA	2.27	118.83	111.90
19	A	1785	CLA	CAA-CBA-CGA	2.27	119.97	113.32
22	3	1220	BCR	C35-C13-C12	2.28	121.89	118.10
19	B	1759	CLA	CMB-C2B-C1B	2.28	132.13	128.36
19	2	1224	CLA	CED-O2D-CGD	2.28	121.33	115.99
19	L	1167	CLA	CAC-C3C-C4C	2.28	128.14	124.83
20	A	7031	LMU	O5'-C5'-C6'	2.28	112.12	106.36
20	A	7041	LMU	O5'-C5'-C4'	2.29	114.58	109.75
19	B	1746	CLA	CED-O2D-CGD	2.29	121.35	115.99
19	B	1786	CLA	O2A-CGA-CBA	2.29	118.87	111.90
19	A	1785	CLA	CMC-C2C-C1C	2.29	128.56	125.02
19	B	1750	CLA	CMC-C2C-C1C	2.29	128.56	125.02
19	2	1224	CLA	CMB-C2B-C3B	2.29	129.57	125.09
19	B	1766	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	A	1772	CLA	O2A-CGA-CBA	2.29	118.88	111.90
21	H	1080	SUC	O5-C5-C6	2.29	112.15	106.36
20	B	1782	LMU	O5'-C5'-C4'	2.29	114.59	109.75
19	L	1168	CLA	CMC-C2C-C1C	2.29	128.57	125.02
19	A	1786	CLA	CBA-CAA-C2A	2.30	120.21	113.73
19	A	1816	CLA	CHB-C4A-NA	2.30	127.69	124.51
20	A	7026	LMU	O5'-C5'-C4'	2.30	114.60	109.75
21	B	8055	SUC	O5-C5-C4	2.30	114.00	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1225	LMU	O5'-C5'-C6'	2.30	112.17	106.36
19	A	1783	CLA	C4-C3-C5	2.30	118.92	115.41
21	B	8060	SUC	O2'-C5'-C6'	2.30	115.54	108.57
19	1	1198	CLA	O2A-CGA-CBA	2.31	118.92	111.90
21	B	8056	SUC	C6'-C5'-C4'	2.31	120.54	115.08
20	A	7043	LMU	O4'-C4B-C5B	2.31	115.35	109.24
21	B	8061	SUC	O5-C1-O1	2.31	117.71	109.96
19	A	1812	CLA	CED-O2D-CGD	2.31	121.40	115.99
19	2	1224	CLA	CAC-C3C-C4C	2.31	128.18	124.83
20	A	7028	LMU	O1B-C4'-C5'	2.31	115.39	109.32
20	A	7024	LMU	C1B-O5B-C5B	2.31	118.23	113.75
22	B	1779	BCR	C35-C13-C12	2.31	121.94	118.10
19	2	1215	CLA	CED-O2D-CGD	2.31	121.41	115.99
19	A	1774	CLA	CED-O2D-CGD	2.31	121.42	115.99
20	A	7022	LMU	O5B-C5B-C4B	2.31	114.03	109.68
19	A	1767	CLA	C3A-C2A-C1A	2.31	105.42	101.50
20	A	7017	LMU	O1B-C1B-C2B	2.32	113.75	108.10
19	4	1209	CLA	CMB-C2B-C3B	2.32	129.63	125.09
19	4	1201	CLA	C5-C3-C2	2.33	125.46	121.05
19	A	1780	CLA	C14-C13-C12	2.33	120.02	111.08
19	B	1738	CLA	C4A-NA-C1A	2.33	109.37	106.36
19	1	1200	CLA	CED-O2D-CGD	2.33	121.45	115.99
22	L	1170	BCR	C23-C22-C21	2.33	122.74	118.98
20	A	7017	LMU	O5'-C5'-C4'	2.33	114.67	109.75
19	H	1079	CLA	C4-C3-C5	2.33	118.97	115.41
19	B	1766	CLA	CED-O2D-CGD	2.34	121.47	115.99
23	A	1802	PQN	O1-C1-C2	2.34	123.19	120.27
19	4	1206	CLA	C2B-C3B-C4B	2.34	108.33	106.29
19	4	1202	CLA	C2B-C3B-C4B	2.34	108.34	106.29
19	2	1213	CLA	CAC-C3C-C4C	2.34	128.23	124.83
20	A	7027	LMU	O5'-C1'-C2'	2.35	115.10	110.28
19	1	1195	CLA	CMB-C2B-C1B	2.35	132.25	128.36
20	A	7023	LMU	C1'-C2'-C3'	2.35	114.61	109.97
19	A	1816	CLA	CMB-C2B-C3B	2.36	129.69	125.09
21	B	8062	SUC	O1-C1-C2	2.36	116.22	108.36
19	A	1773	CLA	C4-C3-C5	2.36	119.01	115.41
19	A	1761	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	2	1221	CLA	C3D-C2D-C1D	2.36	108.38	106.30
19	2	1212	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	B	1755	CLA	CHB-C4A-NA	2.37	127.79	124.51
21	2	1226	SUC	O3-C3-C4	2.37	115.67	110.34
20	A	7027	LMU	C1'-O5'-C5'	2.37	118.34	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1794	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	1	1189	CLA	CAC-C3C-C4C	2.37	128.27	124.83
20	A	1810	LMU	C1'-C2'-C3'	2.38	114.66	109.97
20	A	7025	LMU	O2B-C2B-C1B	2.38	115.23	110.02
22	B	1776	BCR	C1-C6-C7	2.38	122.47	115.82
20	A	7019	LMU	C3'-C4'-C5'	2.38	116.22	110.84
19	3	3008	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	A	1809	LMU	C3B-C4B-C5B	2.38	114.35	110.20
19	3	3007	CLA	CED-O2D-CGD	2.38	121.58	115.99
19	4	4014	CLA	CHB-C4A-NA	2.38	127.81	124.51
20	A	7026	LMU	O5B-C1B-C2B	2.39	115.17	110.28
19	A	1800	CLA	CMB-C2B-C1B	2.39	132.31	128.36
22	B	1776	BCR	C33-C5-C4	2.39	117.95	113.43
20	A	7013	LMU	O1'-C1'-C2'	2.39	111.06	108.04
19	J	1045	CLA	O2A-CGA-CBA	2.39	119.19	111.90
19	B	1742	CLA	CAC-C3C-C4C	2.39	128.30	124.83
19	A	1764	CLA	CAA-CBA-CGA	2.39	120.33	113.32
19	A	1759	CLA	C5-C3-C4	2.40	120.53	114.64
21	B	8052	SUC	O2'-C5'-C6'	2.40	115.82	108.57
19	B	1744	CLA	CAC-C3C-C4C	2.40	128.31	124.83
19	A	1816	CLA	CHC-C1C-NC	2.40	128.18	123.67
20	A	7025	LMU	O4'-C4B-C3B	2.40	115.74	110.34
19	H	1079	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	B	1781	BCR	C20-C19-C18	2.40	133.40	126.32
22	L	1170	BCR	C2-C1-C6	2.40	114.17	110.36
19	B	1760	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	A	7028	LMU	O3'-C3'-C2'	2.41	115.76	110.34
19	A	1771	CLA	CMB-C2B-C3B	2.41	129.80	125.09
19	A	1791	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	F	1156	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	2	1223	CLA	C4A-NA-C1A	2.41	109.47	106.36
19	A	1770	CLA	CMB-C2B-C1B	2.41	132.35	128.36
19	A	1797	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	B	1749	CLA	CAA-C2A-C1A	2.41	120.99	112.47
19	A	1786	CLA	CHB-C4A-NA	2.41	127.85	124.51
20	A	7022	LMU	O5'-C5'-C4'	2.42	114.85	109.75
19	B	1756	CLA	CHB-C4A-NA	2.42	127.85	124.51
19	B	1771	CLA	CMB-C2B-C1B	2.42	132.37	128.36
19	L	1168	CLA	CAA-C2A-C1A	2.42	121.00	112.47
19	3	1212	CLA	CMB-C2B-C3B	2.42	130.09	125.14
19	A	1792	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	2	1220	CLA	C4-C3-C5	2.42	119.11	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1055	CLA	CED-O2D-CGD	2.42	121.67	115.99
21	B	8062	SUC	O1-C2'-O2'	2.43	118.22	110.52
19	A	1776	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	A	1795	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	B	8054	SUC	O5-C1-C2	2.43	115.26	110.28
20	B	1782	LMU	C2'-C3'-C4'	2.43	114.94	109.60
19	J	1043	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	3	1219	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	B	1740	CLA	O2A-CGA-CBA	2.44	119.32	111.90
20	A	1810	LMU	C1B-C2B-C3B	2.44	114.77	109.97
19	2	1220	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	4	1196	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	B	1757	CLA	CMB-C2B-C3B	2.44	129.86	125.09
20	A	7022	LMU	O4'-C4B-C5B	2.44	115.71	109.24
19	A	1781	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	B	1735	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	B	1743	CLA	O2A-CGA-CBA	2.45	119.36	111.90
19	4	1205	CLA	C3D-C2D-C1D	2.45	108.46	106.30
19	A	1815	CLA	C3B-C4B-NB	2.45	112.38	109.21
19	L	1505	CLA	C6-C5-C3	2.45	117.86	112.48
19	A	1761	CLA	CAC-C3C-C4C	2.45	128.39	124.83
19	B	1761	CLA	CMC-C2C-C1C	2.45	128.82	125.02
19	A	1793	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	A	1782	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	4	1204	CLA	O2A-CGA-CBA	2.46	119.38	111.90
19	B	1749	CLA	O2A-CGA-CBA	2.46	119.38	111.90
19	A	1770	CLA	CED-O2D-CGD	2.46	121.75	115.99
19	A	1796	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	A	1784	CLA	CGD-CBD-CAD	2.46	118.95	110.62
19	J	1044	CLA	CED-O2D-CGD	2.46	121.76	115.99
20	A	7042	LMU	O5B-C5B-C6B	2.46	112.57	106.36
19	A	1811	CLA	CHC-C1C-NC	2.46	128.30	123.67
19	B	1745	CLA	CED-O2D-CGD	2.46	121.76	115.99
19	A	1787	CLA	CBA-CAA-C2A	2.46	120.68	113.73
22	B	1781	BCR	C8-C9-C10	2.46	122.95	118.98
21	B	8061	SUC	O2'-C2'-C1'	2.47	114.69	107.98
19	4	1201	CLA	C3B-C4B-NB	2.47	112.40	109.21
22	B	1779	BCR	C12-C13-C14	2.47	122.96	118.98
19	G	1099	CLA	CMB-C2B-C3B	2.47	129.92	125.09
22	3	1220	BCR	C33-C5-C4	2.47	118.12	113.43
19	K	1142	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	A	1813	CLA	O2A-CGA-CBA	2.48	119.45	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1782	LMU	O1B-C4'-C3'	2.48	113.56	107.17
19	4	1208	CLA	C3D-C2D-C1D	2.48	108.48	106.30
19	K	1146	CLA	C5-C3-C4	2.48	120.74	114.64
19	4	1200	CLA	CED-O2D-CGD	2.48	121.81	115.99
19	1	1194	CLA	C2B-C3B-C4B	2.49	108.46	106.29
20	A	7013	LMU	O1B-C4'-C5'	2.49	115.86	109.32
19	K	1085	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	A	1784	CLA	C4-C3-C5	2.49	119.21	115.41
19	3	1216	CLA	C3D-C4D-ND	2.49	112.34	110.13
19	A	1784	CLA	O2A-CGA-CBA	2.49	119.49	111.90
19	4	4007	CLA	CED-O2D-CGD	2.49	121.84	115.99
19	B	1767	CLA	O2A-CGA-CBA	2.49	119.50	111.90
19	A	1764	CLA	CMB-C2B-C3B	2.49	129.97	125.09
20	A	7025	LMU	O1'-C1'-C2'	2.49	111.19	108.04
20	A	7039	LMU	C1'-O5'-C5'	2.50	118.59	113.75
19	4	1201	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	1	1200	CLA	CMB-C2B-C3B	2.50	129.97	125.09
19	4	1201	CLA	C1C-NC-C4C	2.50	109.30	106.27
20	A	7022	LMU	C1'-C2'-C3'	2.50	114.90	109.97
19	A	1774	CLA	CMB-C2B-C3B	2.50	129.99	125.09
19	K	3009	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	A	7034	LMU	C1B-C2B-C3B	2.51	114.91	109.97
19	A	1815	CLA	CGD-CBD-CAD	2.51	119.13	110.62
19	3	3011	CLA	CAC-C3C-C4C	2.51	128.47	124.83
19	3	3008	CLA	CAA-C2A-C3A	2.51	120.43	113.22
19	A	1778	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	B	1748	CLA	CAC-C3C-C4C	2.52	128.48	124.83
19	1	1189	CLA	CHC-C1C-NC	2.52	128.41	123.67
19	3	1212	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	B	1766	CLA	O2A-CGA-CBA	2.52	119.58	111.90
20	A	7028	LMU	O4'-C4B-C3B	2.52	116.02	110.34
19	A	1775	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	A	7027	LMU	O5'-C5'-C6'	2.53	112.74	106.36
21	B	8054	SUC	C3-C4-C5	2.53	114.60	110.20
20	A	7033	LMU	C4B-C3B-C2B	2.53	115.51	110.79
19	A	1763	CLA	CAC-C3C-C4C	2.53	128.50	124.83
19	G	1099	CLA	O2A-CGA-CBA	2.53	119.61	111.90
19	B	1770	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	A	7035	LMU	O5'-C5'-C6'	2.53	112.75	106.36
21	2	1226	SUC	O1'-C1'-C2'	2.53	120.01	111.91
19	B	1786	CLA	CAA-C2A-C1A	2.53	121.40	112.47
19	L	1168	CLA	O2A-CGA-CBA	2.54	119.63	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1785	CLA	CGD-CBD-CAD	2.54	119.22	110.62
22	I	1032	BCR	C23-C22-C21	2.54	123.08	118.98
22	L	1170	BCR	C11-C10-C9	2.54	130.87	127.20
19	B	1752	CLA	CAC-C3C-C4C	2.54	128.52	124.83
19	A	1773	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	B	1742	CLA	C6-C5-C3	2.55	118.08	112.48
20	R	1057	LMU	O5B-C5B-C6B	2.55	112.80	106.36
22	L	1169	BCR	C30-C25-C24	2.55	122.97	115.82
22	B	1779	BCR	C7-C8-C9	2.55	130.11	126.22
19	1	1189	CLA	CHB-C4A-NA	2.56	128.05	124.51
19	H	1079	CLA	CAC-C3C-C4C	2.56	128.54	124.83
22	B	1776	BCR	C32-C1-C6	2.56	114.32	110.30
19	K	3009	CLA	CMC-C2C-C1C	2.56	128.98	125.02
19	B	1743	CLA	C4-C3-C5	2.56	119.32	115.41
19	B	1771	CLA	O2D-CGD-CBD	2.56	114.81	111.30
19	B	1747	CLA	CED-O2D-CGD	2.57	122.01	115.99
19	4	4007	CLA	CMB-C2B-C3B	2.57	130.11	125.09
19	3	3002	CLA	C3D-C2D-C1D	2.57	108.56	106.30
19	B	1754	CLA	CMC-C2C-C1C	2.57	129.00	125.02
19	B	1744	CLA	CED-O2D-CGD	2.58	122.04	115.99
19	A	1790	CLA	O2A-CGA-CBA	2.58	119.76	111.90
19	B	1740	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	H	1080	SUC	O2'-C2'-C1'	2.58	115.01	107.98
19	B	1738	CLA	CAC-C3C-C4C	2.59	128.58	124.83
19	L	1168	CLA	CHC-C1C-NC	2.59	128.54	123.67
19	A	1817	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	A	1786	CLA	CAC-C3C-C4C	2.59	128.59	124.83
19	2	1213	CLA	CHB-C4A-NA	2.59	128.09	124.51
21	2	1226	SUC	O5-C1-C2	2.59	115.59	110.28
19	B	1744	CLA	O2A-CGA-CBA	2.59	119.79	111.90
19	A	1778	CLA	CAA-C2A-C3A	2.59	120.64	114.13
19	4	1199	CLA	O2A-CGA-CBA	2.59	119.80	111.90
19	A	1817	CLA	CAA-C2A-C1A	2.59	121.61	112.47
19	3	3014	CLA	C2B-C3B-C4B	2.59	108.55	106.29
19	A	1813	CLA	CGD-CBD-CAD	2.59	119.41	110.62
19	R	1055	CLA	CAA-CBA-CGA	2.59	120.91	113.32
20	A	7035	LMU	O1B-C4'-C5'	2.59	116.14	109.32
22	B	1781	BCR	C40-C30-C25	2.60	114.38	110.30
19	A	1759	CLA	O2A-CGA-CBA	2.60	119.82	111.90
19	A	1761	CLA	C4-C3-C5	2.60	119.38	115.41
21	B	8054	SUC	O2-C2-C1	2.60	115.73	110.02
19	J	1044	CLA	CMB-C2B-C3B	2.60	130.18	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1200	CLA	CAC-C3C-C4C	2.61	128.61	124.83
19	A	1772	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	A	1801	CLA	CHC-C1C-NC	2.61	128.59	123.67
19	2	1218	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	A	1811	CLA	CMB-C2B-C3B	2.62	130.21	125.09
19	B	1754	CLA	C2C-C1C-NC	2.62	112.19	110.24
19	B	1737	CLA	C4-C3-C5	2.62	119.41	115.41
19	3	1214	CLA	C2B-C3B-C4B	2.62	108.58	106.29
20	A	7043	LMU	O1B-C1B-C2B	2.62	114.49	108.10
19	R	1055	CLA	CMB-C2B-C1B	2.63	132.71	128.36
19	3	3008	CLA	CED-O2D-CGD	2.63	122.15	115.99
20	A	7027	LMU	C3'-C4'-C5'	2.63	116.78	110.84
19	3	3007	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	1	1193	CLA	O2A-CGA-CBA	2.63	119.92	111.90
19	B	1738	CLA	CMB-C2B-C1B	2.63	132.72	128.36
22	B	1779	BCR	C39-C30-C25	2.64	114.44	110.30
19	G	1099	CLA	CED-O2D-CGD	2.64	122.19	115.99
20	A	7033	LMU	O5'-C5'-C6'	2.65	113.04	106.36
19	B	1745	CLA	CHB-C4A-NA	2.65	128.17	124.51
19	B	1747	CLA	CMB-C2B-C3B	2.65	130.27	125.09
20	A	7025	LMU	O5'-C5'-C4'	2.65	115.35	109.75
19	A	1788	CLA	C4-C3-C5	2.65	119.46	115.41
19	4	1197	CLA	CHB-C4A-NA	2.65	128.18	124.51
19	1	1197	CLA	C4A-NA-C1A	2.66	109.79	106.36
20	A	7038	LMU	O1B-C1B-C2B	2.66	114.57	108.10
19	L	1167	CLA	CED-O2D-CGD	2.66	122.22	115.99
19	A	1782	CLA	O2A-CGA-CBA	2.67	120.04	111.90
19	B	1786	CLA	CMC-C2C-C1C	2.67	129.16	125.02
19	B	1772	CLA	CMC-C2C-C1C	2.68	129.16	125.02
19	B	1749	CLA	CHC-C1C-NC	2.68	128.71	123.67
19	K	3009	CLA	CHC-C1C-NC	2.68	128.71	123.67
20	A	7017	LMU	O2B-C2B-C3B	2.68	116.37	110.34
19	4	1199	CLA	C4-C3-C5	2.68	119.50	115.41
19	4	4014	CLA	O2A-CGA-CBA	2.68	120.08	111.90
19	F	1157	CLA	C2C-C1C-NC	2.69	112.24	110.24
19	A	1800	CLA	CMC-C2C-C1C	2.69	129.18	125.02
19	1	1193	CLA	CMB-C2B-C3B	2.69	130.35	125.09
19	3	1214	CLA	C3D-C4D-ND	2.69	112.52	110.13
19	B	1761	CLA	O2A-CGA-CBA	2.69	120.11	111.90
19	B	1758	CLA	C4A-NA-C1A	2.69	109.84	106.36
20	A	7043	LMU	C1B-O5B-C5B	2.70	118.98	113.75
19	A	1761	CLA	CED-O2D-CGD	2.70	122.31	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7043	LMU	C1'-O5'-C5'	2.70	118.98	113.75
19	A	1780	CLA	CAC-C3C-C4C	2.70	128.75	124.83
19	B	1772	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	2	1215	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	3	1219	CLA	O2A-CGA-CBA	2.70	120.13	111.90
20	L	1171	LMU	O5B-C5B-C4B	2.70	114.75	109.68
19	A	1796	CLA	O2A-CGA-CBA	2.70	120.14	111.90
19	B	1761	CLA	CED-O2D-CGD	2.70	122.33	115.99
20	A	7023	LMU	O5B-C5B-C6B	2.70	113.19	106.36
19	A	1759	CLA	CMB-C2B-C3B	2.70	130.38	125.09
19	4	1204	CLA	CED-O2D-CGD	2.71	122.34	115.99
19	J	1045	CLA	CED-O2D-CGD	2.71	122.34	115.99
19	A	1781	CLA	O2A-CGA-CBA	2.71	120.15	111.90
19	A	1785	CLA	CED-O2D-CGD	2.71	122.34	115.99
19	A	1797	CLA	O2A-CGA-CBA	2.71	120.16	111.90
22	B	1779	BCR	C24-C25-C26	2.71	127.58	121.37
19	A	1792	CLA	O2A-CGA-CBA	2.71	120.17	111.90
19	A	1793	CLA	O2A-CGA-CBA	2.71	120.17	111.90
21	2	1226	SUC	O3-C3-C2	2.71	116.45	110.34
19	J	1043	CLA	O2A-CGA-CBA	2.71	120.17	111.90
19	A	1794	CLA	O2A-CGA-CBA	2.71	120.17	111.90
19	B	1735	CLA	O2A-CGA-CBA	2.71	120.17	111.90
19	I	1031	CLA	CHB-C4A-NA	2.72	128.27	124.51
20	A	7026	LMU	O3'-C3'-C2'	2.72	116.46	110.34
19	A	1795	CLA	O2A-CGA-CBA	2.72	120.18	111.90
22	B	1781	BCR	C15-C16-C17	2.72	129.40	123.39
20	A	7043	LMU	O5'-C5'-C6'	2.72	113.23	106.36
19	2	1212	CLA	O2A-CGA-CBA	2.72	120.19	111.90
20	B	1782	LMU	O5B-C5B-C4B	2.72	114.79	109.68
19	1	1197	CLA	CHB-C4A-NA	2.72	128.28	124.51
19	A	1789	CLA	CHB-C4A-NA	2.72	128.28	124.51
19	B	1756	CLA	O2A-CGA-CBA	2.72	120.20	111.90
19	A	1799	CLA	CHB-C4A-NA	2.72	128.28	124.51
19	4	1196	CLA	O2A-CGA-CBA	2.73	120.21	111.90
20	A	7021	LMU	O1B-C1B-C2B	2.73	114.74	108.10
19	2	1218	CLA	O2A-CGA-CBA	2.73	120.22	111.90
24	B	1783	LMG	O8-C28-C29	2.73	120.22	111.90
19	K	1085	CLA	O2A-CGA-CBA	2.73	120.22	111.90
19	4	1205	CLA	C3D-C4D-ND	2.73	112.56	110.13
20	A	7013	LMU	O5'-C5'-C6'	2.74	113.28	106.36
19	B	1755	CLA	O2A-CGA-CBA	2.74	120.26	111.90
20	A	7033	LMU	C6B-C5B-C4B	2.74	119.78	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1189	CLA	O2A-CGA-CBA	2.74	120.26	111.90
19	B	1741	CLA	CAC-C3C-C4C	2.75	128.82	124.83
19	A	1780	CLA	CMB-C2B-C3B	2.75	130.46	125.09
19	B	1747	CLA	O2A-CGA-CBA	2.75	120.27	111.90
19	A	1768	CLA	O2A-CGA-CBA	2.75	120.28	111.90
19	A	1787	CLA	O2A-CGA-CBA	2.75	120.28	111.90
19	B	1745	CLA	CMB-C2B-C3B	2.75	130.48	125.09
19	3	1215	CLA	C3D-C4D-ND	2.76	112.58	110.13
19	A	1788	CLA	CHB-C4A-NA	2.76	128.33	124.51
20	K	1086	LMU	O3B-C3B-C2B	2.76	116.55	110.34
21	B	8056	SUC	O1-C2'-C3'	2.76	117.66	108.04
19	B	1737	CLA	O2A-CGA-CBA	2.76	120.32	111.90
19	2	1224	CLA	C4-C3-C5	2.76	119.63	115.41
19	A	1776	CLA	CED-O2D-CGD	2.77	122.48	115.99
19	A	1788	CLA	CMB-C2B-C3B	2.77	130.50	125.09
19	B	1763	CLA	CMB-C2B-C3B	2.77	130.50	125.09
20	A	7038	LMU	O3'-C3'-C2'	2.77	116.57	110.34
19	B	1743	CLA	CMB-C2B-C3B	2.77	130.51	125.09
19	4	1204	CLA	CHC-C1C-NC	2.77	128.89	123.67
19	1	1188	CLA	C3A-C2A-C1A	2.77	106.20	101.50
19	A	1811	CLA	O2A-CGA-CBA	2.78	120.36	111.90
19	L	1167	CLA	O2A-CGA-CBA	2.78	120.36	111.90
22	B	1776	BCR	C36-C18-C19	2.78	122.72	118.10
19	A	1789	CLA	C2C-C1C-NC	2.78	112.32	110.24
19	3	3015	CLA	C3D-C4D-ND	2.79	112.60	110.13
20	A	7032	LMU	C3'-C4'-C5'	2.79	117.15	110.84
19	H	1079	CLA	CMC-C2C-C1C	2.79	129.34	125.02
19	A	1798	CLA	CHB-C4A-NA	2.79	128.38	124.51
19	3	1213	CLA	C3D-C2D-C1D	2.79	108.76	106.30
19	B	1744	CLA	CMC-C2C-C1C	2.79	129.34	125.02
19	A	1771	CLA	CGD-CBD-CAD	2.79	120.09	110.62
19	3	1218	CLA	CAC-C3C-C2C	2.80	132.41	127.51
19	3	1215	CLA	C2B-C3B-C4B	2.80	108.73	106.29
21	B	8059	SUC	O4-C4-C3	2.80	116.64	110.34
20	A	7017	LMU	O5'-C5'-C6'	2.80	113.44	106.36
19	B	1746	CLA	CHB-C4A-NA	2.80	128.39	124.51
19	1	1188	CLA	CHB-C4A-NA	2.80	128.39	124.51
19	1	1188	CLA	O2D-CGD-CBD	2.81	115.15	111.30
20	B	1782	LMU	C3B-C4B-C5B	2.81	115.09	110.20
19	2	1221	CLA	C2B-C3B-C4B	2.81	108.74	106.29
19	B	1771	CLA	CHB-C4A-NA	2.81	128.40	124.51
19	A	1767	CLA	CAA-CBA-CGA	2.81	121.55	113.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1789	CLA	CED-O2D-CGD	2.82	122.60	115.99
19	B	1750	CLA	O2A-CGA-CBA	2.82	120.49	111.90
19	A	1801	CLA	CMC-C2C-C1C	2.82	129.38	125.02
19	H	1079	CLA	O2A-CGA-CBA	2.82	120.50	111.90
21	B	8059	SUC	O2-C2-C3	2.82	116.69	110.34
20	A	7042	LMU	O6'-C6'-C5'	2.83	120.67	111.33
19	A	1813	CLA	CHC-C1C-NC	2.83	129.00	123.67
20	A	7023	LMU	O1B-C1B-C2B	2.83	115.00	108.10
21	3	1221	SUC	O2-C2-C3	2.83	116.72	110.34
19	A	1762	CLA	O2A-CGA-CBA	2.84	120.54	111.90
19	A	1760	CLA	CMB-C2B-C3B	2.84	130.64	125.09
19	A	1779	CLA	CAC-C3C-C4C	2.84	128.95	124.83
19	A	1779	CLA	CMC-C2C-C1C	2.84	129.42	125.02
20	A	7030	LMU	O1'-C1'-C2'	2.84	111.63	108.04
19	1	1194	CLA	C3D-C4D-ND	2.85	112.66	110.13
19	B	1762	CLA	CHB-C4A-NA	2.85	128.45	124.51
19	A	1817	CLA	C3A-C2A-C1A	2.85	106.33	101.50
20	A	1809	LMU	C3'-C4'-C5'	2.86	117.30	110.84
19	1	1192	CLA	CAC-C3C-C4C	2.86	128.98	124.83
20	A	7036	LMU	C1B-O5B-C5B	2.86	119.29	113.75
19	B	1742	CLA	CHB-C4A-NA	2.86	128.47	124.51
20	A	7019	LMU	O5'-C5'-C4'	2.86	115.80	109.75
20	A	7034	LMU	C3B-C4B-C5B	2.86	115.19	110.20
19	A	1763	CLA	CMC-C2C-C1C	2.87	129.46	125.02
19	J	1046	CLA	C3D-C4D-ND	2.87	112.68	110.13
19	B	1741	CLA	O2A-CGA-CBA	2.87	120.65	111.90
21	B	8054	SUC	O1-C2'-C3'	2.88	118.06	108.04
19	3	3011	CLA	C4-C3-C5	2.88	119.80	115.41
19	F	1157	CLA	O2A-CGA-CBA	2.88	120.67	111.90
19	3	1216	CLA	C3D-C2D-C1D	2.88	108.84	106.30
19	B	1754	CLA	CHC-C1C-NC	2.88	129.09	123.67
20	A	7015	LMU	C4B-C3B-C2B	2.88	116.17	110.79
19	B	1772	CLA	CHC-C1C-NC	2.89	129.10	123.67
19	B	1761	CLA	CHB-C4A-NA	2.89	128.50	124.51
19	J	1044	CLA	C3A-C2A-C1A	2.90	106.41	101.50
19	A	1765	CLA	C2C-C1C-NC	2.90	112.40	110.24
21	B	8061	SUC	O6'-C6'-C5'	2.90	120.91	111.33
19	1	1193	CLA	CAA-CBA-CGA	2.90	121.81	113.32
19	B	1764	CLA	CHC-C1C-NC	2.90	129.13	123.67
20	A	7038	LMU	O3B-C3B-C2B	2.90	116.87	110.34
19	B	1749	CLA	CMC-C2C-C1C	2.90	129.51	125.02
19	3	1215	CLA	C3D-C2D-C1D	2.90	108.86	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3002	CLA	C3D-C4D-ND	2.90	112.71	110.13
19	A	1800	CLA	CHC-C1C-NC	2.91	129.14	123.67
20	A	1810	LMU	O3B-C3B-C2B	2.91	116.88	110.34
19	2	1227	CLA	CHC-C1C-NC	2.91	128.98	123.78
19	G	1099	CLA	CHB-C4A-NA	2.91	128.54	124.51
19	G	1099	CLA	CHC-C1C-NC	2.91	129.15	123.67
20	A	7024	LMU	O5B-C5B-C6B	2.91	113.72	106.36
19	B	1767	CLA	CMC-C2C-C1C	2.92	129.54	125.02
20	A	1810	LMU	C1B-O5B-C5B	2.92	119.41	113.75
19	I	1033	CLA	O2A-CGA-CBA	2.92	120.80	111.90
19	4	1203	CLA	C3D-C4D-ND	2.92	112.72	110.13
19	B	1785	CLA	O2A-CGA-CBA	2.92	120.80	111.90
20	A	7017	LMU	O5'-C1'-C2'	2.92	116.27	110.28
19	A	1784	CLA	CHB-C4A-NA	2.92	128.55	124.51
19	A	1762	CLA	CHB-C4A-NA	2.93	128.56	124.51
19	B	1748	CLA	CHB-C4A-NA	2.93	128.56	124.51
19	B	1766	CLA	CHC-C1C-NC	2.93	129.19	123.67
22	B	1779	BCR	C33-C5-C4	2.93	118.99	113.43
19	2	1221	CLA	C3D-C4D-ND	2.93	112.73	110.13
20	A	7040	LMU	O2B-C2B-C1B	2.93	116.45	110.02
22	L	1169	BCR	C33-C5-C4	2.94	118.99	113.43
19	A	1783	CLA	CHC-C1C-NC	2.94	129.20	123.67
19	B	1770	CLA	CMB-C2B-C3B	2.94	130.84	125.09
19	2	1219	CLA	C3D-C2D-C1D	2.94	108.89	106.30
19	3	1213	CLA	C3D-C4D-ND	2.94	112.74	110.13
20	A	7033	LMU	O2'-C2'-C1'	2.94	116.47	110.02
19	4	1207	CLA	CMC-C2C-C1C	2.95	129.58	125.02
22	B	1779	BCR	C23-C22-C21	2.96	123.74	118.98
19	A	1780	CLA	CHB-C4A-NA	2.96	128.60	124.51
19	1	1199	CLA	C3D-C2D-C1D	2.96	108.91	106.30
19	4	4007	CLA	CHB-C4A-NA	2.96	128.61	124.51
20	A	7035	LMU	O5'-C1'-C2'	2.96	116.36	110.28
20	A	7022	LMU	O1B-C4'-C3'	2.97	114.83	107.17
19	A	1761	CLA	O2A-CGA-CBA	2.97	120.95	111.90
19	2	1218	CLA	CGD-CBD-CAD	2.97	120.70	110.62
19	1	1191	CLA	CHB-C4A-NA	2.97	128.62	124.51
19	A	1777	CLA	CHB-C4A-NA	2.98	128.63	124.51
19	K	3009	CLA	O2A-CGA-CBA	2.98	120.97	111.90
21	B	8056	SUC	O4'-C4'-C5'	2.98	119.98	111.05
19	A	1779	CLA	CHB-C4A-NA	2.98	128.64	124.51
19	4	1209	CLA	CHC-C1C-NC	2.98	129.29	123.67
19	A	1797	CLA	C4-C3-C5	2.99	119.97	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1190	CLA	CGD-CBD-CAD	2.99	120.75	110.62
19	A	1799	CLA	CAC-C3C-C4C	2.99	129.17	124.83
19	J	1046	CLA	C3D-C2D-C1D	2.99	108.93	106.30
20	A	7043	LMU	O3B-C3B-C2B	2.99	117.07	110.34
19	B	1771	CLA	CAA-CBA-CGA	3.00	122.09	113.32
19	3	1214	CLA	C3D-C2D-C1D	3.00	108.94	106.30
19	A	1763	CLA	CHC-C1C-NC	3.00	129.32	123.67
20	A	7021	LMU	O1'-C1'-C2'	3.00	111.83	108.04
19	4	4003	CLA	C3D-C4D-ND	3.00	112.79	110.13
21	B	8060	SUC	O5-C1-C2	3.00	116.43	110.28
19	B	1749	CLA	C4-C3-C5	3.00	119.99	115.41
19	A	1800	CLA	CAC-C3C-C4C	3.00	129.19	124.83
19	B	1767	CLA	CHC-C1C-NC	3.01	129.33	123.67
20	L	1171	LMU	O5'-C5'-C6'	3.01	113.95	106.36
19	A	1796	CLA	C4-C3-C5	3.01	120.00	115.41
19	A	1768	CLA	CHB-C4A-NA	3.01	128.67	124.51
19	4	1202	CLA	C3D-C2D-C1D	3.01	108.95	106.30
19	A	1760	CLA	O2D-CGD-CBD	3.01	115.43	111.30
19	L	1505	CLA	O2A-CGA-CBA	3.01	121.07	111.90
20	A	7019	LMU	C1'-C2'-C3'	3.01	115.91	109.97
19	1	1191	CLA	CHC-C1C-NC	3.01	129.34	123.67
19	B	1745	CLA	CHC-C1C-NC	3.01	129.34	123.67
19	A	1798	CLA	CED-O2D-CGD	3.02	123.06	115.99
19	A	1793	CLA	C4-C3-C5	3.02	120.01	115.41
19	A	1781	CLA	C4-C3-C5	3.02	120.02	115.41
19	4	1196	CLA	C4-C3-C5	3.02	120.02	115.41
19	B	1756	CLA	C4-C3-C5	3.02	120.02	115.41
19	3	1219	CLA	C4-C3-C5	3.02	120.02	115.41
19	A	1782	CLA	C4-C3-C5	3.02	120.03	115.41
19	B	1735	CLA	C4-C3-C5	3.02	120.03	115.41
19	A	1774	CLA	O2A-CGA-CBA	3.03	121.12	111.90
19	J	1043	CLA	C4-C3-C5	3.03	120.03	115.41
19	B	1755	CLA	C4-C3-C5	3.04	120.05	115.41
19	A	1777	CLA	O2A-CGA-CBA	3.04	121.16	111.90
20	A	7026	LMU	C6B-C5B-C4B	3.04	120.52	113.02
19	3	3011	CLA	CMB-C2B-C3B	3.04	131.04	125.09
19	K	3009	CLA	C4-C3-C5	3.05	120.06	115.41
19	B	1740	CLA	O2D-CGD-CBD	3.05	115.48	111.30
19	1	1192	CLA	C4-C3-C5	3.05	120.06	115.41
20	A	7030	LMU	O1B-C4'-C3'	3.05	115.05	107.17
22	L	1170	BCR	C32-C1-C6	3.05	115.09	110.30
20	A	7028	LMU	O5B-C5B-C6B	3.06	114.08	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7026	LMU	O5'-C5'-C6'	3.06	114.08	106.36
19	B	1757	CLA	CHB-C4A-NA	3.06	128.74	124.51
19	B	1761	CLA	CHC-C1C-NC	3.06	129.43	123.67
19	2	1223	CLA	O2A-CGA-CBA	3.07	121.25	111.90
20	A	1810	LMU	C2'-C3'-C4'	3.07	116.34	109.60
19	A	1767	CLA	CHB-C4A-NA	3.07	128.76	124.51
20	R	1057	LMU	O2B-C2B-C1B	3.07	116.75	110.02
19	A	1776	CLA	CGD-CBD-CAD	3.08	121.05	110.62
20	A	7013	LMU	O1B-C4'-C3'	3.08	115.13	107.17
19	A	1789	CLA	O2A-CGA-CBA	3.08	121.30	111.90
20	A	7030	LMU	C1B-O5B-C5B	3.09	119.73	113.75
19	A	1817	CLA	CGD-CBD-CAD	3.09	121.08	110.62
20	A	7031	LMU	O1B-C4'-C3'	3.09	115.14	107.17
19	A	1760	CLA	CBA-CAA-C2A	3.09	122.45	113.73
19	2	1222	CLA	CHB-C4A-NA	3.09	128.79	124.51
20	A	7023	LMU	C1B-C2B-C3B	3.09	116.06	109.97
19	A	1772	CLA	CAC-C3C-C4C	3.10	129.34	124.83
22	I	1032	BCR	C24-C25-C26	3.10	128.48	121.37
20	A	7023	LMU	O1'-C1'-C2'	3.11	111.96	108.04
19	A	1764	CLA	CHC-C1C-NC	3.11	129.51	123.67
20	R	1057	LMU	C1B-C2B-C3B	3.11	116.09	109.97
19	2	1220	CLA	O2A-CGA-CBA	3.11	121.36	111.90
20	A	7024	LMU	C2'-C3'-C4'	3.11	116.44	109.60
20	A	7037	LMU	O1B-C4'-C3'	3.12	115.22	107.17
22	L	1169	BCR	C15-C14-C13	3.12	131.70	127.20
21	3	1221	SUC	O4-C4-C5	3.12	117.51	109.24
19	A	1776	CLA	C4-C3-C5	3.12	120.18	115.41
19	B	1771	CLA	CHC-C1C-NC	3.12	129.55	123.67
19	A	1773	CLA	CED-O2D-CGD	3.13	123.32	115.99
19	1	1189	CLA	CMC-C2C-C1C	3.13	129.86	125.02
19	H	1079	CLA	CMB-C2B-C3B	3.13	131.21	125.09
20	A	7021	LMU	O5B-C5B-C4B	3.13	115.56	109.68
19	I	1033	CLA	CED-O2D-CGD	3.13	123.34	115.99
20	A	7024	LMU	O5'-C5'-C6'	3.14	114.28	106.36
19	B	1753	CLA	CBA-CAA-C2A	3.14	122.60	113.73
19	B	1771	CLA	C4-C3-C5	3.14	120.21	115.41
19	B	1760	CLA	CED-O2D-CGD	3.14	123.36	115.99
19	2	1224	CLA	O2A-CGA-CBA	3.15	121.48	111.90
19	3	1213	CLA	C3B-C4B-NB	3.15	112.91	110.09
22	B	1776	BCR	C23-C22-C21	3.15	124.06	118.98
19	4	1208	CLA	CHC-C1C-NC	3.15	129.41	123.78
20	A	7040	LMU	C1'-C2'-C3'	3.15	116.19	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7013	LMU	O4'-C4B-C5B	3.15	117.59	109.24
20	2	1225	LMU	O1B-C4'-C3'	3.16	115.32	107.17
19	1	1192	CLA	CHC-C1C-NC	3.16	129.62	123.67
19	4	1201	CLA	CED-O2D-CGD	3.16	123.40	115.99
19	1	1196	CLA	CHC-C1C-NC	3.16	129.62	123.67
19	B	1787	CLA	O2A-CGA-CBA	3.16	121.54	111.90
19	A	1762	CLA	CMB-C2B-C3B	3.16	131.28	125.09
20	A	7042	LMU	O2'-C2'-C1'	3.17	116.96	110.02
20	A	7019	LMU	O5B-C5B-C6B	3.17	114.36	106.36
19	3	1218	CLA	O2A-CGA-CBA	3.17	121.56	111.90
21	B	8056	SUC	O2'-C2'-C1'	3.17	116.61	107.98
20	A	1809	LMU	C2'-C3'-C4'	3.18	116.58	109.60
20	A	7025	LMU	O1B-C1B-C2B	3.18	115.84	108.10
19	A	1779	CLA	CHC-C1C-NC	3.18	129.66	123.67
22	I	1032	BCR	C19-C18-C17	3.19	124.12	118.98
19	R	1055	CLA	CHC-C1C-NC	3.19	129.67	123.67
19	B	1754	CLA	O2A-CGA-CBA	3.20	121.65	111.90
19	1	1197	CLA	CMB-C2B-C1B	3.20	133.66	128.36
19	2	1214	CLA	C3D-C2D-C1D	3.21	109.12	106.30
19	B	1744	CLA	CHB-C4A-NA	3.21	128.95	124.51
19	A	1775	CLA	CHC-C1C-NC	3.21	129.71	123.67
21	B	8061	SUC	O2'-C5'-C6'	3.21	118.29	108.57
20	A	7020	LMU	O5B-C1B-C2B	3.21	116.86	110.28
19	3	3001	CLA	C3D-C4D-ND	3.21	112.98	110.13
23	A	1802	PQN	C2M-C2-C1	3.21	121.48	116.27
19	B	1736	CLA	CHB-C4A-NA	3.21	128.96	124.51
19	B	1762	CLA	CHC-C1C-NC	3.21	129.72	123.67
19	1	1201	CLA	C3D-C2D-C1D	3.22	109.14	106.30
19	A	1779	CLA	C4-C3-C5	3.22	120.32	115.41
19	4	4003	CLA	C3D-C2D-C1D	3.22	109.14	106.30
19	A	1811	CLA	CHB-C4A-NA	3.22	128.96	124.51
19	A	1790	CLA	CHC-C1C-NC	3.22	129.73	123.67
19	I	1031	CLA	CHC-C1C-NC	3.22	129.73	123.67
19	B	1744	CLA	CHC-C1C-NC	3.23	129.74	123.67
19	2	1223	CLA	CAA-C2A-C1A	3.23	123.86	112.47
19	1	1190	CLA	CHC-C1C-NC	3.23	129.75	123.67
19	A	1790	CLA	CHB-C4A-NA	3.23	128.98	124.51
19	A	1783	CLA	CHB-C4A-NA	3.23	128.98	124.51
20	A	1809	LMU	C1B-O5B-C5B	3.24	120.03	113.75
19	B	1745	CLA	C4-C3-C5	3.24	120.35	115.41
19	A	1801	CLA	O2A-CGA-CBA	3.24	121.77	111.90
19	L	1505	CLA	CED-O2D-CGD	3.25	123.61	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1213	CLA	C4-C3-C5	3.25	120.37	115.41
19	3	3011	CLA	CHC-C1C-NC	3.26	129.80	123.67
20	R	1057	LMU	O5'-C1'-O1'	3.26	117.89	110.05
19	4	1202	CLA	C3D-C4D-ND	3.26	113.02	110.13
19	B	1751	CLA	CHC-C1C-NC	3.26	129.80	123.67
20	A	7031	LMU	O5'-C1'-O1'	3.26	117.90	110.05
20	A	7017	LMU	C4B-C3B-C2B	3.26	116.88	110.79
19	A	1783	CLA	O2A-CGA-CBA	3.26	121.84	111.90
19	R	1054	CLA	CED-O2D-CGD	3.26	123.65	115.99
19	2	1223	CLA	CHC-C1C-NC	3.27	129.81	123.67
20	A	7035	LMU	O3'-C3'-C4'	3.27	117.60	109.87
19	4	1200	CLA	CHC-C1C-NC	3.27	129.82	123.67
19	B	1753	CLA	CMC-C2C-C1C	3.27	130.08	125.02
19	L	1166	CLA	CHC-C1C-NC	3.27	129.83	123.67
20	A	7026	LMU	O1B-C1B-C2B	3.27	116.06	108.10
19	B	1785	CLA	CHB-C4A-NA	3.28	129.04	124.51
19	B	1770	CLA	C4-C3-C5	3.28	120.41	115.41
22	L	1170	BCR	C29-C30-C25	3.28	115.56	110.36
19	A	1798	CLA	CHC-C1C-NC	3.29	129.87	123.67
19	A	1777	CLA	CHC-C1C-NC	3.30	129.87	123.67
20	A	7030	LMU	O5B-C5B-C6B	3.30	114.69	106.36
20	A	7025	LMU	C1'-O5'-C5'	3.30	120.14	113.75
20	A	7027	LMU	C1'-C2'-C3'	3.30	116.48	109.97
19	B	1764	CLA	CED-O2D-CGD	3.30	123.73	115.99
19	4	1206	CLA	CHC-C1C-NC	3.30	129.68	123.78
19	1	1199	CLA	C3D-C4D-ND	3.30	113.06	110.13
19	B	1763	CLA	O2A-CGA-CBA	3.30	121.97	111.90
19	A	1777	CLA	C4-C3-C5	3.31	119.43	115.68
19	B	1768	CLA	O2A-CGA-CBA	3.31	121.97	111.90
19	B	1760	CLA	CHC-C1C-NC	3.31	129.89	123.67
19	1	1195	CLA	CHC-C1C-NC	3.31	129.90	123.67
19	B	1750	CLA	CHC-C1C-NC	3.31	129.90	123.67
19	B	1740	CLA	CMB-C2B-C3B	3.31	131.57	125.09
19	B	1763	CLA	CED-O2D-CGD	3.32	123.77	115.99
19	B	1745	CLA	O2A-CGA-CBA	3.32	122.02	111.90
19	B	1764	CLA	CHB-C4A-NA	3.33	129.11	124.51
19	A	1787	CLA	CHC-C1C-NC	3.33	129.94	123.67
19	B	1760	CLA	CAC-C3C-C4C	3.34	129.68	124.83
19	4	1197	CLA	CMB-C2B-C3B	3.34	131.97	125.14
19	A	1771	CLA	O2A-CGA-CBA	3.34	122.07	111.90
20	A	7037	LMU	O3'-C3'-C4'	3.34	117.78	109.87
19	B	1758	CLA	CHC-C1C-NC	3.34	129.96	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1054	CLA	CHC-C1C-NC	3.34	129.96	123.67
19	B	1742	CLA	C5-C3-C2	3.35	127.40	121.05
20	A	7017	LMU	O5B-C5B-C6B	3.35	114.82	106.36
19	1	1188	CLA	CMB-C2B-C3B	3.35	131.64	125.09
19	A	1759	CLA	CHC-C1C-NC	3.35	129.98	123.67
19	H	1079	CLA	CHC-C1C-NC	3.35	129.98	123.67
19	B	1754	CLA	CHB-C4A-NA	3.36	129.16	124.51
19	I	1031	CLA	O2A-CGA-CBA	3.36	122.13	111.90
19	B	1740	CLA	CHC-C1C-NC	3.36	129.99	123.67
19	2	1224	CLA	CHC-C1C-NC	3.36	129.99	123.67
19	A	1774	CLA	C4-C3-C5	3.36	120.54	115.41
19	A	1766	CLA	CMB-C2B-C3B	3.36	131.66	125.09
19	4	1197	CLA	CHC-C1C-NC	3.36	130.00	123.67
19	B	1765	CLA	CHC-C1C-NC	3.37	130.00	123.67
20	A	7036	LMU	O3'-C3'-C2'	3.37	117.92	110.34
19	B	1763	CLA	CHC-C1C-NC	3.37	130.01	123.67
22	B	1779	BCR	C38-C26-C27	3.37	119.83	113.43
19	B	1757	CLA	CHC-C1C-NC	3.38	130.03	123.67
20	A	7020	LMU	C1B-O5B-C5B	3.38	120.30	113.75
19	A	1780	CLA	CHC-C1C-NC	3.38	130.03	123.67
19	1	1194	CLA	CHC-C1C-NC	3.38	129.82	123.78
19	4	1207	CLA	CHC-C1C-NC	3.38	130.04	123.67
19	1	1193	CLA	CHC-C1C-NC	3.39	130.04	123.67
19	A	1786	CLA	O2A-CGA-CBA	3.39	122.22	111.90
19	B	1760	CLA	CGD-CBD-CAD	3.39	122.10	110.62
19	R	1054	CLA	C4-C3-C5	3.39	120.58	115.41
21	B	8061	SUC	O3-C3-C2	3.39	117.98	110.34
19	B	1752	CLA	CED-O2D-CGD	3.39	123.95	115.99
19	1	1192	CLA	O2A-CGA-CBA	3.40	122.26	111.90
19	A	1764	CLA	CHB-C4A-NA	3.41	129.22	124.51
19	2	1221	CLA	CHC-C1C-NC	3.41	129.87	123.78
19	A	1815	CLA	O2A-CGA-CBA	3.41	122.28	111.90
22	B	1778	BCR	C33-C5-C4	3.41	119.90	113.43
19	J	1044	CLA	CHC-C1C-NC	3.41	130.09	123.67
20	A	7043	LMU	C1'-C2'-C3'	3.42	116.71	109.97
19	A	1785	CLA	CHC-C1C-NC	3.42	130.12	123.67
19	A	1799	CLA	CHC-C1C-NC	3.43	130.12	123.67
20	A	7027	LMU	C2'-C3'-C4'	3.43	117.13	109.60
19	B	1754	CLA	CAC-C3C-C4C	3.43	129.81	124.83
22	3	1220	BCR	C38-C26-C27	3.43	119.94	113.43
19	2	1223	CLA	CHB-C4A-NA	3.43	129.26	124.51
19	3	1218	CLA	C4-C3-C5	3.44	120.65	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1775	BCR	C38-C26-C27	3.44	119.95	113.43
22	A	1808	BCR	C33-C5-C4	3.44	119.95	113.43
22	A	1807	BCR	C38-C26-C27	3.44	119.95	113.43
19	1	1198	CLA	CHC-C1C-NC	3.44	130.15	123.67
19	4	1209	CLA	CHB-C4A-NA	3.44	129.27	124.51
19	4	1199	CLA	CHB-C4A-NA	3.44	129.28	124.51
19	A	1773	CLA	CHC-C1C-NC	3.45	130.16	123.67
22	A	1804	BCR	C33-C5-C4	3.45	119.96	113.43
19	2	1215	CLA	CHC-C1C-NC	3.45	130.16	123.67
22	B	1781	BCR	C33-C5-C4	3.45	119.97	113.43
22	B	1780	BCR	C33-C5-C4	3.46	119.98	113.43
20	A	7027	LMU	O1B-C1B-C2B	3.46	116.52	108.10
20	A	7037	LMU	O5'-C5'-C6'	3.46	115.10	106.36
19	A	1817	CLA	CBA-CAA-C2A	3.46	123.50	113.73
22	A	1803	BCR	C33-C5-C4	3.46	119.99	113.43
19	B	1786	CLA	CHC-C1C-NC	3.46	130.19	123.67
19	J	1044	CLA	CHB-C4A-NA	3.46	129.30	124.51
19	A	1780	CLA	O2A-CGA-CBA	3.46	122.45	111.90
22	A	1806	BCR	C33-C5-C4	3.46	120.00	113.43
22	B	1775	BCR	C33-C5-C4	3.47	120.00	113.43
22	A	1806	BCR	C38-C26-C27	3.47	120.01	113.43
19	A	1765	CLA	C4-C3-C5	3.47	120.71	115.41
22	B	1777	BCR	C33-C5-C4	3.47	120.02	113.43
19	A	1813	CLA	CHB-C4A-NA	3.48	129.32	124.51
19	A	1789	CLA	CAC-C3C-C4C	3.48	129.88	124.83
22	A	1804	BCR	C38-C26-C27	3.48	120.03	113.43
22	B	1780	BCR	C38-C26-C27	3.48	120.03	113.43
22	A	1808	BCR	C38-C26-C27	3.48	120.03	113.43
22	B	1774	BCR	C33-C5-C4	3.48	120.03	113.43
