



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:26 AM GMT

PDB ID : 2WSF  
Title : Improved Model of Plant Photosystem I  
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.  
Deposited on : 2009-09-05  
Resolution : 3.48 Å(reported)

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

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

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

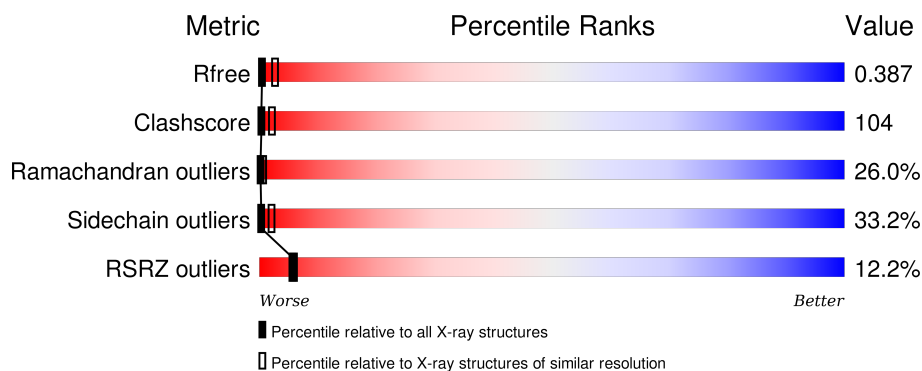
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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

Mol	Chain	Length	Quality of chain
1	1	241	<div> <div>17%</div> <div>27%</div> <div>29%</div> <div>10%</div> <div>•</div> <div>32%</div> </div>
2	2	269	<div> <div>14%</div> <div>10%</div> <div>23%</div> <div>23%</div> <div>10%</div> <div>35%</div> </div>
3	3	276	<div> <div>11%</div> <div>15%</div> <div>21%</div> <div>13%</div> <div>5%</div> <div>45%</div> </div>
4	4	251	<div> <div>5%</div> <div>7%</div> <div>22%</div> <div>25%</div> <div>12%</div> <div>34%</div> </div>
5	A	758	<div> <div>7%</div> <div>10%</div> <div>50%</div> <div>30%</div> <div>7%</div> <div>•</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	1014	X	-	-	-
19	CLA	1	1142	X	-	-	-
19	CLA	1	1143	X	-	X	-
19	CLA	1	1145	X	-	-	-
19	CLA	1	1146	X	-	-	-
19	CLA	1	1148	X	-	-	-
19	CLA	1	1149	X	-	-	-
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	-	-	-
19	CLA	1	1192	X	-	-	-
19	CLA	1	1193	X	-	-	-
19	CLA	1	1194	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	1195	X	-	-	-
19	CLA	1	1196	X	-	-	-
19	CLA	1	1197	X	-	-	X
19	CLA	1	1198	X	-	-	-
19	CLA	1	1199	X	-	-	-
19	CLA	1	1200	X	-	-	-
19	CLA	1	1307	X	-	-	-
19	CLA	1	1308	X	-	-	-
19	CLA	1	1309	X	-	-	-
19	CLA	1	1505	X	-	-	-
19	CLA	2	1212	X	-	-	-
19	CLA	2	1213	X	-	X	-
19	CLA	2	1214	X	-	-	-
19	CLA	2	1215	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	-	-	-
19	CLA	2	1221	X	-	X	-
19	CLA	2	1222	X	-	-	-
19	CLA	2	1223	X	-	-	-
19	CLA	2	2006	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	3	1212	X	-	-	X
19	CLA	3	1213	X	-	-	-
19	CLA	3	1214	X	-	-	-
19	CLA	3	1215	X	-	-	-
19	CLA	3	1216	X	-	-	-
19	CLA	3	1217	X	-	-	-
19	CLA	3	1218	X	-	-	-
19	CLA	3	1219	X	-	-	-
19	CLA	3	1220	X	-	-	-
19	CLA	3	1221	X	-	-	-
19	CLA	3	1222	X	-	-	-
19	CLA	3	3001	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	1198	X	-	-	-
19	CLA	4	1199	X	-	X	-
19	CLA	4	1200	X	-	-	X
19	CLA	4	1201	X	-	-	-
19	CLA	4	1202	X	-	-	-
19	CLA	4	1203	X	-	-	-
19	CLA	4	1204	X	-	-	-
19	CLA	4	1205	X	-	X	-
19	CLA	4	1206	X	-	-	-
19	CLA	4	1207	X	-	-	-
19	CLA	4	1208	X	-	-	-
19	CLA	4	1209	X	-	-	-
19	CLA	4	1210	X	-	-	-
19	CLA	4	1211	X	-	-	-
19	CLA	4	4007	X	-	-	-
19	CLA	4	4014	X	-	-	-
19	CLA	A	1759	X	-	-	-
19	CLA	A	1760	X	-	X	-
19	CLA	A	1761	X	-	-	-
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	-	-	-
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	X
19	CLA	A	1777	X	-	-	-
19	CLA	A	1778	X	-	-	-
19	CLA	A	1779	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	X	-
19	CLA	A	1790	X	-	-	-
19	CLA	A	1791	X	-	-	-
19	CLA	A	1792	X	-	-	X
19	CLA	A	1793	X	-	-	-
19	CLA	A	1794	X	-	-	-
19	CLA	A	1795	X	-	-	-
19	CLA	A	1796	X	-	X	-
19	CLA	A	1797	X	-	X	-
19	CLA	A	1798	X	-	-	-
19	CLA	A	1799	X	-	-	-
19	CLA	A	1800	X	-	X	-
19	CLA	A	1801	X	-	-	X
19	CLA	A	1813	X	-	X	-
19	CLA	A	1814	X	-	X	-
19	CLA	A	1815	X	-	X	-
19	CLA	A	1816	X	-	-	-
19	CLA	A	1817	X	-	X	-
19	CLA	B	1735	X	-	X	-
19	CLA	B	1736	X	-	-	-
19	CLA	B	1737	X	-	X	-
19	CLA	B	1738	X	-	X	-
19	CLA	B	1739	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
19	CLA	B	1747	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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1755	X	-	X	-
19	CLA	B	1756	X	-	X	-
19	CLA	B	1757	X	-	-	-
19	CLA	B	1758	X	-	X	-
19	CLA	B	1759	X	-	X	-
19	CLA	B	1760	X	-	-	-
19	CLA	B	1761	X	-	X	-
19	CLA	B	1762	X	-	X	-
19	CLA	B	1763	X	-	-	-
19	CLA	B	1764	X	-	X	-
19	CLA	B	1765	X	-	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	-	-	-
19	CLA	B	1771	X	-	-	-
19	CLA	B	1772	X	-	-	-
19	CLA	B	1784	X	-	-	-
19	CLA	F	1155	X	-	-	-
19	CLA	F	1156	X	-	-	-
19	CLA	F	1157	X	-	-	-
19	CLA	G	1099	X	-	-	X
19	CLA	H	1079	X	-	X	-
19	CLA	H	1080	X	-	-	-
19	CLA	H	1081	X	-	-	-
19	CLA	I	1031	X	-	-	-
19	CLA	J	1043	X	-	-	-
19	CLA	L	1167	X	-	X	-
19	CLA	L	1168	X	-	-	-
19	CLA	R	1054	X	-	-	-
19	CLA	R	1055	X	-	-	-
20	LMU	2	1224	-	-	X	-
20	LMU	A	7008	-	-	X	-
20	LMU	A	7016	-	-	X	-
20	LMU	A	7042	-	-	X	-
21	SUC	2	1225	X	-	X	-
21	SUC	3	1223	X	-	-	-
21	SUC	B	8051	X	-	-	-
21	SUC	B	8052	X	-	-	-
21	SUC	B	8053	X	-	-	-
21	SUC	B	8054	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	SUC	B	8055	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	1082	X	-	X	-
22	PQN	A	1802	X	-	-	-
22	PQN	B	1773	X	-	X	-
23	BCR	A	1803	-	-	X	X
23	BCR	A	1804	-	-	X	X
23	BCR	A	1805	-	-	X	-
23	BCR	A	1806	-	-	X	-
23	BCR	A	1808	-	-	X	-
23	BCR	B	1774	-	-	-	X
23	BCR	B	1777	-	-	X	-
23	BCR	B	1778	-	-	X	-
23	BCR	B	1779	-	-	X	-
23	BCR	B	1780	-	-	X	-
23	BCR	I	1032	-	-	X	X
23	BCR	L	1169	-	-	X	X
25	SF4	B	1783	-	-	X	-
25	SF4	C	1082	-	-	X	-



## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36033 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	153	Total	C	N	O	S	0	0	0
			1186	781	193	207	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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	162	Total	C	N	O	S	0	0	0
			1215	800	194	216	5			

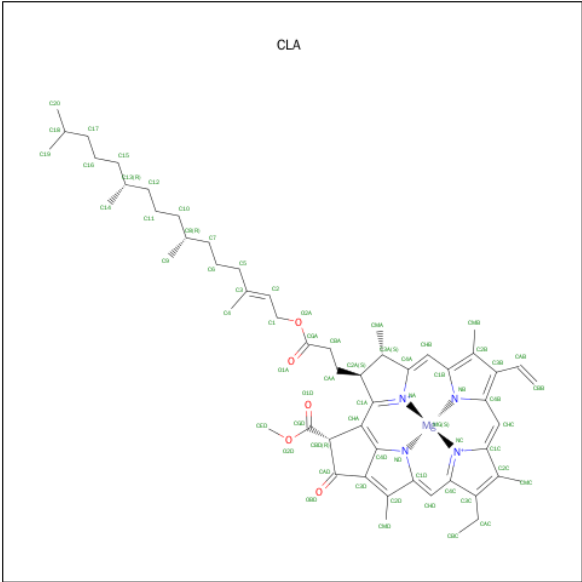
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
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		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
			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
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
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	O	0	0
			42	34	1	4	3		
19	3	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
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			

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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	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		0	0
			25	20	1	4			
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
			65	55	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
			46	36	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
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			56	46	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
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	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
			58	48	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
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	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
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			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
			59	49	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		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	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		
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
			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
			25	20	1	4			
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
			60	50	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
			53	43	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
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		

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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
			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		
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
			59	49	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		

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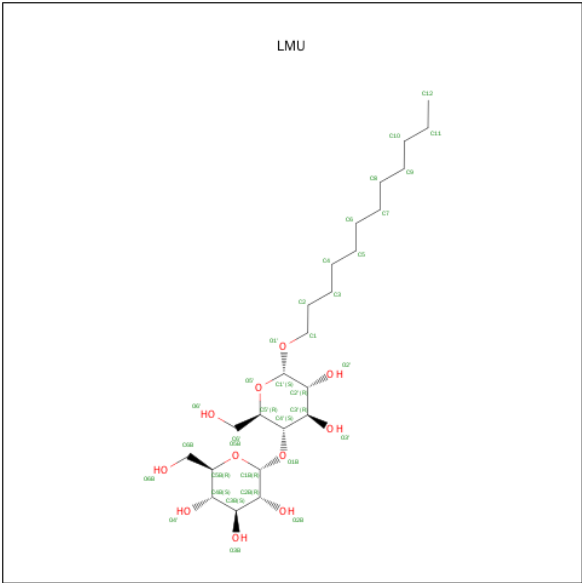
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			50	40	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	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	1	1	Total	C	Mg	N	O	0	0
			51	41	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
			50	40	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			48	38	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
			55	45	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
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	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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



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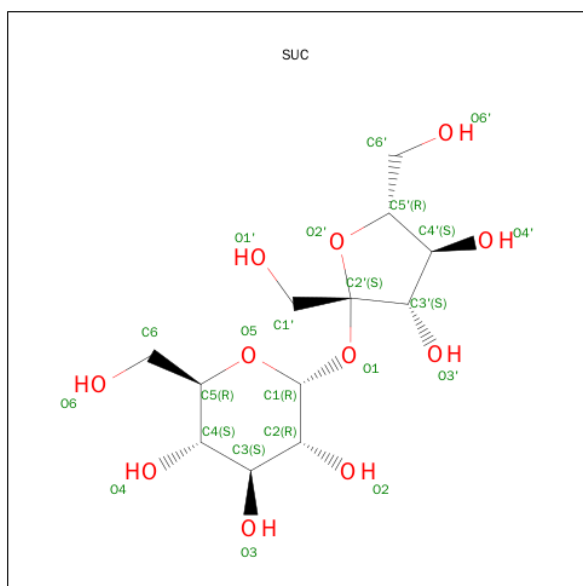
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

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



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

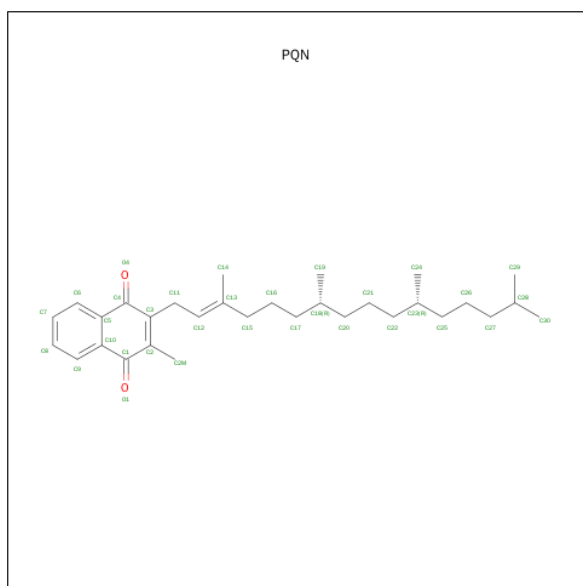
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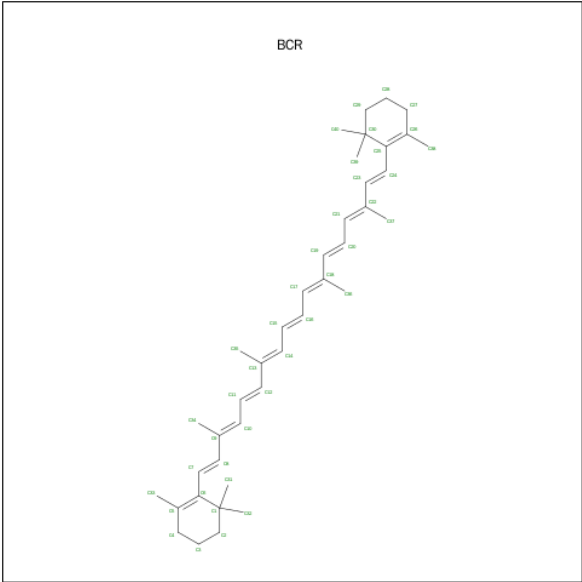
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



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

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



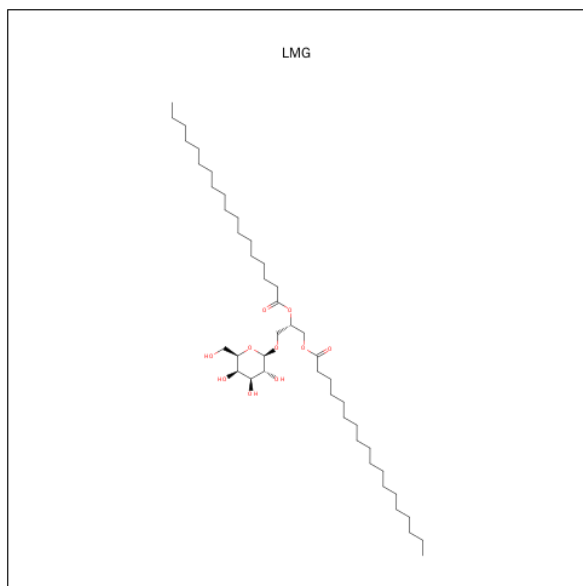
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 39 39	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0

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

- 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 49 39 10	0	0

- 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		

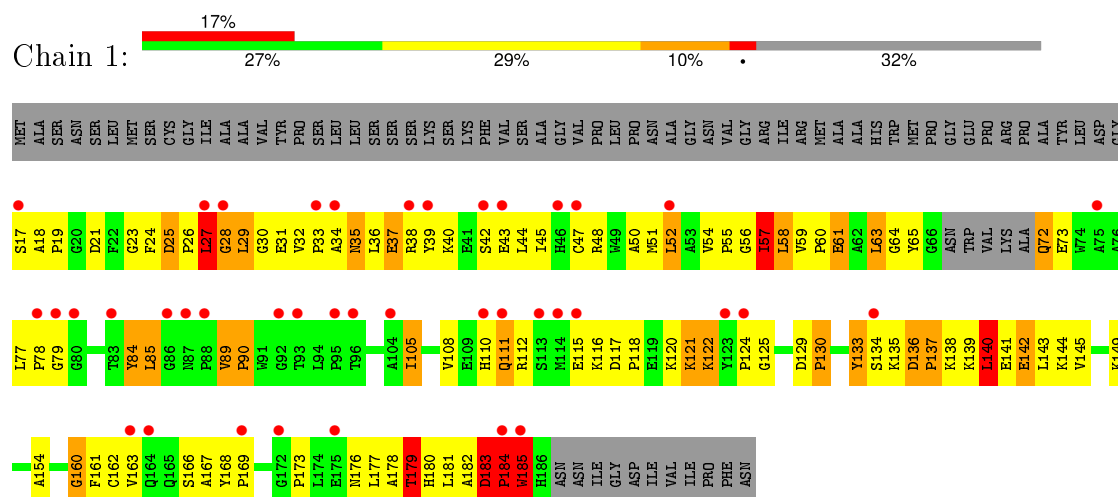
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

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

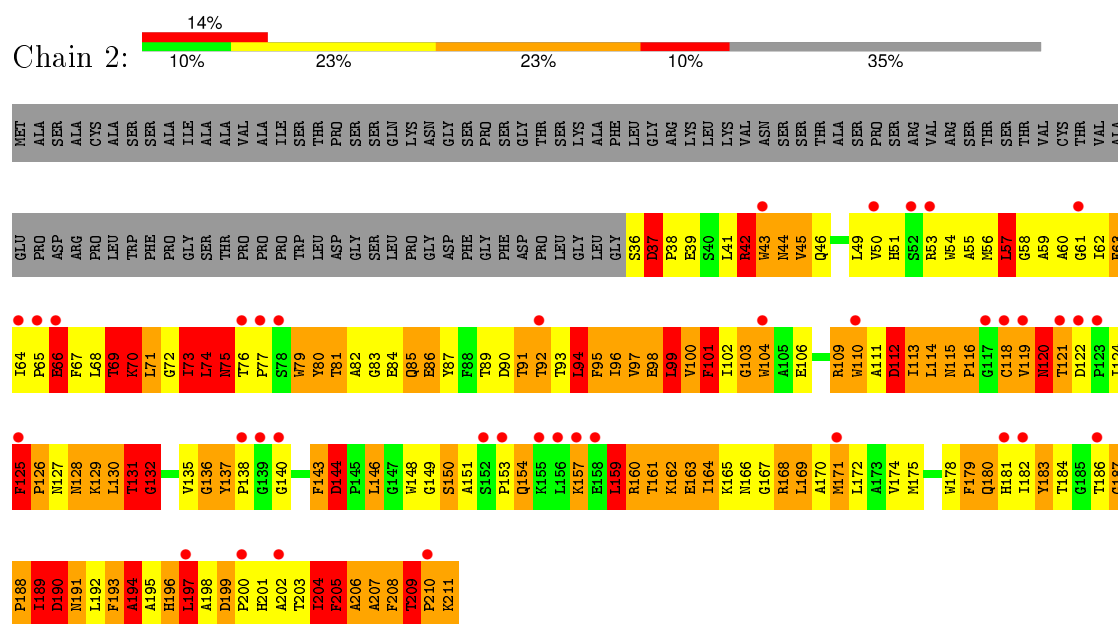
### 3 Residue-property plots

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.

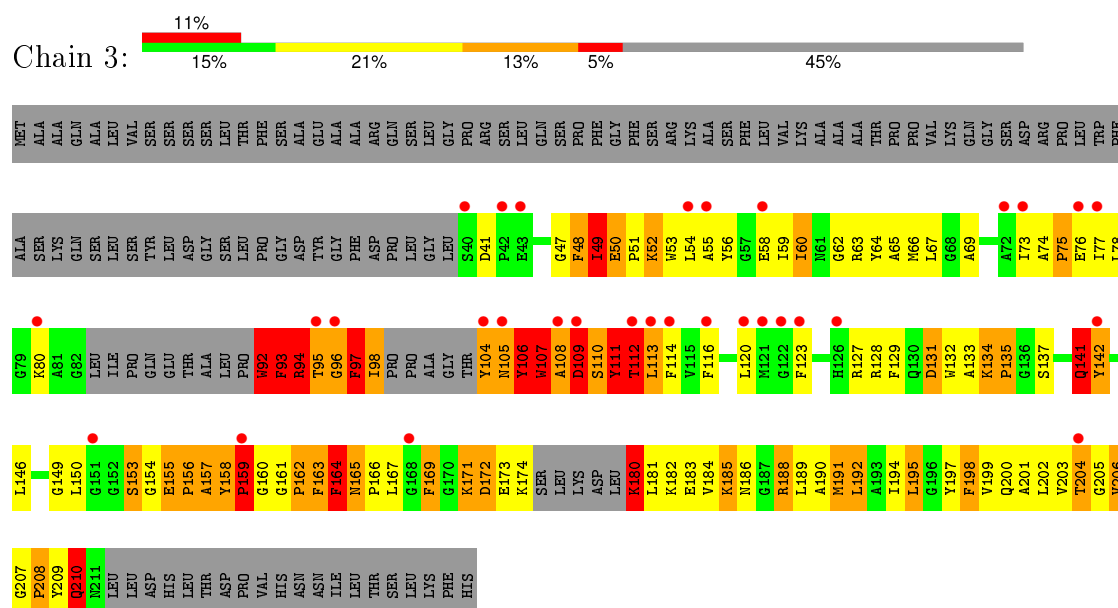
#### • Molecule 1: AT3G54890



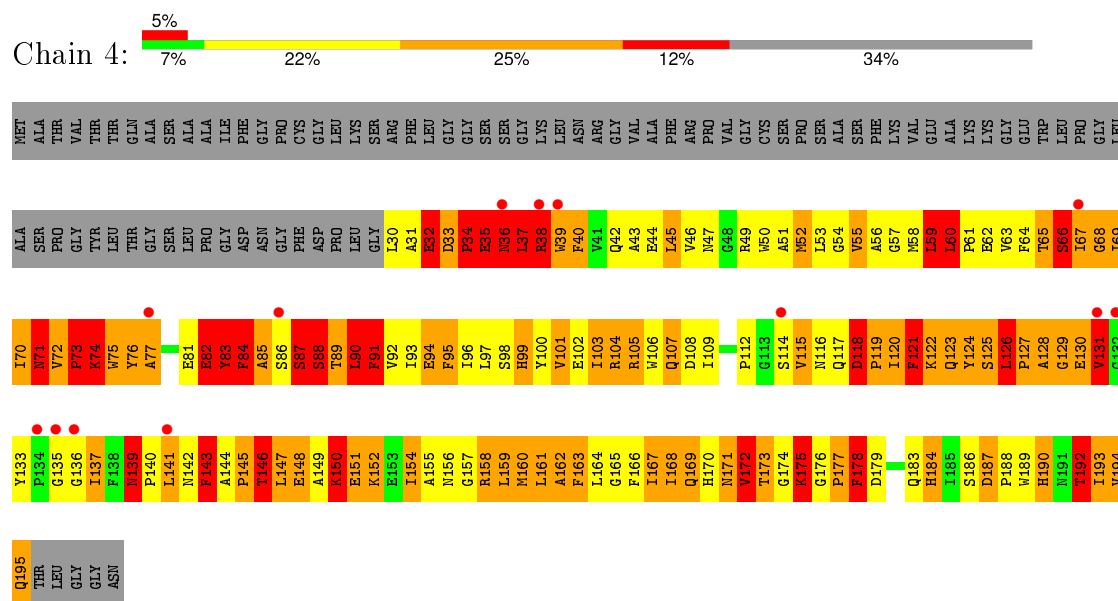
#### • Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I



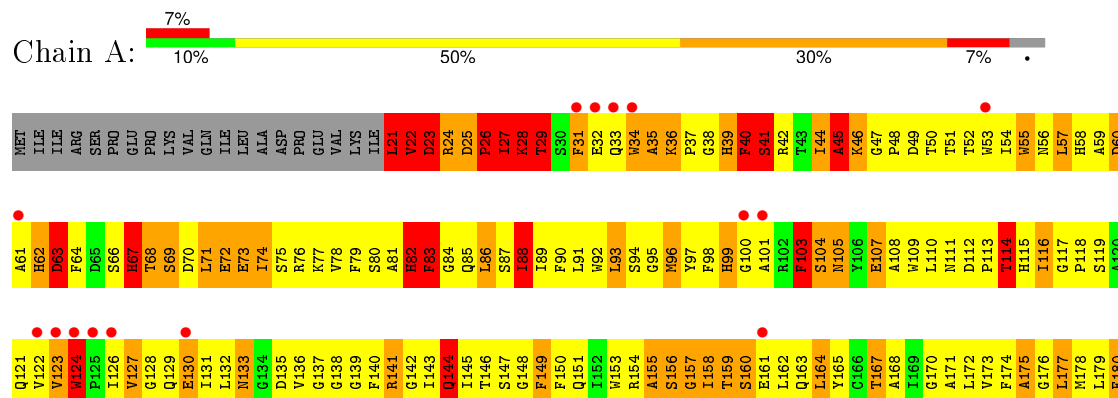
#### • Molecule 3: LHCA3

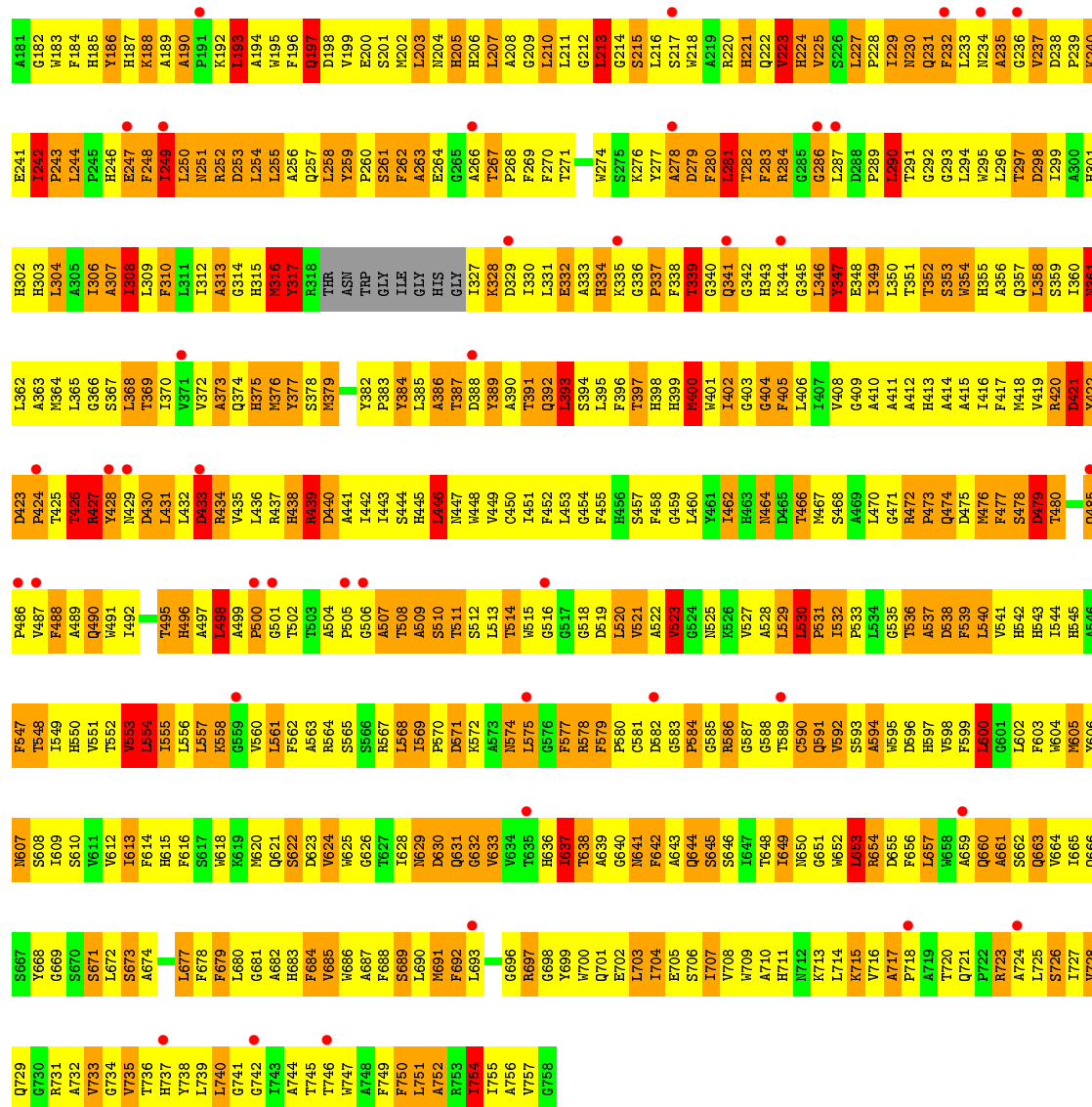


• Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC

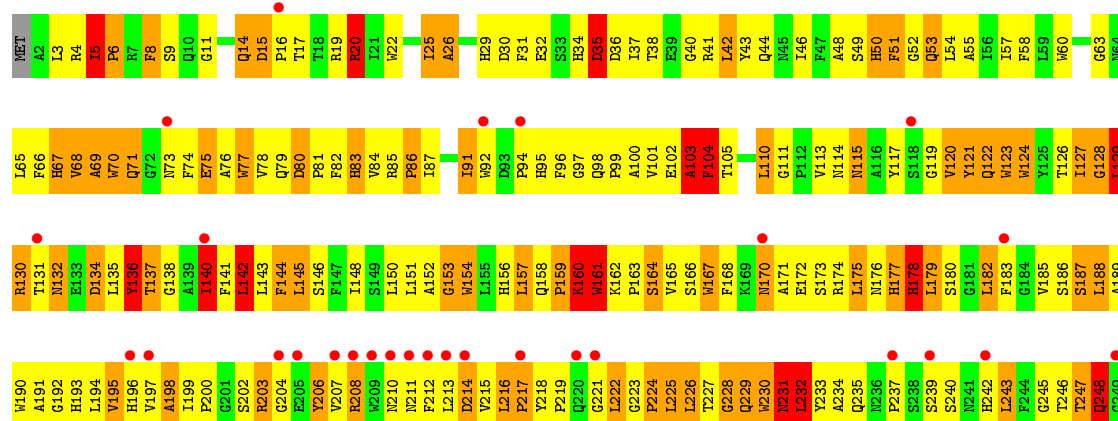
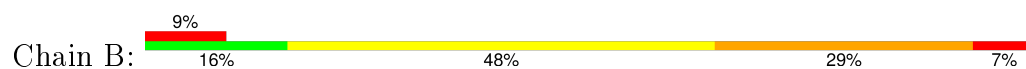