19	2	1222	CLA	CHC-C1C-NC	3.49	130.23	123.67
19	K	1146	CLA	CHB-C4A-NA	3.49	129.33	124.51
19	3	3001	CLA	CHC-C1C-NC	3.49	130.02	123.78
19	J	1045	CLA	CHB-C4A-NA	3.49	129.34	124.51
22	A	1805	BCR	C33-C5-C4	3.49	120.05	113.43
22	B	1774	BCR	C38-C26-C27	3.49	120.05	113.43
22	B	1778	BCR	C38-C26-C27	3.49	120.05	113.43
22	B	1777	BCR	C38-C26-C27	3.49	120.05	113.43
22	B	1781	BCR	C19-C18-C17	3.49	124.61	118.98
20	A	7016	LMU	C2'-C3'-C4'	3.50	117.28	109.60
22	A	1807	BCR	C33-C5-C4	3.50	120.06	113.43
22	A	1803	BCR	C38-C26-C27	3.50	120.07	113.43
22	A	1805	BCR	C38-C26-C27	3.50	120.07	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1768	CLA	CHC-C1C-NC	3.50	130.26	123.67
19	A	1788	CLA	O2A-CGA-CBA	3.50	122.58	111.90
20	A	7024	LMU	C1'-C2'-C3'	3.51	116.88	109.97
19	B	1741	CLA	CHC-C1C-NC	3.51	130.27	123.67
19	L	1166	CLA	CED-O2D-CGD	3.51	124.22	115.99
19	A	1767	CLA	O2D-CGD-CBD	3.51	116.11	111.30
19	B	1740	CLA	CGD-CBD-CAD	3.51	122.52	110.62
19	A	1812	CLA	CHB-C4A-NA	3.51	129.37	124.51
22	L	1170	BCR	C1-C6-C7	3.51	125.66	115.82
19	B	1740	CLA	C4-C3-C5	3.51	120.77	115.41
19	1	1190	CLA	CED-O2D-CGD	3.52	124.25	115.99
19	1	1187	CLA	CMC-C2C-C1C	3.52	130.47	125.02
20	A	7033	LMU	O1'-C1'-C2'	3.52	112.49	108.04
19	B	1752	CLA	O2D-CGD-CBD	3.52	116.13	111.30
19	A	1788	CLA	CHC-C1C-NC	3.53	130.31	123.67
20	A	7017	LMU	C1'-C2'-C3'	3.53	116.92	109.97
19	B	1748	CLA	O2A-CGA-CBA	3.53	122.66	111.90
19	2	1213	CLA	O2A-CGA-CBA	3.53	122.66	111.90
19	A	1769	CLA	CHB-C4A-NA	3.53	129.40	124.51
20	A	7037	LMU	C1'-C2'-C3'	3.54	116.94	109.97
19	A	1770	CLA	CHC-C1C-NC	3.54	130.33	123.67
19	A	1812	CLA	CHC-C1C-NC	3.54	130.33	123.67
20	K	1086	LMU	O1B-C4'-C5'	3.54	118.62	109.32
19	A	1772	CLA	CHC-C1C-NC	3.54	130.34	123.67
19	3	1212	CLA	CHC-C1C-NC	3.55	130.34	123.67
19	4	4003	CLA	CHC-C1C-NC	3.55	130.13	123.78
19	I	1033	CLA	CHC-C1C-NC	3.55	130.36	123.67
19	F	1155	CLA	CHB-C4A-NA	3.56	129.43	124.51
20	A	7037	LMU	O1B-C1B-O5B	3.56	119.70	110.68
19	L	1505	CLA	CHC-C1C-NC	3.56	130.38	123.67
19	2	1217	CLA	CHC-C1C-NC	3.57	130.38	123.67
19	3	3008	CLA	O2A-CGA-CBA	3.57	122.78	111.90
19	1	1194	CLA	C3D-C2D-C1D	3.57	109.44	106.30
19	1	1199	CLA	CHC-C1C-NC	3.57	130.17	123.78
20	A	7039	LMU	O1B-C1B-O5B	3.58	119.74	110.68
19	A	1776	CLA	CHC-C1C-NC	3.58	130.41	123.67
19	3	1218	CLA	CHC-C1C-NC	3.58	130.41	123.67
20	A	7038	LMU	O5B-C5B-C6B	3.58	115.42	106.36
20	A	7032	LMU	O5B-C5B-C6B	3.59	115.43	106.36
19	L	1167	CLA	CHC-C1C-NC	3.59	130.43	123.67
19	B	1742	CLA	CHC-C1C-NC	3.60	130.44	123.67
19	B	1739	CLA	CHB-C4A-NA	3.60	129.49	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1202	CLA	CHC-C1C-NC	3.60	130.21	123.78
20	A	7038	LMU	C1'-O5'-C5'	3.60	120.73	113.75
19	3	3014	CLA	CHC-C1C-NC	3.60	130.22	123.78
19	J	1044	CLA	O2A-CGA-CBA	3.61	122.88	111.90
19	A	1779	CLA	O2D-CGD-CBD	3.61	116.25	111.30
20	A	7031	LMU	O1B-C1B-C2B	3.61	116.88	108.10
19	A	1762	CLA	CHC-C1C-NC	3.61	130.47	123.67
19	1	1200	CLA	CAA-C2A-C1A	3.61	125.22	112.47
19	A	1774	CLA	CHC-C1C-NC	3.62	130.47	123.67
19	J	1043	CLA	CHC-C1C-NC	3.62	130.48	123.67
19	B	1786	CLA	CAC-C3C-C4C	3.62	130.08	124.83
19	4	1196	CLA	CHC-C1C-NC	3.62	130.48	123.67
19	A	1767	CLA	CMB-C2B-C1B	3.62	134.36	128.36
19	3	3007	CLA	CAC-C3C-C4C	3.63	130.10	124.83
19	4	4014	CLA	CHC-C1C-NC	3.63	130.51	123.67
19	B	1746	CLA	CHC-C1C-NC	3.64	130.52	123.67
20	A	7036	LMU	O5B-C5B-C6B	3.64	115.56	106.36
19	4	1200	CLA	O2A-CGA-CBA	3.64	123.00	111.90
19	A	1781	CLA	CHC-C1C-NC	3.65	130.53	123.67
19	K	1085	CLA	CHC-C1C-NC	3.66	130.55	123.67
19	A	1797	CLA	CHC-C1C-NC	3.66	130.56	123.67
19	A	1792	CLA	CHC-C1C-NC	3.66	130.56	123.67
19	A	1793	CLA	CHC-C1C-NC	3.67	130.57	123.67
19	A	1791	CLA	CHC-C1C-NC	3.67	130.57	123.67
19	A	1784	CLA	CHC-C1C-NC	3.67	130.57	123.67
19	2	1213	CLA	CHC-C1C-NC	3.67	130.57	123.67
19	A	1771	CLA	CHC-C1C-NC	3.67	130.58	123.67
19	J	1044	CLA	CAC-C3C-C4C	3.67	130.16	124.83
19	A	1794	CLA	CHC-C1C-NC	3.67	130.58	123.67
19	A	1795	CLA	CHC-C1C-NC	3.67	130.58	123.67
19	A	1796	CLA	CHC-C1C-NC	3.67	130.58	123.67
19	B	1739	CLA	O2A-CGA-CBA	3.67	123.10	111.90
19	A	1815	CLA	CHC-C1C-NC	3.67	130.59	123.67
20	A	1809	LMU	O5'-C5'-C4'	3.68	117.52	109.75
19	B	1735	CLA	CHC-C1C-NC	3.68	130.59	123.67
19	B	1738	CLA	O2A-CGA-CBA	3.68	123.11	111.90
19	B	1785	CLA	O2D-CGD-CBD	3.68	116.35	111.30
19	2	1212	CLA	CHC-C1C-NC	3.68	130.60	123.67
19	A	1811	CLA	CMC-C2C-C1C	3.68	130.72	125.02
20	A	1810	LMU	O5B-C1B-C2B	3.68	117.84	110.28
19	A	1782	CLA	CHC-C1C-NC	3.69	130.61	123.67
19	B	1755	CLA	CHC-C1C-NC	3.70	130.62	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1142	CLA	CHC-C1C-NC	3.70	130.62	123.67
19	B	1756	CLA	CHC-C1C-NC	3.70	130.63	123.67
22	B	1776	BCR	C38-C26-C27	3.70	120.44	113.43
19	B	1759	CLA	CHC-C1C-NC	3.70	130.63	123.67
19	I	1033	CLA	CHB-C4A-NA	3.71	129.64	124.51
20	A	7026	LMU	O3'-C3'-C4'	3.71	118.65	109.87
19	2	1220	CLA	CHC-C1C-NC	3.72	130.67	123.67
19	3	1219	CLA	CHC-C1C-NC	3.72	130.68	123.67
19	2	1222	CLA	CAC-C3C-C4C	3.73	130.25	124.83
19	A	1816	CLA	O2A-CGA-CBA	3.74	123.29	111.90
19	1	1188	CLA	O2A-CGA-CBA	3.74	123.29	111.90
19	B	1768	CLA	C4-C3-C5	3.74	121.12	115.41
19	J	1045	CLA	CHC-C1C-NC	3.74	130.71	123.67
20	A	7016	LMU	C1B-C2B-C3B	3.74	117.35	109.97
19	F	1156	CLA	CHC-C1C-NC	3.75	130.72	123.67
19	2	2010	CLA	CHC-C1C-NC	3.75	130.49	123.78
19	3	1216	CLA	CHC-C1C-NC	3.75	130.49	123.78
19	4	1207	CLA	CHB-C4A-NA	3.76	129.71	124.51
19	A	1801	CLA	C4-C3-C5	3.76	121.15	115.41
19	3	3007	CLA	CHC-C1C-NC	3.76	130.75	123.67
19	3	3011	CLA	CHB-C4A-NA	3.77	129.72	124.51
20	K	1086	LMU	O5B-C5B-C6B	3.77	115.88	106.36
19	3	3008	CLA	CHC-C1C-NC	3.78	130.78	123.67
20	A	7020	LMU	C1B-C2B-C3B	3.78	117.42	109.97
19	2	1217	CLA	CED-O2D-CGD	3.78	124.86	115.99
20	4	1210	LMU	O1'-C1'-C2'	3.78	112.82	108.04
21	B	8051	SUC	O5-C5-C4	3.78	116.78	109.68
19	A	1766	CLA	CHC-C1C-NC	3.78	130.79	123.67
19	A	1799	CLA	O2D-CGD-CBD	3.79	116.49	111.30
20	A	7033	LMU	O5'-C1'-C2'	3.79	118.05	110.28
20	A	7026	LMU	O5B-C5B-C6B	3.79	115.94	106.36
19	4	1201	CLA	CGD-CBD-CAD	3.80	123.49	110.62
20	A	7038	LMU	O5B-C5B-C4B	3.80	116.81	109.68
19	B	1752	CLA	CHC-C1C-NC	3.80	130.82	123.67
19	A	1792	CLA	C4-C3-C5	3.80	119.99	115.68
19	4	1199	CLA	CAC-C3C-C4C	3.81	130.35	124.83
19	2	1212	CLA	C4-C3-C5	3.81	120.00	115.68
19	B	1758	CLA	CHB-C4A-NA	3.82	129.80	124.51
19	4	1205	CLA	CHC-C1C-NC	3.82	130.62	123.78
19	A	1795	CLA	C4-C3-C5	3.84	120.03	115.68
20	A	7015	LMU	C1B-C2B-C3B	3.84	117.54	109.97
19	F	1155	CLA	CMB-C2B-C3B	3.84	132.99	125.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1778	CLA	CHC-C1C-NC	3.84	130.90	123.67
19	A	1817	CLA	CED-O2D-CGD	3.84	125.00	115.99
19	B	1736	CLA	CHC-C1C-NC	3.85	130.91	123.67
23	B	1773	PQN	C2M-C2-C1	3.85	122.52	116.27
19	B	1739	CLA	CHC-C1C-NC	3.85	130.92	123.67
19	A	1812	CLA	CAA-C2A-C1A	3.85	126.06	112.47
19	B	1743	CLA	CHC-C1C-NC	3.85	130.92	123.67
19	2	1217	CLA	C4-C3-C5	3.86	121.30	115.41
19	B	1786	CLA	C6-C5-C3	3.87	120.97	112.48
19	4	1203	CLA	CHC-C1C-NC	3.87	130.69	123.78
19	B	1751	CLA	CHB-C4A-NA	3.87	129.86	124.51
19	A	1760	CLA	CHC-C1C-NC	3.87	130.96	123.67
19	A	1812	CLA	O2A-CGA-CBA	3.88	123.71	111.90
20	A	7027	LMU	C6B-C5B-C4B	3.88	122.60	113.02
19	A	1811	CLA	CED-O2D-CGD	3.89	125.11	115.99
19	A	1780	CLA	O2D-CGD-CBD	3.90	116.64	111.30
19	B	1758	CLA	O2A-CGA-CBA	3.90	123.78	111.90
19	B	1770	CLA	O2A-CGA-CBA	3.90	123.79	111.90
19	B	1785	CLA	CHC-C1C-NC	3.91	131.03	123.67
19	A	1785	CLA	C4-C3-C5	3.91	121.38	115.41
19	3	1217	CLA	C3D-C2D-C1D	3.91	109.75	106.30
19	4	1203	CLA	C3D-C2D-C1D	3.92	109.76	106.30
19	B	1768	CLA	CHC-C1C-NC	3.93	131.06	123.67
19	A	1772	CLA	C4-C3-C5	3.93	121.40	115.41
19	B	1747	CLA	CHC-C1C-NC	3.93	131.06	123.67
19	B	1762	CLA	C4-C3-C5	3.93	121.41	115.41
19	4	1198	CLA	O2A-CGA-CBA	3.94	123.90	111.90
19	4	1206	CLA	C3D-C4D-ND	3.94	113.63	110.13
19	4	4007	CLA	CHC-C1C-NC	3.95	131.09	123.67
19	3	3002	CLA	CHC-C1C-NC	3.95	130.84	123.78
19	2	1214	CLA	CHC-C1C-NC	3.95	130.84	123.78
19	B	1769	CLA	CHC-C1C-NC	3.96	131.11	123.67
22	I	1032	BCR	C30-C25-C24	3.96	126.90	115.82
19	1	1188	CLA	CHC-C1C-NC	3.96	131.13	123.67
19	1	1187	CLA	CHC-C1C-NC	3.96	131.13	123.67
19	A	1773	CLA	O2A-CGA-CBA	3.97	123.99	111.90
20	A	7025	LMU	O3B-C3B-C4B	3.97	119.28	110.34
19	A	1786	CLA	CHC-C1C-NC	3.97	131.15	123.67
19	2	1219	CLA	C3D-C4D-ND	3.98	113.66	110.13
19	2	1214	CLA	C3D-C4D-ND	3.98	113.67	110.13
22	B	1781	BCR	C31-C1-C6	3.99	116.56	110.30
20	4	1210	LMU	C1B-O5B-C5B	3.99	121.50	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1787	CLA	CMB-C2B-C3B	4.00	132.91	125.09
19	4	1201	CLA	O2D-CGD-CBD	4.00	116.79	111.30
24	B	1783	LMG	O7-C10-C11	4.01	120.23	111.53
19	4	1204	CLA	C4-C3-C5	4.01	121.53	115.41
19	J	1046	CLA	CHC-C1C-NC	4.01	130.95	123.78
21	3	1221	SUC	O5-C1-C2	4.01	118.50	110.28
19	4	1208	CLA	C2B-C1B-NB	4.02	113.70	110.09
21	B	8055	SUC	O5-C5-C6	4.02	116.52	106.36
19	J	1045	CLA	C4-C3-C5	4.02	121.55	115.41
19	F	1155	CLA	CHC-C1C-NC	4.03	131.26	123.67
20	A	7033	LMU	C3B-C4B-C5B	4.03	117.23	110.20
19	A	1765	CLA	O2A-CGA-CBA	4.04	124.20	111.90
19	2	1218	CLA	CHC-C1C-NC	4.05	131.30	123.67
19	B	1752	CLA	C4-C3-C5	4.06	121.60	115.41
19	K	1146	CLA	O2A-CGA-CBA	4.06	124.26	111.90
19	B	1748	CLA	CHC-C1C-NC	4.06	131.30	123.67
22	B	1776	BCR	C8-C9-C10	4.06	125.53	118.98
19	L	1167	CLA	CHB-C4A-NA	4.08	130.15	124.51
19	3	3015	CLA	CHC-C1C-NC	4.09	131.09	123.78
20	A	7038	LMU	C1B-O5B-C5B	4.09	121.69	113.75
20	K	1086	LMU	O2'-C2'-C1'	4.09	118.99	110.02
20	A	7022	LMU	O2B-C2B-C1B	4.09	119.00	110.02
19	I	1033	CLA	C4-C3-C5	4.10	121.67	115.41
19	A	1778	CLA	CAA-C2A-C1A	4.11	121.24	112.14
20	A	7021	LMU	O2B-C2B-C1B	4.12	119.05	110.02
19	A	1789	CLA	CHC-C1C-NC	4.12	131.43	123.67
20	A	7026	LMU	O4'-C4B-C3B	4.12	119.62	110.34
20	A	7021	LMU	C1B-O5B-C5B	4.12	121.75	113.75
19	4	1207	CLA	CAC-C3C-C4C	4.13	131.41	125.02
19	1	1187	CLA	CED-O2D-CGD	4.14	125.70	115.99
19	1	1200	CLA	O2A-CGA-CBA	4.15	124.55	111.90
19	A	1815	CLA	CHB-C4A-NA	4.16	130.27	124.51
19	A	1817	CLA	CAC-C3C-C4C	4.18	130.90	124.83
19	1	1187	CLA	C4A-NA-C1A	4.18	111.76	106.36
20	A	7023	LMU	C2'-C3'-C4'	4.19	118.80	109.60
19	B	1787	CLA	CGD-CBD-CAD	4.19	124.81	110.62
19	1	1201	CLA	CHC-C1C-NC	4.19	131.27	123.78
19	A	1815	CLA	CED-O2D-CGD	4.20	125.84	115.99
19	B	1786	CLA	CHB-C4A-NA	4.22	130.35	124.51
19	3	1217	CLA	CHC-C1C-NC	4.22	131.33	123.78
19	B	1787	CLA	CHC-C1C-NC	4.23	131.63	123.67
20	A	7040	LMU	O1B-C1B-C2B	4.26	118.46	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1206	CLA	C3D-C2D-C1D	4.26	110.05	106.30
19	2	1217	CLA	O2D-CGD-CBD	4.27	117.16	111.30
20	A	1810	LMU	O1'-C1'-C2'	4.28	113.44	108.04
19	K	1146	CLA	CHC-C1C-NC	4.28	131.73	123.67
19	A	1817	CLA	CHC-C1C-NC	4.29	131.74	123.67
19	2	1219	CLA	CHC-C1C-NC	4.29	131.45	123.78
19	3	1214	CLA	CHC-C1C-NC	4.29	131.46	123.78
20	A	7047	LMU	O1B-C4'-C5'	4.30	120.62	109.32
22	B	1781	BCR	C38-C26-C27	4.30	121.59	113.43
19	4	1201	CLA	O2A-CGA-CBA	4.31	125.05	111.90
19	3	3001	CLA	C3D-C2D-C1D	4.31	110.10	106.30
19	B	1770	CLA	CHC-C1C-NC	4.32	131.80	123.67
19	3	1215	CLA	CHC-C1C-NC	4.32	131.51	123.78
19	2	1227	CLA	C3D-C2D-C1D	4.33	110.12	106.30
19	3	3014	CLA	C3D-C2D-C1D	4.35	110.13	106.30
19	3	3014	CLA	C3D-C4D-ND	4.35	113.99	110.13
19	4	1199	CLA	CHC-C1C-NC	4.35	131.86	123.67
20	A	7037	LMU	O1B-C1B-C2B	4.35	118.70	108.10
19	K	1146	CLA	CMB-C2B-C3B	4.36	133.61	125.09
20	A	7019	LMU	C2'-C3'-C4'	4.36	119.17	109.60
19	R	1055	CLA	O2A-CGA-CBA	4.37	125.23	111.90
22	B	1779	BCR	C34-C9-C8	4.38	125.38	118.10
20	A	7037	LMU	O3B-C3B-C2B	4.39	120.21	110.34
19	B	1748	CLA	O2D-CGD-CBD	4.39	117.32	111.30
20	A	7020	LMU	O1'-C1'-C2'	4.39	113.58	108.04
19	A	1817	CLA	O2A-CGA-CBA	4.39	125.29	111.90
19	L	1505	CLA	O2D-CGD-CBD	4.40	117.33	111.30
19	1	1197	CLA	CHC-C1C-NC	4.40	131.95	123.67
19	B	1757	CLA	O2A-CGA-CBA	4.40	125.32	111.90
19	B	1737	CLA	CHB-C4A-NA	4.41	130.61	124.51
19	1	1188	CLA	CED-O2D-CGD	4.43	126.38	115.99
21	B	8061	SUC	C1-O5-C5	4.43	122.35	113.75
19	1	1193	CLA	CAA-C2A-C3A	4.43	125.97	113.22
20	A	7026	LMU	O4'-C4B-C5B	4.45	121.02	109.24
23	A	1802	PQN	C14-C13-C15	4.48	122.25	115.41
19	R	1054	CLA	O2A-CGA-CBA	4.49	125.58	111.90
19	B	1771	CLA	O2A-CGA-CBA	4.50	125.62	111.90
20	L	1171	LMU	C3B-C4B-C5B	4.51	118.05	110.20
20	A	7038	LMU	O5'-C5'-C6'	4.51	117.75	106.36
22	L	1169	BCR	C36-C18-C19	4.51	125.61	118.10
20	A	7032	LMU	C2'-C3'-C4'	4.52	119.53	109.60
20	A	7021	LMU	C1B-O1B-C4'	4.53	129.83	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1188	CLA	CAA-C2A-C1A	4.53	128.45	112.47
20	A	7024	LMU	O5B-C1B-C2B	4.55	119.61	110.28
20	A	7024	LMU	O1'-C1'-C2'	4.55	113.79	108.04
19	A	1812	CLA	O2D-CGD-CBD	4.56	117.55	111.30
19	B	1738	CLA	CHB-C4A-NA	4.56	130.82	124.51
19	A	1783	CLA	O2D-CGD-CBD	4.56	117.56	111.30
19	A	1765	CLA	CAC-C3C-C4C	4.57	131.47	124.83
21	B	8061	SUC	O5-C5-C6	4.57	117.92	106.36
19	A	1767	CLA	CHC-C1C-NC	4.58	132.29	123.67
21	B	8051	SUC	C1-O5-C5	4.58	122.64	113.75
19	A	1798	CLA	C4-C3-C5	4.60	122.43	115.41
20	A	7038	LMU	O1B-C4'-C3'	4.60	119.05	107.17
19	B	1787	CLA	O2D-CGD-CBD	4.61	117.62	111.30
19	R	1055	CLA	O2D-CGD-CBD	4.63	117.65	111.30
22	I	1032	BCR	C7-C6-C5	4.64	132.00	121.37
19	A	1769	CLA	CHC-C1C-NC	4.64	132.41	123.67
19	2	1216	CLA	CHC-C1C-NC	4.65	132.09	123.78
19	A	1780	CLA	C4-C3-C5	4.66	122.52	115.41
19	B	1737	CLA	CHC-C1C-NC	4.66	132.45	123.67
20	A	7017	LMU	C1'-O5'-C5'	4.67	122.81	113.75
19	B	1738	CLA	CHC-C1C-NC	4.68	132.47	123.67
19	G	1099	CLA	C4-C3-C5	4.68	120.98	115.68
19	4	1204	CLA	O2D-CGD-CBD	4.69	117.73	111.30
19	B	1787	CLA	CHB-C4A-NA	4.69	131.00	124.51
19	A	1761	CLA	O2D-CGD-CBD	4.71	117.76	111.30
19	A	1761	CLA	CHC-C1C-NC	4.71	132.53	123.67
19	A	1760	CLA	O2A-CGA-CBA	4.71	126.25	111.90
19	4	4003	CLA	C2B-C1B-NB	4.75	114.35	110.09
21	2	1226	SUC	C1-C2-C3	4.78	119.40	109.97
19	2	1216	CLA	C3D-C2D-C1D	4.78	110.51	106.30
19	A	1774	CLA	O2D-CGD-CBD	4.80	117.88	111.30
20	A	7037	LMU	O4'-C4B-C5B	4.80	121.95	109.24
19	A	1789	CLA	C4-C3-C5	4.81	122.76	115.41
22	L	1169	BCR	C38-C26-C27	4.82	122.56	113.43
20	A	7026	LMU	O3B-C3B-C2B	4.82	121.19	110.34
20	A	7031	LMU	O1'-C1'-C2'	4.83	114.14	108.04
20	B	1782	LMU	O1'-C1'-C2'	4.83	114.14	108.04
19	1	1200	CLA	CHC-C1C-NC	4.84	132.78	123.67
19	F	1157	CLA	O2D-CGD-CBD	4.85	117.95	111.30
20	A	7038	LMU	O2'-C2'-C3'	4.85	121.26	110.34
19	B	1745	CLA	O2D-CGD-CBD	4.87	117.98	111.30
20	A	7042	LMU	O1B-C4'-C5'	4.88	122.14	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	1086	LMU	C1B-C2B-C3B	4.89	119.60	109.97
20	A	7039	LMU	O3B-C3B-C4B	4.90	121.36	110.34
22	L	1170	BCR	C33-C5-C4	4.90	122.72	113.43
19	B	1753	CLA	O2D-CGD-CBD	4.93	118.06	111.30
20	A	7026	LMU	O3B-C3B-C4B	4.94	121.46	110.34
19	4	1201	CLA	CMB-C2B-C3B	4.94	134.75	125.09
19	4	1201	CLA	C3A-C2A-C1A	4.98	109.94	101.50
19	A	1771	CLA	O2D-CGD-CBD	4.99	118.14	111.30
19	1	1187	CLA	CAC-C3C-C4C	5.00	132.08	124.83
22	I	1032	BCR	C15-C14-C13	5.01	134.43	127.20
21	B	8059	SUC	O3-C3-C4	5.04	121.69	110.34
19	3	3015	CLA	C2B-C1B-NB	5.05	114.62	110.09
19	A	1765	CLA	CHC-C1C-NC	5.08	133.23	123.67
19	B	1751	CLA	O2D-CGD-CBD	5.11	118.31	111.30
19	B	1764	CLA	O2D-CGD-CBD	5.12	118.32	111.30
19	F	1157	CLA	C4-C3-C5	5.12	123.23	115.41
19	1	1197	CLA	CBA-CAA-C2A	5.13	128.19	113.73
20	A	7021	LMU	O1B-C4'-C3'	5.15	120.47	107.17
19	A	1788	CLA	O2D-CGD-CBD	5.15	118.37	111.30
22	L	1170	BCR	C36-C18-C19	5.16	126.68	118.10
19	3	1218	CLA	CED-O2D-CGD	5.18	128.13	115.99
19	3	1217	CLA	C3D-C4D-ND	5.19	114.74	110.13
19	J	1046	CLA	C2B-C1B-NB	5.19	114.75	110.09
19	1	1187	CLA	CHB-C4A-NA	5.19	131.69	124.51
19	B	1760	CLA	O2D-CGD-CBD	5.20	118.43	111.30
19	B	1744	CLA	O2D-CGD-CBD	5.21	118.45	111.30
19	2	1227	CLA	C3D-C4D-ND	5.22	114.77	110.13
19	L	1505	CLA	C4-C3-C5	5.26	123.44	115.41
19	B	1766	CLA	C4-C3-C5	5.26	121.64	115.68
19	3	1213	CLA	CHC-C1C-NC	5.28	133.22	123.78
22	I	1032	BCR	C15-C16-C17	5.28	135.07	123.39
19	2	2010	CLA	C2B-C1B-NB	5.29	114.84	110.09
20	A	7043	LMU	C1B-C2B-C3B	5.29	120.40	109.97
19	3	1214	CLA	C2B-C1B-NB	5.31	114.85	110.09
20	A	7035	LMU	O1B-C4'-C3'	5.32	120.90	107.17
20	A	7022	LMU	O1B-C1B-C2B	5.33	121.07	108.10
19	2	1216	CLA	C2B-C1B-NB	5.33	114.88	110.09
19	3	1215	CLA	C2B-C1B-NB	5.34	114.88	110.09
20	A	7043	LMU	O5B-C5B-C4B	5.35	119.72	109.68
19	2	1216	CLA	C3D-C4D-ND	5.37	114.90	110.13
20	A	7047	LMU	O1'-C1'-C2'	5.39	114.85	108.04
21	B	8062	SUC	C6-C5-C4	5.40	126.33	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1219	CLA	C2B-C1B-NB	5.43	114.96	110.09
22	I	1032	BCR	C7-C8-C9	5.43	134.50	126.22
19	4	1203	CLA	C2B-C1B-NB	5.45	114.98	110.09
20	A	7042	LMU	O1'-C1'-C2'	5.46	114.93	108.04
20	A	7040	LMU	O1'-C1'-C2'	5.47	114.94	108.04
19	3	3002	CLA	C2B-C1B-NB	5.47	115.00	110.09
20	A	7016	LMU	O1'-C1'-C2'	5.47	114.95	108.04
20	A	7034	LMU	O1'-C1'-C2'	5.50	114.99	108.04
19	4	1201	CLA	CAA-C2A-C1A	5.51	131.89	112.47
19	1	1201	CLA	C3D-C4D-ND	5.51	115.02	110.13
19	B	1742	CLA	O2D-CGD-CBD	5.51	118.86	111.30
19	A	1787	CLA	C4-C3-C5	5.51	123.83	115.41
20	A	7039	LMU	O1B-C1B-C2B	5.52	121.53	108.10
19	4	1201	CLA	CHC-C1C-NC	5.54	134.10	123.67
20	A	7015	LMU	O1'-C1'-C2'	5.56	115.06	108.04
19	B	1743	CLA	O2D-CGD-CBD	5.56	118.93	111.30
19	4	1198	CLA	CHC-C1C-NC	5.63	134.27	123.67
19	1	1197	CLA	O2A-CGA-CBA	5.69	129.24	111.90
19	2	1215	CLA	O2D-CGD-CBD	5.70	119.12	111.30
20	A	7026	LMU	C1'-O5'-C5'	5.72	124.84	113.75
22	B	1781	BCR	C30-C25-C24	5.73	131.87	115.82
19	R	1054	CLA	O2D-CGD-CBD	5.74	119.17	111.30
19	3	3001	CLA	C2B-C1B-NB	5.75	115.25	110.09
21	3	1221	SUC	O3-C3-C2	5.77	123.32	110.34
19	3	1216	CLA	C2B-C1B-NB	5.80	115.29	110.09
19	H	1079	CLA	O2D-CGD-CBD	5.80	119.26	111.30
19	A	1768	CLA	O2D-CGD-CBD	5.81	119.27	111.30
20	A	7039	LMU	O4'-C4B-C3B	5.83	123.47	110.34
19	A	1817	CLA	CAA-C2A-C3A	5.84	130.01	113.22
19	2	1214	CLA	C2B-C1B-NB	5.85	115.34	110.09
19	4	4007	CLA	O2D-CGD-CBD	5.86	119.33	111.30
19	4	1206	CLA	C2B-C1B-NB	5.87	115.36	110.09
19	J	1045	CLA	O2D-CGD-CBD	5.92	119.42	111.30
22	I	1032	BCR	C8-C9-C10	5.93	128.53	118.98
20	A	7027	LMU	O1'-C1'-C2'	5.97	115.58	108.04
20	R	1057	LMU	O1'-C1'-C2'	6.00	115.62	108.04
19	4	1205	CLA	C2B-C1B-NB	6.01	115.48	110.09
19	A	1790	CLA	O2D-CGD-CBD	6.04	119.58	111.30
19	4	1202	CLA	C2B-C1B-NB	6.06	115.53	110.09
19	1	1199	CLA	C2B-C1B-NB	6.07	115.53	110.09
19	1	1194	CLA	C2B-C1B-NB	6.09	115.55	110.09
19	1	1192	CLA	O2D-CGD-CBD	6.17	119.77	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1213	CLA	C2B-C1B-NB	6.18	115.64	110.09
19	1	1200	CLA	C4-C3-C5	6.20	122.70	115.68
19	B	1750	CLA	O2D-CGD-CBD	6.21	119.82	111.30
19	3	3008	CLA	O2D-CGD-CBD	6.24	119.86	111.30
22	I	1032	BCR	C38-C26-C27	6.24	125.26	113.43
19	A	1769	CLA	O2D-CGD-CBD	6.28	119.91	111.30
19	F	1155	CLA	CBD-CHA-C1A	6.28	131.47	128.59
19	4	1198	CLA	O2D-CGD-CBD	6.34	119.99	111.30
19	2	1221	CLA	C2B-C1B-NB	6.42	115.85	110.09
19	F	1156	CLA	O2D-CGD-CBD	6.43	120.12	111.30
19	B	1755	CLA	O2D-CGD-CBD	6.43	120.12	111.30
19	4	1196	CLA	O2D-CGD-CBD	6.43	120.13	111.30
19	A	1797	CLA	O2D-CGD-CBD	6.44	120.14	111.30
19	A	1796	CLA	O2D-CGD-CBD	6.44	120.14	111.30
19	A	1762	CLA	O2D-CGD-CBD	6.45	120.14	111.30
19	A	1794	CLA	O2D-CGD-CBD	6.45	120.15	111.30
19	3	1219	CLA	O2D-CGD-CBD	6.45	120.15	111.30
19	B	1756	CLA	O2D-CGD-CBD	6.45	120.16	111.30
19	B	1735	CLA	O2D-CGD-CBD	6.46	120.16	111.30
19	4	4014	CLA	O2D-CGD-CBD	6.46	120.17	111.30
19	A	1793	CLA	O2D-CGD-CBD	6.47	120.18	111.30
19	J	1043	CLA	O2D-CGD-CBD	6.47	120.18	111.30
19	A	1791	CLA	O2D-CGD-CBD	6.47	120.18	111.30
19	K	1142	CLA	O2D-CGD-CBD	6.47	120.18	111.30
19	K	1085	CLA	O2D-CGD-CBD	6.47	120.18	111.30
19	2	1212	CLA	O2D-CGD-CBD	6.47	120.18	111.30
19	A	1792	CLA	O2D-CGD-CBD	6.47	120.18	111.30
19	A	1795	CLA	O2D-CGD-CBD	6.48	120.19	111.30
19	A	1781	CLA	O2D-CGD-CBD	6.48	120.19	111.30
22	L	1170	BCR	C8-C9-C10	6.50	129.45	118.98
19	4	1200	CLA	O2D-CGD-CBD	6.51	120.23	111.30
19	A	1816	CLA	C4-C3-C5	6.52	125.36	115.41
19	A	1782	CLA	O2D-CGD-CBD	6.53	120.25	111.30
19	B	1766	CLA	O2D-CGD-CBD	6.54	120.28	111.30
19	A	1815	CLA	O2D-CGD-CBD	6.54	120.28	111.30
19	2	1220	CLA	O2D-CGD-CBD	6.55	120.28	111.30
19	3	3011	CLA	O2D-CGD-CBD	6.55	120.28	111.30
19	3	3014	CLA	C2B-C1B-NB	6.67	116.08	110.09
19	2	1227	CLA	C2B-C1B-NB	6.69	116.09	110.09
19	3	3007	CLA	O2D-CGD-CBD	6.70	120.50	111.30
19	A	1777	CLA	O2D-CGD-CBD	6.80	120.63	111.30
19	A	1776	CLA	O2D-CGD-CBD	6.80	120.63	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7032	LMU	C1B-O5B-C5B	6.84	127.03	113.75
20	R	1057	LMU	O2B-C2B-C3B	6.85	125.75	110.34
19	A	1764	CLA	O2D-CGD-CBD	6.85	120.70	111.30
19	B	1747	CLA	O2D-CGD-CBD	6.88	120.74	111.30
19	A	1772	CLA	O2D-CGD-CBD	6.91	120.78	111.30
20	R	1057	LMU	O1B-C1B-C2B	6.96	125.04	108.10
19	A	1773	CLA	O2D-CGD-CBD	6.98	120.88	111.30
19	B	1786	CLA	C4-C3-C5	6.99	126.08	115.41
19	3	1217	CLA	C2B-C1B-NB	7.02	116.39	110.09
19	2	1223	CLA	O2D-CGD-CBD	7.03	120.95	111.30
20	K	1086	LMU	O1'-C1'-C2'	7.07	116.97	108.04
19	A	1765	CLA	O2D-CGD-CBD	7.10	121.03	111.30
19	1	1193	CLA	C3A-C2A-C1A	7.20	113.71	101.50
19	A	1800	CLA	O2D-CGD-CBD	7.25	121.25	111.30
19	G	1099	CLA	O2D-CGD-CBD	7.26	121.26	111.30
19	3	1212	CLA	CBD-CHA-C1A	7.26	131.92	128.59
19	A	1770	CLA	O2D-CGD-CBD	7.33	121.35	111.30
19	1	1187	CLA	O2D-CGD-CBD	7.35	121.39	111.30
19	B	1765	CLA	O2D-CGD-CBD	7.37	121.41	111.30
19	2	1222	CLA	O2D-CGD-CBD	7.39	121.44	111.30
19	K	3009	CLA	O2D-CGD-CBD	7.39	121.44	111.30
19	2	1224	CLA	O2D-CGD-CBD	7.44	121.50	111.30
19	B	1746	CLA	O2D-CGD-CBD	7.55	121.66	111.30
19	1	1201	CLA	C2B-C1B-NB	7.55	116.86	110.09
19	B	1737	CLA	O2D-CGD-CBD	7.57	121.69	111.30
19	A	1813	CLA	O2D-CGD-CBD	7.59	121.72	111.30
19	2	1213	CLA	O2D-CGD-CBD	7.62	121.76	111.30
19	B	1762	CLA	O2D-CGD-CBD	7.62	121.76	111.30
19	L	1167	CLA	O2D-CGD-CBD	7.70	121.86	111.30
19	A	1787	CLA	O2D-CGD-CBD	7.72	121.90	111.30
19	1	1196	CLA	CBD-CHA-C1A	7.81	132.17	128.59
19	B	1770	CLA	O2D-CGD-CBD	7.83	122.04	111.30
19	B	1786	CLA	O2D-CGD-CBD	7.90	122.14	111.30
19	I	1031	CLA	O2D-CGD-CBD	7.91	122.16	111.30
19	A	1798	CLA	O2D-CGD-CBD	7.95	122.21	111.30
19	1	1198	CLA	O2D-CGD-CBD	8.02	122.30	111.30
19	B	1761	CLA	O2D-CGD-CBD	8.03	122.32	111.30
19	A	1763	CLA	O2D-CGD-CBD	8.10	122.41	111.30
19	1	1189	CLA	O2D-CGD-CBD	8.15	122.48	111.30
19	B	1763	CLA	O2D-CGD-CBD	8.17	122.51	111.30
19	A	1775	CLA	CBD-CHA-C1A	8.26	132.37	128.59
19	A	1766	CLA	O2D-CGD-CBD	8.27	122.65	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1200	CLA	O2D-CGD-CBD	8.28	122.65	111.30
19	A	1801	CLA	O2D-CGD-CBD	8.30	122.69	111.30
19	B	1741	CLA	O2D-CGD-CBD	8.33	122.73	111.30
19	B	1738	CLA	O2D-CGD-CBD	8.44	122.88	111.30
19	A	1816	CLA	O2D-CGD-CBD	8.51	122.97	111.30
19	J	1044	CLA	O2D-CGD-CBD	8.52	122.99	111.30
19	B	1769	CLA	O2D-CGD-CBD	8.61	123.12	111.30
19	B	1757	CLA	O2D-CGD-CBD	8.71	123.25	111.30
19	A	1778	CLA	O2D-CGD-CBD	8.72	123.26	111.30
19	A	1789	CLA	O2D-CGD-CBD	8.73	123.27	111.30
19	4	1198	CLA	CGD-CBD-CAD	8.76	140.30	110.62
19	K	1146	CLA	O2D-CGD-CBD	8.80	123.37	111.30
19	I	1033	CLA	O2D-CGD-CBD	8.83	123.42	111.30
19	A	1785	CLA	O2D-CGD-CBD	8.83	123.42	111.30
19	L	1166	CLA	O2D-CGD-CBD	8.86	123.45	111.30
19	B	1754	CLA	O2D-CGD-CBD	8.87	123.46	111.30
19	A	1817	CLA	O2D-CGD-CBD	8.89	123.50	111.30
19	3	1218	CLA	O2D-CGD-CBD	9.01	123.66	111.30
19	B	1767	CLA	O2D-CGD-CBD	9.02	123.67	111.30
22	B	1781	BCR	C23-C22-C21	9.02	133.51	118.98
19	1	1193	CLA	O2D-CGD-CBD	9.05	123.72	111.30
19	4	1199	CLA	O2D-CGD-CBD	9.08	123.76	111.30
19	1	1190	CLA	O2D-CGD-CBD	9.12	123.81	111.30
19	B	1768	CLA	O2D-CGD-CBD	9.42	124.23	111.30
19	B	1749	CLA	O2D-CGD-CBD	9.45	124.26	111.30
19	1	1195	CLA	CBD-CHA-C1A	9.46	132.92	128.59
19	B	1736	CLA	O2D-CGD-CBD	9.59	124.46	111.30
19	2	1218	CLA	O2D-CGD-CBD	9.62	124.50	111.30
19	4	1209	CLA	O2D-CGD-CBD	9.77	124.71	111.30
19	B	1759	CLA	O2D-CGD-CBD	9.84	124.80	111.30
19	A	1786	CLA	O2D-CGD-CBD	9.87	124.84	111.30
19	A	1784	CLA	O2D-CGD-CBD	10.04	125.07	111.30
19	B	1758	CLA	O2D-CGD-CBD	10.18	125.27	111.30
19	B	1739	CLA	O2D-CGD-CBD	10.26	125.38	111.30
19	1	1191	CLA	CBD-CHA-C1A	10.60	133.44	128.59
19	B	1772	CLA	CBD-CHA-C1A	10.72	133.50	128.59
19	A	1759	CLA	O2D-CGD-CBD	11.53	127.12	111.30
19	L	1168	CLA	O2D-CGD-CBD	12.10	127.90	111.30
19	4	1207	CLA	CBD-CHA-C1A	12.94	134.52	128.59
22	B	1781	BCR	C21-C20-C19	13.79	165.16	123.13
22	B	1776	BCR	C21-C20-C19	15.21	169.48	123.13
22	L	1170	BCR	C21-C20-C19	17.32	175.92	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1760	CLA	C3B-CAB-CBB	17.33	161.77	126.32
22	I	1032	BCR	C21-C20-C19	17.51	176.51	123.13
22	B	1779	BCR	C21-C20-C19	17.74	177.20	123.13
19	A	1769	CLA	C3B-CAB-CBB	17.79	162.72	126.32
19	B	1769	CLA	C3B-CAB-CBB	18.02	163.19	126.32
22	L	1169	BCR	C21-C20-C19	18.04	178.12	123.13
22	3	1220	BCR	C21-C20-C19	18.12	178.35	123.13
19	A	1774	CLA	C3B-CAB-CBB	18.49	164.15	126.32
19	B	1760	CLA	C3B-CAB-CBB	18.53	164.22	126.32
22	B	1775	BCR	C21-C20-C19	18.62	179.89	123.13
22	A	1804	BCR	C21-C20-C19	18.62	179.90	123.13
22	B	1774	BCR	C21-C20-C19	18.62	179.90	123.13
22	B	1778	BCR	C21-C20-C19	18.63	179.93	123.13
22	A	1808	BCR	C21-C20-C19	18.63	179.93	123.13
22	B	1777	BCR	C21-C20-C19	18.64	179.94	123.13
22	B	1780	BCR	C21-C20-C19	18.64	179.94	123.13
22	A	1806	BCR	C21-C20-C19	18.64	179.95	123.13
22	A	1807	BCR	C21-C20-C19	18.64	179.97	123.13
22	A	1803	BCR	C21-C20-C19	18.65	179.97	123.13
22	A	1805	BCR	C21-C20-C19	18.65	179.98	123.13
19	A	1768	CLA	C3B-CAB-CBB	18.65	164.48	126.32
19	B	1736	CLA	C3B-CAB-CBB	18.83	164.85	126.32
19	A	1816	CLA	C3B-CAB-CBB	18.88	164.94	126.32
19	1	1192	CLA	C3B-CAB-CBB	18.97	165.14	126.32
19	2	1222	CLA	C3B-CAB-CBB	19.10	165.39	126.32
19	A	1770	CLA	C3B-CAB-CBB	19.11	165.42	126.32
19	A	1785	CLA	C3B-CAB-CBB	19.34	165.90	126.32
19	2	1215	CLA	C3B-CAB-CBB	19.72	166.68	126.32
19	B	1742	CLA	C3B-CAB-CBB	20.00	167.24	126.32
19	B	1763	CLA	C3B-CAB-CBB	20.20	167.65	126.32
19	2	1213	CLA	C3B-CAB-CBB	20.32	167.89	126.32
19	2	1224	CLA	C3B-CAB-CBB	20.33	167.92	126.32
19	4	1200	CLA	C3B-CAB-CBB	20.40	168.06	126.32
19	2	1223	CLA	C3B-CAB-CBB	20.43	168.11	126.32
19	A	1778	CLA	C3B-CAB-CBB	20.58	168.42	126.32
19	B	1747	CLA	C3B-CAB-CBB	20.60	168.47	126.32
19	A	1765	CLA	C3B-CAB-CBB	20.82	168.92	126.32
19	A	1766	CLA	C3B-CAB-CBB	20.84	168.97	126.32
19	B	1757	CLA	C3B-CAB-CBB	20.90	169.08	126.32
19	B	1786	CLA	C3B-CAB-CBB	21.00	169.29	126.32
19	B	1743	CLA	C3B-CAB-CBB	21.05	169.39	126.32
19	B	1750	CLA	C3B-CAB-CBB	21.06	169.40	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1744	CLA	C3B-CAB-CBB	21.06	169.41	126.32
19	A	1776	CLA	C3B-CAB-CBB	21.17	169.63	126.32
19	B	1758	CLA	C3B-CAB-CBB	21.39	170.09	126.32
19	4	1198	CLA	C3B-CAB-CBB	21.40	170.11	126.32
19	B	1766	CLA	C3B-CAB-CBB	21.56	170.44	126.32
19	1	1193	CLA	C3B-CAB-CBB	21.56	170.44	126.32
19	A	1790	CLA	C3B-CAB-CBB	21.58	170.48	126.32
19	B	1746	CLA	C3B-CAB-CBB	21.63	170.56	126.32
19	G	1099	CLA	C3B-CAB-CBB	21.68	170.67	126.32
19	4	1199	CLA	C3B-CAB-CBB	21.69	170.70	126.32
19	A	1784	CLA	C3B-CAB-CBB	21.69	170.70	126.32
19	A	1780	CLA	C3B-CAB-CBB	21.81	170.95	126.32
19	I	1033	CLA	C3B-CAB-CBB	21.88	171.09	126.32
19	B	1737	CLA	C3B-CAB-CBB	22.09	171.52	126.32
19	B	1768	CLA	C3B-CAB-CBB	22.10	171.53	126.32
19	B	1751	CLA	C3B-CAB-CBB	22.43	172.21	126.32
19	A	1801	CLA	C3B-CAB-CBB	22.47	172.28	126.32
19	2	1218	CLA	C3B-CAB-CBB	22.52	172.40	126.32
19	A	1761	CLA	C3B-CAB-CBB	22.54	172.43	126.32
19	A	1764	CLA	C3B-CAB-CBB	22.67	172.71	126.32
19	1	1190	CLA	C3B-CAB-CBB	22.69	172.75	126.32
19	B	1748	CLA	C3B-CAB-CBB	22.74	172.85	126.32
19	A	1783	CLA	C3B-CAB-CBB	22.77	172.91	126.32
19	F	1157	CLA	C3B-CAB-CBB	22.78	172.93	126.32
19	4	1201	CLA	C3B-CAB-CBB	22.79	172.95	126.32
19	1	1188	CLA	C3B-CAB-CBB	22.84	173.05	126.32
19	B	1749	CLA	C3B-CAB-CBB	22.85	173.08	126.32
19	B	1785	CLA	C3B-CAB-CBB	22.86	173.08	126.32
19	A	1786	CLA	C3B-CAB-CBB	22.96	173.30	126.32
19	A	1771	CLA	C3B-CAB-CBB	23.07	173.53	126.32
19	B	1764	CLA	C3B-CAB-CBB	23.14	173.66	126.32
19	B	1787	CLA	C3B-CAB-CBB	23.26	173.90	126.32
19	A	1789	CLA	C3B-CAB-CBB	23.35	174.10	126.32
19	A	1815	CLA	C3B-CAB-CBB	23.42	174.24	126.32
19	1	1189	CLA	C3B-CAB-CBB	23.49	174.37	126.32
19	2	1217	CLA	C3B-CAB-CBB	23.49	174.38	126.32
19	B	1754	CLA	C3B-CAB-CBB	23.53	174.46	126.32
19	3	3007	CLA	C3B-CAB-CBB	23.55	174.51	126.32
19	A	1759	CLA	C3B-CAB-CBB	23.56	174.52	126.32
19	B	1767	CLA	C3B-CAB-CBB	23.64	174.68	126.32
19	A	1800	CLA	C3B-CAB-CBB	23.64	174.68	126.32
19	L	1167	CLA	C3B-CAB-CBB	23.66	174.72	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1799	CLA	C3B-CAB-CBB	23.69	174.78	126.32
19	B	1745	CLA	C3B-CAB-CBB	23.69	174.80	126.32
19	R	1055	CLA	C3B-CAB-CBB	23.71	174.84	126.32
19	H	1079	CLA	C3B-CAB-CBB	23.76	174.93	126.32
19	B	1770	CLA	C3B-CAB-CBB	23.80	175.02	126.32
19	A	1779	CLA	C3B-CAB-CBB	23.84	175.10	126.32
19	A	1767	CLA	C3B-CAB-CBB	23.88	175.18	126.32
19	3	1218	CLA	C3B-CAB-CBB	23.89	175.19	126.32
19	1	1197	CLA	C3B-CAB-CBB	23.89	175.20	126.32
19	L	1505	CLA	C3B-CAB-CBB	23.94	175.30	126.32
19	B	1771	CLA	C3B-CAB-CBB	24.05	175.52	126.32
19	A	1773	CLA	C3B-CAB-CBB	24.10	175.64	126.32
19	4	1204	CLA	C3B-CAB-CBB	24.24	175.91	126.32
19	B	1738	CLA	C3B-CAB-CBB	24.24	175.91	126.32
19	1	1187	CLA	C3B-CAB-CBB	24.24	175.92	126.32
19	A	1763	CLA	C3B-CAB-CBB	24.30	176.03	126.32
19	A	1812	CLA	C3B-CAB-CBB	24.31	176.05	126.32
19	A	1777	CLA	C3B-CAB-CBB	24.47	176.39	126.32
19	B	1753	CLA	C3B-CAB-CBB	24.52	176.49	126.32
19	A	1811	CLA	C3B-CAB-CBB	24.52	176.49	126.32
19	4	1209	CLA	C3B-CAB-CBB	24.56	176.57	126.32
19	4	4007	CLA	C3B-CAB-CBB	24.58	176.62	126.32
19	R	1054	CLA	C3B-CAB-CBB	24.58	176.62	126.32
19	B	1761	CLA	C3B-CAB-CBB	24.66	176.78	126.32
22	B	1781	BCR	C20-C21-C22	24.70	162.87	127.20
19	A	1788	CLA	C3B-CAB-CBB	24.73	176.91	126.32
19	A	1787	CLA	C3B-CAB-CBB	24.81	177.07	126.32
19	A	1772	CLA	C3B-CAB-CBB	24.82	177.09	126.32
19	1	1198	CLA	C3B-CAB-CBB	24.85	177.16	126.32
19	L	1166	CLA	C3B-CAB-CBB	24.96	177.39	126.32
19	B	1762	CLA	C3B-CAB-CBB	25.15	177.78	126.32
19	A	1798	CLA	C3B-CAB-CBB	25.21	177.89	126.32
19	B	1739	CLA	C3B-CAB-CBB	25.27	178.03	126.32
19	B	1759	CLA	C3B-CAB-CBB	25.27	178.03	126.32
19	3	3011	CLA	C3B-CAB-CBB	25.30	178.09	126.32
19	2	1220	CLA	C3B-CAB-CBB	25.34	178.17	126.32
19	1	1200	CLA	C3B-CAB-CBB	25.40	178.29	126.32
19	B	1765	CLA	C3B-CAB-CBB	25.46	178.41	126.32
19	B	1752	CLA	C3B-CAB-CBB	25.46	178.41	126.32
19	B	1740	CLA	C3B-CAB-CBB	25.47	178.43	126.32
19	K	3009	CLA	C3B-CAB-CBB	25.52	178.53	126.32
19	A	1762	CLA	C3B-CAB-CBB	25.53	178.56	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	1146	CLA	C3B-CAB-CBB	25.54	178.57	126.32
19	A	1813	CLA	C3B-CAB-CBB	25.58	178.66	126.32
19	J	1044	CLA	C3B-CAB-CBB	25.58	178.66	126.32
19	I	1031	CLA	C3B-CAB-CBB	25.60	178.70	126.32
19	J	1045	CLA	C3B-CAB-CBB	25.72	178.94	126.32
19	L	1168	CLA	C3B-CAB-CBB	25.72	178.95	126.32
19	3	3008	CLA	C3B-CAB-CBB	26.01	179.53	126.32
19	A	1781	CLA	C3B-CAB-CBB	26.16	179.84	126.32
19	F	1156	CLA	C3B-CAB-CBB	26.17	179.87	126.32
19	B	1755	CLA	C3B-CAB-CBB	26.18	179.89	126.32
19	K	1142	CLA	C3B-CAB-CBB	26.19	179.90	126.32
19	B	1756	CLA	C3B-CAB-CBB	26.20	179.91	126.32
19	K	1085	CLA	C3B-CAB-CBB	26.20	179.92	126.32
19	A	1794	CLA	C3B-CAB-CBB	26.20	179.92	126.32
19	B	1735	CLA	C3B-CAB-CBB	26.20	179.92	126.32
19	4	1196	CLA	C3B-CAB-CBB	26.20	179.93	126.32
19	3	1219	CLA	C3B-CAB-CBB	26.20	179.93	126.32
19	4	4014	CLA	C3B-CAB-CBB	26.21	179.94	126.32
19	J	1043	CLA	C3B-CAB-CBB	26.21	179.95	126.32
19	2	1212	CLA	C3B-CAB-CBB	26.21	179.96	126.32
19	A	1782	CLA	C3B-CAB-CBB	26.22	179.96	126.32
19	A	1795	CLA	C3B-CAB-CBB	26.22	179.96	126.32
19	A	1797	CLA	C3B-CAB-CBB	26.22	179.96	126.32
19	A	1791	CLA	C3B-CAB-CBB	26.22	179.96	126.32
19	A	1792	CLA	C3B-CAB-CBB	26.22	179.96	126.32
19	A	1793	CLA	C3B-CAB-CBB	26.23	179.98	126.32
19	A	1796	CLA	C3B-CAB-CBB	26.23	179.99	126.32
22	B	1776	BCR	C20-C21-C22	29.81	170.25	127.20
22	I	1032	BCR	C20-C21-C22	33.82	176.05	127.20
22	B	1779	BCR	C20-C21-C22	34.40	176.88	127.20
22	L	1169	BCR	C20-C21-C22	34.69	177.30	127.20
22	L	1170	BCR	C20-C21-C22	34.82	177.48	127.20
22	3	1220	BCR	C20-C21-C22	35.32	178.21	127.20
22	B	1777	BCR	C20-C21-C22	36.44	179.84	127.20
22	B	1775	BCR	C20-C21-C22	36.45	179.84	127.20
22	B	1774	BCR	C20-C21-C22	36.47	179.88	127.20
22	A	1803	BCR	C20-C21-C22	36.48	179.88	127.20
22	B	1778	BCR	C20-C21-C22	36.48	179.89	127.20
22	A	1807	BCR	C20-C21-C22	36.50	179.91	127.20
22	A	1804	BCR	C20-C21-C22	36.51	179.93	127.20
22	A	1806	BCR	C20-C21-C22	36.52	179.95	127.20
22	A	1805	BCR	C20-C21-C22	36.53	179.95	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1808	BCR	C20-C21-C22	36.54	179.97	127.20
22	B	1780	BCR	C20-C21-C22	36.55	179.99	127.20

All (630) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1760	CLA	C8
19	A	1760	CLA	NC
19	A	1760	CLA	ND
19	A	1760	CLA	NA
19	A	1785	CLA	C8
19	A	1785	CLA	NC
19	A	1785	CLA	ND
19	A	1785	CLA	NA
19	3	1218	CLA	C8
19	3	1218	CLA	NC
19	3	1218	CLA	ND
19	3	1218	CLA	NA
19	4	1204	CLA	C8
19	4	1204	CLA	NC
19	4	1204	CLA	ND
19	4	1204	CLA	NA
19	L	1168	CLA	CBD
19	L	1168	CLA	NC
19	L	1168	CLA	ND
19	L	1168	CLA	NA
19	4	1201	CLA	NC
19	4	1201	CLA	C2A
19	4	1201	CLA	ND
19	4	1201	CLA	NA
19	1	1195	CLA	NC
19	1	1195	CLA	ND
19	1	1195	CLA	NA
19	K	1142	CLA	NC
19	K	1142	CLA	ND
19	K	1142	CLA	NA
19	J	1045	CLA	C8
19	J	1045	CLA	NC
19	J	1045	CLA	ND
19	J	1045	CLA	NA
19	3	1216	CLA	NC
19	3	1216	CLA	ND

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Mol	Chain	Res	Type	Atom
19	3	1216	CLA	NA
19	L	1505	CLA	C8
19	L	1505	CLA	NC
19	L	1505	CLA	ND
19	L	1505	CLA	NA
19	3	3014	CLA	NC
19	3	3014	CLA	ND
19	3	3014	CLA	NA
21	B	8062	SUC	C2'
19	A	1778	CLA	NC
19	A	1778	CLA	ND
19	A	1778	CLA	NA
21	B	8051	SUC	C2'
19	A	1781	CLA	C8
19	A	1781	CLA	NC
19	A	1781	CLA	ND
19	A	1781	CLA	NA
21	3	1221	SUC	C2'
19	B	1753	CLA	NC
19	B	1753	CLA	ND
19	B	1753	CLA	NA
19	A	1791	CLA	NC
19	A	1791	CLA	ND
19	A	1791	CLA	NA
21	B	8059	SUC	C2'
19	B	1743	CLA	C8
19	B	1743	CLA	NC
19	B	1743	CLA	ND
19	B	1743	CLA	NA
19	B	1742	CLA	C8
19	B	1742	CLA	NC
19	B	1742	CLA	ND
19	B	1742	CLA	NA
19	B	1754	CLA	NC
19	B	1754	CLA	ND
19	B	1754	CLA	NA
19	2	1218	CLA	C8
19	2	1218	CLA	NC
19	2	1218	CLA	ND
19	2	1218	CLA	NA
19	4	1207	CLA	NC
19	4	1207	CLA	ND