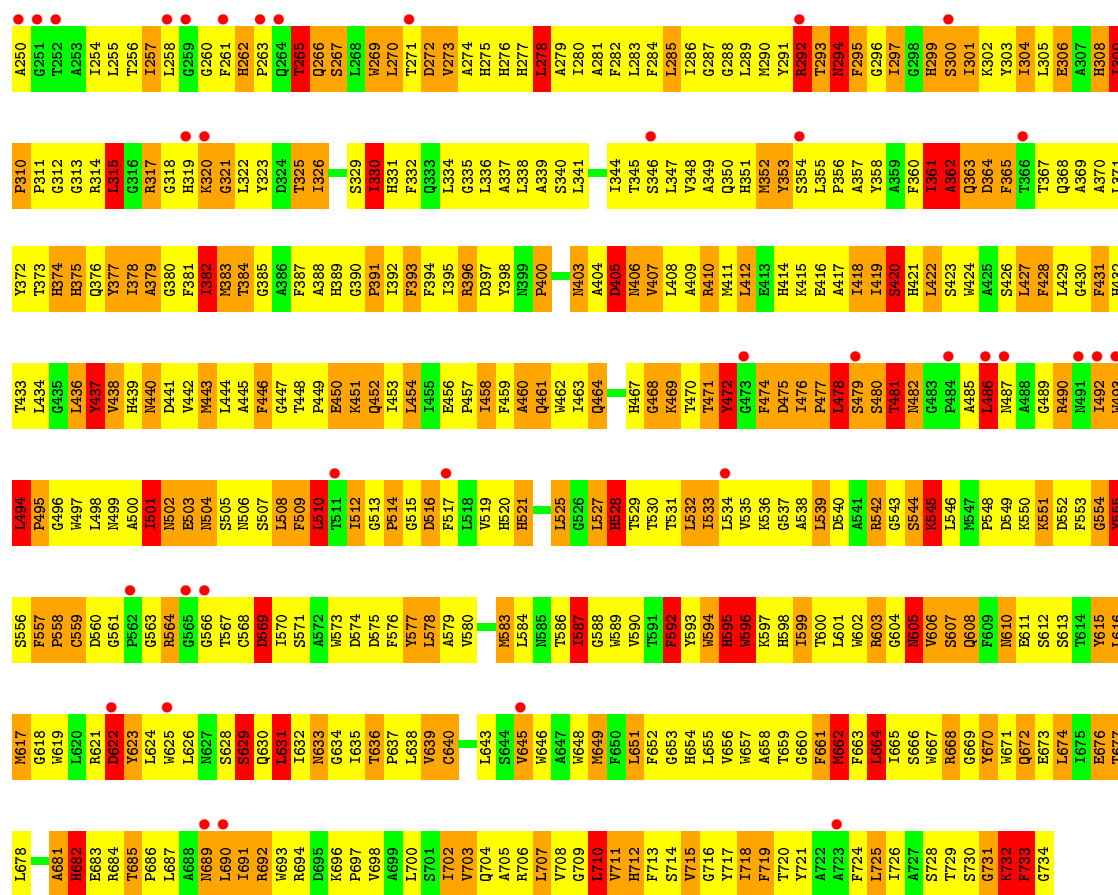
• Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



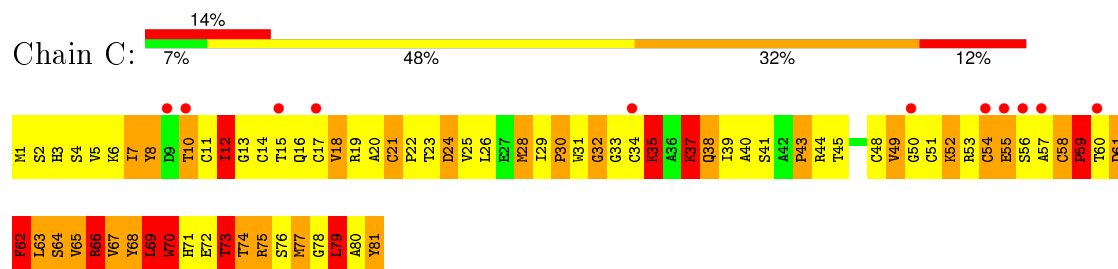


• Molecule 6: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

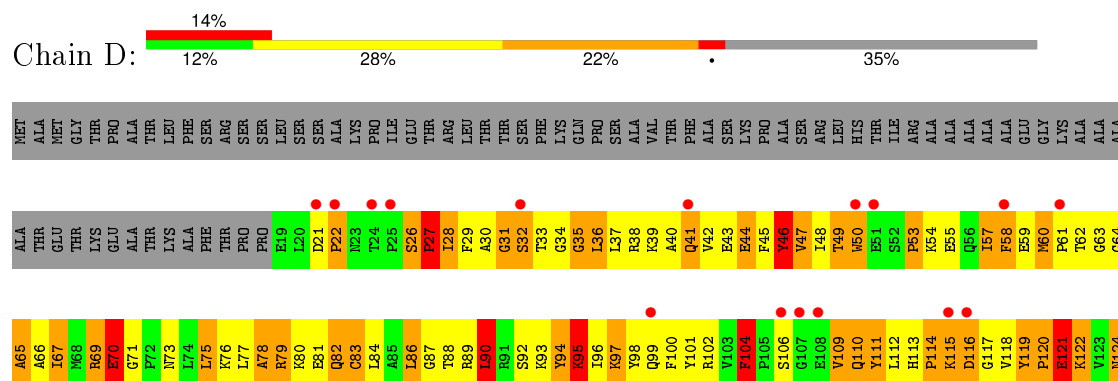




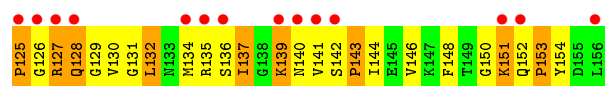
### • Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



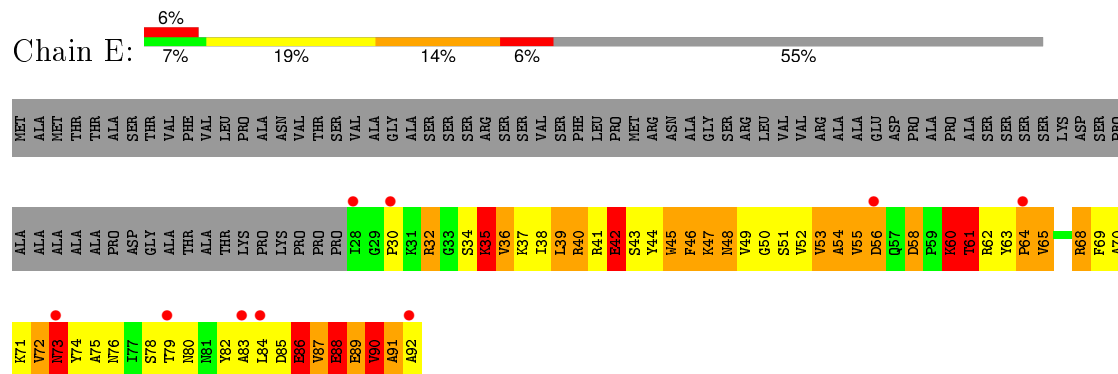
### • Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC



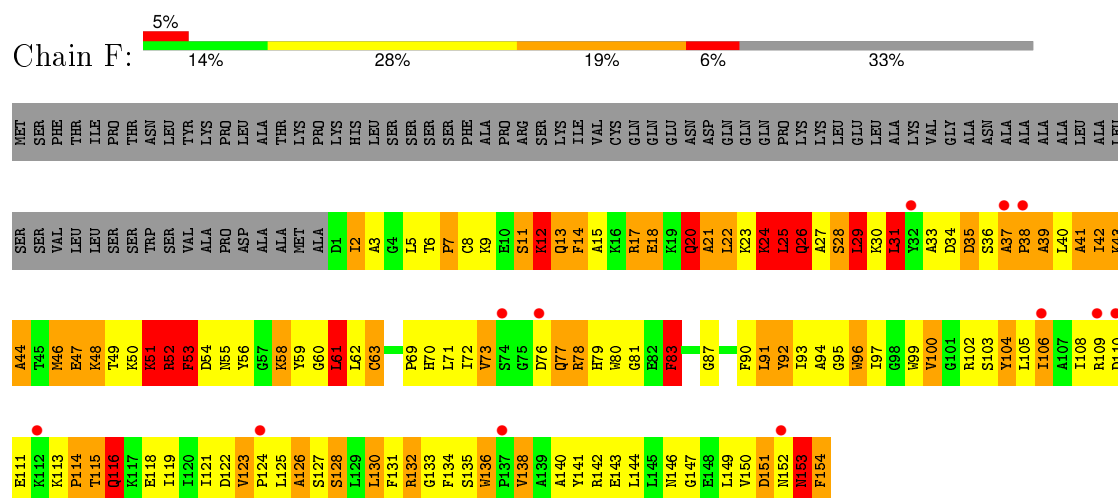




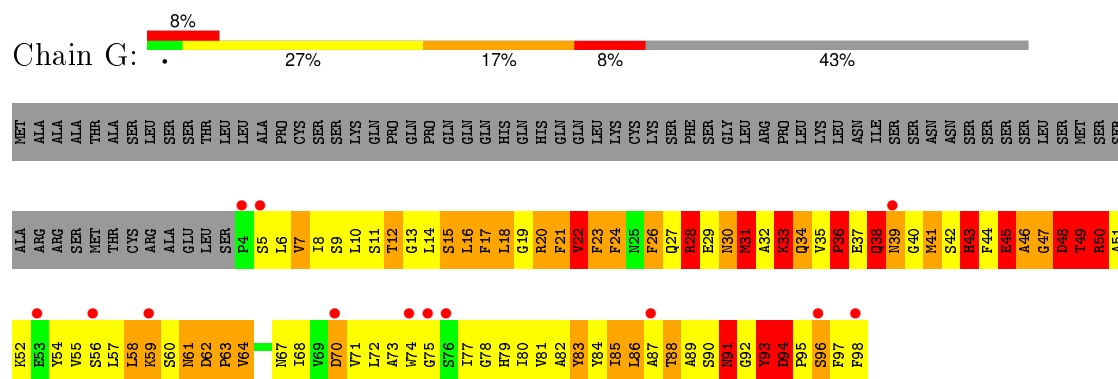
- Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC



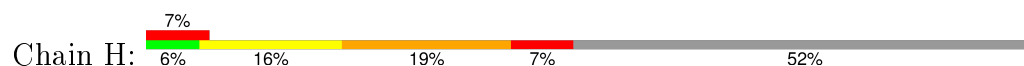
- Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

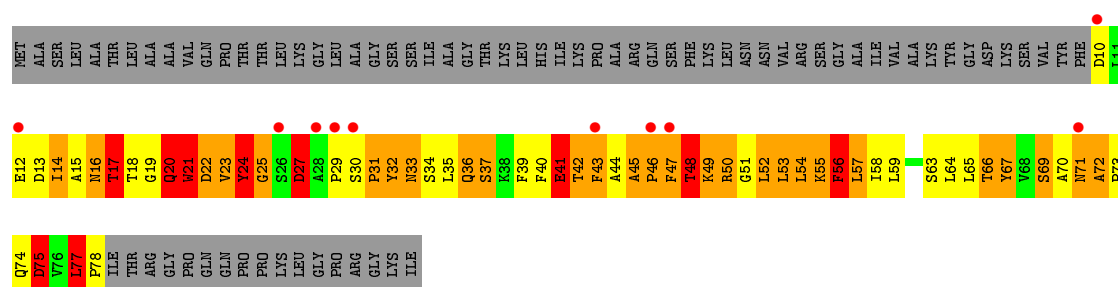


- Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

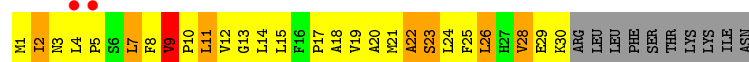


- Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC





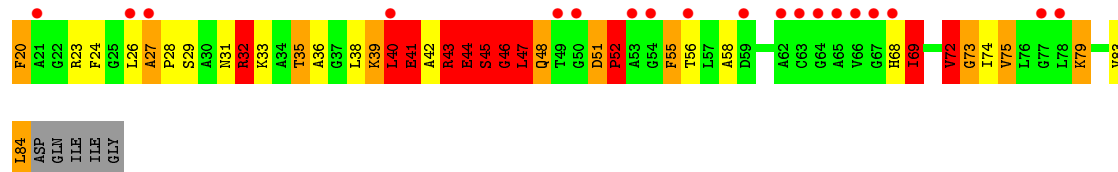
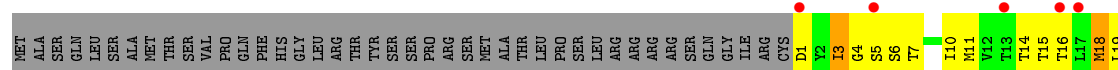
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



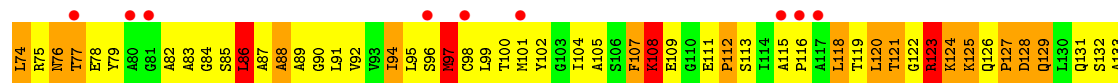
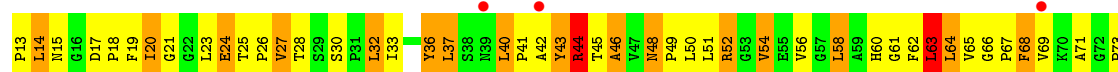
• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

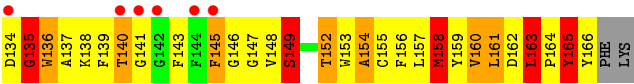


• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

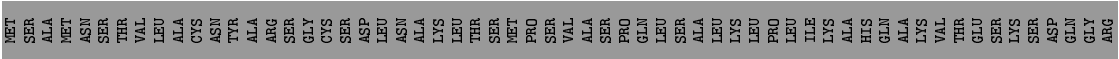
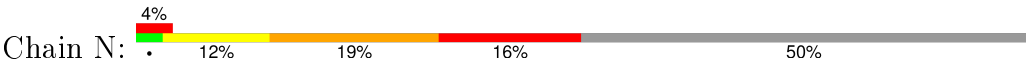


• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

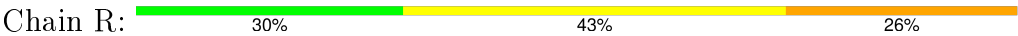




● Molecule 17: PHOTOSYSTEM I-N SUBUNIT



● Molecule 18: PHOTOSYSTEM I-N SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.20Å 190.20Å 130.30Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	50.00 – 3.48 49.46 – 3.47	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-3.48) 96.2 (49.46-3.47)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.391 , 0.425 0.383 , 0.387	Depositor DCC
$R_{free}$ test set	1456 reflections (2.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.09 , 30.0	EDS
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 72533 reflections	Xtriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	36033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.55	1/1303 (0.1%)	0.73	1/1774 (0.1%)
2	2	0.67	0/1420	1.10	7/1943 (0.4%)
3	3	0.60	0/1221	0.91	2/1642 (0.1%)
4	4	0.77	0/1359	1.12	10/1851 (0.5%)
5	A	0.61	1/5938 (0.0%)	0.88	9/8104 (0.1%)
6	B	0.58	0/6058	0.86	8/8278 (0.1%)
7	C	0.78	0/632	1.05	1/856 (0.1%)
8	D	0.71	0/1122	0.91	0/1514
9	E	0.70	0/530	0.95	1/718 (0.1%)
10	F	0.67	0/1250	0.88	0/1687
11	G	0.84	1/760 (0.1%)	1.20	7/1031 (0.7%)
12	H	0.70	0/543	1.02	0/741
13	I	0.62	0/235	0.80	0/320
14	J	0.65	0/349	0.91	0/475
15	K	0.65	1/599 (0.2%)	0.88	1/810 (0.1%)
16	L	0.69	1/1251 (0.1%)	0.94	2/1709 (0.1%)
17	N	0.89	0/699	1.22	5/936 (0.5%)
All	All	0.65	5/25269 (0.0%)	0.93	54/34389 (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	17
3	3	0	17
4	4	0	20
5	A	0	20
6	B	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1
8	D	0	1
9	E	0	3
10	F	0	7
11	G	1	13
12	H	0	9
15	K	0	6
16	L	0	2
17	N	0	22
18	R	0	16
All	All	1	169

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	165	TYR	CE2-CZ	-6.04	1.30	1.38
11	G	15	SER	CB-OG	5.83	1.49	1.42
1	1	185	TRP	CB-CG	-5.34	1.40	1.50
15	K	41	GLU	CG-CD	5.15	1.59	1.51
5	A	22	VAL	CA-CB	-5.05	1.44	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	180	LYS	C-N-CA	-10.34	95.85	121.70
11	G	46	ALA	N-CA-C	-10.20	83.47	111.00
6	B	731	GLY	N-CA-C	-7.75	93.73	113.10
11	G	16	LEU	CA-CB-CG	7.25	131.98	115.30
6	B	315	LEU	CA-CB-CG	7.00	131.41	115.30
5	A	23	ASP	CB-CG-OD1	6.86	124.47	118.30
17	N	33	TYR	N-CA-C	-6.69	92.95	111.00
4	4	40	PHE	CB-CA-C	6.54	123.48	110.40
5	A	93	LEU	CA-CB-CG	6.51	130.28	115.30
6	B	486	LEU	CA-CB-CG	6.46	130.15	115.30
2	2	74	LEU	N-CA-C	-6.43	93.63	111.00
6	B	494	LEU	CA-CB-CG	6.42	130.05	115.30
11	G	51	ALA	N-CA-C	6.41	128.32	111.00
7	C	69	LEU	CA-CB-CG	6.36	129.92	115.30
4	4	39	TRP	CA-CB-CG	6.34	125.74	113.70
4	4	126	LEU	N-CA-C	6.33	128.10	111.00
5	A	316	MET	N-CA-C	-6.27	94.07	111.00
4	4	161	LEU	CA-CB-CG	6.24	129.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	478	LEU	CA-CB-CG	6.19	129.53	115.30
5	A	540	LEU	CA-CB-CG	6.16	129.47	115.30
17	N	24	THR	N-CA-C	-6.14	94.42	111.00
5	A	653	LEU	CA-CB-CG	6.08	129.28	115.30
11	G	50	ARG	N-CA-C	6.05	127.35	111.00
2	2	101	PHE	N-CA-CB	6.04	121.47	110.60
16	L	86	LEU	CA-CB-CG	6.02	129.15	115.30
4	4	143	PHE	N-CA-C	5.96	127.09	111.00
6	B	710	LEU	N-CA-C	-5.91	95.03	111.00
1	1	183	ASP	C-N-CD	-5.89	107.64	120.60
2	2	132	GLY	N-CA-C	5.80	127.61	113.10
4	4	88	SER	N-CA-C	5.74	126.50	111.00
4	4	66	SER	N-CA-C	5.71	126.43	111.00
5	A	530	LEU	CA-CB-CG	5.63	128.26	115.30
2	2	57	LEU	CA-CB-CG	5.63	128.24	115.30
4	4	37	LEU	N-CA-C	5.59	126.10	111.00
2	2	121	THR	N-CA-C	5.58	126.08	111.00
17	N	27	ALA	N-CA-C	-5.56	95.98	111.00
15	K	40	LEU	O-C-N	-5.51	113.89	122.70
5	A	554	LEU	CA-CB-CG	5.46	127.87	115.30
4	4	39	TRP	C-N-CA	-5.43	108.12	121.70
11	G	21	PHE	N-CA-C	5.42	125.65	111.00
6	B	104	PHE	N-CA-C	-5.37	96.51	111.00
2	2	125	PHE	N-CA-C	5.35	125.44	111.00
16	L	135	GLY	N-CA-C	-5.34	99.75	113.10
4	4	124	TYR	N-CA-C	-5.33	96.60	111.00
2	2	94	LEU	CA-CB-CG	5.31	127.52	115.30
11	G	91	ASN	N-CA-C	5.31	125.33	111.00
17	N	60	PHE	C-N-CA	-5.28	108.49	121.70
17	N	16	LEU	N-CA-C	-5.23	96.88	111.00
11	G	45	GLU	N-CA-C	5.21	125.07	111.00
5	A	271	THR	N-CA-C	-5.13	97.14	111.00
3	3	111	TYR	CA-CB-CG	5.08	123.06	113.40
6	B	631	LEU	CA-CB-CG	5.06	126.93	115.30
9	E	60	LYS	N-CA-C	5.06	124.65	111.00
5	A	600	LEU	CA-CB-CG	5.04	126.89	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

All (169) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide
1	1	185	TRP	Peptide
1	1	72	GLN	Peptide
2	2	111	ALA	Peptide
2	2	112	ASP	Peptide
2	2	120	ASN	Peptide
2	2	126	PRO	Peptide
2	2	131	THR	Peptide
2	2	144	ASP	Peptide
2	2	194	ALA	Peptide
2	2	197	LEU	Peptide
2	2	209	THR	Peptide
2	2	42	ARG	Peptide
2	2	73	ILE	Peptide
2	2	74	LEU	Peptide
2	2	75	ASN	Peptide
2	2	80	TYR	Peptide
2	2	84	GLU	Peptide
2	2	92	THR	Peptide
2	2	99	LEU	Peptide
3	3	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
3	3	159	PRO	Peptide
3	3	169	PHE	Peptide
3	3	172	ASP	Peptide
3	3	180	LYS	Peptide
3	3	49	ILE	Peptide
3	3	92	TRP	Peptide
3	3	93	PHE	Peptide
3	3	95	THR	Peptide
3	3	96	GLY	Peptide
4	4	143	PHE	Peptide
4	4	146	THR	Peptide
4	4	152	LYS	Peptide
4	4	190	HIS	Peptide
4	4	192	THR	Peptide

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Mol	Chain	Res	Type	Group
4	4	194	VAL	Peptide
4	4	34	PRO	Peptide
4	4	35	GLU	Peptide
4	4	36	ASN	Peptide
4	4	37	LEU	Peptide
4	4	38	ARG	Peptide
4	4	63	VAL	Peptide
4	4	65	THR	Peptide
4	4	68	GLY	Peptide
4	4	74	LYS	Peptide
4	4	83	TYR	Peptide
4	4	87	SER	Peptide
4	4	88	SER	Peptide
4	4	89	THR	Peptide
4	4	90	LEU	Peptide
5	A	103	PHE	Peptide
5	A	117	GLY	Peptide
5	A	123	VAL	Peptide
5	A	197	GLN	Peptide
5	A	21	LEU	Peptide
5	A	23	ASP	Peptide
5	A	240	LYS	Peptide
5	A	242	ILE	Peptide
5	A	26	PRO	Peptide
5	A	27	ILE	Peptide
5	A	28	LYS	Peptide
5	A	29	THR	Peptide
5	A	316	MET	Peptide
5	A	347	TYR	Peptide
5	A	393	LEU	Peptide
5	A	41	SER	Peptide
5	A	427	ARG	Peptide
5	A	45	ALA	Peptide
5	A	55	TRP	Peptide
5	A	67	HIS	Peptide
6	B	103	ALA	Peptide
6	B	104	PHE	Peptide
6	B	232	LEU	Peptide
6	B	265	THR	Peptide
6	B	304	ILE	Peptide
6	B	362	ALA	Peptide
6	B	377	TYR	Peptide

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Mol	Chain	Res	Type	Group
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
7	C	79	LEU	Peptide
8	D	90	LEU	Peptide
9	E	86	GLU	Peptide
9	E	88	GLU	Peptide
9	E	91	ALA	Peptide
10	F	136	TRP	Peptide
10	F	20	GLN	Peptide
10	F	24	LYS	Peptide
10	F	31	LEU	Peptide
10	F	41	ALA	Peptide
10	F	51	LYS	Peptide
10	F	56	TYR	Peptide
11	G	15	SER	Peptide
11	G	22	VAL	Peptide
11	G	26	PHE	Peptide
11	G	36	PRO	Peptide
11	G	39	ASN	Peptide
11	G	43	HIS	Peptide
11	G	45	GLU	Mainchain
11	G	48	ASP	Peptide
11	G	49	THR	Peptide
11	G	50	ARG	Peptide
11	G	90	SER	Peptide
11	G	93	TYR	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	24	TYR	Peptide
12	H	25	GLY	Peptide
12	H	27	ASP	Peptide
12	H	43	PHE	Peptide
12	H	48	THR	Peptide
15	K	41	GLU	Peptide
15	K	43	ARG	Peptide
15	K	44	GLU	Peptide

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Mol	Chain	Res	Type	Group
15	K	45	SER	Peptide
15	K	46	GLY	Peptide
15	K	47	LEU	Peptide
16	L	160	VAL	Peptide
16	L	165	TYR	Peptide
17	N	12	THR	Peptide
17	N	15	GLU	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	44	GLU	Peptide
17	N	46	PHE	Peptide
17	N	48	GLY	Peptide
17	N	50	GLN	Peptide
17	N	52	LEU	Peptide
17	N	54	LYS	Peptide
17	N	60	PHE	Peptide
17	N	63	ASP	Peptide
17	N	67	LEU	Peptide
17	N	7	LEU	Peptide
17	N	70	GLU	Peptide
17	N	75	TYR	Peptide
17	N	79	SER	Peptide
17	N	84	LYS	Peptide
18	R	28	UNK	Peptide
18	R	31	UNK	Peptide
18	R	32	UNK	Peptide
18	R	33	UNK	Peptide
18	R	34	UNK	Peptide
18	R	35	UNK	Peptide
18	R	36	UNK	Peptide
18	R	37	UNK	Peptide
18	R	40	UNK	Peptide
18	R	41	UNK	Peptide
18	R	42	UNK	Peptide
18	R	45	UNK	Peptide
18	R	46	UNK	Peptide
18	R	48	UNK	Peptide
18	R	51	UNK	Peptide

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Mol	Chain	Res	Type	Group
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	1229	137	3
2	2	1374	0	1331	301	2
3	3	1186	0	1147	291	6
4	4	1319	0	1282	609	3
5	A	5745	0	5597	1350	0
6	B	5848	0	5655	1211	5
7	C	619	0	608	204	0
8	D	1095	0	1112	189	0
9	E	520	0	528	128	0
10	F	1221	0	1249	201	0
11	G	740	0	708	190	1
12	H	529	0	514	106	0
13	I	229	0	252	55	0
14	J	338	0	340	64	0
15	K	593	0	619	110	0
16	L	1215	0	1222	311	3
17	N	685	0	668	320	1
18	R	265	0	68	78	0
19	1	1072	0	710	174	1
19	2	596	0	409	136	0
19	3	604	0	376	84	0
19	4	759	0	514	177	0
19	A	2610	0	2341	814	0
19	B	2157	0	1981	654	0
19	F	130	0	86	17	0
19	G	51	0	40	4	0
19	H	163	0	140	43	0
19	I	60	0	58	12	0
19	J	61	0	60	14	0
19	L	97	0	72	36	0
19	R	122	0	123	14	0
20	2	35	0	46	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	4	35	0	46	1	0
20	A	1503	0	1967	302	18
20	B	25	0	23	1	0
20	L	35	0	46	1	0
20	R	35	0	46	9	1
21	2	22	0	19	10	0
21	3	23	0	22	6	0
21	B	229	0	217	35	17
21	H	23	0	22	14	0
22	A	33	0	46	7	0
22	B	33	0	46	28	0
23	A	279	0	375	178	0
23	B	280	0	378	155	0
23	I	40	0	54	38	0
23	L	40	0	54	36	0
24	B	49	0	71	17	0
25	B	8	0	0	17	0
25	C	16	0	0	5	0
26	B	23	0	0	1	0
All	All	36033	0	34517	7355	31

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 104.