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Mol	Chain	Res	Type	Atom
19	4	1207	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
19	A	1776	CLA	C8
19	A	1776	CLA	NC
19	A	1776	CLA	ND
19	A	1776	CLA	NA
19	A	1788	CLA	C8
19	A	1788	CLA	NC
19	A	1788	CLA	ND
19	A	1788	CLA	NA
19	B	1758	CLA	C8
19	B	1758	CLA	NC
19	B	1758	CLA	ND
19	B	1758	CLA	NA
19	B	1757	CLA	C8
19	B	1757	CLA	NC
19	B	1757	CLA	ND
19	B	1757	CLA	NA
19	A	1812	CLA	C8
19	A	1812	CLA	NC
19	A	1812	CLA	ND
19	A	1812	CLA	NA
19	A	1777	CLA	NC
19	A	1777	CLA	ND
19	A	1777	CLA	NA
19	A	1764	CLA	C8
19	A	1764	CLA	NC
19	A	1764	CLA	ND
19	A	1764	CLA	NA
19	4	1208	CLA	NC
19	4	1208	CLA	ND
19	4	1208	CLA	NA
19	4	1203	CLA	NC
19	4	1203	CLA	ND
19	4	1203	CLA	NA
19	A	1811	CLA	C8
19	A	1811	CLA	NC