All (7355) 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:CE	19:4:1201:CLA:HBB2	1.18	1.65
4:4:69:ILE:HD11	4:4:175:LYS:CB	1.26	1.65
3:3:97:PHE:CD2	3:3:98:ILE:HG23	1.33	1.62
1:1:185:TRP:CH2	19:1:1199:CLA:H12	1.38	1.59
3:3:97:PHE:CE2	3:3:98:ILE:HD13	1.42	1.55
17:N:41:LYS:CG	17:N:42:PHE:HB3	1.31	1.55
3:3:132:TRP:CZ3	3:3:155:GLU:HG2	1.37	1.55
19:A:1782:CLA:CBB	19:A:1790:CLA:HMA2	1.36	1.53
17:N:45:ASN:HD22	17:N:54:LYS:CG	1.21	1.52
7:C:5:VAL:CG2	7:C:65:VAL:HG13	1.35	1.51
3:3:92:TRP:HA	3:3:95:THR:CG2	1.33	1.51
23:A:1808:BCR:C33	19:L:1167:CLA:C4B	1.86	1.49
19:A:1759:CLA:HBB2	19:A:1760:CLA:C3C	1.41	1.49
3:3:132:TRP:CZ3	3:3:155:GLU:CG	1.91	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:185:TRP:CH2	19:1:1199:CLA:C1	1.97	1.45
7:C:5:VAL:HG21	7:C:65:VAL:CG1	1.44	1.45
17:N:45:ASN:HB3	17:N:57:LYS:NZ	1.18	1.43
23:A:1808:BCR:H333	19:L:1167:CLA:C4B	1.42	1.43
4:4:160:MET:SD	19:4:1201:CLA:HBB2	1.55	1.43
5:A:27:ILE:HG22	5:A:28:LYS:CG	1.50	1.42
17:N:72:LYS:CG	17:N:74:LYS:HG3	1.50	1.42
6:B:732:LYS:HB3	6:B:733:PHE:CA	1.47	1.41
11:G:37:GLU:CD	11:G:42:SER:HB3	1.39	1.40
19:A:1759:CLA:HBB2	19:A:1760:CLA:C2C	1.49	1.39
16:L:163:LEU:CG	16:L:164:PRO:HD3	1.51	1.39
4:4:106:TRP:CD1	19:4:1196:CLA:HED3	1.58	1.38
19:A:1779:CLA:C4C	23:A:1804:BCR:H19C	1.52	1.38
16:L:164:PRO:HG3	16:L:165:TYR:CE1	1.57	1.37
1:1:185:TRP:CZ3	19:1:1199:CLA:H12	1.59	1.36
11:G:94:ASP:H	11:G:95:PRO:CD	1.34	1.36
1:1:183:ASP:CG	1:1:184:PRO:HD2	1.45	1.36
4:4:37:LEU:C	4:4:39:TRP:HB3	1.43	1.35
4:4:160:MET:CE	19:4:1201:CLA:CBB	2.01	1.35
6:B:403:ASN:O	6:B:406:ASN:HB3	1.22	1.35
4:4:95:PHE:CE2	19:4:1210:CLA:C3C	2.10	1.34
4:4:106:TRP:NE1	19:4:1196:CLA:HED3	1.38	1.34
22:B:1773:PQN:H162	23:B:1780:BCR:C33	1.57	1.34
1:1:27:LEU:HD11	6:B:314:ARG:CZ	1.54	1.33
16:L:164:PRO:HA	16:L:165:TYR:CG	1.61	1.33
3:3:94:ARG:NH2	3:3:98:ILE:HG21	1.42	1.32
19:B:1742:CLA:HAC2	19:B:1743:CLA:CBB	1.60	1.32
7:C:14:CYS:HA	7:C:17:CYS:SG	1.68	1.31
17:N:61:LEU:HD11	17:N:63:ASP:O	1.18	1.31
18:R:39:UNK:HA	18:R:42:UNK:CB	1.59	1.31
4:4:122:LYS:HB2	4:4:143:PHE:CD2	1.65	1.31
17:N:45:ASN:HD22	17:N:54:LYS:CD	1.42	1.31
15:K:79:LYS:HE3	15:K:84:LEU:O	1.21	1.31
17:N:72:LYS:CB	17:N:73:ASP:HA	1.49	1.31
4:4:128:ALA:HB2	4:4:143:PHE:CE2	1.65	1.30
4:4:95:PHE:HE2	19:4:1210:CLA:C3C	1.41	1.30
4:4:106:TRP:CE2	19:4:1196:CLA:HED3	1.65	1.30
17:N:62:SER:HB3	17:N:66:ASP:CB	1.60	1.30
19:A:1782:CLA:HBB2	19:A:1790:CLA:CMA	1.60	1.30
3:3:97:PHE:HE2	3:3:98:ILE:CD1	1.42	1.29
4:4:69:ILE:HD11	4:4:175:LYS:CG	1.61	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:94:ARG:HG3	3:3:97:PHE:CZ	1.67	1.29
4:4:122:LYS:CD	4:4:150:LYS:HD3	1.61	1.29
4:4:107:GLN:C	19:4:1196:CLA:HMA3	1.52	1.29
22:B:1773:PQN:C19	23:B:1780:BCR:H10C	1.62	1.28
11:G:44:PHE:O	11:G:47:GLY:HA3	1.32	1.28
11:G:94:ASP:N	11:G:95:PRO:HD3	1.48	1.28
19:2:2006:CLA:C5	19:2:2006:CLA:HMA2	1.62	1.28
16:L:163:LEU:HD12	16:L:164:PRO:CD	1.62	1.28
17:N:58:VAL:HB	17:N:59:PRO:CD	1.63	1.27
16:L:164:PRO:HA	16:L:165:TYR:CB	1.39	1.26
5:A:331:LEU:HD21	5:A:343:HIS:O	1.11	1.26
11:G:37:GLU:CD	11:G:42:SER:CB	2.03	1.26
11:G:44:PHE:C	11:G:47:GLY:HA3	1.53	1.26
4:4:36:ASN:O	4:4:39:TRP:HB2	1.25	1.26
3:3:80:LYS:NZ	3:3:92:TRP:CD1	2.03	1.26
17:N:72:LYS:HB3	17:N:73:ASP:CA	1.65	1.26
15:K:44:GLU:CG	15:K:45:SER:HA	1.64	1.26
17:N:6:TYR:O	17:N:8:GLU:N	1.66	1.26
17:N:72:LYS:HE2	17:N:74:LYS:CE	1.66	1.26
3:3:132:TRP:CH2	3:3:155:GLU:CG	2.12	1.26
3:3:94:ARG:CA	3:3:97:PHE:HE1	1.49	1.25
7:C:1:MET:N	7:C:4:SER:HB3	1.50	1.25
6:B:25:ILE:HG21	23:L:1169:BCR:C29	1.66	1.24
4:4:124:TYR:O	4:4:127:PRO:HD2	1.32	1.24
4:4:107:GLN:CA	19:4:1196:CLA:HMA3	1.65	1.24
5:A:567:ARG:NH1	8:D:35:GLY:HA2	1.51	1.24
12:H:69:SER:OG	19:H:1079:CLA:H2	1.27	1.24
16:L:164:PRO:HG3	16:L:165:TYR:CD1	1.71	1.24
19:A:1796:CLA:H141	23:A:1805:BCR:C2	1.67	1.23
17:N:72:LYS:CE	17:N:74:LYS:HE2	1.69	1.23
4:4:36:ASN:HB2	4:4:39:TRP:CE3	1.71	1.23
4:4:160:MET:HE3	19:4:1201:CLA:CBB	1.62	1.23
11:G:45:GLU:O	11:G:49:THR:HG23	1.32	1.23
15:K:44:GLU:HG3	15:K:45:SER:CA	1.67	1.23
3:3:97:PHE:CE2	3:3:98:ILE:HG23	1.74	1.23
17:N:45:ASN:ND2	17:N:54:LYS:CG	2.01	1.23
16:L:164:PRO:CB	16:L:165:TYR:HD1	1.50	1.23
4:4:40:PHE:HB3	4:4:43:ALA:CB	1.69	1.23
4:4:94:GLU:HG2	4:4:95:PHE:CD1	1.74	1.22
7:C:5:VAL:CB	7:C:65:VAL:HG13	1.69	1.22
5:A:744:ALA:CB	23:A:1805:BCR:H391	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:1205:CLA:CGD	19:4:1205:CLA:HBA2	1.68	1.22
4:4:174:GLY:O	4:4:175:LYS:HG3	1.37	1.22
4:4:36:ASN:HB2	4:4:39:TRP:CZ3	1.73	1.22
19:B:1765:CLA:HMB1	23:B:1777:BCR:C29	1.67	1.22
5:A:27:ILE:CG2	5:A:28:LYS:HD3	1.68	1.22
7:C:5:VAL:CG2	7:C:65:VAL:CG1	2.04	1.22
1:1:112:ARG:HH12	19:1:1196:CLA:CGD	1.52	1.22
23:A:1808:BCR:C33	19:L:1167:CLA:CHC	2.18	1.21
21:B:8052:SUC:C5'	21:B:8052:SUC:H1	1.70	1.21
5:A:24:ARG:NH1	5:A:29:THR:HB	1.54	1.21
19:A:1776:CLA:CMD	19:A:1778:CLA:HBB2	1.71	1.21
17:N:72:LYS:HE2	17:N:74:LYS:CG	1.68	1.21
5:A:27:ILE:C	5:A:28:LYS:HG2	1.48	1.20
3:3:48:PHE:CD2	3:3:49:ILE:HG22	1.74	1.20
19:B:1765:CLA:CMB	23:B:1777:BCR:H292	1.70	1.20
5:A:331:LEU:CD2	5:A:343:HIS:O	1.90	1.20
17:N:45:ASN:CB	17:N:54:LYS:HG2	1.69	1.20
3:3:94:ARG:HD2	3:3:97:PHE:CE1	1.77	1.20
3:3:205:GLY:N	5:A:252:ARG:HH22	1.38	1.20
19:B:1742:CLA:CAC	19:B:1743:CLA:HBB2	1.70	1.19
12:H:69:SER:HB2	19:H:1079:CLA:H61	1.25	1.19
19:2:1217:CLA:CBB	19:2:1217:CLA:H71	1.71	1.19
4:4:192:THR:CG2	4:4:195:GLN:H	1.55	1.19
5:A:25:ASP:HB2	5:A:26:PRO:CA	1.71	1.19
1:1:27:LEU:HD11	6:B:314:ARG:NH1	1.58	1.19
3:3:132:TRP:CZ3	3:3:155:GLU:CD	2.06	1.18
4:4:121:PHE:O	4:4:122:LYS:HD2	1.39	1.18
7:C:54:CYS:HB2	25:C:1082:SF4:S1	1.83	1.18
4:4:69:ILE:CD1	4:4:175:LYS:CB	2.21	1.18
3:3:74:ALA:HA	19:3:1216:CLA:C3D	1.73	1.18
19:A:1797:CLA:CMA	19:A:1797:CLA:HBA1	1.70	1.18
19:A:1774:CLA:H121	19:A:1774:CLA:HBB2	1.26	1.18
17:N:72:LYS:HB3	17:N:74:LYS:N	1.59	1.18
12:H:73:PRO:HD3	21:H:1082:SUC:C6'	1.73	1.18
3:3:94:ARG:HA	3:3:97:PHE:CE1	1.77	1.18
17:N:41:LYS:CD	17:N:42:PHE:HB3	1.74	1.18
19:B:1755:CLA:HBB2	19:B:1769:CLA:CMB	1.73	1.17
17:N:61:LEU:HD11	17:N:63:ASP:C	1.64	1.17
5:A:744:ALA:HB2	23:A:1805:BCR:C39	1.75	1.17
19:B:1735:CLA:H191	10:F:104:TYR:HB3	1.18	1.17
6:B:493:TRP:CE2	19:B:1765:CLA:O1A	1.96	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:25:ASP:HB2	5:A:26:PRO:HA	1.24	1.17
19:2:1213:CLA:HHD	19:2:1213:CLA:HBC3	1.24	1.17
1:1:24:PHE:HB3	6:B:314:ARG:NH2	1.60	1.17
17:N:45:ASN:ND2	17:N:53:ALA:O	1.78	1.16
19:B:1768:CLA:CBB	19:B:1768:CLA:H93	1.74	1.16
6:B:25:ILE:CG2	23:L:1169:BCR:H292	1.75	1.16
4:4:69:ILE:HD11	4:4:175:LYS:HB2	1.28	1.16
3:3:132:TRP:HH2	3:3:155:GLU:OE2	0.82	1.16
16:L:163:LEU:HB3	16:L:164:PRO:CD	1.75	1.16
20:A:7016:LMU:C2	20:A:7016:LMU:H81	1.74	1.16
4:4:122:LYS:HD3	4:4:150:LYS:CD	1.75	1.16
4:4:160:MET:SD	19:4:1201:CLA:CBB	2.33	1.16
5:A:28:LYS:HB3	5:A:28:LYS:NZ	1.50	1.16
5:A:269:PHE:CE1	15:K:14:THR:HG21	1.80	1.16
11:G:6:LEU:HB3	11:G:9:SER:CB	1.76	1.16
19:B:1761:CLA:HBC3	19:B:1761:CLA:HHD	1.17	1.16
19:4:1199:CLA:HMC1	19:4:1199:CLA:HBC3	1.27	1.16
19:B:1768:CLA:C9	19:B:1768:CLA:HBB2	1.76	1.16
4:4:36:ASN:C	4:4:39:TRP:HB2	1.65	1.16
4:4:39:TRP:C	4:4:40:PHE:HD1	1.48	1.16
3:3:205:GLY:H	5:A:252:ARG:NH2	1.44	1.16
19:A:1774:CLA:C12	19:A:1774:CLA:HBB2	1.74	1.15
19:1:1190:CLA:HBC2	19:1:1190:CLA:HMC1	1.28	1.15
2:2:102:ILE:C	19:2:1221:CLA:HBB2	1.67	1.15
4:4:171:ASN:O	4:4:173:THR:N	1.79	1.15
4:4:69:ILE:HD11	4:4:175:LYS:HB3	1.27	1.15
1:1:144:LYS:NZ	19:1:1187:CLA:HED3	1.32	1.15
13:I:7:LEU:HD12	23:I:1032:BCR:H333	1.28	1.15
3:3:94:ARG:CZ	3:3:97:PHE:CE2	2.29	1.15
3:3:132:TRP:HH2	3:3:155:GLU:CD	1.21	1.15
16:L:164:PRO:CG	16:L:165:TYR:CD1	2.29	1.15
16:L:164:PRO:CB	16:L:165:TYR:CD1	2.30	1.15
5:A:316:MET:HG2	5:A:317:TYR:CD1	1.82	1.15
10:F:102:ARG:HG2	10:F:106:ILE:HD11	1.27	1.15
4:4:107:GLN:C	19:4:1196:CLA:CMA	2.16	1.15
19:L:1168:CLA:HBC3	19:L:1168:CLA:HHD	1.28	1.15
17:N:62:SER:HB3	17:N:66:ASP:CA	1.75	1.15
3:3:94:ARG:CD	3:3:97:PHE:CZ	2.30	1.15
19:1:1191:CLA:CAB	19:1:1197:CLA:HBC2	1.76	1.15
23:A:1809:BCR:H393	23:A:1809:BCR:H23C	1.26	1.15
17:N:45:ASN:HB2	17:N:57:LYS:NZ	1.57	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:27:ILE:HG22	5:A:28:LYS:CD	1.74	1.15
19:1:1143:CLA:HAC2	20:A:7001:LMU:O3B	1.43	1.15
3:3:110:SER:C	3:3:111:TYR:HD2	1.49	1.15
20:A:7020:LMU:H6E	20:A:7020:LMU:H5B	1.20	1.15
20:A:7022:LMU:C2'	20:A:7022:LMU:H21	1.74	1.15
5:A:51:THR:HG21	19:A:1795:CLA:HBB2	1.22	1.14
16:L:164:PRO:CA	16:L:165:TYR:CD1	2.29	1.14
19:1:1191:CLA:HMC1	19:1:1194:CLA:HHD	1.21	1.14
6:B:120:VAL:HA	6:B:123:TRP:CD1	1.81	1.14
1:1:24:PHE:CB	6:B:314:ARG:HH21	1.60	1.14
19:A:1781:CLA:HED1	19:A:1782:CLA:C2D	1.77	1.14
3:3:94:ARG:CG	3:3:97:PHE:CE1	2.28	1.14
15:K:44:GLU:O	15:K:47:LEU:HG	1.46	1.14
3:3:97:PHE:CD2	3:3:98:ILE:CG2	2.30	1.14
2:2:169:LEU:HD22	19:2:1215:CLA:CAB	1.77	1.14
4:4:122:LYS:CD	4:4:150:LYS:CD	2.24	1.14
6:B:732:LYS:HB3	6:B:733:PHE:C	1.68	1.13
17:N:72:LYS:CE	17:N:74:LYS:HG2	1.77	1.13
12:H:20:GLN:CB	12:H:22:ASP:HB3	1.77	1.13
6:B:323:TYR:HE2	11:G:48:ASP:O	1.27	1.13
3:3:94:ARG:CG	3:3:97:PHE:CZ	2.30	1.13
3:3:110:SER:O	3:3:111:TYR:HD2	1.31	1.13
19:3:1217:CLA:HAC2	19:3:1218:CLA:H72	1.29	1.13
17:N:45:ASN:HB2	17:N:54:LYS:HG2	1.16	1.13
17:N:57:LYS:O	17:N:60:PHE:O	1.64	1.13
21:B:8052:SUC:H5'	21:B:8052:SUC:H1	1.23	1.13
12:H:73:PRO:HG3	21:H:1082:SUC:H5'	1.14	1.13
11:G:6:LEU:CB	11:G:9:SER:HB3	1.76	1.13
11:G:43:HIS:HB2	11:G:44:PHE:CD1	1.84	1.13
3:3:94:ARG:CD	3:3:97:PHE:CE1	2.30	1.13
4:4:104:ARG:HH11	4:4:105:ARG:CB	1.61	1.12
4:4:34:PRO:HA	4:4:35:GLU:HB2	1.31	1.12
19:B:1761:CLA:CBC	19:B:1761:CLA:HHD	1.76	1.12
17:N:41:LYS:CG	17:N:42:PHE:CB	2.26	1.12
19:1:1308:CLA:HBD	19:1:1308:CLA:HBA2	1.12	1.12
16:L:157:LEU:O	16:L:158:MET:O	1.67	1.12
19:A:1781:CLA:HED1	19:A:1782:CLA:CMD	1.79	1.12
19:A:1783:CLA:H203	23:A:1806:BCR:H17C	1.17	1.12
23:I:1032:BCR:HC8	23:I:1032:BCR:C31	1.74	1.12
23:A:1806:BCR:H393	23:A:1806:BCR:H23C	1.18	1.12
19:B:1753:CLA:HMD2	19:B:1754:CLA:HBB2	1.30	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:310:PRO:HG3	19:B:1753:CLA:HMA1	1.13	1.12
17:N:72:LYS:HE2	17:N:74:LYS:CD	1.79	1.12
16:L:163:LEU:CD1	16:L:164:PRO:HD3	1.77	1.12
5:A:452:PHE:CE1	19:A:1793:CLA:HBB2	1.84	1.12
19:A:1776:CLA:HMD3	19:A:1778:CLA:HBB2	1.20	1.12
19:B:1755:CLA:HBC2	19:B:1755:CLA:HHD	1.31	1.12
22:B:1773:PQN:H162	23:B:1780:BCR:H333	1.12	1.12
7:C:62:PHE:CE2	9:E:42:GLU:OE1	2.02	1.12
23:A:1808:BCR:H333	19:L:1167:CLA:CHC	1.79	1.12
7:C:1:MET:HB3	7:C:4:SER:OG	1.50	1.12
1:1:27:LEU:CD1	6:B:314:ARG:NH1	2.12	1.12
11:G:8:ILE:O	11:G:12:THR:OG1	1.66	1.12
15:K:38:LEU:HG	15:K:39:LYS:HD3	1.17	1.12
5:A:402:ILE:HG13	19:A:1784:CLA:HBB2	1.14	1.11
7:C:1:MET:H1	7:C:4:SER:CB	1.60	1.11
17:N:45:ASN:ND2	17:N:54:LYS:HD3	1.65	1.11
5:A:22:VAL:HG23	5:A:23:ASP:N	1.50	1.11
3:3:158:TYR:HB3	3:3:159:PRO:HD2	1.32	1.11
5:A:707:ILE:HG22	5:A:711:HIS:NE2	1.65	1.11
4:4:69:ILE:CD1	4:4:175:LYS:HG2	1.79	1.11
5:A:423:ASP:HB3	5:A:424:PRO:HD3	1.26	1.11
5:A:588:GLY:CA	6:B:668:ARG:HD3	1.81	1.11
19:4:1201:CLA:HMA2	19:4:1201:CLA:HBA1	1.21	1.11
3:3:94:ARG:CA	3:3:97:PHE:CE1	2.29	1.11
2:2:169:LEU:CD2	19:2:1215:CLA:HBB2	1.79	1.11
2:2:51:HIS:HB2	19:2:1221:CLA:CAD	1.80	1.11
4:4:104:ARG:HD2	19:4:1208:CLA:C2C	1.80	1.11
11:G:33:LYS:CE	11:G:33:LYS:HA	1.74	1.11
16:L:163:LEU:CD1	16:L:164:PRO:CD	2.29	1.11
15:K:44:GLU:HG3	15:K:45:SER:HA	1.17	1.11
3:3:52:LYS:O	3:3:56:TYR:CD2	2.03	1.11
19:4:1198:CLA:HAA2	19:4:1198:CLA:HED3	1.20	1.11
19:B:1739:CLA:H92	19:B:1739:CLA:HBB2	1.11	1.11
6:B:732:LYS:HB3	6:B:733:PHE:HA	1.15	1.11
23:B:1779:BCR:C8	23:B:1779:BCR:H321	1.71	1.11
19:1:1190:CLA:HED3	19:1:1190:CLA:HAA1	1.16	1.11
19:3:1218:CLA:H41	19:3:1218:CLA:C8	1.81	1.11
2:2:128:ASN:C	2:2:130:LEU:H	1.48	1.11
23:A:1803:BCR:HC8	23:A:1803:BCR:H311	1.22	1.10
6:B:596:TRP:CH2	6:B:612:SER:O	2.04	1.10
19:A:1776:CLA:H92	23:A:1804:BCR:C37	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:421:HIS:NE2	19:B:1761:CLA:ND	1.98	1.10
11:G:37:GLU:OE2	11:G:42:SER:HB3	0.93	1.10
4:4:95:PHE:CE2	19:4:1210:CLA:C2C	2.34	1.10
5:A:25:ASP:CB	5:A:26:PRO:HA	1.81	1.10
16:L:164:PRO:HA	16:L:165:TYR:CD1	1.86	1.10
15:K:44:GLU:CD	15:K:45:SER:HA	1.71	1.10
4:4:93:ILE:HA	4:4:96:ILE:HD12	1.34	1.10
4:4:40:PHE:CB	4:4:43:ALA:HB2	1.79	1.10
18:R:34:UNK:CB	18:R:35:UNK:CB	2.30	1.10
4:4:142:ASN:C	4:4:150:LYS:NZ	2.04	1.10
23:A:1805:BCR:HC8	23:A:1805:BCR:H311	1.31	1.10
1:1:24:PHE:CD2	6:B:314:ARG:NH2	2.20	1.10
15:K:43:ARG:HG3	15:K:43:ARG:HH11	1.00	1.10
18:R:46:UNK:CB	18:R:47:UNK:CB	2.30	1.10
19:A:1779:CLA:CHD	23:A:1804:BCR:H19C	1.81	1.09
22:B:1773:PQN:H191	23:B:1780:BCR:H10C	1.16	1.09
5:A:342:GLY:CA	5:A:430:ASP:HB2	1.80	1.09
17:N:57:LYS:HG3	17:N:58:VAL:N	1.49	1.09
3:3:92:TRP:HA	3:3:95:THR:HG23	1.10	1.09
17:N:72:LYS:CD	17:N:74:LYS:CG	2.30	1.09
18:R:39:UNK:C	18:R:41:UNK:CB	2.30	1.09
18:R:41:UNK:CB	18:R:42:UNK:CB	2.30	1.09
5:A:328:LYS:HG2	5:A:332:GLU:HB2	1.23	1.09
19:A:1782:CLA:CBB	19:A:1790:CLA:CMA	2.20	1.09
19:A:1791:CLA:HMA2	19:A:1797:CLA:HBB1	1.32	1.09
4:4:107:GLN:HA	19:4:1196:CLA:HMA3	1.34	1.09
6:B:131:THR:HB	6:B:134:ASP:HB2	1.29	1.09
6:B:87:ILE:HA	6:B:115:ASN:HA	1.34	1.09
17:N:45:ASN:ND2	17:N:54:LYS:CD	2.12	1.09
4:4:52:MET:HG3	4:4:160:MET:HG3	1.27	1.09
19:A:1774:CLA:O1A	19:A:1784:CLA:H71	1.52	1.09
23:B:1779:BCR:HC8	23:B:1779:BCR:C32	1.80	1.09
6:B:561:GLY:HA3	7:C:52:LYS:HG2	1.17	1.09
9:E:40:ARG:NE	9:E:86:GLU:OE1	1.85	1.09
3:3:92:TRP:CA	3:3:95:THR:CG2	2.30	1.09
5:A:27:ILE:CG2	5:A:28:LYS:CG	2.30	1.09
5:A:27:ILE:CG2	5:A:28:LYS:CD	2.29	1.09
16:L:163:LEU:CB	16:L:164:PRO:HD3	1.83	1.09
6:B:58:PHE:HB2	6:B:146:SER:HB3	1.31	1.09
19:B:1764:CLA:ND	19:B:1765:CLA:HBB2	1.65	1.09
17:N:41:LYS:HG3	17:N:42:PHE:CB	1.81	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:52:UNK:CB	18:R:53:UNK:CB	2.30	1.09
20:A:7021:LMU:H22	20:A:7021:LMU:H62	1.30	1.09
4:4:106:TRP:CD1	19:4:1196:CLA:CED	2.36	1.08
4:4:94:GLU:HG2	4:4:95:PHE:CE1	1.87	1.08
19:A:1797:CLA:H122	19:A:1797:CLA:H71	1.11	1.08
17:N:72:LYS:HG3	17:N:74:LYS:CG	1.82	1.08
11:G:93:TYR:HA	11:G:94:ASP:CB	1.81	1.08
20:A:7016:LMU:H22	20:A:7016:LMU:H61	1.32	1.08
1:1:144:LYS:HZ2	19:1:1187:CLA:CED	1.66	1.08
3:3:107:TRP:CD1	3:3:108:ALA:N	2.21	1.08
6:B:493:TRP:NE1	19:B:1765:CLA:O1A	1.85	1.08
19:A:1760:CLA:H12	19:A:1767:CLA:H61	1.30	1.08
5:A:435:VAL:O	5:A:438:HIS:O	1.69	1.08
3:3:97:PHE:HD2	3:3:97:PHE:C	1.57	1.08
23:A:1808:BCR:H331	19:L:1167:CLA:CHC	1.82	1.08
20:A:7020:LMU:H6E	20:A:7020:LMU:C5B	1.82	1.08
19:3:1218:CLA:C4	19:3:1218:CLA:H8	1.82	1.08
4:4:122:LYS:HB3	4:4:143:PHE:CB	1.83	1.08
4:4:122:LYS:HB3	4:4:143:PHE:HB2	1.28	1.08
4:4:149:ALA:HB3	4:4:151:GLU:HG2	1.35	1.08
7:C:1:MET:N	7:C:4:SER:CB	2.14	1.08
19:A:1759:CLA:CBB	19:A:1760:CLA:C2C	2.32	1.08
19:A:1815:CLA:HMD3	6:B:578:LEU:HD23	1.29	1.08
6:B:382:ILE:HG22	6:B:383:MET:H	1.06	1.08
18:R:39:UNK:CA	18:R:42:UNK:CB	2.30	1.08
1:1:144:LYS:HE3	19:1:1187:CLA:O2D	1.48	1.08
20:A:7021:LMU:H31	20:A:7021:LMU:H1'	1.32	1.08
3:3:198:PHE:HA	3:3:201:ALA:HB2	1.36	1.08
4:4:122:LYS:CB	4:4:143:PHE:HB2	1.83	1.08
17:N:72:LYS:CE	17:N:74:LYS:CG	2.32	1.08
16:L:164:PRO:HA	16:L:165:TYR:HB3	1.30	1.08
19:B:1751:CLA:HBC2	19:B:1751:CLA:HHD	1.36	1.07
17:N:45:ASN:ND2	17:N:54:LYS:HG2	1.62	1.07
1:1:24:PHE:HD2	6:B:314:ARG:NH2	1.49	1.07
15:K:84:LEU:H	15:K:84:LEU:CD2	1.66	1.07
8:D:78:ALA:HB3	8:D:82:GLN:HE22	1.15	1.07
5:A:466:THR:HG22	19:B:1740:CLA:HHC	1.13	1.07
5:A:342:GLY:HA3	5:A:430:ASP:CB	1.83	1.07
16:L:163:LEU:HG	16:L:164:PRO:HD3	1.35	1.07
19:2:2006:CLA:HBA1	19:2:2006:CLA:HBD	1.36	1.07
4:4:69:ILE:CD1	4:4:175:LYS:CG	2.33	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:CD1	17:N:63:ASP:O	2.02	1.07
19:2:2006:CLA:HBD	19:2:2006:CLA:CBA	1.83	1.07
3:3:180:LYS:O	3:3:182:LYS:N	1.87	1.07
19:1:1197:CLA:O1D	19:1:1197:CLA:HAA2	1.53	1.07
20:A:7039:LMU:H3'	20:A:7039:LMU:H6'2	1.33	1.07
5:A:472:ARG:HH12	16:L:74:LEU:HG	1.10	1.07
11:G:93:TYR:HA	11:G:94:ASP:HB2	1.11	1.07
11:G:12:THR:HG22	11:G:72:LEU:HG	1.07	1.07
6:B:672:GLN:HA	6:B:672:GLN:HE21	1.14	1.07
4:4:119:PRO:HG3	19:4:1208:CLA:C2D	1.85	1.07
19:A:1770:CLA:HHC	23:A:1803:BCR:H17C	1.26	1.07
5:A:58:HIS:HE1	19:A:1759:CLA:ND	1.51	1.07
16:L:163:LEU:CB	16:L:164:PRO:CD	2.30	1.07
15:K:84:LEU:N	15:K:84:LEU:HD23	1.54	1.07
19:2:1213:CLA:ND	19:2:1213:CLA:H43	1.67	1.07
4:4:104:ARG:HH11	4:4:105:ARG:HB2	1.20	1.06
4:4:160:MET:HE3	19:4:1201:CLA:HBB2	1.08	1.06
17:N:45:ASN:HD22	17:N:54:LYS:HG2	1.15	1.06
16:L:82:ALA:HB2	16:L:86:LEU:HD13	1.34	1.06
9:E:52:VAL:O	9:E:53:VAL:CG2	2.04	1.06
3:3:92:TRP:CA	3:3:95:THR:HG23	1.85	1.06
6:B:608:GLN:HA	6:B:608:GLN:HE21	1.14	1.06
17:N:57:LYS:CG	17:N:58:VAL:H	1.69	1.06
17:N:63:ASP:H	17:N:64:ASP:HB3	1.17	1.06
19:2:1223:CLA:H8	19:2:1223:CLA:H41	1.38	1.06
6:B:663:PHE:O	6:B:664:LEU:HB2	1.55	1.06
4:4:147:LEU:HD13	4:4:148:GLU:H	1.12	1.06
6:B:531:THR:HG22	19:B:1755:CLA:HMC2	1.36	1.06
4:4:74:LYS:N	4:4:75:TRP:HA	1.70	1.06
5:A:581:CYS:HB2	5:A:590:CYS:HA	1.34	1.06
19:H:1080:CLA:CAC	23:I:1032:BCR:HC31	1.86	1.06
15:K:44:GLU:CG	15:K:45:SER:CA	2.30	1.06
5:A:249:ILE:HG12	5:A:250:LEU:H	0.94	1.06
19:1:1142:CLA:CED	19:1:1143:CLA:HMB2	1.86	1.06
4:4:99:HIS:CE1	4:4:103:ILE:CD1	2.37	1.05
4:4:101:VAL:HG13	4:4:104:ARG:NH2	1.71	1.05
6:B:558:PRO:HG2	6:B:703:VAL:HB	1.34	1.05
1:1:185:TRP:HH2	19:1:1199:CLA:C2	1.68	1.05
19:A:1759:CLA:CBB	19:A:1760:CLA:C3C	2.34	1.05
17:N:45:ASN:HB2	17:N:54:LYS:CG	1.83	1.05
17:N:72:LYS:HE2	17:N:74:LYS:HG2	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:1217:CLA:HMC1	19:3:1217:CLA:HBC3	1.38	1.05
19:4:1206:CLA:H12	19:4:1206:CLA:HAA1	1.36	1.05
19:A:1781:CLA:HED1	19:A:1782:CLA:C3D	1.85	1.05
17:N:57:LYS:C	17:N:60:PHE:O	1.94	1.05
6:B:247:THR:HA	6:B:250:ALA:HB2	1.14	1.05
19:A:1796:CLA:H141	23:A:1805:BCR:HC22	1.33	1.05
16:L:164:PRO:CA	16:L:165:TYR:CB	2.30	1.05
10:F:24:LYS:HE2	10:F:24:LYS:N	1.71	1.05
5:A:466:THR:CG2	19:B:1740:CLA:HHC	1.86	1.05
17:N:40:CYS:H	17:N:41:LYS:HA	1.16	1.05
15:K:79:LYS:CE	15:K:84:LEU:O	2.05	1.05
20:A:7001:LMU:H81	20:A:7001:LMU:H42	1.32	1.05
12:H:20:GLN:HB3	12:H:22:ASP:HB3	1.06	1.05
5:A:116:ILE:HG23	5:A:137:GLY:HA3	1.38	1.05
5:A:331:LEU:HD11	5:A:346:LEU:HB3	1.33	1.05
6:B:493:TRP:O	6:B:495:PRO:HD3	1.57	1.05
4:4:36:ASN:O	4:4:39:TRP:CB	2.04	1.05
19:2:1213:CLA:C1D	19:2:1213:CLA:H43	1.86	1.05
12:H:73:PRO:HD3	21:H:1082:SUC:H6'2	1.12	1.05
15:K:38:LEU:HG	15:K:39:LYS:CD	1.87	1.05
6:B:302:LYS:O	6:B:303:TYR:HB2	1.57	1.05
6:B:474:PHE:HE2	6:B:476:ILE:HG13	1.13	1.05
1:1:184:PRO:C	1:1:185:TRP:CD1	2.30	1.04
19:A:1816:CLA:H93	19:A:1817:CLA:H91	1.34	1.04
4:4:122:LYS:CE	4:4:150:LYS:HD3	1.87	1.04
4:4:128:ALA:CB	4:4:143:PHE:CE2	2.39	1.04
11:G:42:SER:OG	11:G:46:ALA:HB2	1.57	1.04
16:L:108:LYS:O	16:L:132:SER:HB2	1.54	1.04
5:A:370:ILE:HG23	5:A:403:GLY:HA3	1.39	1.04
6:B:340:SER:HA	19:B:1756:CLA:H51	1.39	1.04
20:A:7013:LMU:H91	20:A:7049:LMU:O3'	1.56	1.04
23:A:1809:BCR:H23C	23:A:1809:BCR:C39	1.88	1.04
5:A:21:LEU:HD12	5:A:21:LEU:N	1.66	1.04
4:4:36:ASN:OD1	4:4:37:LEU:HA	1.57	1.04
19:1:1143:CLA:CAC	20:A:7001:LMU:O3B	2.05	1.04
6:B:323:TYR:CE2	11:G:48:ASP:O	2.10	1.04
4:4:69:ILE:HG22	4:4:70:ILE:H	0.91	1.04
19:2:1223:CLA:H3A	19:2:1223:CLA:O1A	1.57	1.04
10:F:23:LYS:O	10:F:26:GLN:HB2	1.57	1.04
7:C:39:ILE:HG12	7:C:40:ALA:H	1.23	1.04
2:2:205:PHE:CD1	2:2:206:ALA:N	2.25	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:5:LEU:HG	10:F:6:THR:H	0.92	1.04
19:A:1781:CLA:HBC2	19:A:1781:CLA:HHD	1.35	1.04
11:G:37:GLU:OE1	11:G:42:SER:HB2	1.54	1.04
5:A:28:LYS:HB3	5:A:28:LYS:HZ3	0.99	1.04
19:2:1217:CLA:H71	19:2:1217:CLA:HBB2	1.05	1.04
3:3:110:SER:O	3:3:111:TYR:CD2	2.10	1.04
20:A:7020:LMU:C6'	20:A:7020:LMU:H5B	1.86	1.04
10:F:25:LEU:CD2	10:F:46:MET:HB3	1.88	1.04
2:2:196:HIS:CE1	21:2:1225:SUC:O3	2.11	1.04
7:C:74:THR:OG1	7:C:80:ALA:HB2	1.57	1.03
4:4:122:LYS:HB2	4:4:143:PHE:HD2	0.88	1.03
19:B:1755:CLA:HBB2	19:B:1769:CLA:HMB3	1.40	1.03
6:B:422:LEU:HD13	6:B:535:VAL:HG11	1.39	1.03
19:3:1217:CLA:CAC	19:3:1218:CLA:H72	1.88	1.03
5:A:197:GLN:HA	5:A:197:GLN:HE21	0.88	1.03
20:A:7037:LMU:H72	20:A:7037:LMU:H32	1.40	1.03
9:E:86:GLU:HG3	9:E:87:VAL:N	1.68	1.03
6:B:293:THR:O	11:G:38:GLN:OE1	1.76	1.03
17:N:72:LYS:CB	17:N:73:ASP:CA	2.30	1.03
19:2:1217:CLA:C7	19:2:1217:CLA:HBB2	1.87	1.03
20:A:7014:LMU:H11	20:A:7014:LMU:H62	1.39	1.03
20:A:7032:LMU:C1B	20:A:7032:LMU:H31	1.86	1.03
19:B:1761:CLA:HMC2	19:B:1769:CLA:CBC	1.88	1.03
19:B:1768:CLA:H152	23:B:1779:BCR:C31	1.88	1.03
17:N:67:LEU:HB2	17:N:68:GLU:HG2	1.37	1.03
15:K:84:LEU:H	15:K:84:LEU:HD23	0.87	1.03
15:K:44:GLU:HG3	15:K:45:SER:N	1.73	1.03
5:A:316:MET:HB3	5:A:317:TYR:HB2	1.35	1.03
2:2:211:LYS:HG2	3:3:113:LEU:HD11	1.36	1.03
13:I:11:LEU:CD1	23:I:1032:BCR:H10C	1.87	1.03
19:A:1797:CLA:HHD	19:A:1797:CLA:CBC	1.87	1.03
6:B:269:TRP:HB2	6:B:497:TRP:HH2	1.22	1.03
1:1:24:PHE:HB3	6:B:314:ARG:HH21	0.86	1.03
5:A:251:ASN:O	5:A:253:ASP:N	1.89	1.03
5:A:588:GLY:HA3	6:B:668:ARG:HD3	1.40	1.03
20:A:7042:LMU:H32	20:A:7042:LMU:C6'	1.87	1.03
20:A:7005:LMU:H32	20:A:7005:LMU:H81	1.05	1.03
12:H:44:ALA:HB2	16:L:145:PHE:CD1	1.93	1.03
4:4:122:LYS:HZ3	4:4:150:LYS:HD2	1.23	1.03
6:B:58:PHE:CB	6:B:146:SER:HB3	1.87	1.03
5:A:22:VAL:HG23	5:A:23:ASP:CA	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7023:LMU:H21	20:A:7023:LMU:H91	1.39	1.03
20:2:1224:LMU:H21	20:2:1224:LMU:H6D	1.40	1.03
4:4:122:LYS:CE	4:4:150:LYS:CD	2.36	1.02
5:A:81:ALA:HB2	19:A:1760:CLA:CMA	1.88	1.02
5:A:368:LEU:CD2	19:A:1774:CLA:H93	1.89	1.02
19:A:1783:CLA:H203	23:A:1806:BCR:C17	1.88	1.02
9:E:86:GLU:HG3	9:E:87:VAL:H	0.90	1.02
4:4:40:PHE:HB3	4:4:43:ALA:HB2	1.33	1.02
20:A:7016:LMU:H21	20:A:7016:LMU:C8	1.89	1.02
4:4:142:ASN:O	4:4:150:LYS:HE2	1.57	1.02
5:A:81:ALA:CB	19:A:1760:CLA:CMA	2.37	1.02
6:B:594:TRP:O	6:B:595:HIS:HB3	1.54	1.02
7:C:66:ARG:HH21	7:C:66:ARG:HG2	1.21	1.02
7:C:62:PHE:CZ	9:E:42:GLU:OE1	2.12	1.02
11:G:49:THR:OG1	11:G:50:ARG:HG2	1.59	1.02
19:A:1796:CLA:H141	23:A:1805:BCR:HC21	1.36	1.02
18:R:33:UNK:C	18:R:36:UNK:CB	2.37	1.02
10:F:47:GLU:HG3	10:F:51:LYS:HE3	1.40	1.02
19:1:1149:CLA:HBC2	19:1:1149:CLA:HMC1	1.40	1.02
19:B:1735:CLA:HMD3	23:B:1778:BCR:HC41	1.37	1.02
17:N:40:CYS:N	17:N:41:LYS:HA	1.71	1.02
5:A:27:ILE:CG2	5:A:28:LYS:HG2	1.89	1.02
19:1:1190:CLA:HED3	19:1:1190:CLA:CAA	1.89	1.02
4:4:93:ILE:HA	4:4:96:ILE:CD1	1.89	1.02
13:I:11:LEU:HD12	23:I:1032:BCR:H10C	1.03	1.02
19:4:1196:CLA:HHD	19:4:1196:CLA:HBC2	1.38	1.02
23:A:1808:BCR:H333	19:L:1167:CLA:NB	1.74	1.02
3:3:97:PHE:CE2	3:3:98:ILE:CG2	2.42	1.02
3:3:94:ARG:CB	3:3:97:PHE:HE1	1.73	1.02
5:A:25:ASP:HB2	5:A:26:PRO:C	1.79	1.02
18:R:41:UNK:CB	18:R:42:UNK:CA	2.38	1.02
2:2:169:LEU:HD22	19:2:1215:CLA:CBB	1.90	1.02
19:A:1797:CLA:C12	19:A:1797:CLA:H71	1.89	1.01
4:4:91:PHE:CD2	19:4:1207:CLA:C3C	2.43	1.01
5:A:590:CYS:SG	25:B:1783:SF4:S1	2.58	1.01
5:A:702:GLU:OE2	6:B:550:LYS:NZ	1.93	1.01
11:G:28:ARG:HG2	11:G:28:ARG:HH21	1.23	1.01
17:N:72:LYS:NZ	17:N:74:LYS:HE2	1.72	1.01
17:N:72:LYS:CE	17:N:74:LYS:CE	2.30	1.01
4:4:35:GLU:HB3	4:4:36:ASN:HB3	1.41	1.01
4:4:193:ILE:HG22	4:4:194:VAL:H	1.25	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:68:ILE:HG23	11:G:72:LEU:HD13	1.42	1.01
10:F:130:LEU:HG	10:F:131:PHE:H	1.24	1.01
3:3:92:TRP:HA	3:3:95:THR:HG21	1.37	1.01
4:4:34:PRO:HA	4:4:35:GLU:CB	1.89	1.01
5:A:269:PHE:HE1	15:K:14:THR:HG21	1.18	1.01
10:F:5:LEU:HG	10:F:6:THR:N	1.74	1.01
19:B:1766:CLA:CBC	19:B:1766:CLA:HHD	1.91	1.01
19:R:1055:CLA:HBA2	19:R:1055:CLA:HBD	1.38	1.01
19:4:1198:CLA:HAA2	19:4:1198:CLA:CED	1.89	1.01
19:4:1200:CLA:HBC2	19:4:1200:CLA:HMC1	1.43	1.01
5:A:335:LYS:HG2	5:A:336:GLY:H	1.21	1.01
19:B:1738:CLA:HHB	19:B:1759:CLA:HBB2	1.41	1.01
4:4:106:TRP:NE1	19:4:1196:CLA:CED	2.22	1.01
19:A:1770:CLA:C4B	23:A:1803:BCR:H19C	1.90	1.01
16:L:164:PRO:HB3	16:L:165:TYR:HD1	1.23	1.01
7:C:17:CYS:HB2	7:C:58:CYS:SG	2.01	1.01
17:N:6:TYR:C	17:N:8:GLU:N	2.09	1.01
3:3:205:GLY:HA3	5:A:252:ARG:HH12	1.24	1.01
5:A:452:PHE:HE1	19:A:1793:CLA:HBB2	1.17	1.01
3:3:95:THR:N	3:3:97:PHE:CE1	2.29	1.01
19:A:1791:CLA:CMA	19:A:1797:CLA:HBB1	1.90	1.01
23:A:1808:BCR:C33	19:L:1167:CLA:C3B	2.38	1.01
5:A:541:VAL:HG11	5:A:615:HIS:CD2	1.94	1.01
1:1:112:ARG:NH1	19:1:1196:CLA:CGD	2.22	1.01
19:1:1191:CLA:CMC	19:1:1194:CLA:HHD	1.89	1.01
15:K:1:ASP:HA	15:K:5:SER:HB3	1.43	1.01
14:J:11:ALA:HB1	14:J:12:PRO:HD2	1.42	1.01
5:A:454:GLY:H	5:A:457:SER:HB3	1.24	1.00
4:4:106:TRP:CG	19:4:1196:CLA:HED3	1.94	1.00
6:B:202:SER:O	6:B:245:GLY:HA2	1.60	1.00
17:N:58:VAL:HB	17:N:59:PRO:HD2	1.04	1.00
5:A:249:ILE:HG12	5:A:250:LEU:N	1.73	1.00
20:A:7022:LMU:H21	20:A:7022:LMU:H2'	1.05	1.00
20:A:7032:LMU:O5B	20:A:7032:LMU:H3'	1.60	1.00
4:4:122:LYS:CG	4:4:150:LYS:HD3	1.91	1.00
4:4:128:ALA:N	4:4:143:PHE:HZ	1.58	1.00
5:A:402:ILE:CG1	19:A:1784:CLA:HBB2	1.90	1.00
5:A:246:HIS:HE1	19:A:1798:CLA:HMA3	1.27	1.00
5:A:81:ALA:CB	19:A:1760:CLA:HMA1	1.90	1.00
1:1:25:ASP:H	6:B:314:ARG:HH22	1.07	1.00
3:3:48:PHE:HD2	3:3:49:ILE:HG22	0.85	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:26:GLN:HA	10:F:26:GLN:OE1	1.55	1.00
20:A:7005:LMU:C3	20:A:7005:LMU:H81	1.90	1.00
20:2:1224:LMU:H41	20:2:1224:LMU:H82	1.35	1.00
17:N:32:ALA:HB1	17:N:35:VAL:HG22	1.42	1.00
1:1:183:ASP:CG	1:1:184:PRO:CD	2.29	1.00
19:B:1753:CLA:H151	19:B:1753:CLA:H102	1.37	1.00
19:A:1781:CLA:CED	19:A:1782:CLA:HMD1	1.90	1.00
3:3:94:ARG:NH1	3:3:97:PHE:CD2	2.29	1.00
17:N:72:LYS:HB3	17:N:73:ASP:HA	1.05	1.00
16:L:163:LEU:CG	16:L:164:PRO:CD	2.40	1.00
8:D:44:GLU:HB2	8:D:46:TYR:HE2	1.24	1.00
19:A:1776:CLA:C9	23:A:1804:BCR:H373	1.91	1.00
6:B:697:PRO:O	7:C:79:LEU:CD1	2.09	1.00
6:B:119:GLY:HA3	19:B:1758:CLA:HED1	1.01	1.00
1:1:27:LEU:CD1	6:B:314:ARG:CZ	2.39	1.00
4:4:170:HIS:O	4:4:171:ASN:O	1.79	1.00
1:1:179:THR:CG2	4:4:87:SER:HB3	1.91	1.00
4:4:142:ASN:O	4:4:150:LYS:CE	2.10	1.00
19:A:1781:CLA:CED	19:A:1782:CLA:CMD	2.40	1.00
3:3:94:ARG:NH1	3:3:97:PHE:CE2	2.29	1.00
16:L:163:LEU:HB3	16:L:164:PRO:HD2	1.44	1.00
19:1:1143:CLA:H3A	19:1:1143:CLA:O1A	1.62	1.00
8:D:117:GLY:O	8:D:118:VAL:HG23	1.60	1.00
6:B:103:ALA:O	6:B:104:PHE:HB2	1.58	0.99
19:B:1739:CLA:HBB2	19:B:1739:CLA:C9	1.92	0.99
23:B:1777:BCR:H382	23:B:1777:BCR:H23C	1.41	0.99
6:B:732:LYS:CB	6:B:733:PHE:CA	2.35	0.99
17:N:41:LYS:HB2	17:N:42:PHE:HA	1.43	0.99
4:4:34:PRO:CA	4:4:35:GLU:HB2	1.91	0.99
15:K:44:GLU:CD	15:K:45:SER:CA	2.30	0.99
19:A:1783:CLA:C20	23:A:1806:BCR:H17C	1.92	0.99
5:A:645:SER:HB3	6:B:637:PRO:HG3	1.42	0.99
6:B:119:GLY:CA	19:B:1758:CLA:HED1	1.92	0.99
17:N:72:LYS:CD	17:N:74:LYS:HG3	1.89	0.99
5:A:27:ILE:CA	5:A:28:LYS:HG2	1.91	0.99
16:L:163:LEU:HD12	16:L:164:PRO:N	1.75	0.99
5:A:197:GLN:NE2	5:A:197:GLN:HA	1.69	0.99
5:A:25:ASP:CB	5:A:26:PRO:CA	2.29	0.99
19:1:1148:CLA:H12	19:1:1148:CLA:O1D	1.62	0.99
20:A:7036:LMU:H71	20:A:7036:LMU:H31	1.41	0.99
3:3:74:ALA:HB3	3:3:75:PRO:HD3	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7043:LMU:H62	20:A:7043:LMU:H102	1.44	0.99
19:1:1145:CLA:CMA	19:1:1145:CLA:H61	1.93	0.99
4:4:121:PHE:CE2	4:4:122:LYS:O	2.16	0.99
11:G:33:LYS:HE3	11:G:33:LYS:HA	1.41	0.99
16:L:164:PRO:CA	16:L:165:TYR:CG	2.46	0.99
5:A:208:ALA:HA	5:A:310:PHE:O	1.60	0.99
19:B:1752:CLA:HBB2	19:B:1752:CLA:H72	1.43	0.99
4:4:69:ILE:CG2	4:4:70:ILE:H	1.76	0.99
3:3:97:PHE:C	3:3:97:PHE:CD2	2.29	0.99
17:N:72:LYS:HB2	17:N:73:ASP:HA	1.43	0.99
5:A:27:ILE:C	5:A:28:LYS:CG	2.28	0.99
19:3:1222:CLA:H102	19:3:1222:CLA:H142	1.45	0.99
8:D:32:SER:O	16:L:21:GLY:HA2	1.62	0.98
3:3:94:ARG:NE	3:3:97:PHE:CZ	2.29	0.98
4:4:37:LEU:O	4:4:39:TRP:HB3	1.61	0.98
19:A:1781:CLA:H72	19:A:1782:CLA:CED	1.91	0.98
23:B:1780:BCR:H382	23:B:1780:BCR:H23C	1.45	0.98
11:G:42:SER:O	11:G:46:ALA:HB3	1.61	0.98
5:A:27:ILE:HG22	5:A:28:LYS:HG2	1.42	0.98
6:B:247:THR:CA	6:B:250:ALA:HB2	1.92	0.98
12:H:44:ALA:CB	16:L:145:PHE:HD1	1.75	0.98
4:4:106:TRP:CD2	19:4:1196:CLA:HED3	1.96	0.98
16:L:56:VAL:HA	19:L:1167:CLA:HED2	1.45	0.98
3:3:98:ILE:O	17:N:63:ASP:O	1.81	0.98
2:2:70:LYS:HG3	2:2:73:ILE:CG1	1.92	0.98
5:A:267:THR:O	5:A:269:PHE:HD2	1.45	0.98
19:4:1201:CLA:CGD	19:4:1201:CLA:HAA2	1.93	0.98
4:4:95:PHE:CE2	19:4:1210:CLA:C4C	2.46	0.98
1:1:144:LYS:NZ	19:1:1187:CLA:CED	2.15	0.98
5:A:394:SER:HB2	19:A:1783:CLA:HMA1	1.44	0.98
23:I:1032:BCR:H313	23:I:1032:BCR:HC8	1.02	0.98
4:4:69:ILE:HD12	4:4:175:LYS:HG2	1.45	0.98
2:2:70:LYS:HG3	2:2:73:ILE:HG13	1.42	0.98
5:A:24:ARG:H	5:A:24:ARG:CD	1.76	0.98
19:4:1206:CLA:H151	19:4:1206:CLA:C19	1.94	0.98
10:F:42:ILE:HG13	10:F:43:LYS:H	1.27	0.98
17:N:63:ASP:H	17:N:64:ASP:CB	1.77	0.98
15:K:46:GLY:O	15:K:47:LEU:HD12	1.64	0.98
4:4:128:ALA:HB2	4:4:143:PHE:CZ	1.99	0.98
5:A:401:TRP:CD1	19:A:1783:CLA:HHC	1.98	0.98
9:E:39:LEU:H	9:E:40:ARG:NH1	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:64:LEU:HB3	16:L:68:PHE:HE1	1.28	0.98
2:2:174:VAL:O	2:2:178:TRP:CD1	2.16	0.98
3:3:173:GLU:HG2	3:3:174:LYS:H	1.29	0.98
19:A:1774:CLA:CBB	19:A:1774:CLA:C12	2.42	0.97
19:B:1768:CLA:HBC1	10:F:83:PHE:CZ	2.00	0.97
17:N:72:LYS:CB	17:N:74:LYS:H	1.77	0.97
17:N:72:LYS:CD	17:N:74:LYS:HG2	1.89	0.97
7:C:14:CYS:HA	7:C:17:CYS:HG	1.27	0.97
19:2:1215:CLA:H2	19:2:1217:CLA:HMD3	1.46	0.97
5:A:316:MET:CG	5:A:317:TYR:CD1	2.47	0.97
11:G:12:THR:HG22	11:G:72:LEU:CG	1.94	0.97
5:A:715:LYS:HD2	10:F:153:ASN:OD1	1.64	0.97
19:H:1079:CLA:CGA	19:H:1079:CLA:HMA2	1.93	0.97
19:3:1222:CLA:C10	19:3:1222:CLA:H142	1.94	0.97
4:4:69:ILE:HG22	4:4:70:ILE:N	1.73	0.97
4:4:118:ASP:OD1	4:4:123:GLN:HB2	1.63	0.97
19:A:1797:CLA:HMA2	19:A:1797:CLA:CBA	1.94	0.97
13:I:11:LEU:HD12	23:I:1032:BCR:C10	1.93	0.97
17:N:79:SER:HA	17:N:80:ASN:O	1.63	0.97
19:A:1776:CLA:HMD3	19:A:1778:CLA:CBB	1.94	0.97
19:A:1797:CLA:HMA2	19:A:1797:CLA:HBA1	0.99	0.97
5:A:195:TRP:CZ2	19:A:1766:CLA:HMA1	2.00	0.97
6:B:58:PHE:HB2	6:B:146:SER:CB	1.92	0.97
16:L:122:GLY:C	16:L:124:LYS:H	1.67	0.97
4:4:106:TRP:CE2	19:4:1196:CLA:CED	2.46	0.97
17:N:41:LYS:HG3	17:N:42:PHE:HB3	0.99	0.97
19:1:1014:CLA:HAA2	19:1:1014:CLA:O1D	1.61	0.97
6:B:517:PHE:CD2	6:B:517:PHE:O	2.18	0.97
7:C:7:ILE:HG22	7:C:65:VAL:CG2	1.94	0.97
5:A:304:LEU:HD22	19:A:1772:CLA:CBB	1.95	0.97
6:B:596:TRP:HH2	6:B:612:SER:O	1.40	0.97
23:I:1032:BCR:H313	23:I:1032:BCR:C8	1.93	0.97
13:I:8:PHE:HB2	19:I:1031:CLA:OBD	1.64	0.97
5:A:365:LEU:HD23	19:A:1761:CLA:HED3	1.45	0.97
19:B:1753:CLA:H43	19:B:1753:CLA:HAA1	1.46	0.97
17:N:47:THR:HG21	17:N:54:LYS:NZ	1.77	0.97
10:F:22:LEU:H	10:F:22:LEU:HD12	1.30	0.97
7:C:74:THR:OG1	7:C:80:ALA:CB	2.12	0.97
2:2:55:ALA:HB3	2:2:56:MET:CE	1.95	0.97
15:K:40:LEU:O	15:K:41:GLU:HB2	1.63	0.97
7:C:7:ILE:HG22	7:C:65:VAL:HG21	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:39:TRP:C	4:4:40:PHE:CD1	2.38	0.96
19:2:1223:CLA:C4	19:2:1223:CLA:H8	1.94	0.96
19:A:1801:CLA:HMA3	16:L:27:VAL:HA	1.47	0.96
5:A:599:PHE:CE2	5:A:735:VAL:HG21	2.00	0.96
3:3:158:TYR:OH	19:3:1214:CLA:C3B	2.13	0.96
11:G:44:PHE:C	11:G:47:GLY:CA	2.34	0.96
2:2:169:LEU:CD2	19:2:1215:CLA:CBB	2.43	0.96
4:4:147:LEU:CD1	4:4:148:GLU:H	1.78	0.96
6:B:551:LYS:NZ	8:D:140:ASN:O	1.98	0.96
11:G:12:THR:CG2	11:G:72:LEU:HG	1.95	0.96
20:A:7037:LMU:H51	20:A:7037:LMU:H12	1.47	0.96
5:A:462:ILE:HD11	19:A:1816:CLA:H51	1.46	0.96
7:C:1:MET:H1	7:C:4:SER:CA	1.79	0.96
4:4:142:ASN:CA	4:4:150:LYS:HZ3	1.79	0.96
5:A:22:VAL:CB	5:A:23:ASP:CA	2.41	0.96
5:A:316:MET:CB	5:A:317:TYR:CD1	2.49	0.96
19:4:1211:CLA:HBD	19:4:1211:CLA:HBA1	1.47	0.96
5:A:78:VAL:HG11	19:A:1761:CLA:HBC3	1.48	0.96
19:A:1800:CLA:HMD3	23:B:1780:BCR:HC31	1.46	0.96
4:4:192:THR:HG22	4:4:195:GLN:H	1.27	0.96
6:B:5:ILE:HB	6:B:6:PRO:HD2	1.48	0.96
6:B:697:PRO:O	7:C:79:LEU:HD13	1.65	0.96
16:L:88:ALA:C	16:L:90:GLY:H	1.67	0.96
18:R:40:UNK:N	18:R:41:UNK:CB	2.29	0.96
3:3:94:ARG:HG3	3:3:97:PHE:CE1	1.95	0.96