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Mol	Chain	Res	Type	Atom
19	A	1811	CLA	ND
19	A	1811	CLA	NA
19	2	1227	CLA	NC
19	2	1227	CLA	ND
19	2	1227	CLA	NA
21	B	8061	SUC	C2'
19	B	1766	CLA	NC
19	B	1766	CLA	ND
19	B	1766	CLA	NA
19	J	1046	CLA	NC
19	J	1046	CLA	ND
19	J	1046	CLA	NA
19	R	1054	CLA	C8
19	R	1054	CLA	NC
19	R	1054	CLA	ND
19	R	1054	CLA	NA
19	B	1750	CLA	NC
19	B	1750	CLA	ND
19	B	1750	CLA	NA
19	A	1799	CLA	NC
19	A	1799	CLA	ND
19	A	1799	CLA	NA
19	B	1751	CLA	NC
19	B	1751	CLA	ND
19	B	1751	CLA	NA
19	A	1790	CLA	NC
19	A	1790	CLA	ND
19	A	1790	CLA	NA
19	1	1197	CLA	CBD
19	1	1197	CLA	NC
19	1	1197	CLA	ND
19	1	1197	CLA	NA
19	B	1746	CLA	NC
19	B	1746	CLA	ND
19	B	1746	CLA	NA
19	3	1213	CLA	NC
19	3	1213	CLA	ND
19	3	1213	CLA	NA
19	B	1737	CLA	C8
19	B	1737	CLA	NC
19	B	1737	CLA	ND
19	B	1737	CLA	NA