17:N:45:ASN:CG	17:N:54:LYS:HG2	1.86	0.96
12:H:73:PRO:CG	21:H:1082:SUC:H5'	1.96	0.96
7:C:44:ARG:HH21	8:D:127:ARG:HB3	1.25	0.96
23:A:1805:BCR:C31	19:A:1815:CLA:H143	1.96	0.96
19:B:1755:CLA:H11	19:B:1769:CLA:HED3	1.46	0.96
19:H:1080:CLA:HAC2	23:I:1032:BCR:HC31	1.46	0.96
5:A:365:LEU:CD2	19:A:1761:CLA:HED3	1.96	0.95
4:4:94:GLU:CG	4:4:95:PHE:CD1	2.49	0.95
6:B:269:TRP:HB2	6:B:497:TRP:CH2	2.02	0.95
6:B:732:LYS:HD2	6:B:734:GLY:N	1.80	0.95
18:R:34:UNK:N	18:R:36:UNK:CB	2.29	0.95
4:4:142:ASN:C	4:4:150:LYS:HZ3	1.65	0.95
5:A:58:HIS:CE1	19:A:1759:CLA:ND	2.34	0.95
19:A:1776:CLA:H92	23:A:1804:BCR:H373	0.97	0.95
5:A:606:TYR:O	5:A:610:SER:HB2	1.66	0.95
19:B:1753:CLA:C2	19:B:1753:CLA:H71	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1779:BCR:H321	23:B:1779:BCR:HC8	0.98	0.95
4:4:75:TRP:HB2	19:4:1205:CLA:HMD3	1.44	0.95
19:1:1149:CLA:O1D	19:1:1149:CLA:HAA1	1.66	0.95
4:4:91:PHE:CG	19:4:1207:CLA:C3C	2.49	0.95
5:A:27:ILE:O	5:A:27:ILE:HG23	1.66	0.95
10:F:23:LYS:HD3	10:F:23:LYS:N	1.78	0.95
23:A:1804:BCR:H382	23:A:1804:BCR:H23C	1.48	0.95
19:B:1753:CLA:H43	19:B:1753:CLA:C1A	1.96	0.95
3:3:94:ARG:HH22	3:3:98:ILE:CG2	1.78	0.95
6:B:403:ASN:O	6:B:406:ASN:CB	2.14	0.95
19:1:1308:CLA:HBA2	19:1:1308:CLA:CBD	1.95	0.95
12:H:44:ALA:HB2	16:L:145:PHE:HD1	1.26	0.95
5:A:217:SER:OG	23:A:1803:BCR:C17	2.15	0.95
6:B:266:GLN:O	6:B:267:SER:HB3	1.65	0.95
3:3:92:TRP:N	3:3:93:PHE:CB	2.30	0.95
4:4:36:ASN:CB	4:4:39:TRP:CE3	2.49	0.95
5:A:453:LEU:HB3	5:A:547:PHE:HB2	1.48	0.95
19:B:1755:CLA:HBB2	19:B:1769:CLA:HMB2	1.48	0.95
19:B:1764:CLA:O2A	19:B:1765:CLA:HMB3	1.67	0.95
19:B:1735:CLA:C19	10:F:104:TYR:HB3	1.96	0.95
17:N:75:TYR:O	17:N:76:LYS:O	1.84	0.95
18:R:34:UNK:CB	18:R:36:UNK:N	2.29	0.95
4:4:95:PHE:CZ	19:4:1210:CLA:C4C	2.50	0.95
9:E:86:GLU:CG	9:E:87:VAL:H	1.72	0.95
17:N:41:LYS:HD2	17:N:42:PHE:CB	1.97	0.95
19:A:1782:CLA:CAB	19:A:1790:CLA:CMA	2.45	0.95
23:A:1805:BCR:H313	19:A:1815:CLA:H143	1.46	0.95
3:3:110:SER:C	3:3:111:TYR:CD2	2.40	0.95
6:B:561:GLY:HA3	7:C:52:LYS:CG	1.97	0.95
7:C:78:GLY:O	7:C:81:TYR:HE1	1.50	0.95
2:2:118:CYS:O	2:2:119:VAL:HG13	1.67	0.95
3:3:94:ARG:CZ	3:3:97:PHE:CZ	2.49	0.94
17:N:41:LYS:CD	17:N:42:PHE:CB	2.45	0.94
5:A:24:ARG:NH1	5:A:29:THR:CB	2.29	0.94
19:3:1221:CLA:HBC3	19:3:1221:CLA:HHD	1.49	0.94
19:A:1774:CLA:CBB	19:A:1774:CLA:H122	1.97	0.94
11:G:28:ARG:HG2	11:G:29:GLU:N	1.78	0.94
16:L:56:VAL:HA	19:L:1167:CLA:CED	1.97	0.94
17:N:57:LYS:HG3	17:N:58:VAL:H	0.78	0.94
17:N:72:LYS:HB3	17:N:73:ASP:C	1.85	0.94
4:4:40:PHE:CG	4:4:43:ALA:HB2	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:169:LEU:HD23	19:2:1215:CLA:HBB2	1.46	0.94
2:2:73:ILE:O	2:2:74:LEU:HG	1.67	0.94
17:N:72:LYS:HE2	17:N:74:LYS:HE2	1.25	0.94
4:4:37:LEU:C	4:4:39:TRP:CB	2.36	0.94
20:A:7042:LMU:H32	20:A:7042:LMU:H6D	1.47	0.94
19:A:1797:CLA:C7	19:A:1797:CLA:H122	1.92	0.94
19:A:1814:CLA:HMB3	19:B:1784:CLA:H18	1.49	0.94
5:A:362:LEU:HD11	19:A:1785:CLA:HBB2	1.48	0.94
5:A:79:PHE:CE2	5:A:185:HIS:CD2	2.55	0.94
22:B:1773:PQN:C16	23:B:1780:BCR:C33	2.44	0.94
17:N:72:LYS:NZ	17:N:74:LYS:CE	2.30	0.94
10:F:153:ASN:C	10:F:153:ASN:HD22	1.69	0.94
26:B:8057:UNL:O6	26:B:8057:UNL:O4'	1.85	0.94
4:4:122:LYS:NZ	4:4:150:LYS:HD2	1.82	0.94
4:4:160:MET:HE2	4:4:163:PHE:HD2	1.33	0.94
4:4:94:GLU:HB3	4:4:95:PHE:CE1	2.03	0.94
5:A:76:ARG:CZ	5:A:192:LYS:HG2	1.98	0.94
6:B:25:ILE:CG2	23:L:1169:BCR:H282	1.97	0.94
4:4:147:LEU:CD2	4:4:148:GLU:HG3	1.97	0.94
1:1:163:VAL:HA	1:1:166:SER:HB3	1.47	0.94
6:B:119:GLY:HA3	19:B:1758:CLA:CED	1.94	0.94
2:2:54:TRP:CZ2	2:2:109:ARG:HD2	2.02	0.94
4:4:122:LYS:CB	4:4:143:PHE:CD2	2.50	0.94
4:4:75:TRP:CE3	4:4:76:TYR:N	2.35	0.94
17:N:67:LEU:C	17:N:68:GLU:HG3	1.87	0.94
12:H:20:GLN:HB3	12:H:22:ASP:CB	1.98	0.94
5:A:328:LYS:CG	5:A:332:GLU:HB2	1.95	0.94
19:3:1222:CLA:HBC3	19:3:1222:CLA:HMC1	1.49	0.94
9:E:52:VAL:O	9:E:53:VAL:HG23	1.65	0.94
23:A:1808:BCR:H332	19:L:1167:CLA:C3B	1.97	0.94
5:A:160:SER:O	5:A:163:GLN:HG2	1.66	0.94
6:B:708:VAL:O	6:B:712:HIS:HB2	1.65	0.94
16:L:163:LEU:HD12	16:L:164:PRO:CG	1.98	0.94
4:4:38:ARG:HG3	4:4:39:TRP:N	1.82	0.94
7:C:14:CYS:CA	7:C:17:CYS:SG	2.55	0.94
4:4:147:LEU:HD21	4:4:148:GLU:HG3	1.48	0.94
7:C:20:ALA:O	7:C:21:CYS:HB2	1.64	0.94
19:A:1770:CLA:CHC	23:A:1803:BCR:H17C	1.98	0.94
19:A:1817:CLA:HHB	19:A:1817:CLA:H43	1.50	0.94
7:C:54:CYS:CB	25:C:1082:SF4:S1	2.55	0.94
19:2:1217:CLA:H93	19:2:1217:CLA:H41	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:178:TRP:O	2:2:182:ILE:HG13	1.66	0.94
16:L:161:LEU:CD1	16:L:162:ASP:O	2.15	0.94
4:4:169:GLN:NE2	19:4:1199:CLA:HHD	1.83	0.94
4:4:122:LYS:CB	4:4:143:PHE:HD2	1.80	0.94
19:A:1774:CLA:H71	19:A:1774:CLA:CAB	1.97	0.94
5:A:368:LEU:HD21	19:A:1774:CLA:H93	1.48	0.94
5:A:511:THR:HG23	19:A:1773:CLA:O1A	1.68	0.94
19:B:1739:CLA:H92	19:B:1739:CLA:CBB	1.98	0.94
19:A:1817:CLA:CMC	6:B:661:PHE:HB2	1.97	0.94
7:C:1:MET:H3	7:C:4:SER:HB3	1.10	0.94
3:3:92:TRP:HA	3:3:95:THR:CB	1.98	0.94
20:A:7036:LMU:H22	20:A:7036:LMU:H82	1.50	0.94
6:B:5:ILE:HB	6:B:6:PRO:CD	1.98	0.94
3:3:92:TRP:N	3:3:93:PHE:CD1	2.36	0.93
5:A:22:VAL:CG2	5:A:23:ASP:CA	2.45	0.93
4:4:149:ALA:CB	4:4:151:GLU:HG2	1.98	0.93
4:4:154:ILE:HG13	4:4:155:ALA:H	1.34	0.93
6:B:432:HIS:HE1	19:B:1762:CLA:NB	1.65	0.93
4:4:192:THR:HG21	4:4:195:GLN:H	1.31	0.93
16:L:161:LEU:HD12	16:L:162:ASP:O	1.68	0.93
19:A:1764:CLA:CHC	19:A:1765:CLA:HMD2	1.98	0.93
19:B:1769:CLA:HMC1	19:B:1769:CLA:CBC	1.98	0.93
4:4:192:THR:HG22	4:4:193:ILE:C	1.88	0.93
3:3:74:ALA:HA	19:3:1216:CLA:C4D	1.96	0.93
2:2:50:VAL:O	2:2:54:TRP:HD1	1.51	0.93
6:B:732:LYS:CB	6:B:733:PHE:C	2.37	0.93
6:B:25:ILE:HG21	23:L:1169:BCR:H292	0.94	0.93
3:3:94:ARG:HG3	3:3:97:PHE:HZ	1.14	0.93
7:C:59:PRO:O	25:C:1083:SF4:S3	2.26	0.93
2:2:211:LYS:HA	2:2:211:LYS:HE2	1.50	0.93
25:B:1783:SF4:S1	25:B:1783:SF4:S2	2.66	0.93
6:B:294:ASN:HB3	11:G:36:PRO:HD2	1.50	0.93
19:4:4014:CLA:CBC	19:4:4014:CLA:HMC1	1.99	0.93
19:3:3011:CLA:H3A	19:3:3011:CLA:CGA	1.98	0.93
19:A:1782:CLA:HBA1	19:A:1782:CLA:O1D	1.68	0.93
17:N:62:SER:HB3	17:N:66:ASP:HB3	1.47	0.93
16:L:37:LEU:O	16:L:42:ALA:HB3	1.68	0.93
2:2:110:TRP:O	2:2:113:ILE:HG12	1.69	0.93
6:B:474:PHE:CE2	6:B:476:ILE:HG13	2.03	0.93
5:A:242:ILE:HG12	5:A:243:PRO:HD3	1.50	0.93
19:B:1753:CLA:HMD2	19:B:1754:CLA:CBB	1.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:110:TRP:HD1	2:2:113:ILE:HG21	1.33	0.93
6:B:310:PRO:HG2	6:B:311:PRO:HD2	1.51	0.93
19:H:1079:CLA:O1A	19:H:1079:CLA:H43	1.67	0.93
3:3:92:TRP:N	3:3:93:PHE:HB2	1.84	0.93
17:N:66:ASP:O	17:N:67:LEU:HG	1.69	0.93
5:A:27:ILE:HG22	5:A:28:LYS:HG3	1.48	0.93
6:B:732:LYS:CB	6:B:733:PHE:HA	1.97	0.93
7:C:1:MET:H1	7:C:4:SER:N	1.66	0.93
11:G:49:THR:OG1	11:G:50:ARG:CG	2.13	0.93
6:B:127:ILE:HD13	6:B:198:ALA:HB2	1.51	0.92
6:B:612:SER:HA	6:B:615:TYR:HE1	1.33	0.92
19:A:1814:CLA:H11	6:B:616:LEU:HG	1.51	0.92
23:A:1808:BCR:H332	19:L:1167:CLA:C4B	1.97	0.92
18:R:35:UNK:C	18:R:38:UNK:CB	2.46	0.92
9:E:51:SER:HB3	9:E:68:ARG:CZ	1.99	0.92
9:E:72:VAL:O	9:E:73:ASN:HB3	1.68	0.92
23:A:1805:BCR:H313	19:A:1815:CLA:C14	1.99	0.92
5:A:370:ILE:HG22	5:A:400:MET:HA	1.51	0.92
5:A:390:ALA:HB2	5:A:754:ILE:HB	1.52	0.92
19:B:1757:CLA:O1D	19:B:1758:CLA:HMA1	1.68	0.92
25:B:1783:SF4:S4	25:B:1783:SF4:S2	2.67	0.92
2:2:129:LYS:O	2:2:132:GLY:N	2.01	0.92
12:H:27:ASP:O	12:H:29:PRO:HD3	1.68	0.92
4:4:124:TYR:O	4:4:127:PRO:CD	2.17	0.92
3:3:94:ARG:NH2	3:3:98:ILE:CG2	2.30	0.92
23:A:1805:BCR:H393	23:A:1805:BCR:H23C	1.49	0.92
9:E:56:ASP:HB2	9:E:64:PRO:HB3	1.49	0.92
6:B:493:TRP:CZ2	19:B:1765:CLA:HBA1	2.05	0.92
5:A:669:GLY:H	6:B:445:ALA:HA	1.31	0.92
5:A:705:GLU:HB3	6:B:545:LYS:HZ1	1.33	0.92
2:2:94:LEU:O	2:2:98:GLU:HB3	1.69	0.92
10:F:5:LEU:CG	10:F:6:THR:H	1.81	0.92
4:4:142:ASN:CA	4:4:150:LYS:NZ	2.33	0.92
19:A:1789:CLA:C4	16:L:64:LEU:HD23	1.99	0.92
5:A:246:HIS:CE1	19:A:1798:CLA:HMA3	2.04	0.92
19:B:1752:CLA:HBC2	19:B:1753:CLA:HBA1	1.51	0.92
19:B:1753:CLA:O2D	19:B:1753:CLA:H2A	1.70	0.92
19:B:1758:CLA:H142	23:B:1776:BCR:H10C	1.49	0.92
17:N:72:LYS:CG	17:N:74:LYS:CG	2.41	0.92
19:3:1218:CLA:HHD	19:3:1218:CLA:HBC3	1.51	0.92
19:A:1789:CLA:H51	16:L:67:PRO:HB3	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:6:TYR:C	17:N:8:GLU:H	1.70	0.92
16:L:163:LEU:CD1	16:L:164:PRO:N	2.31	0.92
7:C:14:CYS:SG	7:C:18:VAL:O	2.28	0.92
20:A:7016:LMU:H22	20:A:7016:LMU:C6	1.89	0.92
19:B:1755:CLA:CBB	19:B:1769:CLA:HMB3	1.99	0.92
13:I:11:LEU:HG	23:I:1032:BCR:C7	2.00	0.92
5:A:472:ARG:NH1	16:L:74:LEU:HG	1.84	0.92
17:N:76:LYS:HG3	17:N:77:CYS:H	1.34	0.92
2:2:128:ASN:C	2:2:130:LEU:N	2.16	0.92
6:B:361:ILE:HG23	6:B:368:GLN:OE1	1.69	0.91
6:B:442:VAL:HG21	19:B:1763:CLA:HAC2	1.52	0.91
7:C:74:THR:CB	7:C:80:ALA:HB2	2.00	0.91
13:I:26:LEU:HA	13:I:29:GLU:O	1.70	0.91
2:2:64:ILE:O	2:2:68:LEU:HB2	1.69	0.91
4:4:151:GLU:C	4:4:154:ILE:H	1.71	0.91
17:N:61:LEU:C	17:N:61:LEU:HD12	1.88	0.91
18:R:34:UNK:H	18:R:36:UNK:C	1.82	0.91
5:A:316:MET:HB3	5:A:317:TYR:CB	2.00	0.91
10:F:22:LEU:O	10:F:25:LEU:HB2	1.70	0.91
5:A:22:VAL:CG2	5:A:23:ASP:N	2.29	0.91
11:G:60:SER:HA	11:G:63:PRO:HD2	1.53	0.91
1:1:179:THR:HG21	4:4:87:SER:HB3	1.49	0.91
5:A:51:THR:CG2	19:A:1795:CLA:HBB2	1.99	0.91
5:A:340:GLY:O	5:A:343:HIS:HB2	1.70	0.91
3:3:74:ALA:HA	19:3:1216:CLA:C2D	2.01	0.91
2:2:96:ILE:HG13	2:2:97:VAL:H	1.35	0.91
5:A:98:PHE:CZ	19:A:1763:CLA:HMD3	2.04	0.91
5:A:302:HIS:O	5:A:306:ILE:HG12	1.70	0.91
19:B:1761:CLA:HMC2	19:B:1769:CLA:HBC1	1.52	0.91
6:B:382:ILE:CG2	6:B:383:MET:H	1.83	0.91
4:4:74:LYS:H	4:4:75:TRP:HA	1.36	0.91
5:A:316:MET:HG2	5:A:317:TYR:CE1	2.05	0.91
20:A:7008:LMU:C6'	20:A:7008:LMU:H22	2.00	0.91
19:A:1782:CLA:CAB	19:A:1790:CLA:HMA2	2.00	0.91
6:B:247:THR:HA	6:B:250:ALA:CB	2.00	0.91
5:A:22:VAL:CA	5:A:23:ASP:C	2.38	0.91
5:A:197:GLN:HE21	5:A:197:GLN:CA	1.80	0.91
1:1:185:TRP:HH2	19:1:1199:CLA:C1	1.57	0.91
5:A:648:THR:HG23	5:A:651:GLY:H	1.36	0.91
11:G:26:PHE:HB2	11:G:27:GLN:HE21	1.35	0.91
5:A:342:GLY:HA3	5:A:430:ASP:HB2	0.93	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1782:CLA:HMC1	19:A:1782:CLA:HBC2	1.51	0.90
19:B:1746:CLA:HHD	19:B:1746:CLA:HBC2	1.53	0.90
6:B:279:ALA:O	19:B:1746:CLA:HMB3	1.71	0.90
5:A:22:VAL:HB	5:A:23:ASP:CA	2.01	0.90
1:1:37:GLU:HA	1:1:40:LYS:HB2	1.50	0.90
1:1:185:TRP:CH2	19:1:1199:CLA:C2	2.49	0.90
19:4:1199:CLA:CBC	19:4:1199:CLA:HMC1	2.01	0.90
4:4:102:GLU:OE2	19:4:1209:CLA:C4B	2.18	0.90
19:A:1781:CLA:HBA2	19:A:1794:CLA:HED1	1.53	0.90
5:A:40:PHE:HE1	5:A:53:TRP:CD1	1.89	0.90
12:H:69:SER:HB2	19:H:1079:CLA:C6	2.02	0.90
19:H:1080:CLA:C4C	23:I:1032:BCR:HC22	2.01	0.90
18:R:52:UNK:CA	18:R:53:UNK:CB	2.48	0.90
4:4:145:PRO:O	4:4:147:LEU:HA	1.70	0.90
1:1:184:PRO:C	1:1:185:TRP:CG	2.44	0.90
19:A:1762:CLA:H43	19:A:1785:CLA:H11	1.50	0.90
7:C:73:THR:OG1	7:C:76:SER:HB3	1.70	0.90
20:A:7016:LMU:H1'	20:A:7016:LMU:H31	1.53	0.90
1:1:89:VAL:HB	1:1:90:PRO:HD3	1.50	0.90
19:4:1201:CLA:CBA	19:4:1201:CLA:HMA2	2.00	0.90
19:B:1739:CLA:HMC2	23:B:1780:BCR:H281	1.53	0.90
17:N:58:VAL:CB	17:N:59:PRO:CD	2.48	0.90
2:2:102:ILE:C	19:2:1221:CLA:CBB	2.40	0.90
5:A:114:THR:HG22	5:A:115:HIS:CE1	2.05	0.90
15:K:83:VAL:O	15:K:84:LEU:O	1.88	0.90
19:2:1213:CLA:C4	19:2:1213:CLA:C4C	2.50	0.90
11:G:68:ILE:CG2	11:G:72:LEU:HD13	2.02	0.90
19:2:1212:CLA:HBC2	19:2:1212:CLA:HHD	1.54	0.90
6:B:666:SER:HB3	6:B:671:TRP:HE1	1.34	0.90
5:A:451:ILE:HD12	19:A:1788:CLA:HED3	1.53	0.90
5:A:73:GLU:O	5:A:76:ARG:N	2.05	0.90
19:B:1737:CLA:C9	19:B:1754:CLA:O1D	2.19	0.90
19:B:1753:CLA:HBC3	19:B:1753:CLA:HMC1	1.52	0.90
3:3:92:TRP:N	3:3:93:PHE:CG	2.40	0.90
5:A:27:ILE:HG23	5:A:28:LYS:HD3	1.52	0.90
19:3:1218:CLA:H41	19:3:1218:CLA:H8	0.92	0.90
20:A:7037:LMU:H12	20:A:7037:LMU:C5	2.01	0.90
19:3:3011:CLA:O1A	19:3:3011:CLA:H3A	1.72	0.90
5:A:466:THR:HG22	19:B:1740:CLA:CHC	2.01	0.90
8:D:113:HIS:H	8:D:114:PRO:HD2	1.34	0.90
5:A:162:LEU:O	5:A:165:TYR:HB3	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1791:CLA:H3A	19:A:1797:CLA:CBB	2.02	0.90
23:A:1806:BCR:H23C	23:A:1806:BCR:C39	2.02	0.90
22:B:1773:PQN:H162	23:B:1780:BCR:H331	1.53	0.90
16:L:163:LEU:HD11	16:L:165:TYR:CZ	2.06	0.90
2:2:127:ASN:HB3	14:J:1:MET:O	1.70	0.90
20:A:7030:LMU:H4'	20:A:7030:LMU:O2B	1.71	0.90
19:A:1770:CLA:C3B	23:A:1803:BCR:H19C	2.01	0.89
9:E:42:GLU:HG2	9:E:43:SER:N	1.87	0.89
9:E:45:TRP:CH2	9:E:78:SER:OG	2.24	0.89
4:4:194:VAL:HB	4:4:195:GLN:C	1.93	0.89
1:1:144:LYS:CE	19:1:1187:CLA:O2D	2.16	0.89
5:A:626:GLY:HA3	5:A:636:HIS:HA	1.54	0.89
9:E:83:ALA:O	9:E:86:GLU:HG2	1.72	0.89
8:D:124:ASN:HB3	8:D:125:PRO:HD3	1.54	0.89
4:4:40:PHE:CB	4:4:43:ALA:CB	2.45	0.89
18:R:41:UNK:CB	18:R:42:UNK:HA	2.02	0.89
19:B:1768:CLA:H161	23:B:1779:BCR:H313	1.54	0.89
7:C:5:VAL:HG21	7:C:65:VAL:HG11	1.50	0.89
17:N:62:SER:CB	17:N:66:ASP:CB	2.47	0.89
5:A:28:LYS:CB	5:A:28:LYS:NZ	2.30	0.89
15:K:42:ALA:O	15:K:43:ARG:HD3	1.71	0.89
20:2:1224:LMU:H62	20:2:1224:LMU:H12	1.53	0.89
5:A:586:ARG:HG3	7:C:49:VAL:HG21	1.54	0.89
5:A:555:ILE:HG21	19:A:1817:CLA:HMD1	1.55	0.89
19:B:1735:CLA:H191	10:F:104:TYR:CB	2.01	0.89
18:R:34:UNK:CA	18:R:36:UNK:N	2.36	0.89
11:G:13:GLY:HA2	11:G:16:LEU:HG	1.54	0.89
19:B:1768:CLA:H152	23:B:1779:BCR:H312	1.51	0.89
6:B:25:ILE:CG2	23:L:1169:BCR:C29	2.41	0.89
13:I:12:VAL:O	13:I:17:PRO:HD3	1.73	0.89
2:2:59:ALA:HB3	2:2:172:LEU:HD13	1.54	0.89
1:1:144:LYS:HZ2	19:1:1187:CLA:HED3	0.75	0.89
20:A:7023:LMU:H91	20:A:7023:LMU:C2	2.02	0.89
4:4:118:ASP:HA	4:4:123:GLN:N	1.87	0.89
4:4:128:ALA:CB	4:4:143:PHE:HE2	1.85	0.89
4:4:149:ALA:HB3	4:4:151:GLU:CG	2.02	0.89
4:4:94:GLU:CG	4:4:95:PHE:CE1	2.55	0.89
5:A:335:LYS:HG2	5:A:336:GLY:N	1.88	0.89
6:B:292:ARG:NE	6:B:292:ARG:HA	1.87	0.89
17:N:41:LYS:CB	17:N:42:PHE:HB3	2.03	0.89
2:2:116:PRO:O	2:2:131:THR:HB	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:148:VAL:O	16:L:149:SER:HB3	1.72	0.89
6:B:574:ASP:HA	6:B:577:TYR:HB3	1.52	0.89
6:B:608:GLN:HA	6:B:608:GLN:NE2	1.88	0.89
19:A:1781:CLA:CED	19:A:1782:CLA:CAD	2.50	0.89
5:A:79:PHE:CE2	5:A:185:HIS:NE2	2.41	0.89
19:B:1761:CLA:CBC	19:B:1761:CLA:CHD	2.51	0.89
11:G:16:LEU:HD23	11:G:68:ILE:HG23	1.54	0.89
5:A:368:LEU:CD2	19:A:1774:CLA:C9	2.50	0.89
22:B:1773:PQN:H192	23:B:1780:BCR:H10C	1.52	0.89
23:A:1808:BCR:H331	19:L:1167:CLA:C4B	2.00	0.89
11:G:93:TYR:CA	11:G:94:ASP:HB2	2.01	0.89
21:B:8052:SUC:C1	21:B:8052:SUC:H5'	2.02	0.89
20:A:7016:LMU:H21	20:A:7016:LMU:H81	0.93	0.89
19:A:1769:CLA:HBA1	19:A:1780:CLA:H41	1.54	0.88
18:R:38:UNK:O	18:R:42:UNK:HA	1.73	0.88
6:B:504:ASN:HD22	6:B:504:ASN:H	1.15	0.88
5:A:131:ILE:HG21	6:B:446:PHE:HA	1.55	0.88
5:A:672:LEU:O	5:A:674:ALA:N	2.05	0.88
6:B:561:GLY:CA	7:C:52:LYS:HG2	2.02	0.88
23:I:1032:BCR:C8	23:I:1032:BCR:C31	2.42	0.88
16:L:164:PRO:CA	16:L:165:TYR:HB3	1.91	0.88
2:2:102:ILE:O	19:2:1221:CLA:HBB2	1.71	0.88
20:A:7010:LMU:O2B	20:A:7010:LMU:H3'	1.72	0.88
3:3:205:GLY:CA	5:A:252:ARG:HH12	1.86	0.88
23:A:1809:BCR:C23	23:A:1809:BCR:H393	2.01	0.88
25:B:1783:SF4:S1	25:B:1783:SF4:S4	2.71	0.88
6:B:190:TRP:HA	19:B:1744:CLA:HBB2	1.55	0.88
5:A:22:VAL:CG2	5:A:23:ASP:HA	2.01	0.88
19:2:2006:CLA:HBA2	19:2:2006:CLA:CGD	2.04	0.88
19:1:1142:CLA:HMD1	19:1:1143:CLA:NA	1.87	0.88
5:A:328:LYS:HE3	5:A:332:GLU:HG3	1.52	0.88
9:E:68:ARG:C	9:E:68:ARG:HE	1.76	0.88
17:N:47:THR:OG1	17:N:54:LYS:HD3	1.72	0.88
17:N:18:ASP:HB2	17:N:22:LEU:HG	1.53	0.88
6:B:382:ILE:HG22	6:B:383:MET:N	1.88	0.88
6:B:492:ILE:HD13	6:B:492:ILE:H	1.39	0.88
16:L:163:LEU:HD12	16:L:165:TYR:CD1	2.09	0.88
2:2:55:ALA:HB3	2:2:56:MET:HE2	1.52	0.88
20:A:7013:LMU:C9	20:A:7049:LMU:O3'	2.20	0.88
6:B:212:PHE:HE1	19:B:1744:CLA:HHD	1.37	0.88
17:N:72:LYS:HB3	17:N:74:LYS:H	1.14	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:39:TRP:CG	4:4:40:PHE:N	2.37	0.88
4:4:118:ASP:HA	4:4:122:LYS:C	1.94	0.88
5:A:301:HIS:NE2	19:A:1772:CLA:O1D	2.07	0.88
6:B:230:TRP:CH2	11:G:11:SER:HB2	2.09	0.88
17:N:45:ASN:HB3	17:N:57:LYS:HZ1	1.05	0.88