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Mol	Chain	Res	Type	Atom
19	3	3015	CLA	NC
19	3	3015	CLA	ND
19	3	3015	CLA	NA
19	1	1191	CLA	NC
19	1	1191	CLA	ND
19	1	1191	CLA	NA
19	B	1762	CLA	C8
19	B	1762	CLA	NC
19	B	1762	CLA	ND
19	B	1762	CLA	NA
19	3	1212	CLA	NC
19	3	1212	CLA	ND
19	3	1212	CLA	NA
19	A	1772	CLA	C8
19	A	1772	CLA	NC
19	A	1772	CLA	ND
19	A	1772	CLA	NA
19	1	1193	CLA	C2A
19	1	1193	CLA	NC
19	1	1193	CLA	ND
19	1	1193	CLA	NA
19	3	3001	CLA	NC
19	3	3001	CLA	ND
19	3	3001	CLA	NA
19	2	1223	CLA	NC
19	2	1223	CLA	ND
19	2	1223	CLA	NA
19	B	1786	CLA	C8
19	B	1786	CLA	NC
19	B	1786	CLA	ND
19	B	1786	CLA	NA
20	R	1057	LMU	C2B
21	B	8054	SUC	C2'
19	1	1194	CLA	NC
19	1	1194	CLA	ND
19	1	1194	CLA	NA
19	2	1219	CLA	NC
19	2	1219	CLA	ND
19	2	1219	CLA	NA
19	A	1783	CLA	C8
19	A	1783	CLA	NC
19	A	1783	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1783	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	B	1772	CLA	NC
19	B	1772	CLA	ND
19	B	1772	CLA	NA
19	A	1796	CLA	C8
19	A	1796	CLA	NC
19	A	1796	CLA	ND
19	A	1796	CLA	NA
19	K	1085	CLA	NC
19	K	1085	CLA	ND
19	K	1085	CLA	NA
19	A	1817	CLA	NC
19	A	1817	CLA	C2A
19	A	1817	CLA	ND
19	A	1817	CLA	NA
19	A	1817	CLA	CBD
21	H	1080	SUC	C2'
23	B	1773	PQN	C23
19	A	1761	CLA	C8
19	A	1761	CLA	NC
19	A	1761	CLA	ND
19	A	1761	CLA	NA
19	2	1215	CLA	NC
19	2	1215	CLA	ND
19	2	1215	CLA	NA
19	1	1200	CLA	C2A
19	1	1200	CLA	NC
19	1	1200	CLA	ND
19	1	1200	CLA	NA
19	1	1200	CLA	C3A
19	B	1771	CLA	C8
19	B	1771	CLA	NC
19	B	1771	CLA	ND
19	B	1771	CLA	NA
19	A	1816	CLA	C2A
19	A	1816	CLA	NC
19	A	1816	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1816	CLA	NA
19	A	1816	CLA	C3A
19	A	1793	CLA	C8
19	A	1793	CLA	NC
19	A	1793	CLA	ND
19	A	1793	CLA	NA
19	A	1798	CLA	C8
19	A	1798	CLA	NC
19	A	1798	CLA	ND
19	A	1798	CLA	NA
19	1	1188	CLA	NC
19	1	1188	CLA	ND
19	1	1188	CLA	NA
19	A	1774	CLA	C8
19	A	1774	CLA	NC
19	A	1774	CLA	ND
19	A	1774	CLA	NA
19	B	1740	CLA	C8
19	B	1740	CLA	NC
19	B	1740	CLA	ND
19	B	1740	CLA	NA
19	B	1759	CLA	C8
19	B	1759	CLA	NC
19	B	1759	CLA	ND
19	B	1759	CLA	NA
19	B	1749	CLA	C8
19	B	1749	CLA	NC
19	B	1749	CLA	ND
19	B	1749	CLA	NA
19	1	1199	CLA	NC
19	1	1199	CLA	ND
19	1	1199	CLA	NA
19	2	2010	CLA	NC
19	2	2010	CLA	ND
19	2	2010	CLA	NA
19	3	1219	CLA	C8
19	3	1219	CLA	NC
19	3	1219	CLA	ND
19	3	1219	CLA	NA
19	J	1044	CLA	C8
19	J	1044	CLA	NC
19	J	1044	CLA	ND

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Mol	Chain	Res	Type	Atom
19	J	1044	CLA	NA
19	4	1205	CLA	NC
19	4	1205	CLA	ND
19	4	1205	CLA	NA
19	G	1099	CLA	NC
19	G	1099	CLA	ND
19	G	1099	CLA	NA
19	2	1220	CLA	C8
19	2	1220	CLA	NC
19	2	1220	CLA	ND
19	2	1220	CLA	NA
19	A	1767	CLA	C8
19	A	1767	CLA	NC
19	A	1767	CLA	ND
19	A	1767	CLA	NA
19	B	1769	CLA	NC
19	B	1769	CLA	ND
19	B	1769	CLA	NA
19	B	1744	CLA	C8
19	B	1744	CLA	NC
19	B	1744	CLA	ND
19	B	1744	CLA	NA
19	4	4003	CLA	NC
19	4	4003	CLA	ND
19	4	4003	CLA	NA
19	1	1190	CLA	NC
19	1	1190	CLA	ND
19	1	1190	CLA	NA
19	3	3007	CLA	NC
19	3	3007	CLA	ND
19	3	3007	CLA	NA
19	A	1797	CLA	C8
19	A	1797	CLA	NC
19	A	1797	CLA	ND
19	A	1797	CLA	NA
19	A	1813	CLA	C8
19	A	1813	CLA	NC
19	A	1813	CLA	ND
19	A	1813	CLA	NA
19	A	1780	CLA	C8
19	A	1780	CLA	NC
19	A	1780	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1780	CLA	NA
19	B	1767	CLA	C8
19	B	1767	CLA	NC
19	B	1767	CLA	ND
19	B	1767	CLA	NA
19	L	1166	CLA	NC
19	L	1166	CLA	ND
19	L	1166	CLA	NA
19	B	1787	CLA	C8
19	B	1787	CLA	NC
19	B	1787	CLA	ND
19	B	1787	CLA	NA
19	B	1756	CLA	C8
19	B	1756	CLA	NC
19	B	1756	CLA	ND
19	B	1756	CLA	NA
19	3	1215	CLA	NC
19	3	1215	CLA	ND
19	3	1215	CLA	NA
19	2	1212	CLA	NC
19	2	1212	CLA	ND
19	2	1212	CLA	NA
19	1	1189	CLA	NC
19	1	1189	CLA	ND
19	1	1189	CLA	NA
19	B	1738	CLA	C8
19	B	1738	CLA	NC
19	B	1738	CLA	ND
19	B	1738	CLA	NA
23	A	1802	PQN	C23
21	B	8060	SUC	C2'
19	2	1217	CLA	C8
19	2	1217	CLA	NC
19	2	1217	CLA	ND
19	2	1217	CLA	NA
21	B	8052	SUC	C2'
19	F	1156	CLA	NC
19	F	1156	CLA	ND
19	F	1156	CLA	NA
19	A	1800	CLA	C8
19	A	1800	CLA	NC
19	A	1800	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1800	CLA	NA
19	K	3009	CLA	C8
19	K	3009	CLA	NC
19	K	3009	CLA	ND
19	K	3009	CLA	NA
19	A	1768	CLA	NC
19	A	1768	CLA	ND
19	A	1768	CLA	NA
19	I	1033	CLA	C8
19	I	1033	CLA	NC
19	I	1033	CLA	ND
19	I	1033	CLA	NA
19	B	1770	CLA	C8
19	B	1770	CLA	NC
19	B	1770	CLA	ND
19	B	1770	CLA	NA
19	1	1187	CLA	NC
19	1	1187	CLA	ND
19	1	1187	CLA	NA
19	A	1784	CLA	C8
19	A	1784	CLA	NC
19	A	1784	CLA	ND
19	A	1784	CLA	NA
19	2	1213	CLA	C8
19	2	1213	CLA	NC
19	2	1213	CLA	ND
19	2	1213	CLA	NA
19	4	1199	CLA	C8
19	4	1199	CLA	NC
19	4	1199	CLA	ND
19	4	1199	CLA	NA
19	J	1043	CLA	C8
19	J	1043	CLA	NC
19	J	1043	CLA	ND
19	J	1043	CLA	NA
19	4	1209	CLA	NC
19	4	1209	CLA	ND
19	4	1209	CLA	NA
19	A	1771	CLA	NC
19	A	1771	CLA	ND
19	A	1771	CLA	NA
19	2	1216	CLA	NC

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Mol	Chain	Res	Type	Atom
19	2	1216	CLA	ND
19	2	1216	CLA	NA
19	B	1763	CLA	NC
19	B	1763	CLA	ND
19	B	1763	CLA	NA
19	3	3011	CLA	C8
19	3	3011	CLA	NC
19	3	3011	CLA	ND
19	3	3011	CLA	NA
19	1	1192	CLA	C8
19	1	1192	CLA	NC
19	1	1192	CLA	ND
19	1	1192	CLA	NA
19	A	1815	CLA	C8
19	A	1815	CLA	CBD
19	A	1815	CLA	NC
19	A	1815	CLA	ND
19	A	1815	CLA	NA
19	A	1782	CLA	C8
19	A	1782	CLA	NC
19	A	1782	CLA	ND
19	A	1782	CLA	NA
19	2	1214	CLA	NC
19	2	1214	CLA	ND
19	2	1214	CLA	NA
19	A	1762	CLA	C8
19	A	1762	CLA	NC
19	A	1762	CLA	ND
19	A	1762	CLA	NA
19	R	1055	CLA	C8
19	R	1055	CLA	NC
19	R	1055	CLA	ND
19	R	1055	CLA	NA
19	4	1206	CLA	NC
19	4	1206	CLA	ND
19	4	1206	CLA	NA
19	A	1794	CLA	NC
19	A	1794	CLA	ND
19	A	1794	CLA	NA
21	B	8056	SUC	C2'
19	B	1761	CLA	NC
19	B	1761	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	1761	CLA	NA
19	B	1739	CLA	C8
19	B	1739	CLA	NC
19	B	1739	CLA	ND
19	B	1739	CLA	NA
19	2	1222	CLA	NC
19	2	1222	CLA	ND
19	2	1222	CLA	NA
19	1	1198	CLA	C8
19	1	1198	CLA	NC
19	1	1198	CLA	ND
19	1	1198	CLA	NA
19	A	1779	CLA	C8
19	A	1779	CLA	NC
19	A	1779	CLA	ND
19	A	1779	CLA	NA
21	B	8053	SUC	C2'
19	4	1197	CLA	NC
19	4	1197	CLA	ND
19	4	1197	CLA	NA
19	F	1155	CLA	NC
19	F	1155	CLA	ND
19	F	1155	CLA	NA
19	B	1736	CLA	NC
19	B	1736	CLA	ND
19	B	1736	CLA	NA
19	A	1765	CLA	C8
19	A	1765	CLA	NC
19	A	1765	CLA	ND
19	A	1765	CLA	NA
19	A	1801	CLA	C8
19	A	1801	CLA	NC
19	A	1801	CLA	ND
19	A	1801	CLA	NA
19	B	1748	CLA	C8
19	B	1748	CLA	NC
19	B	1748	CLA	ND
19	B	1748	CLA	NA
19	4	1200	CLA	NC
19	4	1200	CLA	ND
19	4	1200	CLA	NA
19	A	1795	CLA	NC

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Mol	Chain	Res	Type	Atom
19	A	1795	CLA	ND
19	A	1795	CLA	NA
19	L	1167	CLA	NC
19	L	1167	CLA	ND
19	L	1167	CLA	NA
19	2	1224	CLA	C8
19	2	1224	CLA	NC
19	2	1224	CLA	ND
19	2	1224	CLA	NA
19	B	1785	CLA	C8
19	B	1785	CLA	NC
19	B	1785	CLA	ND
19	B	1785	CLA	NA
19	B	1768	CLA	C8
19	B	1768	CLA	NC
19	B	1768	CLA	ND
19	B	1768	CLA	NA
19	4	1196	CLA	C8
19	4	1196	CLA	NC
19	4	1196	CLA	ND
19	4	1196	CLA	NA
19	4	4007	CLA	NC
19	4	4007	CLA	ND
19	4	4007	CLA	NA
19	I	1031	CLA	C8
19	I	1031	CLA	NC
19	I	1031	CLA	ND
19	I	1031	CLA	NA
19	B	1741	CLA	C8
19	B	1741	CLA	NC
19	B	1741	CLA	ND
19	B	1741	CLA	NA
19	3	1214	CLA	NC
19	3	1214	CLA	ND
19	3	1214	CLA	NA
19	1	1196	CLA	NC
19	1	1196	CLA	ND
19	1	1196	CLA	NA
19	1	1201	CLA	NC
19	1	1201	CLA	ND
19	1	1201	CLA	NA
19	2	1221	CLA	NC

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Mol	Chain	Res	Type	Atom
19	2	1221	CLA	ND
19	2	1221	CLA	NA
19	B	1765	CLA	NC
19	B	1765	CLA	ND
19	B	1765	CLA	NA
19	A	1787	CLA	C8
19	A	1787	CLA	NC
19	A	1787	CLA	ND
19	A	1787	CLA	NA
19	B	1764	CLA	NC
19	B	1764	CLA	ND
19	B	1764	CLA	NA
19	B	1755	CLA	C8
19	B	1755	CLA	NC
19	B	1755	CLA	ND
19	B	1755	CLA	NA
19	B	1735	CLA	C8
19	B	1735	CLA	NC
19	B	1735	CLA	ND
19	B	1735	CLA	NA
21	2	1226	SUC	C2'
19	A	1759	CLA	NC
19	A	1759	CLA	ND
19	A	1759	CLA	NA
19	3	3008	CLA	NC
19	3	3008	CLA	ND
19	3	3008	CLA	NA
19	A	1786	CLA	NC
19	A	1786	CLA	ND
19	A	1786	CLA	NA
19	A	1789	CLA	C8
19	A	1789	CLA	NC
19	A	1789	CLA	ND
19	A	1789	CLA	NA
19	A	1773	CLA	NC
19	A	1773	CLA	ND
19	A	1773	CLA	NA
19	4	4014	CLA	NC
19	4	4014	CLA	ND
19	4	4014	CLA	NA
19	3	3002	CLA	NC
19	3	3002	CLA	ND

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Mol	Chain	Res	Type	Atom
19	3	3002	CLA	NA
19	3	1217	CLA	NC
19	3	1217	CLA	ND
19	3	1217	CLA	NA
19	H	1079	CLA	C8
19	H	1079	CLA	NC
19	H	1079	CLA	ND
19	H	1079	CLA	NA
19	B	1752	CLA	C8
19	B	1752	CLA	NC
19	B	1752	CLA	ND
19	B	1752	CLA	NA
19	A	1792	CLA	NC
19	A	1792	CLA	ND
19	A	1792	CLA	NA
19	B	1745	CLA	C8
19	B	1745	CLA	NC
19	B	1745	CLA	ND
19	B	1745	CLA	NA
19	A	1770	CLA	NC
19	A	1770	CLA	ND
19	A	1770	CLA	NA
19	A	1775	CLA	NC
19	A	1775	CLA	ND
19	A	1775	CLA	NA
19	K	1146	CLA	NC
19	K	1146	CLA	ND
19	K	1146	CLA	NA
19	A	1766	CLA	NC
19	A	1766	CLA	ND
19	A	1766	CLA	NA
21	B	8055	SUC	C2'
19	A	1769	CLA	NC
19	A	1769	CLA	ND
19	A	1769	CLA	NA
19	A	1763	CLA	NC
19	A	1763	CLA	ND
19	A	1763	CLA	NA
19	4	1202	CLA	NC
19	4	1202	CLA	ND
19	4	1202	CLA	NA
19	B	1747	CLA	C8

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Mol	Chain	Res	Type	Atom
19	B	1747	CLA	NC
19	B	1747	CLA	ND
19	B	1747	CLA	NA
19	B	1760	CLA	NC
19	B	1760	CLA	ND
19	B	1760	CLA	NA

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	1778	BCR	C21-C20-C19-C18
22	3	1220	BCR	C21-C20-C19-C18
22	I	1032	BCR	C20-C21-C22-C23
22	L	1169	BCR	C20-C21-C22-C37
22	A	1803	BCR	C21-C20-C19-C18
22	L	1169	BCR	C20-C21-C22-C23
22	B	1775	BCR	C21-C20-C19-C18
22	A	1803	BCR	C20-C21-C22-C23
22	A	1803	BCR	C20-C21-C22-C37
20	A	7032	LMU	C1-O1'-C1'-O5'
22	B	1780	BCR	C21-C20-C19-C18
22	A	1808	BCR	C21-C20-C19-C18
19	B	1755	CLA	CED-O2D-CGD-CBD
19	B	1737	CLA	CGA-O2A-C1-C2
19	L	1166	CLA	CED-O2D-CGD-CBD
19	R	1054	CLA	CED-O2D-CGD-CBD
20	A	1810	LMU	C1'-O1'-C1-C2
19	J	1045	CLA	CED-O2D-CGD-CBD
19	A	1781	CLA	CED-O2D-CGD-CBD
19	1	1197	CLA	CED-O2D-CGD-CBD
19	J	1043	CLA	CED-O2D-CGD-CBD
19	B	1760	CLA	CED-O2D-CGD-CBD
19	1	1190	CLA	CED-O2D-CGD-CBD
19	A	1798	CLA	CED-O2D-CGD-CBD
19	A	1812	CLA	CED-O2D-CGD-CBD
19	F	1157	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

234 monomers are involved in 3581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1187	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1188	CLA	7	0
19	1	1189	CLA	11	0
19	1	1190	CLA	5	0
19	1	1191	CLA	10	0
19	1	1192	CLA	9	0
19	1	1193	CLA	6	1
19	1	1194	CLA	5	0
19	1	1195	CLA	4	0
19	1	1196	CLA	6	0
19	1	1197	CLA	20	0
19	1	1198	CLA	20	0
19	1	1199	CLA	2	0
19	1	1200	CLA	11	0
20	1	1202	LMU	5	0
20	1	7004	LMU	10	0
19	2	1212	CLA	18	0
19	2	1213	CLA	13	0
19	2	1214	CLA	7	0
19	2	1215	CLA	24	0
19	2	1217	CLA	9	0
19	2	1218	CLA	7	0
19	2	1220	CLA	74	0
19	2	1222	CLA	14	0
19	2	1223	CLA	4	0
19	2	1224	CLA	7	0
20	2	1225	LMU	1	1
21	2	1226	SUC	10	0
20	2	7003	LMU	3	0
20	2	7006	LMU	11	0
19	3	1212	CLA	9	0
19	3	1213	CLA	1	0
19	3	1214	CLA	3	0
19	3	1215	CLA	17	0
19	3	1216	CLA	7	0
19	3	1217	CLA	8	0
19	3	1218	CLA	25	0
19	3	1219	CLA	18	0
22	3	1220	BCR	21	0
21	3	1221	SUC	14	0
19	3	3007	CLA	2	0
19	3	3008	CLA	17	0
19	3	3011	CLA	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	7005	LMU	3	0
19	4	1196	CLA	34	0
19	4	1197	CLA	2	0
19	4	1198	CLA	25	0
19	4	1199	CLA	22	0
19	4	1200	CLA	3	0
19	4	1201	CLA	25	0
19	4	1202	CLA	4	0
19	4	1204	CLA	8	0
19	4	1205	CLA	3	0
19	4	1206	CLA	2	0
19	4	1207	CLA	5	0
19	4	1208	CLA	8	0
19	4	1209	CLA	5	0
19	4	4014	CLA	11	0
19	A	1759	CLA	20	0
19	A	1760	CLA	29	0
19	A	1761	CLA	32	0
19	A	1762	CLA	18	0
19	A	1763	CLA	31	0
19	A	1764	CLA	26	0
19	A	1765	CLA	25	0
19	A	1766	CLA	5	0
19	A	1767	CLA	23	0
19	A	1768	CLA	4	0
19	A	1769	CLA	22	0
19	A	1770	CLA	27	0
19	A	1771	CLA	13	0
19	A	1772	CLA	34	0
19	A	1773	CLA	11	0
19	A	1774	CLA	31	0
19	A	1776	CLA	47	0
19	A	1777	CLA	13	0
19	A	1778	CLA	11	0
19	A	1779	CLA	35	0
19	A	1780	CLA	17	0
19	A	1781	CLA	85	0
19	A	1782	CLA	81	0
19	A	1783	CLA	61	0
19	A	1784	CLA	18	0
19	A	1785	CLA	17	0
19	A	1786	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1787	CLA	26	0
19	A	1788	CLA	40	0
19	A	1789	CLA	20	0
19	A	1790	CLA	16	0
19	A	1791	CLA	24	1
19	A	1792	CLA	22	0
19	A	1793	CLA	35	0
19	A	1794	CLA	21	0
19	A	1795	CLA	40	0
19	A	1796	CLA	63	0
19	A	1797	CLA	35	0
19	A	1798	CLA	29	0
19	A	1799	CLA	7	0
19	A	1800	CLA	31	0
19	A	1801	CLA	15	0
23	A	1802	PQN	12	0
22	A	1803	BCR	41	0
22	A	1804	BCR	22	0
22	A	1805	BCR	48	0
22	A	1806	BCR	36	0
22	A	1807	BCR	62	0
22	A	1808	BCR	43	0
20	A	1809	LMU	4	0
20	A	1810	LMU	4	0
19	A	1811	CLA	20	0
19	A	1812	CLA	35	0
19	A	1813	CLA	33	0
19	A	1815	CLA	19	0
19	A	1816	CLA	35	0
19	A	1817	CLA	9	0
20	A	7009	LMU	9	0
20	A	7010	LMU	8	0
20	A	7013	LMU	9	0
20	A	7016	LMU	42	0
20	A	7017	LMU	3	0
20	A	7019	LMU	2	0
20	A	7020	LMU	21	0
20	A	7021	LMU	24	0
20	A	7022	LMU	11	0
20	A	7023	LMU	26	0
20	A	7025	LMU	1	0
20	A	7026	LMU	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	28	0
20	A	7033	LMU	19	0
20	A	7034	LMU	1	0
20	A	7036	LMU	19	0
20	A	7037	LMU	24	0
20	A	7038	LMU	13	0
20	A	7039	LMU	19	0
20	A	7040	LMU	4	0
20	A	7041	LMU	9	0
20	A	7042	LMU	35	0
20	A	7043	LMU	16	0
19	B	1735	CLA	33	0
19	B	1736	CLA	9	0
19	B	1737	CLA	24	0
19	B	1738	CLA	19	0
19	B	1739	CLA	22	0
19	B	1740	CLA	20	0
19	B	1741	CLA	6	0
19	B	1742	CLA	9	0
19	B	1743	CLA	29	0
19	B	1744	CLA	20	0
19	B	1745	CLA	12	0
19	B	1746	CLA	23	0
19	B	1747	CLA	23	0
19	B	1748	CLA	14	0
19	B	1749	CLA	18	0
19	B	1750	CLA	9	0
19	B	1751	CLA	16	0
19	B	1752	CLA	14	0
19	B	1753	CLA	40	0
19	B	1754	CLA	23	0
19	B	1755	CLA	62	0
19	B	1756	CLA	46	0
19	B	1757	CLA	21	0
19	B	1758	CLA	34	0
19	B	1759	CLA	34	0
19	B	1760	CLA	10	0
19	B	1761	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1762	CLA	28	0
19	B	1763	CLA	13	0
19	B	1764	CLA	21	0
19	B	1765	CLA	20	0
19	B	1766	CLA	3	0
19	B	1767	CLA	15	0
19	B	1768	CLA	48	0
19	B	1769	CLA	25	0
19	B	1770	CLA	24	0
19	B	1771	CLA	24	0
19	B	1772	CLA	2	0
23	B	1773	PQN	33	0
22	B	1774	BCR	8	0
22	B	1775	BCR	20	0
22	B	1776	BCR	20	0
22	B	1777	BCR	31	0
22	B	1778	BCR	30	0
22	B	1779	BCR	46	0
22	B	1780	BCR	53	0
22	B	1781	BCR	17	0
20	B	1782	LMU	1	0
24	B	1783	LMG	30	0
25	B	1784	SF4	18	0
19	B	1785	CLA	22	0
19	B	1786	CLA	43	0
19	B	1787	CLA	50	0
21	B	8052	SUC	15	0
21	B	8053	SUC	1	0
21	B	8054	SUC	9	0
21	B	8055	SUC	9	0
21	B	8056	SUC	5	0
21	B	8059	SUC	18	0
21	B	8060	SUC	7	0
21	B	8061	SUC	1	0
21	B	8062	SUC	20	0
25	C	1082	SF4	5	0
25	C	1083	SF4	4	0
19	F	1155	CLA	1	0
19	F	1156	CLA	13	0
19	F	1157	CLA	13	0
19	G	1099	CLA	6	0
19	H	1079	CLA	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	H	1080	SUC	5	0
19	I	1031	CLA	11	0
22	I	1032	BCR	47	0
19	I	1033	CLA	15	0
19	J	1043	CLA	29	0
19	J	1044	CLA	40	0
19	J	1045	CLA	44	0
19	K	1085	CLA	26	0
20	K	1086	LMU	6	0
19	K	1142	CLA	20	1
19	K	1146	CLA	11	0
19	K	3009	CLA	3	0
19	L	1166	CLA	7	0
19	L	1167	CLA	18	0
19	L	1168	CLA	12	0
22	L	1169	BCR	48	0
22	L	1170	BCR	13	0
20	L	1171	LMU	3	0
19	L	1505	CLA	3	0
19	R	1054	CLA	11	0
19	R	1055	CLA	6	0
20	R	1056	LMU	19	0
20	R	1057	LMU	5	0

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, 95th 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 ²)	Q<0.9
1	1	165/241 (68%)	0.85	25 (15%) 3 2	31, 61, 71, 72	0
2	2	176/269 (65%)	0.45	17 (9%) 10 9	33, 52, 64, 68	0
3	3	162/276 (58%)	0.76	22 (13%) 4 3	49, 79, 110, 112	0
4	4	166/251 (66%)	0.62	24 (14%) 3 3	21, 44, 57, 58	0
5	A	730/758 (96%)	0.22	28 (3%) 44 37	20, 20, 20, 20	0
6	B	733/734 (99%)	0.22	13 (1%) 71 65	20, 20, 20, 20	0
7	C	81/81 (100%)	0.75	12 (14%) 3 3	20, 20, 20, 20	0
8	D	138/212 (65%)	0.30	11 (7%) 15 12	20, 20, 20, 20	0
9	E	65/143 (45%)	0.47	7 (10%) 8 6	20, 20, 20, 20	0
10	F	154/231 (66%)	0.19	11 (7%) 19 15	20, 20, 20, 20	0
11	G	95/167 (56%)	0.45	8 (8%) 14 11	20, 20, 20, 20	0
12	H	69/144 (47%)	0.23	3 (4%) 39 32	20, 20, 20, 20	0
13	I	30/40 (75%)	-0.02	0 100 100	20, 20, 20, 20	0
14	J	42/44 (95%)	0.22	1 (2%) 62 55	20, 20, 20, 20	0
15	K	84/131 (64%)	1.41	23 (27%) 1 1	20, 20, 20, 20	0
16	L	161/216 (74%)	0.26	10 (6%) 24 19	20, 20, 20, 20	0
17	N	85/170 (50%)	0.20	3 (3%) 48 40	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3136/4161 (75%)	0.37	218 (6%) 19 16	20, 20, 65, 112	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	13.1
6	B	491	ASN	10.1
1	1	92	GLY	9.3