15:K:43:ARG:HG3	15:K:43:ARG:NH1	1.71	0.88
20:2:1224:LMU:C1	20:2:1224:LMU:H72	2.03	0.88
5:A:425:THR:HG21	8:D:59:GLU:OE2	1.72	0.88
4:4:60:LEU:HG	4:4:61:PRO:HD3	1.56	0.88
5:A:316:MET:CB	5:A:317:TYR:HD1	1.86	0.88
5:A:100:GLY:HA3	5:A:153:TRP:CH2	2.09	0.88
20:A:7042:LMU:H5'	20:A:7042:LMU:O2B	1.74	0.88
16:L:161:LEU:HD12	16:L:162:ASP:N	1.88	0.88
20:A:7008:LMU:H6D	20:A:7008:LMU:H22	1.54	0.88
19:B:1737:CLA:H93	19:B:1754:CLA:O1D	1.74	0.88
6:B:86:PRO:O	6:B:87:ILE:HG13	1.74	0.88
2:2:110:TRP:HA	2:2:113:ILE:HG23	1.56	0.88
10:F:40:LEU:HA	10:F:42:ILE:HG12	1.56	0.88
12:H:25:GLY:HA3	12:H:27:ASP:H	1.38	0.88
4:4:89:THR:O	4:4:92:VAL:HB	1.74	0.87
19:A:1789:CLA:H41	16:L:64:LEU:HD23	1.54	0.87
20:A:7021:LMU:H31	20:A:7021:LMU:C1'	2.02	0.87
4:4:151:GLU:HA	4:4:154:ILE:HG23	1.56	0.87
6:B:174:ARG:HB2	19:B:1743:CLA:CBC	2.03	0.87
2:2:168:ARG:O	2:2:172:LEU:HD12	1.74	0.87
5:A:328:LYS:CE	5:A:332:GLU:HG3	2.04	0.87
5:A:141:ARG:HG3	5:A:141:ARG:HH21	1.38	0.87
5:A:239:PRO:HA	5:A:242:ILE:CD1	2.05	0.87
19:B:1747:CLA:H52	19:B:1756:CLA:HMB1	1.53	0.87
22:B:1773:PQN:H191	23:B:1780:BCR:C10	2.04	0.87
10:F:93:ILE:O	10:F:96:TRP:HD1	1.56	0.87
19:2:1217:CLA:HMD2	19:2:1219:CLA:HMD3	1.54	0.87
19:A:1791:CLA:C3A	19:A:1797:CLA:HBB1	2.05	0.87
23:A:1805:BCR:C31	19:A:1815:CLA:C14	2.51	0.87
5:A:331:LEU:HD11	5:A:346:LEU:CB	2.03	0.87
5:A:114:THR:OG1	5:A:525:ASN:HB2	1.74	0.87
19:A:1788:CLA:H161	23:L:1169:BCR:C36	2.04	0.87
3:3:93:PHE:HB2	3:3:95:THR:HG23	1.52	0.87
4:4:192:THR:CG2	4:4:195:GLN:N	2.37	0.87
5:A:217:SER:OG	23:A:1803:BCR:H17C	1.71	0.87
3:3:94:ARG:HA	3:3:97:PHE:CD1	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:8052:SUC:C1	21:B:8052:SUC:C5'	2.52	0.87
19:2:1213:CLA:HBC3	19:2:1213:CLA:CHD	2.04	0.87
19:A:1772:CLA:HBA2	19:A:1772:CLA:H2	1.55	0.87
25:B:1783:SF4:S4	25:B:1783:SF4:S3	2.72	0.87
19:L:1168:CLA:HAA1	19:L:1168:CLA:CGD	2.04	0.87
17:N:70:GLU:O	17:N:72:LYS:HD3	1.74	0.87
4:4:104:ARG:HH11	4:4:105:ARG:HB3	1.39	0.87
4:4:33:ASP:HB3	4:4:34:PRO:CD	2.03	0.87
19:2:1223:CLA:C4A	19:2:1223:CLA:HBA1	2.03	0.87
6:B:461:GLN:O	6:B:464:GLN:HG2	1.74	0.87
2:2:66:GLU:O	2:2:69:THR:N	2.07	0.87
5:A:412:ALA:HB2	5:A:598:VAL:HG11	1.55	0.87
5:A:204:ASN:O	5:A:205:HIS:HB2	1.73	0.87
5:A:25:ASP:CG	5:A:26:PRO:HA	1.96	0.87
5:A:249:ILE:CG1	5:A:250:LEU:H	1.85	0.87
5:A:382:TYR:OH	19:A:1784:CLA:H42	1.73	0.86
6:B:180:SER:HB2	6:B:288:GLY:HA3	1.57	0.86
6:B:87:ILE:CA	6:B:115:ASN:HA	2.04	0.86
9:E:52:VAL:HG12	9:E:53:VAL:H	1.35	0.86
19:L:1168:CLA:HHD	19:L:1168:CLA:CBC	2.04	0.86
18:R:34:UNK:N	18:R:36:UNK:CA	2.37	0.86
3:3:112:THR:OG1	3:3:113:LEU:N	2.04	0.86
19:A:1759:CLA:HBB2	19:A:1760:CLA:C4C	2.04	0.86
19:A:1797:CLA:HHD	19:A:1797:CLA:HBC2	1.56	0.86
5:A:368:LEU:HD21	19:A:1774:CLA:C9	2.04	0.86
19:B:1764:CLA:HMD2	19:B:1765:CLA:C1C	2.05	0.86
9:E:58:ASP:OD2	9:E:60:LYS:HG2	1.75	0.86
4:4:142:ASN:C	4:4:150:LYS:CE	2.44	0.86
19:B:1743:CLA:H151	19:B:1758:CLA:HMD2	1.57	0.86
6:B:391:PRO:HB3	6:B:538:ALA:HA	1.55	0.86
4:4:122:LYS:HD3	4:4:150:LYS:HD2	1.54	0.86
19:A:1801:CLA:CMA	16:L:27:VAL:HA	2.05	0.86
5:A:470:LEU:CD1	6:B:95:HIS:HB3	2.06	0.86
9:E:40:ARG:NH2	9:E:86:GLU:OE1	2.07	0.86
11:G:37:GLU:CD	11:G:42:SER:HB2	1.91	0.86
3:3:94:ARG:HH22	3:3:98:ILE:HG21	1.05	0.86
11:G:94:ASP:H	11:G:95:PRO:HD3	0.71	0.86
1:1:184:PRO:O	1:1:185:TRP:CD1	2.28	0.86
6:B:398:TYR:O	8:D:143:PRO:HG2	1.74	0.86
4:4:68:GLY:O	4:4:71:ASN:HB2	1.74	0.86
11:G:94:ASP:N	11:G:95:PRO:CD	2.14	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:316:MET:HB3	5:A:317:TYR:CD1	2.10	0.86
5:A:328:LYS:HG2	5:A:332:GLU:CB	2.05	0.86
20:A:7013:LMU:H51	20:A:7049:LMU:H12	1.57	0.86
17:N:72:LYS:HG3	17:N:74:LYS:HG3	0.86	0.86
3:3:132:TRP:HZ3	3:3:155:GLU:HG2	1.07	0.86
19:3:1221:CLA:HBC3	19:3:1221:CLA:CHD	2.06	0.86
7:C:44:ARG:NH2	8:D:127:ARG:HB3	1.88	0.86
20:A:7005:LMU:H32	20:A:7005:LMU:C8	2.00	0.86
7:C:1:MET:N	7:C:3:HIS:C	2.29	0.86
13:I:24:LEU:C	13:I:26:LEU:H	1.78	0.86
4:4:107:GLN:O	19:4:1196:CLA:CMA	2.23	0.86
6:B:374:HIS:HB2	19:B:1757:CLA:C1B	2.06	0.86
7:C:5:VAL:CG2	7:C:65:VAL:HG11	2.05	0.86
17:N:67:LEU:O	17:N:68:GLU:HG3	1.75	0.86
4:4:106:TRP:C	4:4:108:ASP:H	1.77	0.86
4:4:124:TYR:HB3	4:4:143:PHE:CD1	2.11	0.86
19:A:1781:CLA:HED2	19:A:1782:CLA:CAD	2.05	0.86
19:A:1816:CLA:HBB2	19:A:1817:CLA:C1B	2.06	0.86
6:B:588:GLY:O	6:B:592:PHE:HB2	1.76	0.86
8:D:39:LYS:HD2	8:D:42:VAL:CG1	2.05	0.86
19:2:1223:CLA:NA	19:2:1223:CLA:HBA1	1.88	0.86
14:J:2:ARG:HH12	14:J:8:LEU:HD13	1.41	0.86
4:4:160:MET:HE2	4:4:163:PHE:CD2	2.11	0.86
19:A:1763:CLA:C3B	23:A:1806:BCR:H331	2.05	0.86
5:A:599:PHE:CE2	5:A:731:ARG:HB3	2.11	0.86
19:B:1737:CLA:H122	19:B:1737:CLA:OBD	1.74	0.86
6:B:25:ILE:HG21	23:L:1169:BCR:C28	2.05	0.86
8:D:32:SER:H	16:L:23:LEU:HG	1.38	0.86
2:2:103:GLY:N	19:2:1221:CLA:HBB2	1.89	0.86
4:4:147:LEU:HD13	4:4:148:GLU:N	1.89	0.86
5:A:452:PHE:HE1	19:A:1793:CLA:CBB	1.88	0.85
3:3:132:TRP:CH2	3:3:155:GLU:HG3	2.08	0.85
16:L:165:TYR:HA	16:L:166:TYR:O	1.76	0.85
4:4:95:PHE:HD1	4:4:95:PHE:N	1.73	0.85
5:A:114:THR:HG22	5:A:115:HIS:ND1	1.90	0.85
5:A:259:TYR:HB3	5:A:260:PRO:HD2	1.58	0.85
19:B:1761:CLA:HBC3	19:B:1761:CLA:CHD	2.05	0.85
16:L:165:TYR:O	16:L:165:TYR:CD1	2.29	0.85
3:3:63:ARG:HH22	3:3:189:LEU:HD23	1.40	0.85
4:4:169:GLN:NE2	4:4:169:GLN:HA	1.90	0.85
19:A:1760:CLA:HBB2	19:A:1762:CLA:C3D	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:571:SER:OG	6:B:574:ASP:OD1	1.94	0.85
3:3:80:LYS:HD3	3:3:105:ASN:HB2	1.58	0.85
10:F:42:ILE:HG13	10:F:43:LYS:N	1.87	0.85
20:A:7040:LMU:O3'	20:A:7040:LMU:H1B	1.74	0.85
4:4:107:GLN:O	19:4:1196:CLA:HMA3	1.76	0.85
6:B:421:HIS:NE2	19:B:1761:CLA:C4D	2.40	0.85
6:B:545:LYS:HG2	9:E:74:TYR:CE2	2.11	0.85
2:2:91:THR:O	2:2:94:LEU:HB3	1.75	0.85
4:4:169:GLN:CG	19:4:1199:CLA:HAC2	2.06	0.85
5:A:87:SER:HB2	5:A:178:MET:O	1.75	0.85
6:B:295:PHE:H	6:B:295:PHE:HD2	1.19	0.85
16:L:66:GLY:HA3	19:L:1168:CLA:CHC	2.07	0.85
2:2:54:TRP:CE2	2:2:109:ARG:HD2	2.12	0.85
20:A:7033:LMU:H3'	20:A:7033:LMU:C6B	2.07	0.85
19:A:1774:CLA:O1A	19:A:1784:CLA:CMD	2.23	0.85
19:A:1797:CLA:HHD	19:A:1797:CLA:HBC3	1.58	0.85
19:B:1735:CLA:CMD	23:B:1778:BCR:HC41	2.07	0.85
5:A:24:ARG:HD2	5:A:24:ARG:H	1.40	0.85
19:1:1146:CLA:HMC1	19:1:1146:CLA:HBC2	1.57	0.85
8:D:102:ARG:HE	8:D:110:GLN:HB2	1.40	0.85
5:A:723:ARG:HH11	5:A:723:ARG:CG	1.88	0.85
4:4:74:LYS:H	4:4:75:TRP:CA	1.90	0.85
3:3:97:PHE:CD2	3:3:97:PHE:O	2.29	0.85
19:3:1221:CLA:H193	19:3:1221:CLA:H152	1.59	0.85
6:B:715:VAL:HG23	6:B:719:PHE:CD2	2.12	0.85
19:R:1054:CLA:HED3	19:R:1054:CLA:CHA	2.05	0.85
19:B:1735:CLA:HED3	19:B:1735:CLA:H2A	1.56	0.85
6:B:521:HIS:HE1	19:B:1768:CLA:NA	1.74	0.85
5:A:246:HIS:O	5:A:248:PHE:N	2.10	0.85
5:A:599:PHE:CE2	5:A:735:VAL:CG2	2.60	0.85
6:B:282:PHE:HZ	19:B:1746:CLA:C1	1.90	0.85
6:B:174:ARG:HB2	19:B:1743:CLA:HBC2	1.57	0.85
5:A:27:ILE:O	5:A:28:LYS:HG2	1.76	0.85
19:2:1222:CLA:HMC1	19:2:1222:CLA:HBC3	1.58	0.85
4:4:107:GLN:HA	19:4:1196:CLA:CMA	2.05	0.85
9:E:52:VAL:O	9:E:53:VAL:HG22	1.74	0.85
19:H:1079:CLA:HBB2	13:I:13:GLY:O	1.77	0.85
19:2:2006:CLA:HBA2	19:2:2006:CLA:CBD	2.07	0.85
19:B:1755:CLA:CBC	19:B:1755:CLA:HHD	2.06	0.84
4:4:124:TYR:CB	4:4:143:PHE:CD1	2.60	0.84
7:C:5:VAL:HG21	7:C:65:VAL:HG13	0.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:44:GLU:O	15:K:46:GLY:HA2	1.77	0.84
19:1:1145:CLA:HMC1	19:1:1145:CLA:HBC3	1.59	0.84
19:A:1779:CLA:C4C	23:A:1804:BCR:C19	2.49	0.84
6:B:419:ILE:O	6:B:420:SER:OG	1.94	0.84
16:L:14:LEU:HA	16:L:24:GLU:HG3	1.59	0.84
3:3:158:TYR:HB3	3:3:159:PRO:CD	2.06	0.84
4:4:128:ALA:HB2	4:4:143:PHE:HE2	1.40	0.84
19:A:1814:CLA:C3B	6:B:589:TRP:HH2	1.91	0.84
19:B:1753:CLA:H151	19:B:1753:CLA:C10	2.04	0.84
17:N:63:ASP:N	17:N:64:ASP:HB3	1.91	0.84
10:F:151:ASP:O	10:F:154:PHE:HB3	1.76	0.84
19:A:1783:CLA:H43	19:A:1783:CLA:HBA1	1.60	0.84
19:B:1755:CLA:CED	19:B:1756:CLA:HMD1	2.07	0.84
19:B:1767:CLA:HBC3	19:B:1767:CLA:HMC1	1.59	0.84
6:B:353:TYR:CG	6:B:594:TRP:HZ3	1.94	0.84
6:B:656:VAL:HG22	19:B:1771:CLA:HMB3	1.56	0.84
11:G:43:HIS:CE1	11:G:45:GLU:HG2	2.13	0.84
19:H:1080:CLA:HAC1	23:I:1032:BCR:HC31	1.60	0.84
3:3:95:THR:N	3:3:97:PHE:CD1	2.42	0.84
5:A:567:ARG:HH11	8:D:35:GLY:HA2	1.37	0.84
19:1:1187:CLA:HBC3	19:1:1187:CLA:HMC1	1.58	0.84
19:A:1779:CLA:CHD	23:A:1804:BCR:C19	2.54	0.84
6:B:120:VAL:HA	6:B:123:TRP:NE1	1.92	0.84
19:B:1755:CLA:C1	19:B:1769:CLA:HED3	2.06	0.84
3:3:180:LYS:O	3:3:181:LEU:C	2.06	0.84
19:1:1142:CLA:HED1	19:1:1143:CLA:HMB2	1.59	0.84
19:1:1146:CLA:HMA2	19:1:1146:CLA:O1A	1.78	0.84
19:B:1766:CLA:HBC2	19:B:1766:CLA:HHD	1.59	0.84
20:A:7034:LMU:H22	20:A:7034:LMU:O2'	1.77	0.84
1:1:184:PRO:O	1:1:185:TRP:CG	2.30	0.84
6:B:22:TRP:HE1	19:B:1770:CLA:CBB	1.90	0.84
6:B:608:GLN:CA	6:B:608:GLN:HE21	1.91	0.84
7:C:63:LEU:HG	7:C:64:SER:N	1.92	0.84
17:N:41:LYS:HB2	17:N:42:PHE:CA	2.06	0.84
20:A:7022:LMU:C2	20:A:7022:LMU:H2'	2.01	0.84
19:3:1222:CLA:H102	19:3:1222:CLA:C14	2.07	0.84
16:L:123:ARG:HA	16:L:123:ARG:CZ	2.07	0.84
21:B:8056:SUC:H3'	21:B:8056:SUC:O2	1.78	0.84
1:1:183:ASP:CB	1:1:184:PRO:HD2	2.05	0.84
5:A:110:LEU:HD11	5:A:239:PRO:HG2	1.60	0.84
6:B:142:LEU:HD22	23:B:1776:BCR:H333	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:62:SER:CB	17:N:66:ASP:HB3	2.08	0.84
6:B:140:ILE:H	6:B:140:ILE:HD13	1.41	0.84
6:B:393:PHE:HD2	6:B:397:ASP:OD1	1.61	0.84
4:4:107:GLN:CA	19:4:1196:CLA:CMA	2.53	0.84
5:A:131:ILE:O	5:A:671:SER:HA	1.77	0.84
19:A:1774:CLA:O1A	19:A:1784:CLA:HMD2	1.78	0.84
23:A:1805:BCR:C8	23:A:1805:BCR:H311	2.07	0.84
5:A:711:HIS:HB3	5:A:717:ALA:HB2	1.58	0.84
23:B:1779:BCR:C8	23:B:1779:BCR:C32	2.47	0.84
10:F:23:LYS:C	10:F:24:LYS:HE2	1.98	0.84
4:4:103:ILE:HG13	19:4:1197:CLA:HMD1	1.60	0.83
23:A:1805:BCR:C39	23:A:1805:BCR:H23C	2.08	0.83
1:1:39:TYR:CB	19:1:1196:CLA:OBD	2.25	0.83
2:2:196:HIS:NE2	21:2:1225:SUC:O3	2.10	0.83
5:A:711:HIS:CD2	19:A:1795:CLA:HBC1	2.13	0.83
5:A:547:PHE:O	5:A:551:VAL:HG13	1.78	0.83
11:G:17:PHE:O	11:G:20:ARG:HB2	1.76	0.83
4:4:154:ILE:HG13	4:4:155:ALA:N	1.92	0.83
4:4:174:GLY:O	4:4:175:LYS:CG	2.23	0.83
17:N:72:LYS:HD2	17:N:74:LYS:HG2	1.60	0.83
3:3:132:TRP:HZ3	3:3:155:GLU:CG	1.60	0.83
19:2:2006:CLA:HBA2	19:2:2006:CLA:HBD	1.60	0.83
19:2:1213:CLA:C4	19:2:1213:CLA:CHD	2.56	0.83
4:4:118:ASP:CG	4:4:123:GLN:HB2	1.97	0.83
6:B:189:ALA:CB	19:B:1758:CLA:H203	2.07	0.83
8:D:124:ASN:CB	8:D:125:PRO:HD3	2.08	0.83
19:4:1199:CLA:HAA1	19:F:1157:CLA:H42	1.59	0.83
6:B:374:HIS:HB2	19:B:1757:CLA:NB	1.92	0.83
6:B:233:TYR:CD2	19:B:1746:CLA:HED1	2.13	0.83
6:B:560:ASP:OD1	6:B:561:GLY:N	2.12	0.83
6:B:382:ILE:O	6:B:384:THR:N	2.11	0.83
20:A:7016:LMU:C7	20:A:7016:LMU:H112	2.08	0.83
3:3:64:TYR:HB3	19:3:1221:CLA:H42	1.58	0.83
15:K:40:LEU:O	15:K:41:GLU:CB	2.22	0.83
3:3:80:LYS:HD3	3:3:105:ASN:CB	2.07	0.83
2:2:167:GLY:O	2:2:170:ALA:N	2.12	0.83
20:A:7042:LMU:H3'	20:A:7042:LMU:H2B	1.61	0.83
8:D:113:HIS:NE2	8:D:118:VAL:HG11	1.94	0.83
12:H:25:GLY:CA	12:H:27:ASP:H	1.91	0.83
15:K:74:ILE:HG22	15:K:75:VAL:HG22	1.61	0.83
16:L:152:THR:O	16:L:156:PHE:N	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:248:PHE:H	5:A:248:PHE:HD2	1.25	0.83
19:B:1759:CLA:HBC2	19:B:1759:CLA:HMC1	1.58	0.83
6:B:304:ILE:HD11	19:B:1749:CLA:CED	2.08	0.83
24:B:1781:LMG:O3	7:C:70:TRP:NE1	2.12	0.83
12:H:73:PRO:CD	21:H:1082:SUC:C6'	2.57	0.83
20:A:7001:LMU:H81	20:A:7001:LMU:C4	1.97	0.83
4:4:95:PHE:N	4:4:95:PHE:CD1	2.44	0.83
19:A:1817:CLA:HMC3	6:B:661:PHE:HB2	1.58	0.83
6:B:556:SER:C	6:B:558:PRO:HD2	1.99	0.83
5:A:555:ILE:HG22	6:B:670:TYR:CE2	2.14	0.83
17:N:67:LEU:CB	17:N:68:GLU:HG2	2.08	0.83
21:B:8052:SUC:C4'	21:B:8052:SUC:H1	2.03	0.83
19:3:1221:CLA:H2A	19:3:1221:CLA:O1D	1.79	0.83
19:B:1766:CLA:HHD	19:B:1766:CLA:HBC3	1.60	0.83
19:1:1189:CLA:HBD	19:1:1189:CLA:CBA	2.08	0.83
17:N:41:LYS:HD2	17:N:42:PHE:HB2	1.58	0.83
4:4:117:GLN:O	4:4:121:PHE:CE2	2.30	0.82
19:A:1796:CLA:C14	23:A:1805:BCR:HC21	2.09	0.82
5:A:217:SER:OG	23:A:1803:BCR:C15	2.27	0.82
5:A:746:THR:HA	5:A:749:PHE:HB3	1.59	0.82
17:N:4:GLU:OE2	17:N:5:GLU:HB2	1.78	0.82
19:A:1790:CLA:CBC	19:A:1790:CLA:HMC1	2.09	0.82
6:B:203:ARG:HG2	6:B:204:GLY:N	1.94	0.82
6:B:25:ILE:CG2	23:L:1169:BCR:C28	2.56	0.82
12:H:69:SER:HG	19:H:1079:CLA:H2	1.43	0.82
4:4:122:LYS:CB	4:4:143:PHE:CB	2.50	0.82
19:A:1781:CLA:O1A	19:A:1782:CLA:HED3	1.79	0.82
19:H:1080:CLA:C3C	23:I:1032:BCR:C2	2.57	0.82
19:A:1788:CLA:H161	23:L:1169:BCR:H361	1.58	0.82
17:N:67:LEU:C	17:N:68:GLU:CG	2.45	0.82
17:N:70:GLU:C	17:N:72:LYS:H	1.81	0.82
20:A:7025:LMU:O5B	20:A:7025:LMU:H6D	1.77	0.82
4:4:124:TYR:CB	4:4:143:PHE:HD1	1.93	0.82
23:B:1778:BCR:H371	10:F:93:ILE:HG21	1.61	0.82
18:R:34:UNK:CB	18:R:35:UNK:CA	2.53	0.82
17:N:57:LYS:CA	17:N:60:PHE:O	2.27	0.82
16:L:157:LEU:C	16:L:158:MET:O	2.17	0.82
3:3:157:ALA:C	3:3:158:TYR:HD2	1.83	0.82
4:4:121:PHE:O	4:4:122:LYS:CD	2.26	0.82
19:A:1763:CLA:CBA	19:A:1765:CLA:H12	2.10	0.82
19:B:1768:CLA:H93	19:B:1768:CLA:HBB2	0.86	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1788:CLA:H52	23:B:1780:BCR:H343	1.62	0.82
16:L:163:LEU:HD11	16:L:165:TYR:CE2	2.14	0.82
19:4:1206:CLA:C1	19:4:1206:CLA:HAA1	2.08	0.82
19:A:1783:CLA:H171	23:A:1806:BCR:H15C	1.60	0.82
5:A:24:ARG:N	5:A:24:ARG:CD	2.36	0.82
20:2:1224:LMU:H6E	20:2:1224:LMU:O2B	1.79	0.82
4:4:151:GLU:O	4:4:154:ILE:N	2.03	0.82
5:A:668:TYR:OH	6:B:441:ASP:OD1	1.95	0.82
7:C:54:CYS:SG	25:C:1082:SF4:S1	2.78	0.82
6:B:545:LYS:HG2	9:E:74:TYR:HE2	1.43	0.82
19:3:1217:CLA:CAC	19:3:1218:CLA:C7	2.58	0.82
20:A:7033:LMU:H3'	20:A:7033:LMU:H6'2	1.62	0.82
4:4:40:PHE:HB3	4:4:43:ALA:HB3	1.60	0.82
19:1:1143:CLA:H3A	19:1:1143:CLA:CGA	2.09	0.82
8:D:104:PHE:HB3	8:D:106:SER:H	1.43	0.82
14:J:31:ARG:HH22	19:J:1043:CLA:C4B	1.92	0.82
19:1:1192:CLA:HHD	19:1:1192:CLA:CBC	2.09	0.82
7:C:5:VAL:C	7:C:65:VAL:HG22	2.00	0.82
16:L:118:LEU:HD12	16:L:119:THR:H	1.45	0.82
19:A:1763:CLA:C3B	23:A:1806:BCR:C33	2.58	0.81
5:A:308:ILE:CD1	19:A:1772:CLA:H91	2.10	0.81
19:B:1755:CLA:HED1	19:B:1756:CLA:HMD1	1.61	0.81
19:B:1759:CLA:HMC1	19:B:1759:CLA:CBC	2.09	0.81
19:B:1771:CLA:HMC1	19:B:1771:CLA:HBC2	1.61	0.81
19:A:1781:CLA:O1A	19:A:1781:CLA:H2	1.80	0.81
6:B:137:THR:HA	6:B:140:ILE:HG13	1.63	0.81
19:F:1156:CLA:C3B	19:F:1157:CLA:CAC	2.55	0.81
15:K:47:LEU:O	15:K:48:GLN:HG3	1.79	0.81
19:3:1217:CLA:CBA	19:3:1217:CLA:HBD	2.09	0.81
9:E:68:ARG:HH21	9:E:69:PHE:HA	1.43	0.81
15:K:6:SER:O	15:K:10:ILE:HD13	1.78	0.81
4:4:169:GLN:HG2	19:4:1199:CLA:HAC2	1.61	0.81
4:4:96:ILE:O	4:4:99:HIS:HB3	1.79	0.81
19:A:1781:CLA:H72	19:A:1782:CLA:HED1	1.61	0.81
19:A:1791:CLA:C3A	19:A:1797:CLA:CBB	2.59	0.81
5:A:356:ALA:HB2	5:A:417:PHE:CD2	2.15	0.81
5:A:723:ARG:HH11	5:A:723:ARG:HG2	1.45	0.81
4:4:122:LYS:HG2	4:4:150:LYS:HD3	1.59	0.81
5:A:217:SER:HA	23:A:1803:BCR:H351	1.62	0.81
6:B:594:TRP:O	6:B:595:HIS:CB	2.28	0.81
3:3:93:PHE:CB	3:3:94:ARG:O	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:203:VAL:O	5:A:252:ARG:NH2	2.14	0.81
2:2:54:TRP:CZ2	2:2:109:ARG:CD	2.62	0.81
5:A:316:MET:HB3	5:A:317:TYR:CG	2.15	0.81
10:F:102:ARG:CG	10:F:106:ILE:HD11	2.08	0.81
17:N:1:GLY:O	17:N:2:VAL:HG13	1.80	0.81
15:K:27:ALA:HB3	15:K:28:PRO:HD3	1.60	0.81
17:N:67:LEU:HB2	17:N:68:GLU:CG	2.11	0.81
20:A:7032:LMU:C2B	20:A:7032:LMU:H31	2.10	0.81
4:4:99:HIS:CE1	4:4:103:ILE:HD11	2.16	0.81
6:B:370:ALA:O	19:B:1757:CLA:HMA1	1.81	0.81
18:R:38:UNK:C	18:R:42:UNK:O	2.29	0.81
1:1:39:TYR:HB3	19:1:1196:CLA:OBD	1.81	0.81
3:3:52:LYS:O	3:3:56:TYR:HD2	1.63	0.81
19:4:4014:CLA:CBB	20:A:7034:LMU:O3B	2.29	0.81
6:B:174:ARG:HH11	19:B:1754:CLA:HMD1	1.43	0.81
6:B:493:TRP:CZ2	19:B:1765:CLA:O1A	2.32	0.81
9:E:61:THR:HG22	9:E:62:ARG:H	1.46	0.81
17:N:40:CYS:H	17:N:41:LYS:CA	1.88	0.81
5:A:27:ILE:O	5:A:28:LYS:CD	2.29	0.81
15:K:46:GLY:O	15:K:47:LEU:CG	2.29	0.81
17:N:18:ASP:CB	17:N:22:LEU:HG	2.09	0.81
1:1:185:TRP:CH2	19:1:1199:CLA:O2A	2.33	0.81
3:3:92:TRP:CB	3:3:95:THR:OG1	2.29	0.81
3:3:80:LYS:NZ	3:3:92:TRP:HD1	1.73	0.81