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Mol	Chain	Res	Type	RSRZ
3	3	42	PRO	8.7
2	2	123	PRO	8.1
1	1	113	SER	7.3
3	3	40	SER	6.5
16	L	117	ALA	6.5
4	4	67	ILE	6.0
3	3	72	ALA	5.8
11	G	74	TRP	5.7
10	F	152	ASN	5.4
5	A	505	PRO	5.1
1	1	75	ALA	5.0
3	3	58	GLU	4.7
9	E	84	LEU	4.6
4	4	132	GLY	4.6
15	K	21	ALA	4.5
6	B	562	PRO	4.5
3	3	55	ALA	4.5
17	N	77	CYS	4.4
1	1	42	SER	4.4
4	4	114	SER	4.3
15	K	53	ALA	4.2
2	2	122	ASP	4.1
15	K	63	CYS	4.1
1	1	33	PRO	4.1
3	3	91	PRO	4.0
4	4	34	PRO	4.0
4	4	68	GLY	3.9
2	2	117	GLY	3.7
4	4	135	GLY	3.7
2	2	173	ALA	3.7
8	D	151	LYS	3.7
17	N	56	LYS	3.6
9	E	64	PRO	3.6
16	L	116	PRO	3.5
2	2	125	PHE	3.5
15	K	17	LEU	3.5
2	2	139	GLY	3.5
5	A	487	VAL	3.5
8	D	116	ASP	3.5
1	1	93	THR	3.4
15	K	22	GLY	3.3
7	C	34	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
5	A	344	LYS	3.3
15	K	15	THR	3.3
7	C	56	SER	3.2
2	2	207	ALA	3.2
7	C	15	THR	3.2
1	1	164	GLN	3.2
3	3	122	GLY	3.2
2	2	43	TRP	3.2
1	1	80	GLY	3.2
1	1	87	ASN	3.2
15	K	49	THR	3.1
16	L	80	ALA	3.1
5	A	124	TRP	3.1
1	1	79	GLY	3.1
16	L	118	LEU	3.1
6	B	170	ASN	3.1
2	2	116	PRO	3.1
4	4	110	LYS	3.1
15	K	27	ALA	3.1
4	4	147	LEU	3.1
5	A	220	ARG	3.1
5	A	247	GLU	3.0
1	1	173	PRO	3.0
8	D	108	GLU	3.0
1	1	124	PRO	3.0
3	3	90	LEU	3.0
2	2	140	GLY	3.0
4	4	83	TYR	3.0
7	C	54	CYS	3.0
6	B	561	GLY	3.0
15	K	31	ASN	2.9
15	K	77	GLY	2.9
6	B	212	PHE	2.9
1	1	178	ALA	2.9
6	B	210	ASN	2.9
5	A	635	THR	2.9
5	A	506	GLY	2.9
1	1	46	HIS	2.9
15	K	26	LEU	2.9
5	A	659	ALA	2.9
2	2	119	VAL	2.9
1	1	88	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
5	A	500	PRO	2.9
3	3	204	THR	2.9
2	2	92	THR	2.9
4	4	145	PRO	2.8
3	3	202	LEU	2.8
6	B	484	PRO	2.8
4	4	125	SER	2.8
2	2	53	ARG	2.8
9	E	65	VAL	2.8
3	3	54	LEU	2.8
4	4	66	SER	2.8
8	D	115	LYS	2.8
11	G	41	MET	2.8
16	L	96	SER	2.8
15	K	56	THR	2.8
11	G	76	SER	2.8
10	F	38	PRO	2.8
4	4	134	PRO	2.8
6	B	263	PRO	2.8
1	1	175	GLU	2.8
9	E	30	PRO	2.8
15	K	5	SER	2.7
15	K	1	ASP	2.7
5	A	752	ALA	2.7
16	L	49	PRO	2.7
8	D	22	PRO	2.7
1	1	134	SER	2.7
5	A	33	GLN	2.7
4	4	136	GLY	2.7
7	C	80	ALA	2.7
7	C	17	CYS	2.6
2	2	141	LEU	2.6
7	C	55	GLU	2.6
5	A	266	ALA	2.6
3	3	41	ASP	2.6
4	4	146	THR	2.6
6	B	492	ILE	2.6
4	4	131	VAL	2.6
10	F	37	ALA	2.6
5	A	100	GLY	2.6
11	G	87	ALA	2.5
5	A	340	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
5	A	388	ASP	2.5
7	C	37	LYS	2.5
1	1	172	GLY	2.5
10	F	137	PRO	2.5
3	3	73	ILE	2.5
12	H	47	PHE	2.5
1	1	74	TRP	2.5
15	K	65	ALA	2.5
3	3	207	GLY	2.5
9	E	79	THR	2.5
11	G	75	GLY	2.4
3	3	123	PHE	2.4
5	A	494	ASN	2.4
16	L	115	ALA	2.4
16	L	84	GLY	2.4
2	2	78	SER	2.4
4	4	78	ALA	2.4
1	1	24	PHE	2.4
2	2	110	TRP	2.4
4	4	86	SER	2.4
15	K	44	GLU	2.4
3	3	92	TRP	2.4
8	D	21	ASP	2.4
15	K	29	SER	2.4
1	1	95	PRO	2.4
5	A	518	GLY	2.4
14	J	41	PHE	2.4
9	E	34	SER	2.3
15	K	13	THR	2.3
15	K	34	ALA	2.3
6	B	502	ASN	2.3
1	1	177	LEU	2.3
11	G	57	LEU	2.3
4	4	63	VAL	2.3
11	G	4	PRO	2.3
11	G	95	PRO	2.3
5	A	191	PRO	2.3
5	A	486	PRO	2.3
2	2	181	HIS	2.3
16	L	140	THR	2.3
17	N	20	LYS	2.2
10	F	110	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	3	89	ALA	2.2
10	F	135	SER	2.2
10	F	111	GLU	2.2
10	F	124	PRO	2.2
8	D	149	THR	2.2
9	E	92	ALA	2.2
8	D	150	GLY	2.2
15	K	84	LEU	2.2
6	B	487	ASN	2.2
5	A	249	ILE	2.2
8	D	24	THR	2.2
4	4	36	ASN	2.2
10	F	73	VAL	2.2
5	A	662	SER	2.1
12	H	26	SER	2.1
3	3	88	THR	2.1
5	A	484	LEU	2.1
3	3	75	PRO	2.1
1	1	102	PHE	2.1
7	C	50	GLY	2.1
7	C	41	SER	2.1
8	D	141	VAL	2.1
8	D	25	PRO	2.1
12	H	30	SER	2.1
4	4	37	LEU	2.1
4	4	84	PHE	2.1
6	B	558	PRO	2.1
4	4	142	ASN	2.1
5	A	485	GLN	2.1
1	1	72	GLN	2.1
5	A	341	GLN	2.1
5	A	354	TRP	2.1
15	K	50	GLY	2.1
7	C	9	ASP	2.1
3	3	180	LYS	2.1
7	C	36	ALA	2.1
3	3	116	PHE	2.0
6	B	271	THR	2.0
16	L	134	ASP	2.0
10	F	107	ALA	2.0
4	4	39	TRP	2.0
10	F	143	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
5	A	181	ALA	2.0
5	A	265	GLY	2.0
15	K	55	PHE	2.0
3	3	84	ILE	2.0
1	1	140	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
22	BCR	A	1803	40/40	0.57	0.49	9.75	20,20,20,20	0
19	CLA	A	1801	55/65	0.61	0.40	5.26	20,20,20,20	0
19	CLA	2	1217	65/65	0.77	0.37	3.72	20,20,20,20	0
22	BCR	B	1775	40/40	0.80	0.35	3.49	20,20,20,20	0
22	BCR	I	1032	40/40	0.76	0.31	3.39	20,20,20,20	0
19	CLA	4	1202	25/65	0.69	0.34	2.91	20,20,20,20	0
19	CLA	B	1746	46/65	0.67	0.39	2.71	20,20,20,20	0
19	CLA	1	1197	51/65	0.71	0.52	2.69	20,20,20,20	0
19	CLA	A	1793	65/65	0.86	0.28	2.55	20,20,20,20	0
22	BCR	B	1781	40/40	0.87	0.27	2.39	20,20,20,20	0
19	CLA	1	1191	36/65	0.74	0.37	2.33	20,20,20,20	0
22	BCR	A	1806	40/40	0.79	0.35	2.19	20,20,20,20	0
22	BCR	A	1808	40/40	0.68	0.39	2.17	20,20,20,20	0
19	CLA	A	1777	51/65	0.82	0.40	2.06	20,20,20,20	0
19	CLA	4	1200	50/65	0.69	0.44	2.00	20,20,20,20	0
19	CLA	B	1755	58/65	0.68	0.41	1.89	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	B	1772	36/65	0.77	0.30	1.86	20,20,20,20	0
22	BCR	B	1779	40/40	0.83	0.31	1.75	20,20,20,20	0
19	CLA	H	1079	65/65	0.79	0.29	1.68	20,20,20,20	0
22	BCR	L	1170	40/40	0.88	0.26	1.62	20,20,20,20	0
19	CLA	A	1781	65/65	0.80	0.30	1.56	20,20,20,20	0
19	CLA	A	1776	65/65	0.82	0.32	1.52	20,20,20,20	0
24	LMG	B	1783	49/55	0.77	0.34	1.51	20,20,20,20	0
22	BCR	L	1169	40/40	0.72	0.42	1.48	20,20,20,20	0
22	BCR	B	1777	40/40	0.85	0.33	1.47	20,20,20,20	0
19	CLA	A	1787	65/65	0.81	0.28	1.46	20,20,20,20	0
22	BCR	B	1778	40/40	0.85	0.32	1.46	20,20,20,20	0
22	BCR	A	1804	40/40	0.76	0.33	1.35	20,20,20,20	0
19	CLA	A	1785	65/65	0.83	0.31	1.33	20,20,20,20	0
19	CLA	A	1764	65/65	0.90	0.33	1.30	20,20,20,20	0
22	BCR	A	1805	40/40	0.74	0.34	1.25	20,20,20,20	0
19	CLA	B	1759	65/65	0.87	0.32	1.23	20,20,20,20	0
19	CLA	B	1749	61/65	0.86	0.28	1.18	20,20,20,20	0
19	CLA	A	1774	65/65	0.82	0.32	1.17	20,20,20,20	0
22	BCR	B	1780	40/40	0.80	0.36	1.17	20,20,20,20	0
19	CLA	B	1764	45/65	0.79	0.29	1.16	20,20,20,20	0
19	CLA	B	1771	65/65	0.86	0.33	1.16	20,20,20,20	0
19	CLA	B	1735	65/65	0.83	0.30	1.14	20,20,20,20	0
19	CLA	A	1762	57/65	0.85	0.30	1.13	20,20,20,20	0
19	CLA	A	1795	51/65	0.85	0.26	1.06	20,20,20,20	0
19	CLA	A	1760	55/65	0.84	0.29	1.01	20,20,20,20	0
19	CLA	B	1762	65/65	0.80	0.32	0.99	20,20,20,20	0
19	CLA	A	1780	65/65	0.78	0.34	0.95	20,20,20,20	0
19	CLA	B	1787	65/65	0.86	0.31	0.94	20,20,20,20	0
19	CLA	3	1212	36/65	0.73	0.36	0.93	20,20,20,20	0
22	BCR	A	1807	40/40	0.80	0.37	0.93	20,20,20,20	0
19	CLA	I	1031	60/65	0.85	0.23	0.83	20,20,20,20	0
19	CLA	B	1748	60/65	0.88	0.30	0.83	20,20,20,20	0
19	CLA	B	1751	46/65	0.75	0.34	0.81	20,20,20,20	0
19	CLA	A	1775	36/65	0.70	0.29	0.79	20,20,20,20	0
19	CLA	L	1167	47/65	0.86	0.23	0.77	20,20,20,20	0
19	CLA	B	1757	65/65	0.90	0.28	0.75	20,20,20,20	0
19	CLA	B	1741	54/65	0.82	0.30	0.73	20,20,20,20	0
19	CLA	A	1770	45/65	0.70	0.39	0.72	20,20,20,20	0
19	CLA	B	1740	65/65	0.85	0.30	0.72	20,20,20,20	0
19	CLA	B	1758	65/65	0.89	0.30	0.72	20,20,20,20	0
19	CLA	L	1166	50/65	0.81	0.27	0.70	20,20,20,20	0
19	CLA	B	1739	65/65	0.90	0.28	0.68	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	BCR	B	1774	40/40	0.79	0.34	0.68	20,20,20,20	0
19	CLA	G	1099	51/65	0.70	0.35	0.67	20,20,20,20	0
19	CLA	A	1792	51/65	0.83	0.28	0.66	20,20,20,20	0
21	SUC	2	1226	22/23	0.77	0.27	0.66	20,20,20,20	0
19	CLA	3	3002	25/65	0.75	0.31	0.64	20,20,20,20	0
19	CLA	A	1779	55/65	0.88	0.23	0.63	20,20,20,20	0
19	CLA	A	1789	65/65	0.85	0.27	0.59	20,20,20,20	0
19	CLA	A	1761	65/65	0.83	0.29	0.57	20,20,20,20	0
19	CLA	B	1770	65/65	0.85	0.30	0.56	20,20,20,20	0
19	CLA	B	1736	45/65	0.81	0.27	0.56	20,20,20,20	0
19	CLA	A	1759	50/65	0.88	0.25	0.56	20,20,20,20	0
19	CLA	A	1783	65/65	0.91	0.30	0.56	20,20,20,20	0
19	CLA	A	1769	54/65	0.83	0.27	0.56	20,20,20,20	0
23	PQN	A	1802	33/33	0.87	0.31	0.56	20,20,20,20	0
19	CLA	B	1744	65/65	0.83	0.30	0.55	20,20,20,20	0
19	CLA	A	1811	65/65	0.89	0.31	0.53	20,20,20,20	0
19	CLA	B	1769	47/65	0.87	0.29	0.51	20,20,20,20	0
19	CLA	B	1786	65/65	0.90	0.27	0.49	20,20,20,20	0
19	CLA	B	1767	60/65	0.84	0.28	0.47	20,20,20,20	0
19	CLA	B	1785	65/65	0.86	0.30	0.45	20,20,20,20	0
19	CLA	A	1763	46/65	0.74	0.36	0.40	20,20,20,20	0
19	CLA	A	1800	65/65	0.86	0.27	0.38	20,20,20,20	0
19	CLA	A	1794	47/65	0.87	0.27	0.38	20,20,20,20	0
19	CLA	B	1737	65/65	0.89	0.25	0.37	20,20,20,20	0
19	CLA	A	1812	65/65	0.85	0.31	0.35	20,20,20,20	0
19	CLA	K	3009	65/65	0.72	0.34	0.33	20,20,20,20	0
19	CLA	4	1204	55/65	0.79	0.24	0.32	20,20,20,20	0
19	CLA	B	1753	65/65	0.85	0.25	0.32	20,20,20,20	0
19	CLA	A	1773	52/65	0.83	0.24	0.29	20,20,20,20	0
19	CLA	B	1756	65/65	0.82	0.32	0.27	20,20,20,20	0
19	CLA	B	1750	50/65	0.83	0.26	0.27	20,20,20,20	0
19	CLA	4	1199	55/65	0.74	0.31	0.27	20,20,20,20	0
20	LMU	L	1171	35/35	0.77	0.24	0.26	20,20,20,20	0
19	CLA	B	1761	50/65	0.85	0.25	0.26	20,20,20,20	0
19	CLA	A	1784	55/65	0.85	0.28	0.26	20,20,20,20	0
19	CLA	B	1760	50/65	0.89	0.24	0.26	20,20,20,20	0
19	CLA	B	1738	65/65	0.90	0.27	0.22	20,20,20,20	0
19	CLA	2	1222	50/65	0.84	0.28	0.20	20,20,20,20	0
19	CLA	A	1813	65/65	0.85	0.29	0.20	20,20,20,20	0
19	CLA	B	1765	45/65	0.67	0.39	0.19	20,20,20,20	0
22	BCR	B	1776	40/40	0.77	0.33	0.18	20,20,20,20	0
20	LMU	A	7047	35/35	0.72	0.25	0.18	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	PQN	B	1773	33/33	0.91	0.29	0.16	20,20,20,20	0
19	CLA	B	1763	50/65	0.84	0.27	0.15	20,20,20,20	0
19	CLA	A	1788	65/65	0.88	0.27	0.15	20,20,20,20	0
19	CLA	B	1745	60/65	0.76	0.31	0.13	20,20,20,20	0
19	CLA	B	1768	65/65	0.89	0.26	0.04	20,20,20,20	0
19	CLA	1	1192	61/65	0.80	0.26	0.04	20,20,20,20	0
19	CLA	B	1742	55/65	0.82	0.26	-0.09	20,20,20,20	0
19	CLA	A	1798	55/65	0.72	0.29	-0.12	20,20,20,20	0
19	CLA	A	1786	50/65	0.88	0.21	-0.12	20,20,20,20	0
19	CLA	A	1772	65/65	0.83	0.23	-0.16	2,35,60,60	0
19	CLA	2	1215	50/65	0.73	0.27	-0.19	20,20,20,20	0
19	CLA	A	1767	65/65	0.85	0.28	-0.19	20,20,20,20	0
19	CLA	1	1189	47/65	0.75	0.27	-0.20	20,20,20,20	0
19	CLA	3	1218	65/65	0.72	0.28	-0.22	20,20,20,20	0
19	CLA	B	1754	54/65	0.90	0.23	-0.24	20,20,20,20	0
19	CLA	A	1790	50/65	0.86	0.23	-0.25	20,20,20,20	0
20	LMU	A	1809	35/35	0.75	0.20	-0.26	20,20,20,20	0
19	CLA	A	1782	65/65	0.86	0.23	-0.28	20,20,20,20	0
19	CLA	A	1771	50/65	0.79	0.29	-0.29	20,20,20,20	0
19	CLA	F	1155	36/65	0.88	0.20	-0.29	20,20,20,20	0
19	CLA	A	1778	42/65	0.72	0.30	-0.29	20,20,20,20	0
19	CLA	B	1747	59/65	0.86	0.24	-0.29	20,20,20,20	0
19	CLA	A	1796	65/65	0.84	0.29	-0.29	20,20,20,20	0
19	CLA	B	1752	55/65	0.86	0.22	-0.31	20,20,20,20	0
19	CLA	2	1221	25/65	0.78	0.31	-0.32	20,20,20,20	0
19	CLA	A	1766	45/65	0.81	0.26	-0.37	20,20,20,20	0
19	CLA	F	1156	41/65	0.74	0.28	-0.38	20,20,20,20	0
19	CLA	A	1765	55/65	0.86	0.26	-0.39	20,20,20,20	0
19	CLA	L	1168	50/65	0.81	0.23	-0.47	20,20,20,20	0
19	CLA	4	1197	36/65	0.81	0.24	-0.51	20,20,20,20	0
19	CLA	3	1214	25/65	0.58	0.27	-0.58	20,20,20,20	0
19	CLA	1	1199	25/65	0.73	0.25	-0.60	20,20,20,20	0
19	CLA	B	1743	65/65	0.89	0.22	-0.62	20,20,20,20	0
20	LMU	A	1810	35/35	0.77	0.17	-0.65	20,20,20,20	0
19	CLA	1	1195	36/65	0.83	0.27	-0.68	20,20,20,20	0
19	CLA	4	1207	36/65	0.85	0.21	-0.70	20,20,20,20	0
19	CLA	3	1215	25/65	0.76	0.26	-0.85	20,20,20,20	0
19	CLA	1	1196	36/65	0.81	0.25	-0.88	20,20,20,20	0
19	CLA	4	1206	25/65	0.88	0.17	-1.04	20,20,20,20	0
19	CLA	4	1201	52/65	0.83	0.20	-1.12	20,20,20,20	0
19	CLA	4	1196	55/65	0.75	0.25	-1.28	20,20,20,20	0
19	CLA	1	1190	46/65	0.82	0.22	-1.33	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	3	1213	25/65	0.78	0.19	-1.70	20,20,20,20	0
25	SF4	B	1784	8/8	0.98	0.06	-1.75	20,20,20,20	0
25	SF4	C	1082	8/8	0.97	0.09	-2.05	20,20,20,20	0
25	SF4	C	1083	8/8	0.98	0.06	-3.35	20,20,20,20	0
19	CLA	2	1223	50/65	0.77	0.26	-	20,20,20,20	0
19	CLA	4	1208	25/65	0.81	0.18	-	20,20,20,20	0
19	CLA	4	1203	25/65	0.75	0.24	-	20,20,20,20	0
20	LMU	R	1057	35/35	0.69	0.38	-	20,20,20,20	0
21	SUC	B	8060	23/23	0.87	0.28	-	20,20,20,20	0
21	SUC	B	8054	23/23	0.72	0.25	-	20,20,20,20	0
20	LMU	A	7033	35/35	0.77	0.21	-	20,20,20,20	0
19	CLA	1	1194	25/65	0.72	0.25	-	20,20,20,20	0
21	SUC	B	8052	23/23	0.72	0.45	-	20,20,20,20	0
20	LMU	A	7039	35/35	0.81	0.19	-	20,20,20,20	0
19	CLA	2	1219	25/65	0.75	0.23	-	20,20,20,20	0
21	SUC	B	8059	23/23	0.86	0.23	-	20,20,20,20	0
19	CLA	A	1768	54/65	0.83	0.23	-	20,20,20,20	0
20	LMU	A	7017	35/35	0.71	0.21	-	20,20,20,20	0
20	LMU	3	7005	35/35	0.71	0.31	-	20,20,20,20	0
19	CLA	4	1198	65/65	0.72	0.26	-	20,20,20,20	0
19	CLA	I	1033	55/65	0.68	0.28	-	20,20,20,20	0
20	LMU	A	7042	35/35	0.73	0.23	-	20,20,20,20	0
19	CLA	2	1227	25/65	0.69	0.56	-	20,20,20,20	0
19	CLA	1	1187	46/65	0.71	0.27	-	20,20,20,20	0
20	LMU	A	7010	35/35	0.73	0.32	-	20,20,20,20	0
21	SUC	B	8061	23/23	0.74	0.32	-	20,20,20,20	0
19	CLA	2	1213	56/65	0.79	0.22	-	20,20,20,20	0
19	CLA	K	1085	50/65	0.78	0.28	-	20,20,20,20	0
19	CLA	J	1043	61/65	0.73	0.30	-	20,20,20,20	0
19	CLA	4	1209	46/65	0.78	0.33	-	20,20,20,20	0
19	CLA	A	1817	46/65	0.72	0.33	-	20,20,20,20	0
19	CLA	2	1216	25/65	0.62	0.30	-	20,20,20,20	0
21	SUC	H	1080	23/23	0.71	0.30	-	20,20,20,20	0
19	CLA	3	3011	65/65	0.81	0.26	-	20,20,20,20	0
20	LMU	A	7032	35/35	0.82	0.33	-	20,20,20,20	0
19	CLA	A	1815	55/65	0.71	0.27	-	20,20,20,20	0
20	LMU	4	1210	35/35	0.77	0.29	-	20,20,20,20	0
19	CLA	2	1214	25/65	0.76	0.41	-	20,20,20,20	0
19	CLA	B	1766	51/65	0.62	0.39	-	20,20,20,20	0
19	CLA	R	1055	65/65	0.72	0.33	-	20,20,20,20	0
20	LMU	A	7038	35/35	0.66	0.37	-	20,20,20,20	0
20	LMU	B	1782	25/35	0.78	0.20	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	J	1046	25/65	0.50	0.56	-	5,42,60,60	0
21	SUC	B	8056	23/23	0.81	0.16	-	20,20,20,20	0
20	LMU	A	7024	35/35	0.80	0.18	-	20,20,20,20	0
19	CLA	1	1200	51/65	0.71	0.37	-	20,20,20,20	0
19	CLA	R	1054	57/65	0.72	0.28	-	20,20,20,20	0
19	CLA	1	1198	61/65	0.70	0.27	-	2,35,60,60	0
19	CLA	A	1816	55/65	0.74	0.32	-	20,20,20,20	0
21	SUC	B	8053	23/23	0.54	0.38	-	3,33,60,60	0
20	LMU	A	7035	35/35	0.81	0.26	-	20,20,20,20	0
20	LMU	A	7030	35/35	0.70	0.35	-	20,20,20,20	0
20	LMU	A	7022	35/35	0.77	0.20	-	20,20,20,20	0
20	LMU	2	1225	35/35	0.59	0.30	-	20,20,20,20	0
20	LMU	A	7020	35/35	0.81	0.23	-	20,20,20,20	0
19	CLA	A	1799	50/65	0.69	0.40	-	20,20,20,20	0
19	CLA	L	1505	55/65	0.62	0.36	-	20,20,20,20	0
20	LMU	A	7043	35/35	0.71	0.19	-	20,20,20,20	0
19	CLA	1	1188	47/65	0.80	0.26	-	20,20,20,20	0
20	LMU	A	7040	35/35	0.75	0.20	-	20,20,20,20	0
20	LMU	R	1056	35/35	0.80	0.22	-	20,20,20,20	0
19	CLA	2	1224	65/65	0.81	0.23	-	20,20,20,20	0
20	LMU	A	7009	34/35	0.69	0.33	-	20,20,20,20	0
19	CLA	2	1218	65/65	0.70	0.28	-	20,20,20,20	0
20	LMU	A	7025	35/35	0.69	0.24	-	20,20,20,20	0
20	LMU	A	7026	35/35	0.75	0.29	-	20,20,20,20	0
20	LMU	A	7023	35/35	0.82	0.24	-	20,20,20,20	0
19	CLA	4	4007	52/65	0.69	0.36	-	20,20,20,20	0
19	CLA	3	3014	25/65	0.66	0.50	-	20,20,20,20	0
19	CLA	F	1157	53/65	0.73	0.37	-	20,20,20,20	0
21	SUC	B	8062	23/23	0.82	0.29	-	20,20,20,20	0
20	LMU	K	1086	35/35	0.77	0.21	-	20,20,20,20	0
26	UNL	B	8057	23/-	0.80	0.17	-	20,20,20,20	0
22	BCR	3	1220	40/40	0.71	0.25	-	20,20,20,20	0
19	CLA	2	2010	25/65	0.76	0.29	-	20,20,20,20	0
19	CLA	1	1201	25/65	0.77	0.27	-	20,20,20,20	0
19	CLA	3	1219	65/65	0.66	0.46	-	20,20,20,20	0
19	CLA	J	1044	61/65	0.66	0.32	-	20,20,20,20	0
20	LMU	A	7036	34/35	0.80	0.28	-	20,20,20,20	0
19	CLA	4	1205	25/65	0.79	0.23	-	20,20,20,20	0
20	LMU	A	7021	35/35	0.72	0.26	-	20,20,20,20	0
19	CLA	2	1220	56/65	0.69	0.27	-	2,36,60,60	0
20	LMU	A	7037	35/35	0.66	0.24	-	20,20,20,20	0
19	CLA	K	1142	45/65	0.69	0.26	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	LMU	1	7004	35/35	0.62	0.43	-	20,20,20,20	0
20	LMU	A	7015	35/35	0.66	0.40	-	20,20,20,20	0
20	LMU	A	7019	35/35	0.78	0.20	-	20,20,20,20	0
19	CLA	4	4003	25/65	0.58	0.31	-	20,20,20,20	0
19	CLA	3	3008	50/65	0.78	0.31	-	20,20,20,20	0
20	LMU	A	7028	35/35	0.81	0.18	-	20,20,20,20	0
19	CLA	3	3015	25/65	0.75	0.33	-	20,20,20,20	0
20	LMU	A	7034	35/35	0.74	0.25	-	20,20,20,20	0
20	LMU	A	7013	35/35	0.57	0.31	-	20,20,20,20	0
19	CLA	3	3007	42/65	0.75	0.30	-	20,20,20,20	0
20	LMU	A	7027	35/35	0.76	0.22	-	20,20,20,20	0
19	CLA	4	4014	47/65	0.68	0.32	-	20,20,20,20	0
21	SUC	B	8051	23/23	0.77	0.33	-	20,20,20,20	0
19	CLA	3	1217	25/65	0.62	0.25	-	20,20,20,20	0
20	LMU	A	7031	35/35	0.70	0.28	-	20,20,20,20	0
19	CLA	A	1797	65/65	0.65	0.27	-	20,20,20,20	0
19	CLA	J	1045	55/65	0.79	0.22	-	2,33,60,60	0
20	LMU	2	7006	35/35	0.78	0.21	-	20,20,20,20	0
21	SUC	3	1221	23/23	0.83	0.30	-	20,20,20,20	0
20	LMU	2	7003	35/35	0.74	0.24	-	20,20,20,20	0
20	LMU	A	7041	35/35	0.66	0.23	-	20,20,20,20	0
19	CLA	K	1146	50/65	0.72	0.30	-	20,20,20,20	0
19	CLA	3	1216	25/65	0.74	0.20	-	20,20,20,20	0
21	SUC	B	8055	23/23	0.86	0.26	-	20,20,20,20	0
20	LMU	A	7016	35/35	0.81	0.24	-	20,20,20,20	0
20	LMU	1	1202	35/35	0.72	0.34	-	20,20,20,20	0
19	CLA	1	1193	51/65	0.74	0.37	-	20,20,20,20	0
19	CLA	A	1791	45/65	0.74	0.27	-	20,20,20,20	0
19	CLA	2	1212	51/65	0.64	0.27	-	20,20,20,20	0
19	CLA	3	3001	25/65	0.78	0.31	-	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.