17:N:72:LYS:HZ1	17:N:74:LYS:HE2	1.45	0.81
4:4:37:LEU:CA	4:4:39:TRP:HB3	2.10	0.81
20:A:7016:LMU:C2	20:A:7016:LMU:H61	2.08	0.81
19:3:1217:CLA:HBC3	19:3:1217:CLA:CMC	2.10	0.81
20:A:7043:LMU:H62	20:A:7043:LMU:C10	2.11	0.81
21:3:1223:SUC:H5	21:3:1223:SUC:O2'	1.79	0.81
19:1:1199:CLA:HMC1	19:1:1199:CLA:HBC2	1.61	0.81
19:A:1780:CLA:H112	19:A:1780:CLA:OBD	1.80	0.81
23:A:1808:BCR:H331	23:A:1808:BCR:C8	2.09	0.81
5:A:331:LEU:O	5:A:331:LEU:HD23	1.81	0.81
11:G:42:SER:OG	11:G:46:ALA:CB	2.28	0.81
5:A:21:LEU:CA	5:A:22:VAL:O	2.29	0.81
11:G:68:ILE:O	11:G:72:LEU:HB3	1.80	0.81
18:R:7:UNK:O	18:R:11:UNK:N	2.14	0.81
4:4:169:GLN:CD	19:4:1199:CLA:HHD	2.01	0.81
19:A:1770:CLA:C4B	23:A:1803:BCR:C19	2.59	0.81
23:A:1808:BCR:H331	23:A:1808:BCR:HC8	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:70:TRP:CD1	6:B:71:GLN:OE1	2.34	0.81
19:2:2006:CLA:CBD	19:2:2006:CLA:CBA	2.58	0.81
4:4:145:PRO:O	4:4:146:THR:C	2.16	0.81
8:D:134:MET:N	8:D:134:MET:SD	2.54	0.81
4:4:165:GLY:O	4:4:169:GLN:HG2	1.81	0.81
5:A:40:PHE:HE1	5:A:53:TRP:HD1	1.29	0.81
6:B:199:ILE:HG23	6:B:270:LEU:HD22	1.63	0.81
6:B:732:LYS:CB	6:B:733:PHE:O	2.29	0.81
5:A:187:HIS:CD2	19:A:1767:CLA:NC	2.38	0.80
19:B:1764:CLA:HBB2	23:B:1777:BCR:H381	1.63	0.80
4:4:74:LYS:N	4:4:75:TRP:CA	2.44	0.80
17:N:45:ASN:O	17:N:46:PHE:O	1.98	0.80
20:A:7021:LMU:C3	20:A:7021:LMU:H1'	2.08	0.80
20:A:7013:LMU:O6B	20:A:7013:LMU:H1B	1.79	0.80
20:2:1224:LMU:C7	20:2:1224:LMU:H12	2.12	0.80
5:A:684:PHE:C	5:A:684:PHE:CD2	2.55	0.80
6:B:275:HIS:O	6:B:279:ALA:N	2.11	0.80
6:B:732:LYS:HD2	6:B:734:GLY:CA	2.10	0.80
17:N:40:CYS:N	17:N:41:LYS:CA	2.44	0.80
4:4:37:LEU:N	4:4:39:TRP:HB2	1.95	0.80
18:R:33:UNK:O	18:R:36:UNK:CB	2.29	0.80
15:K:84:LEU:N	15:K:84:LEU:CD2	2.30	0.80
3:3:107:TRP:CG	3:3:108:ALA:N	2.38	0.80
5:A:472:ARG:HE	5:A:474:GLN:HG3	1.45	0.80
19:B:1768:CLA:C15	23:B:1779:BCR:C31	2.58	0.80
11:G:42:SER:O	11:G:46:ALA:CB	2.29	0.80
19:H:1080:CLA:CAC	23:I:1032:BCR:C3	2.59	0.80
5:A:22:VAL:HB	5:A:23:ASP:C	2.01	0.80
2:2:103:GLY:N	19:2:1221:CLA:CBB	2.44	0.80
19:A:1779:CLA:CBB	23:A:1804:BCR:H351	2.11	0.80
19:B:1765:CLA:HMB1	23:B:1777:BCR:H292	0.83	0.80
15:K:46:GLY:O	15:K:47:LEU:CD1	2.29	0.80
6:B:110:LEU:HD12	6:B:111:GLY:H	1.46	0.80
4:4:150:LYS:CG	4:4:150:LYS:O	2.23	0.80
5:A:497:ALA:HB2	5:A:515:TRP:HB2	1.62	0.80
19:B:1765:CLA:HBB1	23:B:1777:BCR:H281	1.63	0.80
6:B:732:LYS:CG	6:B:733:PHE:O	2.30	0.80
7:C:5:VAL:HB	7:C:65:VAL:HG13	1.64	0.80
3:3:92:TRP:CA	3:3:95:THR:OG1	2.30	0.80
17:N:74:LYS:O	17:N:76:LYS:N	2.13	0.80
5:A:27:ILE:O	5:A:28:LYS:CG	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:165:TYR:CA	16:L:166:TYR:O	2.30	0.80
18:R:38:UNK:CB	18:R:42:UNK:O	2.30	0.80
19:2:2006:CLA:H2	19:2:2006:CLA:HAA1	1.62	0.80
2:2:162:LYS:NZ	19:2:1215:CLA:OBD	2.14	0.80
5:A:488:PHE:CE2	5:A:533:PRO:HB3	2.16	0.80
25:B:1783:SF4:S1	25:B:1783:SF4:S3	2.78	0.80
5:A:22:VAL:CA	5:A:23:ASP:O	2.30	0.80
5:A:25:ASP:OD2	5:A:26:PRO:CD	2.30	0.80
18:R:34:UNK:N	18:R:36:UNK:N	2.29	0.80
19:1:1190:CLA:H2A	19:1:1190:CLA:HED2	1.62	0.80
5:A:100:GLY:HA3	5:A:153:TRP:HH2	1.45	0.80
16:L:115:ALA:H	16:L:116:PRO:HD2	1.44	0.80
5:A:599:PHE:HD1	5:A:600:LEU:HD23	1.44	0.80
5:A:705:GLU:HB3	6:B:545:LYS:NZ	1.96	0.80
19:B:1737:CLA:O1A	19:B:1743:CLA:CGA	2.30	0.80
23:B:1777:BCR:C38	23:B:1777:BCR:H23C	2.09	0.80
15:K:44:GLU:O	15:K:46:GLY:CA	2.29	0.80
15:K:47:LEU:O	15:K:48:GLN:CG	2.29	0.80
15:K:42:ALA:O	15:K:43:ARG:CG	2.30	0.80
19:1:1149:CLA:CGD	19:1:1149:CLA:HAA1	2.12	0.80
4:4:99:HIS:CE1	4:4:103:ILE:HD12	2.14	0.80
19:A:1789:CLA:H51	16:L:67:PRO:CB	2.11	0.80
6:B:388:ALA:C	6:B:391:PRO:HD2	2.00	0.80
6:B:549:ASP:OD1	7:C:63:LEU:HB3	1.82	0.80
4:4:91:PHE:C	4:4:91:PHE:CD2	2.54	0.80
5:A:360:ILE:HD13	23:A:1804:BCR:H371	1.64	0.80
19:B:1747:CLA:CAD	19:B:1756:CLA:HBB2	2.12	0.80
19:B:1755:CLA:CBB	19:B:1769:CLA:CMB	2.58	0.80
19:B:1769:CLA:HBC2	19:B:1769:CLA:HMC1	1.62	0.80
5:A:714:LEU:HD13	23:B:1779:BCR:C39	2.12	0.80
6:B:696:LYS:HG2	7:C:80:ALA:HA	1.64	0.80
15:K:44:GLU:O	15:K:47:LEU:CG	2.30	0.80
3:3:104:TYR:HB2	3:3:106:TYR:N	1.96	0.80
6:B:172:GLU:O	6:B:176:ASN:HB2	1.81	0.80
23:A:1803:BCR:HC8	23:A:1803:BCR:C31	2.04	0.80
19:A:1779:CLA:NC	23:A:1804:BCR:H19C	1.97	0.80
5:A:368:LEU:HD11	19:A:1782:CLA:H61	1.64	0.80
5:A:22:VAL:CB	5:A:23:ASP:HA	2.10	0.80
5:A:22:VAL:HB	5:A:23:ASP:HA	1.63	0.80
18:R:38:UNK:O	18:R:42:UNK:CA	2.28	0.80
19:2:1223:CLA:HHD	19:2:1223:CLA:HBC3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:4014:CLA:HBC2	19:4:4014:CLA:HMC1	1.64	0.80
4:4:166:PHE:O	4:4:169:GLN:HB2	1.81	0.79
6:B:558:PRO:CG	6:B:703:VAL:HB	2.12	0.79
12:H:69:SER:OG	19:H:1079:CLA:C2	2.22	0.79
5:A:24:ARG:HD2	5:A:24:ARG:N	1.96	0.79
15:K:42:ALA:O	15:K:43:ARG:CD	2.30	0.79
19:4:1206:CLA:H151	19:4:1206:CLA:H192	1.64	0.79
1:1:183:ASP:OD2	1:1:184:PRO:CD	2.30	0.79
4:4:124:TYR:HB2	4:4:143:PHE:HD1	1.48	0.79
11:G:37:GLU:OE2	11:G:42:SER:CA	2.29	0.79
3:3:92:TRP:CA	3:3:93:PHE:HB2	2.12	0.79
19:1:1191:CLA:HMC1	19:1:1194:CLA:CHD	2.10	0.79
19:1:1308:CLA:HMA3	19:2:1223:CLA:HED2	1.64	0.79
5:A:151:GLN:NE2	5:A:384:TYR:O	2.15	0.79
21:B:8060:SUC:H5	21:B:8060:SUC:O1'	1.82	0.79
5:A:121:GLN:NE2	19:A:1765:CLA:HMD1	1.97	0.79
19:A:1774:CLA:H121	19:A:1774:CLA:CBB	2.07	0.79
5:A:402:ILE:HG13	19:A:1784:CLA:CBB	2.07	0.79
5:A:618:TRP:O	5:A:622:SER:HB3	1.82	0.79
5:A:81:ALA:HB1	19:A:1761:CLA:HBB2	1.62	0.79
6:B:621:ARG:O	6:B:625:TRP:HB3	1.81	0.79
16:L:164:PRO:HG3	16:L:165:TYR:HE1	1.44	0.79
19:2:1213:CLA:C4	19:2:1213:CLA:C1D	2.59	0.79
19:4:1206:CLA:H151	19:4:1206:CLA:H193	1.61	0.79
6:B:516:ASP:O	6:B:520:HIS:HB2	1.82	0.79
19:B:1744:CLA:HMA1	23:B:1776:BCR:H313	1.63	0.79
6:B:732:LYS:HD2	6:B:733:PHE:C	2.01	0.79
24:B:1781:LMG:O3	7:C:70:TRP:CE2	2.35	0.79
5:A:25:ASP:OD2	5:A:26:PRO:CA	2.30	0.79
14:J:9:SER:O	14:J:10:VAL:HB	1.83	0.79
6:B:128:GLY:HA2	6:B:130:ARG:HE	1.47	0.79
6:B:469:LYS:HG2	6:B:471:THR:OG1	1.83	0.79
18:R:38:UNK:O	18:R:41:UNK:CB	2.30	0.79
11:G:16:LEU:HD23	11:G:68:ILE:CG2	2.12	0.79
20:2:1224:LMU:C6	20:2:1224:LMU:H12	2.12	0.79
19:A:1797:CLA:CHD	19:A:1797:CLA:CBC	2.61	0.79
22:B:1773:PQN:C16	23:B:1780:BCR:H331	2.09	0.79
6:B:293:THR:C	11:G:38:GLN:OE1	2.21	0.79
5:A:22:VAL:HA	5:A:23:ASP:O	1.82	0.79
4:4:37:LEU:CA	4:4:39:TRP:CB	2.60	0.79
19:B:1766:CLA:H2A	19:B:1766:CLA:O1D	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:123:GLN:O	4:4:143:PHE:CD1	2.35	0.79
19:A:1787:CLA:HBB2	19:A:1793:CLA:H203	1.64	0.79
3:3:94:ARG:CZ	3:3:98:ILE:HG21	2.12	0.79
5:A:21:LEU:CD1	5:A:21:LEU:O	2.30	0.79
18:R:32:UNK:CB	18:R:33:UNK:CB	2.59	0.79
18:R:35:UNK:O	18:R:38:UNK:CB	2.30	0.79
5:A:92:TRP:CD1	19:A:1763:CLA:HBB1	2.17	0.79
8:D:30:ALA:O	16:L:18:PRO:HB2	1.82	0.79
17:N:39:SER:OG	17:N:41:LYS:HA	1.83	0.79
12:H:73:PRO:CD	21:H:1082:SUC:H6'2	2.06	0.79
19:1:1142:CLA:CMD	19:1:1143:CLA:NA	2.45	0.79
19:1:1189:CLA:HBD	19:1:1189:CLA:HBA2	1.62	0.79
1:1:185:TRP:CZ3	19:1:1199:CLA:C1	2.47	0.79
5:A:588:GLY:N	6:B:668:ARG:HD3	1.97	0.79
14:J:10:VAL:HG13	14:J:14:LEU:HG	1.64	0.79
19:3:3011:CLA:C3A	19:3:3011:CLA:CGA	2.61	0.79
5:A:239:PRO:HA	5:A:242:ILE:HD11	1.64	0.79
3:3:97:PHE:HD2	3:3:98:ILE:HG23	0.98	0.79
12:H:21:TRP:H	12:H:22:ASP:CA	1.95	0.79
4:4:121:PHE:HD1	4:4:128:ALA:HB3	1.48	0.78
19:A:1787:CLA:O2A	16:L:27:VAL:O	2.00	0.78
19:A:1787:CLA:HAC2	19:A:1801:CLA:HMC3	1.64	0.78
5:A:207:LEU:CB	19:A:1776:CLA:HBB2	2.13	0.78
17:N:70:GLU:HB3	17:N:72:LYS:H	1.48	0.78
8:D:78:ALA:O	8:D:79:ARG:HD3	1.83	0.78
20:A:7016:LMU:C2	20:A:7016:LMU:C6	2.60	0.78
3:3:158:TYR:O	3:3:160:GLY:N	2.16	0.78
5:A:726:SER:O	5:A:728:VAL:N	2.16	0.78
4:4:126:LEU:HD23	4:4:127:PRO:HD3	1.65	0.78
19:A:1816:CLA:HBB2	19:A:1817:CLA:CHB	2.13	0.78
5:A:53:TRP:HA	5:A:56:ASN:HB2	1.66	0.78
24:B:1781:LMG:HC61	7:C:70:TRP:CH2	2.18	0.78
6:B:362:ALA:HB2	6:B:368:GLN:HG2	1.64	0.78
6:B:438:VAL:HG23	19:B:1763:CLA:HAC1	1.65	0.78
9:E:39:LEU:N	9:E:40:ARG:NH1	2.31	0.78
4:4:75:TRP:HE3	4:4:76:TYR:H	1.25	0.78
20:A:7016:LMU:H112	20:A:7016:LMU:H71	1.64	0.78
2:2:178:TRP:C	2:2:182:ILE:HG13	2.03	0.78
1:1:149:LYS:HB3	19:1:1192:CLA:HMC2	1.65	0.78
4:4:128:ALA:N	4:4:143:PHE:CZ	2.48	0.78
6:B:65:LEU:HD22	6:B:124:TRP:HE3	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1773:PQN:C19	23:B:1780:BCR:C10	2.55	0.78
6:B:325:THR:O	6:B:329:SER:HB2	1.83	0.78
1:1:27:LEU:CD1	1:1:28:GLY:H	1.95	0.78
1:1:183:ASP:OD2	1:1:184:PRO:HD2	1.84	0.78
4:4:100:TYR:HA	4:4:103:ILE:CG1	2.14	0.78
4:4:94:GLU:CB	4:4:95:PHE:CE1	2.67	0.78
19:A:1783:CLA:H102	23:A:1805:BCR:H372	1.64	0.78
5:A:397:THR:HB	5:A:613:ILE:CG1	2.13	0.78
5:A:475:ASP:OD2	16:L:74:LEU:HA	1.82	0.78
9:E:60:LYS:HG3	9:E:61:THR:H	1.46	0.78
17:N:44:GLU:O	17:N:46:PHE:N	2.16	0.78
2:2:127:ASN:HD21	14:J:7:TYR:HA	1.49	0.78
12:H:25:GLY:HA3	12:H:27:ASP:CB	2.12	0.78
19:A:1791:CLA:CMA	19:A:1797:CLA:CBB	2.61	0.78
5:A:242:ILE:HG12	5:A:243:PRO:CD	2.13	0.78
6:B:189:ALA:HB2	19:B:1758:CLA:H203	1.63	0.78
7:C:8:TYR:O	7:C:60:THR:HA	1.83	0.78
4:4:75:TRP:CB	19:4:1205:CLA:HMD3	2.13	0.78
19:1:1190:CLA:CMC	19:1:1190:CLA:HBC2	2.12	0.78
20:A:7037:LMU:C7	20:A:7037:LMU:H32	2.10	0.78
20:2:1224:LMU:C4	20:2:1224:LMU:H82	2.13	0.78
8:D:28:ILE:HG12	8:D:67:ILE:HG13	1.66	0.78
5:A:349:ILE:HG23	5:A:352:THR:O	1.82	0.78
19:B:1739:CLA:HBA1	19:B:1757:CLA:OBD	1.84	0.78
11:G:19:GLY:C	11:G:21:PHE:N	2.33	0.78
4:4:69:ILE:CD1	4:4:175:LYS:HB3	1.95	0.78
17:N:72:LYS:HD2	17:N:74:LYS:CG	2.12	0.78
19:J:1043:CLA:O1A	19:J:1043:CLA:H143	1.83	0.78
20:A:7027:LMU:O2'	20:A:7027:LMU:H12	1.82	0.78
5:A:170:GLY:O	5:A:173:VAL:HG22	1.83	0.78
6:B:317:ARG:NH1	6:B:405:ASP:O	2.16	0.78
4:4:171:ASN:O	4:4:172:VAL:C	2.21	0.78
3:3:112:THR:O	3:3:114:PHE:N	2.17	0.78
6:B:174:ARG:NH1	19:B:1754:CLA:HMD1	1.99	0.78
16:L:48:ASN:HB3	16:L:49:PRO:HD2	1.66	0.78
4:4:104:ARG:NH1	4:4:105:ARG:CB	2.45	0.78
4:4:142:ASN:N	4:4:150:LYS:HZ3	1.81	0.78
5:A:81:ALA:HB1	19:A:1760:CLA:HMA1	1.66	0.78
19:A:1789:CLA:HBC3	19:A:1789:CLA:HMC1	1.66	0.78
5:A:345:GLY:O	5:A:347:TYR:N	2.17	0.78
6:B:317:ARG:NE	6:B:317:ARG:HA	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:353:TYR:CG	6:B:594:TRP:CZ3	2.71	0.78
7:C:52:LYS:HG3	7:C:52:LYS:O	1.84	0.78
13:I:9:VAL:HG12	13:I:10:PRO:HD3	1.65	0.78
17:N:45:ASN:HD22	17:N:54:LYS:CB	1.97	0.78
17:N:62:SER:HB3	17:N:66:ASP:CG	2.04	0.78
8:D:113:HIS:N	8:D:114:PRO:HD2	1.99	0.78
6:B:11:GLY:HA3	7:C:71:HIS:HD2	1.49	0.78
2:2:188:PRO:O	2:2:190:ASP:N	2.17	0.78
4:4:128:ALA:CB	4:4:143:PHE:CZ	2.63	0.78
19:A:1765:CLA:CBB	19:B:1763:CLA:HMD2	2.13	0.78
19:B:1753:CLA:C4A	19:B:1753:CLA:H42	2.14	0.78
19:B:1755:CLA:H11	19:B:1769:CLA:CED	2.14	0.78
10:F:100:VAL:HA	10:F:103:SER:OG	1.84	0.78
16:L:36:TYR:CG	16:L:36:TYR:O	2.36	0.78
1:1:179:THR:HG21	4:4:87:SER:CB	2.14	0.78
23:A:1805:BCR:C32	23:A:1806:BCR:H391	2.14	0.77
6:B:91:ILE:HD12	6:B:104:PHE:HE2	1.48	0.77
2:2:205:PHE:HD1	2:2:206:ALA:N	1.80	0.77
4:4:58:MET:O	4:4:61:PRO:HD2	1.84	0.77
15:K:27:ALA:CB	15:K:28:PRO:HD3	2.14	0.77
5:A:442:ILE:HG23	19:A:1786:CLA:HMC3	1.64	0.77
6:B:124:TRP:NE1	6:B:129:LEU:HD22	2.00	0.77
10:F:96:TRP:HZ3	10:F:134:PHE:HB2	1.48	0.77
16:L:95:LEU:HD13	23:L:1169:BCR:C31	2.14	0.77
4:4:36:ASN:CG	4:4:39:TRP:CD2	2.58	0.77
5:A:567:ARG:NH1	8:D:35:GLY:CA	2.42	0.77
15:K:69:ILE:HA	15:K:72:VAL:HG12	1.66	0.77
7:C:26:LEU:H	7:C:43:PRO:HG3	1.50	0.77
4:4:142:ASN:C	4:4:150:LYS:HE2	2.05	0.77
19:B:1756:CLA:H122	23:B:1777:BCR:C14	2.15	0.77
19:B:1764:CLA:HMD2	19:B:1765:CLA:C2C	2.14	0.77
23:B:1779:BCR:H271	23:B:1779:BCR:H403	1.63	0.77
25:B:1783:SF4:S1	25:B:1783:SF4:FE3	1.77	0.77
6:B:310:PRO:CG	6:B:311:PRO:HD2	2.13	0.77
6:B:349:ALA:HB2	6:B:375:HIS:HB3	1.67	0.77
3:3:93:PHE:CA	3:3:94:ARG:O	2.31	0.77
20:A:7022:LMU:C2'	20:A:7022:LMU:C2	2.55	0.77
19:B:1766:CLA:CBC	19:B:1766:CLA:CHD	2.62	0.77
6:B:216:LEU:HD21	6:B:221:GLY:HA2	1.67	0.77
19:1:1199:CLA:HMC1	19:4:1198:CLA:HMB3	1.67	0.77
19:A:1759:CLA:CBB	19:A:1760:CLA:C1C	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:51:THR:HG21	19:A:1795:CLA:CBB	2.11	0.77
5:A:21:LEU:HD12	5:A:21:LEU:O	1.84	0.77
5:A:25:ASP:CB	5:A:26:PRO:C	2.51	0.77
11:G:92:GLY:O	11:G:93:TYR:O	2.03	0.77
20:A:7032:LMU:O5B	20:A:7032:LMU:H31	1.83	0.77
18:R:49:UNK:O	18:R:50:UNK:C	2.30	0.77
5:A:81:ALA:HB1	19:A:1760:CLA:CMA	2.13	0.77
19:A:1781:CLA:CED	19:A:1782:CLA:C3D	2.63	0.77
19:A:1787:CLA:H52	19:A:1801:CLA:HHB	1.66	0.77
5:A:451:ILE:CD1	19:A:1788:CLA:CED	2.62	0.77
5:A:542:HIS:HA	5:A:545:HIS:HD2	1.50	0.77
5:A:700:TRP:O	5:A:704:ILE:HB	1.83	0.77
19:B:1738:CLA:H2A	19:B:1738:CLA:O1D	1.83	0.77
6:B:334:LEU:HB2	19:B:1737:CLA:HMD3	1.64	0.77
5:A:25:ASP:OD2	5:A:26:PRO:HA	1.84	0.77
4:4:192:THR:HG22	4:4:195:GLN:N	1.96	0.77
10:F:130:LEU:HG	10:F:131:PHE:N	2.00	0.77
19:B:1744:CLA:HMB2	23:B:1776:BCR:C8	2.14	0.77
19:B:1753:CLA:C4	19:B:1753:CLA:C4A	2.57	0.77
9:E:40:ARG:HB2	9:E:42:GLU:OE2	1.85	0.77
19:2:2006:CLA:CMA	19:2:2006:CLA:C5	2.55	0.77
19:1:1143:CLA:CBC	20:A:7001:LMU:O3B	2.32	0.77
19:3:1217:CLA:HHD	19:3:1218:CLA:H92	1.66	0.77
19:A:1759:CLA:HBB2	19:A:1760:CLA:C1C	2.12	0.77
19:A:1817:CLA:CGA	19:A:1817:CLA:H3A	2.15	0.77
5:A:22:VAL:CB	5:A:24:ARG:HA	2.14	0.77
19:1:1190:CLA:CED	19:1:1190:CLA:H2A	2.14	0.77
2:2:85:GLN:OE1	2:2:85:GLN:HA	1.83	0.77
19:4:1198:CLA:H151	19:4:1198:CLA:H203	1.66	0.77
19:A:1817:CLA:H3A	19:A:1817:CLA:O2A	1.84	0.77
5:A:76:ARG:NH1	5:A:192:LYS:HG2	1.99	0.77
5:A:246:HIS:O	5:A:248:PHE:HD2	1.67	0.77
5:A:355:HIS:CE1	5:A:416:ILE:HG21	2.18	0.77
19:B:1755:CLA:H72	19:B:1769:CLA:C2D	2.15	0.77
19:B:1768:CLA:H121	23:B:1779:BCR:C31	2.15	0.77
5:A:22:VAL:HB	5:A:24:ARG:HA	1.66	0.77
3:3:48:PHE:HD2	3:3:49:ILE:CG2	1.82	0.77
2:2:42:ARG:O	2:2:44:ASN:N	2.18	0.77
16:L:122:GLY:C	16:L:124:LYS:N	2.36	0.77
15:K:51:ASP:HB3	15:K:52:PRO:CD	2.14	0.77
6:B:8:PHE:O	6:B:35:ASP:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:244:LEU:HD22	5:A:247:GLU:OE2	1.85	0.77
13:I:8:PHE:CB	19:I:1031:CLA:OBD	2.32	0.77
17:N:59:PRO:HB3	17:N:75:TYR:HE1	1.48	0.77
5:A:713:LYS:NZ	19:B:1761:CLA:C4	2.48	0.76
5:A:146:THR:HG21	5:A:751:LEU:HD22	1.66	0.76
19:B:1768:CLA:CMA	19:B:1769:CLA:HED1	2.15	0.76
16:L:63:LEU:HD22	16:L:64:LEU:H	1.50	0.76
17:N:79:SER:HA	17:N:80:ASN:C	2.05	0.76
11:G:68:ILE:O	11:G:72:LEU:CB	2.32	0.76
5:A:146:THR:O	19:A:1783:CLA:HMA2	1.84	0.76
23:B:1776:BCR:H331	23:B:1776:BCR:C8	2.13	0.76
5:A:27:ILE:O	5:A:27:ILE:CG2	2.30	0.76
2:2:126:PRO:CD	2:2:129:LYS:HB2	2.16	0.76
5:A:210:LEU:CD1	19:A:1769:CLA:HMB2	2.16	0.76
2:2:102:ILE:HG13	19:2:1222:CLA:HMD2	1.68	0.76
5:A:217:SER:OG	23:A:1803:BCR:H15C	1.83	0.76
5:A:22:VAL:CB	5:A:23:ASP:C	2.53	0.76
19:A:1789:CLA:H18	19:L:1167:CLA:HMB2	1.67	0.76
6:B:122:GLN:HG3	6:B:361:ILE:HG12	1.67	0.76
8:D:44:GLU:HB2	8:D:46:TYR:CE2	2.16	0.76
5:A:194:ALA:O	5:A:198:ASP:N	2.16	0.76
4:4:122:LYS:HE2	4:4:150:LYS:HD3	1.66	0.76
19:A:1770:CLA:CHC	23:A:1803:BCR:C19	2.64	0.76
5:A:207:LEU:O	5:A:310:PHE:HB3	1.85	0.76
5:A:581:CYS:HB2	5:A:590:CYS:CA	2.13	0.76
7:C:1:MET:H2	7:C:3:HIS:C	1.89	0.76
7:C:7:ILE:O	7:C:8:TYR:O	2.03	0.76
11:G:28:ARG:HH21	11:G:29:GLU:H	1.34	0.76
17:N:59:PRO:HB3	17:N:75:TYR:CE1	2.20	0.76
5:A:22:VAL:HA	5:A:23:ASP:C	2.05	0.76
2:2:168:ARG:NH2	2:2:171:MET:HB2	2.00	0.76
19:A:1772:CLA:HMC1	19:A:1772:CLA:HBC3	1.68	0.76
6:B:586:THR:O	6:B:588:GLY:N	2.19	0.76
9:E:43:SER:HB2	9:E:82:TYR:HE1	1.49	0.76
4:4:192:THR:HG22	4:4:193:ILE:O	1.86	0.76
2:2:116:PRO:HB2	2:2:136:GLY:HA2	1.67	0.76
20:A:7038:LMU:H4'	20:A:7038:LMU:O2B	1.85	0.76
4:4:103:ILE:O	4:4:106:TRP:HB3	1.85	0.76
4:4:128:ALA:O	4:4:130:GLU:N	2.18	0.76
19:A:1781:CLA:C7	19:A:1782:CLA:HED1	2.15	0.76
5:A:393:LEU:O	5:A:397:THR:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:680:LEU:HB3	19:A:1814:CLA:O2A	1.86	0.76
19:B:1755:CLA:HED1	19:B:1756:CLA:CMD	2.15	0.76
6:B:693:TRP:HD1	19:B:1770:CLA:C2D	1.99	0.76
4:4:39:TRP:O	4:4:40:PHE:CD1	2.38	0.76
2:2:189:ILE:HD13	2:2:189:ILE:H	1.48	0.76
19:4:1201:CLA:CMA	19:4:1201:CLA:HBA1	1.94	0.76
23:A:1805:BCR:C31	23:A:1805:BCR:HC8	2.13	0.76
6:B:398:TYR:HD1	6:B:542:ARG:HH21	1.32	0.76
7:C:5:VAL:CB	7:C:65:VAL:CG1	2.55	0.76
19:4:1205:CLA:CBA	19:4:1205:CLA:CGD	2.59	0.76
2:2:73:ILE:H	2:2:73:ILE:HD12	1.51	0.76
8:D:111:TYR:HD2	8:D:114:PRO:HB3	1.50	0.76
4:4:104:ARG:HA	4:4:107:GLN:HB2	1.68	0.76
4:4:160:MET:HE1	19:4:1201:CLA:CBB	2.14	0.76
4:4:91:PHE:CD2	4:4:92:VAL:N	2.54	0.76
4:4:94:GLU:CB	4:4:95:PHE:CD1	2.68	0.76
19:A:1790:CLA:HMC1	19:A:1790:CLA:HBC2	1.68	0.76
19:B:1768:CLA:C20	23:B:1779:BCR:HC41	2.16	0.76
4:4:93:ILE:CA	4:4:96:ILE:HD12	2.13	0.75
19:A:1791:CLA:HMA2	19:A:1797:CLA:CBB	2.14	0.75
5:A:692:PHE:CE2	19:A:1796:CLA:HBC3	2.20	0.75
5:A:362:LEU:HB3	5:A:410:ALA:HB2	1.67	0.75
25:B:1783:SF4:S1	25:B:1783:SF4:FE4	1.77	0.75
4:4:36:ASN:C	4:4:39:TRP:CB	2.52	0.75
19:2:1213:CLA:H2A	19:2:1213:CLA:O1D	1.85	0.75
19:2:1215:CLA:H42	19:2:1217:CLA:HMD1	1.68	0.75
14:J:23:ALA:O	14:J:26:LEU:HB3	1.87	0.75
2:2:196:HIS:O	2:2:197:LEU:HB2	1.85	0.75
3:3:173:GLU:CG	3:3:174:LYS:H	1.98	0.75
19:B:1755:CLA:H52	19:B:1769:CLA:CAD	2.15	0.75
19:A:1800:CLA:HBB2	19:B:1770:CLA:HMD1	1.66	0.75
25:B:1783:SF4:FE1	25:B:1783:SF4:S4	1.78	0.75
9:E:55:VAL:HG23	9:E:65:VAL:HB	1.68	0.75
17:N:56:LYS:O	17:N:60:PHE:HD1	1.68	0.75
1:1:43:GLU:OE2	19:1:1190:CLA:HBC3	1.85	0.75
2:2:110:TRP:CD1	2:2:113:ILE:HG21	2.20	0.75
2:2:116:PRO:O	2:2:131:THR:CB	2.34	0.75
2:2:128:ASN:O	2:2:130:LEU:HD13	1.86	0.75
5:A:629:ASN:HD21	5:A:633:VAL:HG23	1.52	0.75
4:4:142:ASN:O	4:4:150:LYS:NZ	2.14	0.75
19:B:1747:CLA:CBD	19:B:1756:CLA:HBB2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1760:CLA:HMA1	19:B:1761:CLA:O1A	1.87	0.75
6:B:732:LYS:CD	6:B:734:GLY:CA	2.64	0.75
13:I:8:PHE:CE1	19:I:1031:CLA:H43	2.22	0.75
3:3:97:PHE:O	3:3:98:ILE:CG2	2.35	0.75
5:A:423:ASP:CB	5:A:424:PRO:HD3	2.14	0.75
5:A:62:HIS:O	19:A:1785:CLA:HAA2	1.85	0.75
19:A:1770:CLA:CHC	23:A:1803:BCR:C17	2.64	0.75
5:A:356:ALA:HB2	5:A:417:PHE:HD2	1.51	0.75
6:B:351:HIS:HB3	19:B:1747:CLA:HED1	1.68	0.75
6:B:174:ARG:NH1	19:B:1754:CLA:CMD	2.48	0.75
19:B:1764:CLA:CBB	23:B:1777:BCR:H381	2.16	0.75
6:B:299:HIS:CE1	19:B:1752:CLA:HMD1	2.21	0.75
11:G:28:ARG:NH2	11:G:28:ARG:HG2	2.00	0.75
2:2:72:GLY:O	2:2:74:LEU:N	2.18	0.75
2:2:124:ILE:HB	2:2:129:LYS:HB3	1.67	0.75
19:A:1792:CLA:HBA2	19:A:1792:CLA:HBD	1.68	0.75
5:A:578:ARG:CZ	5:A:578:ARG:HB2	2.15	0.75
17:N:47:THR:HG21	17:N:54:LYS:HZ1	1.50	0.75
1:1:25:ASP:H	6:B:314:ARG:NH2	1.83	0.75
19:1:1149:CLA:O1D	19:1:1149:CLA:CAA	2.34	0.75
4:4:126:LEU:HD23	4:4:127:PRO:CD	2.17	0.75
4:4:121:PHE:CD1	4:4:143:PHE:CE2	2.75	0.75
17:N:54:LYS:HB3	17:N:57:LYS:HE2	1.69	0.75
17:N:62:SER:HB3	17:N:66:ASP:HA	1.68	0.75
5:A:316:MET:CB	5:A:317:TYR:HB2	2.14	0.75
12:H:45:ALA:O	12:H:48:THR:N	2.18	0.75
5:A:248:PHE:CD2	5:A:248:PHE:N	2.55	0.75
25:B:1783:SF4:FE4	25:B:1783:SF4:S2	1.77	0.75
6:B:292:ARG:NH1	6:B:296:GLY:H	1.85	0.75
6:B:29:HIS:CG	19:B:1737:CLA:HBB2	2.21	0.75
6:B:85:ARG:O	6:B:86:PRO:O	2.05	0.75
16:L:95:LEU:HA	16:L:98:CYS:HB2	1.68	0.75
5:A:27:ILE:HG23	5:A:28:LYS:CD	2.10	0.75
3:3:205:GLY:HA3	5:A:252:ARG:NH1	2.01	0.75
3:3:183:GLU:HG3	19:3:1217:CLA:OBD	1.87	0.75
20:A:7023:LMU:O3B	20:A:7023:LMU:H6'1	1.87	0.75
4:4:104:ARG:NH1	4:4:105:ARG:HB2	1.98	0.75
23:A:1807:BCR:H342	19:H:1079:CLA:CHD	2.17	0.75
25:B:1783:SF4:FE1	25:B:1783:SF4:S2	1.77	0.75
7:C:63:LEU:HG	7:C:64:SER:H	1.49	0.75
20:A:7008:LMU:O6'	20:A:7008:LMU:H22	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:95:PHE:CZ	19:4:1210:CLA:NC	2.55	0.75
4:4:128:ALA:HB1	4:4:141:LEU:HD23	1.68	0.75
5:A:103:PHE:CE1	19:A:1763:CLA:O1D	2.40	0.75
19:A:1774:CLA:HBB2	19:A:1774:CLA:C8	2.16	0.75
19:A:1814:CLA:HED2	19:A:1814:CLA:CAD	2.16	0.75
19:B:1755:CLA:CHD	19:B:1755:CLA:HBC2	2.15	0.75
10:F:62:LEU:HG	10:F:72:ILE:HD13	1.68	0.75
17:N:72:LYS:CG	17:N:74:LYS:H	2.00	0.75
10:F:24:LYS:CA	10:F:24:LYS:HE2	2.08	0.75
12:H:10:ASP:HB3	12:H:13:ASP:HB2	1.67	0.75
13:I:1:MET:O	13:I:2:ILE:HG22	1.85	0.75
19:1:1199:CLA:CMA	19:1:1199:CLA:HBA2	2.16	0.74
19:A:1759:CLA:CBB	19:A:1760:CLA:C4C	2.64	0.74
23:A:1803:BCR:H23C	23:A:1803:BCR:H402	1.69	0.74
6:B:120:VAL:HA	6:B:123:TRP:HD1	1.46	0.74
6:B:557:PHE:N	6:B:558:PRO:CD	2.49	0.74
6:B:732:LYS:CD	6:B:734:GLY:HA3	2.17	0.74
5:A:28:LYS:CB	5:A:28:LYS:HZ3	1.90	0.74
4:4:33:ASP:HB3	4:4:34:PRO:HD2	1.69	0.74
4:4:36:ASN:OD1	4:4:37:LEU:CA	2.35	0.74
15:K:44:GLU:HA	15:K:44:GLU:OE1	1.87	0.74
3:3:112:THR:OG1	3:3:113:LEU:HG	1.87	0.74
5:A:530:LEU:HB2	5:A:531:PRO:HD2	1.66	0.74
4:4:100:TYR:HA	4:4:103:ILE:HG12	1.67	0.74
19:A:1797:CLA:CMA	19:A:1797:CLA:CBA	2.55	0.74
23:A:1803:BCR:C23	23:A:1803:BCR:H402	2.16	0.74
17:N:47:THR:HG21	17:N:54:LYS:HZ3	1.51	0.74
19:1:1308:CLA:CBA	19:1:1308:CLA:HBD	2.06	0.74
4:4:121:PHE:CZ	4:4:122:LYS:O	2.41	0.74
19:A:1794:CLA:HMC1	19:A:1794:CLA:HBC3	1.69	0.74
19:A:1797:CLA:O2D	19:A:1797:CLA:HAA2	1.87	0.74
6:B:87:ILE:HA	6:B:115:ASN:CA	2.13	0.74
19:B:1755:CLA:C1	19:B:1769:CLA:CED	2.65	0.74
4:4:36:ASN:CG	4:4:39:TRP:CE2	2.61	0.74
1:1:39:TYR:CD2	19:1:1196:CLA:OBD	2.40	0.74
6:B:664:LEU:C	6:B:667:TRP:HZ3	1.89	0.74
6:B:369:ALA:O	6:B:725:LEU:HD11	1.86	0.74
19:A:1782:CLA:CAB	19:A:1790:CLA:HMA1	2.17	0.74
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.68	0.74
19:H:1080:CLA:HAC1	23:I:1032:BCR:C3	2.17	0.74
17:N:58:VAL:HG23	17:N:60:PHE:CE1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:ASN:O	2:2:130:LEU:N	2.19	0.74
7:C:31:TRP:HB2	7:C:39:ILE:HG21	1.69	0.74
11:G:73:ALA:O	11:G:75:GLY:N	2.20	0.74
5:A:25:ASP:HB2	5:A:26:PRO:O	1.86	0.74
5:A:567:ARG:HH12	8:D:35:GLY:HA2	1.46	0.74
5:A:496:HIS:HB3	5:A:515:TRP:CE3	2.23	0.74
19:B:1741:CLA:H62	19:B:1741:CLA:CAD	2.17	0.74
6:B:395:ILE:HD12	6:B:396:ARG:HG2	1.69	0.74
5:A:21:LEU:CB	5:A:22:VAL:O	2.36	0.74
5:A:197:GLN:HE22	5:A:351:THR:HB	1.53	0.74
6:B:11:GLY:HA3	7:C:71:HIS:CD2	2.22	0.74
4:4:94:GLU:HB3	4:4:95:PHE:HE1	1.45	0.74
25:B:1783:SF4:S1	25:B:1783:SF4:FE2	1.79	0.74
7:C:5:VAL:HB	7:C:65:VAL:HA	1.69	0.74
5:A:24:ARG:HH12	5:A:29:THR:CA	2.00	0.74
18:R:38:UNK:CA	18:R:42:UNK:O	2.35	0.74
15:K:44:GLU:CA	15:K:44:GLU:OE1	2.33	0.74
19:2:1213:CLA:CBC	19:2:1213:CLA:HHD	2.11	0.74
6:B:672:GLN:HA	6:B:672:GLN:NE2	1.97	0.74
19:4:1198:CLA:C20	19:4:1198:CLA:H151	2.18	0.74
19:A:1816:CLA:C9	19:A:1817:CLA:H91	2.16	0.74
5:A:401:TRP:CD1	19:A:1783:CLA:CHC	2.69	0.74
6:B:230:TRP:HB3	19:B:1746:CLA:HED3	1.68	0.74
4:4:38:ARG:CG	4:4:39:TRP:N	2.48	0.74
2:2:126:PRO:HD2	2:2:129:LYS:HB2	1.69	0.74
2:2:96:ILE:HG13	2:2:97:VAL:N	2.02	0.74
20:A:7032:LMU:C5B	20:A:7032:LMU:H3'	2.17	0.74
19:1:1199:CLA:HBA2	19:1:1199:CLA:HMA3	1.70	0.74
1:1:183:ASP:CB	1:1:184:PRO:CD	2.61	0.74
19:A:1787:CLA:H3A	6:B:685:THR:OG1	1.88	0.74
5:A:665:ILE:HD13	6:B:621:ARG:HG3	1.70	0.74
6:B:438:VAL:HG22	19:B:1763:CLA:CMC	2.18	0.74
6:B:16:PRO:HG3	7:C:74:THR:CG2	2.17	0.74
19:F:1156:CLA:C3B	19:F:1157:CLA:HAC2	2.16	0.74
5:A:267:THR:O	5:A:269:PHE:CD2	2.35	0.74
20:A:7036:LMU:C7	20:A:7036:LMU:H31	2.15	0.74
17:N:54:LYS:O	17:N:57:LYS:N	2.21	0.74
11:G:8:ILE:O	11:G:8:ILE:HG13	1.88	0.74
7:C:39:ILE:CG1	7:C:40:ALA:H	1.97	0.74
8:D:94:TYR:O	8:D:95:LYS:HG2	1.88	0.74
6:B:378:ILE:O	6:B:380:GLY:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1781:CLA:H2	19:A:1782:CLA:HED3	1.70	0.73
19:B:1751:CLA:CHD	19:B:1751:CLA:HBC2	2.15	0.73
6:B:469:LYS:HE2	6:B:471:THR:OG1	1.87	0.73
16:L:99:LEU:HD11	23:L:1169:BCR:HC7	1.69	0.73
3:3:92:TRP:C	3:3:94:ARG:C	2.47	0.73
6:B:373:THR:HA	6:B:376:GLN:HB2	1.68	0.73
10:F:63:CYS:HA	10:F:69:PRO:HA	1.70	0.73
6:B:211:ASN:HB2	6:B:214:ASP:HB3	1.70	0.73
19:A:1776:CLA:HMD2	19:A:1778:CLA:HBB2	1.67	0.73
5:A:470:LEU:HD13	6:B:95:HIS:HB3	1.68	0.73
5:A:591:GLN:HA	5:A:591:GLN:HE21	1.52	0.73
19:B:1738:CLA:H91	19:B:1738:CLA:H193	1.69	0.73
19:B:1768:CLA:H152	23:B:1779:BCR:H313	1.69	0.73
17:N:54:LYS:O	17:N:56:LYS:N	2.20	0.73
15:K:44:GLU:CD	15:K:45:SER:C	2.46	0.73
15:K:46:GLY:O	15:K:47:LEU:CB	2.36	0.73
19:1:1190:CLA:CBC	19:1:1190:CLA:HMC1	2.14	0.73
2:2:51:HIS:HB2	19:2:1221:CLA:OBD	1.87	0.73
2:2:120:ASN:HB3	2:2:121:THR:HB	1.69	0.73
7:C:29:ILE:HG23	8:D:126:GLY:HA2	1.69	0.73
15:K:24:PHE:HB3	15:K:52:PRO:HG2	1.69	0.73
19:A:1800:CLA:CMD	23:B:1780:BCR:HC31	2.17	0.73
4:4:34:PRO:HA	4:4:35:GLU:CG	2.19	0.73
8:D:78:ALA:HB3	8:D:82:GLN:NE2	1.97	0.73
2:2:55:ALA:HB3	2:2:56:MET:HE1	1.68	0.73
19:A:1764:CLA:HMB1	19:A:1765:CLA:H11	1.71	0.73
5:A:79:PHE:CZ	5:A:185:HIS:NE2	2.54	0.73
6:B:374:HIS:O	6:B:374:HIS:CG	2.41	0.73
6:B:427:LEU:HD23	6:B:431:PHE:CZ	2.24	0.73
17:N:47:THR:O	17:N:48:GLY:O	2.07	0.73
20:2:1224:LMU:C2	20:2:1224:LMU:C6	2.66	0.73
6:B:507:SER:O	6:B:508:LEU:HB2	1.86	0.73
17:N:11:LYS:HD2	17:N:12:THR:O	1.89	0.73
6:B:174:ARG:O	6:B:175:LEU:HB3	1.88	0.73
7:C:5:VAL:HB	7:C:65:VAL:CB	2.18	0.73
10:F:20:GLN:CD	10:F:21:ALA:H	1.92	0.73
17:N:29:PHE:CD1	17:N:32:ALA:HB3	2.24	0.73
5:A:596:ASP:HA	5:A:599:PHE:HB3	1.70	0.73
19:B:1742:CLA:HAC2	19:B:1743:CLA:HBB2	0.80	0.73
6:B:612:SER:HA	6:B:615:TYR:CE1	2.22	0.73
6:B:709:GLY:O	6:B:710:LEU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:1079:CLA:CGA	19:H:1079:CLA:CMA	2.66	0.73
16:L:36:TYR:O	16:L:36:TYR:CD1	2.40	0.73
3:3:208:PRO:HB3	3:3:210:GLN:OE1	1.89	0.73
5:A:108:ALA:HB1	5:A:138:GLY:HA3	1.70	0.73
1:1:57:ILE:HG23	1:1:58:LEU:H	1.53	0.73
1:1:57:ILE:O	1:1:59:VAL:N	2.22	0.73
19:A:1796:CLA:C14	23:A:1805:BCR:C2	2.59	0.73
19:B:1746:CLA:HHD	19:B:1746:CLA:CBC	2.19	0.73
6:B:362:ALA:O	6:B:363:GLN:HG3	1.87	0.73
4:4:144:ALA:HB3	4:4:147:LEU:O	1.89	0.73
20:A:7037:LMU:C1	20:A:7037:LMU:C5	2.67	0.73
19:1:1145:CLA:H2	19:1:1145:CLA:HMA2	1.69	0.73
16:L:49:PRO:HB2	16:L:139:PHE:HB2	1.71	0.73
10:F:7:PRO:HA	10:F:61:LEU:O	1.89	0.73
10:F:147:GLY:CA	10:F:150:VAL:HB	2.19	0.73
19:A:1763:CLA:HBA2	19:A:1765:CLA:H12	1.71	0.73
19:B:1737:CLA:O1A	19:B:1743:CLA:HBA1	1.87	0.73
19:B:1761:CLA:CMC	19:B:1769:CLA:HBC1	2.18	0.73
6:B:255:LEU:HD13	6:B:275:HIS:HB2	1.69	0.73
11:G:28:ARG:NH2	11:G:29:GLU:H	1.86	0.73
3:3:50:GLU:N	3:3:51:PRO:CD	2.52	0.73
2:2:168:ARG:HH21	2:2:171:MET:HB2	1.51	0.73
4:4:193:ILE:HG22	4:4:194:VAL:N	2.02	0.73
20:2:1224:LMU:H6E	20:2:1224:LMU:C2B	2.18	0.73
5:A:289:PRO:O	5:A:290:LEU:HB2	1.89	0.73
16:L:128:ASP:CG	16:L:129:GLN:H	1.91	0.73
5:A:331:LEU:CD1	5:A:346:LEU:HB3	2.15	0.73
6:B:394:PHE:O	6:B:542:ARG:NE	2.19	0.73
16:L:123:ARG:NE	16:L:123:ARG:HA	2.03	0.73
12:H:50:ARG:HH12	12:H:53:LEU:C	1.92	0.73
23:A:1805:BCR:C23	23:A:1805:BCR:H393	2.13	0.73
6:B:50:HIS:CD2	19:B:1737:CLA:HAA2	2.23	0.73
19:B:1756:CLA:H8	23:B:1777:BCR:H12C	1.70	0.73
25:B:1783:SF4:S4	25:B:1783:SF4:FE2	1.81	0.73
10:F:83:PHE:O	10:F:87:GLY:HA3	1.89	0.73
5:A:423:ASP:HB3	5:A:424:PRO:CD	2.12	0.73
5:A:626:GLY:CA	5:A:636:HIS:HA	2.19	0.73
12:H:50:ARG:HG2	16:L:137:ALA:HB1	1.71	0.73
19:A:1760:CLA:HMC3	19:A:1762:CLA:O2D	1.88	0.72
19:A:1795:CLA:C1C	19:B:1735:CLA:HBC2	2.19	0.72
5:A:355:HIS:ND1	5:A:416:ILE:HG21	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1769:CLA:H2A	19:B:1769:CLA:O1D	1.89	0.72
19:B:1759:CLA:H72	24:B:1781:LMG:H311	1.70	0.72
5:A:24:ARG:HD3	5:A:24:ARG:H	1.51	0.72
20:A:7039:LMU:C6B	20:A:7039:LMU:H3'	2.17	0.72
16:L:124:LYS:C	16:L:126:GLN:H	1.92	0.72
4:4:57:GLY:O	4:4:60:LEU:HD23	1.88	0.72
6:B:160:LYS:HZ3	6:B:160:LYS:HB2	1.54	0.72
6:B:50:HIS:HD2	19:B:1737:CLA:HAA2	1.54	0.72
6:B:48:ALA:CB	6:B:157:LEU:HD22	2.19	0.72
6:B:53:GLN:NE2	19:B:1736:CLA:HBB1	2.03	0.72
2:2:70:LYS:HG3	2:2:73:ILE:HG12	1.70	0.72
6:B:635:ILE:O	6:B:636:THR:O	2.07	0.72
21:B:8059:SUC:H3	21:B:8059:SUC:O2'	1.88	0.72
19:A:1774:CLA:CAB	19:A:1774:CLA:C7	2.67	0.72
5:A:451:ILE:CD1	19:A:1788:CLA:HED3	2.20	0.72
6:B:697:PRO:HB3	19:B:1770:CLA:HBC3	1.70	0.72
9:E:87:VAL:O	9:E:89:GLU:N	2.19	0.72
6:B:404:ALA:C	6:B:406:ASN:H	1.92	0.72
18:R:52:UNK:HA	18:R:53:UNK:CB	2.19	0.72
20:A:7023:LMU:H32	20:A:7023:LMU:H82	1.71	0.72
4:4:100:TYR:HA	4:4:103:ILE:HD11	1.72	0.72
5:A:654:ARG:HA	6:B:632:ILE:HD13	1.71	0.72
6:B:75:GLU:HB2	6:B:132:ASN:HB3	1.69	0.72
7:C:78:GLY:O	7:C:81:TYR:CE1	2.38	0.72
4:4:192:THR:HG21	4:4:195:GLN:N	2.00	0.72
19:2:1223:CLA:HED3	19:2:1223:CLA:OBD	1.89	0.72
3:3:106:TYR:CD2	3:3:107:TRP:CD1	2.78	0.72
20:2:1224:LMU:C1	20:2:1224:LMU:H62	2.19	0.72
5:A:368:LEU:HD22	19:A:1774:CLA:C9	2.19	0.72
5:A:91:LEU:O	19:A:1763:CLA:HMC3	1.90	0.72
19:B:1768:CLA:H202	23:B:1779:BCR:HC41	1.72	0.72
25:B:1783:SF4:S2	25:B:1783:SF4:FE3	1.80	0.72
1:1:39:TYR:CG	19:1:1196:CLA:OBD	2.41	0.72
6:B:663:PHE:O	6:B:664:LEU:CB	2.37	0.72
19:1:1192:CLA:HHD	19:1:1192:CLA:HBC2	1.70	0.72
6:B:315:LEU:HD13	6:B:315:LEU:O	1.90	0.72
5:A:309:LEU:HD21	19:A:1776:CLA:CMC	2.20	0.72
5:A:684:PHE:HD2	5:A:685:VAL:N	1.88	0.72
6:B:142:LEU:CD2	23:B:1776:BCR:H333	2.19	0.72
5:A:697:ARG:NH2	6:B:566:GLY:O	2.21	0.72
12:H:69:SER:CB	19:H:1079:CLA:H2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:52:LYS:HA	3:3:55:ALA:HB3	1.70	0.72
19:2:1212:CLA:HBC2	19:2:1212:CLA:CHD	2.19	0.72
5:A:349:ILE:HG22	5:A:349:ILE:O	1.87	0.72
19:4:1200:CLA:HBC2	19:4:1200:CLA:CMC	2.15	0.72
5:A:207:LEU:HD12	5:A:310:PHE:HD1	1.53	0.72
6:B:167:TRP:CD1	11:G:41:MET:HE3	2.24	0.72
5:A:558:LYS:NZ	6:B:674:LEU:HB3	2.05	0.72
11:G:40:GLY:O	11:G:41:MET:SD	2.48	0.72
2:2:73:ILE:O	2:2:74:LEU:CG	2.36	0.72
12:H:23:VAL:HG12	12:H:23:VAL:O	1.88	0.72
10:F:61:LEU:HD23	10:F:69:PRO:CB	2.20	0.72
6:B:493:TRP:HE1	19:B:1746:CLA:HAC2	1.55	0.72
19:B:1769:CLA:HMC1	19:B:1769:CLA:HBC3	1.71	0.72
24:B:1781:LMG:O3	7:C:70:TRP:CZ2	2.43	0.72
19:R:1055:CLA:CBD	19:R:1055:CLA:HBA2	2.20	0.72
5:A:224:HIS:O	5:A:225:VAL:HG22	1.90	0.72
5:A:497:ALA:HB2	5:A:515:TRP:CB	2.20	0.72
6:B:334:LEU:HG	6:B:334:LEU:O	1.90	0.72
6:B:542:ARG:NH2	8:D:141:VAL:O	2.21	0.72
23:B:1778:BCR:H371	10:F:93:ILE:CG2	2.19	0.72
11:G:43:HIS:O	11:G:45:GLU:HG3	1.89	0.72
20:A:7016:LMU:H51	20:A:7016:LMU:O6'	1.89	0.72
2:2:98:GLU:HG3	2:2:99:LEU:HG	1.70	0.72
19:1:1148:CLA:H12	19:1:1148:CLA:CGD	2.17	0.72
12:H:25:GLY:HA3	12:H:27:ASP:HB2	1.71	0.72
20:A:7030:LMU:H21	20:A:7030:LMU:O5'	1.86	0.72
4:4:106:TRP:O	4:4:108:ASP:N	2.22	0.72
4:4:129:GLY:C	4:4:131:VAL:H	1.93	0.72
19:A:1764:CLA:H142	23:A:1806:BCR:C14	2.20	0.72
5:A:454:GLY:H	5:A:457:SER:CB	2.02	0.72
19:B:1757:CLA:HMC1	19:B:1757:CLA:HBC3	1.71	0.72
23:B:1778:BCR:C37	10:F:93:ILE:HG21	2.19	0.72
6:B:438:VAL:CG2	19:B:1763:CLA:HMC1	2.20	0.72
5:A:705:GLU:CB	6:B:545:LYS:NZ	2.53	0.72
6:B:586:THR:C	6:B:588:GLY:H	1.91	0.72
5:A:470:LEU:HD11	6:B:95:HIS:HB3	1.70	0.72
16:L:64:LEU:HB3	16:L:68:PHE:CE1	2.19	0.72
17:N:50:GLN:CA	17:N:51:ASP:O	2.38	0.72
19:1:1142:CLA:HED2	19:1:1143:CLA:HMB2	1.72	0.72
11:G:7:VAL:HG22	11:G:8:ILE:H	1.55	0.72
4:4:44:GLU:O	4:4:47:ASN:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:545:HIS:O	5:A:549:ILE:HG13	1.90	0.71
6:B:347:LEU:HD22	6:B:351:HIS:CE1	2.25	0.71
23:B:1778:BCR:C37	10:F:93:ILE:CG2	2.68	0.71
19:4:1205:CLA:O1D	19:4:1205:CLA:HBA2	1.90	0.71
17:N:77:CYS:O	17:N:79:SER:N	2.23	0.71
19:3:1217:CLA:HAC2	19:3:1218:CLA:C7	2.15	0.71
4:4:114:SER:OG	4:4:120:ILE:HD11	1.90	0.71
19:B:1737:CLA:O1A	19:B:1743:CLA:CBA	2.38	0.71
6:B:174:ARG:CB	19:B:1743:CLA:HBC2	2.20	0.71
5:A:690:LEU:HD21	6:B:661:PHE:HE1	1.55	0.71
6:B:557:PHE:HE2	7:C:66:ARG:HE	1.35	0.71
16:L:88:ALA:C	16:L:90:GLY:N	2.40	0.71
19:4:1205:CLA:CBD	19:4:1205:CLA:HBA2	2.20	0.71
3:3:92:TRP:C	3:3:94:ARG:O	2.29	0.71
5:A:28:LYS:HZ2	5:A:28:LYS:HB3	1.50	0.71
11:G:93:TYR:CA	11:G:94:ASP:CB	2.64	0.71
1:1:27:LEU:HD21	6:B:314:ARG:HG2	1.73	0.71
6:B:504:ASN:ND2	6:B:504:ASN:H	1.87	0.71
19:A:1779:CLA:CBB	23:A:1804:BCR:C35	2.68	0.71
5:A:25:ASP:CA	5:A:26:PRO:C	2.58	0.71
4:4:37:LEU:O	4:4:39:TRP:CD1	2.43	0.71
5:A:284:ARG:HA	5:A:284:ARG:CZ	2.19	0.71
6:B:349:ALA:CB	6:B:375:HIS:HB3	2.21	0.71
16:L:64:LEU:HA	16:L:67:PRO:HG2	1.72	0.71
10:F:25:LEU:HD22	10:F:46:MET:HB3	1.70	0.71
7:C:12:ILE:HB	7:C:39:ILE:HA	1.71	0.71
19:3:1222:CLA:HMA2	19:3:1222:CLA:O1A	1.91	0.71
20:A:7017:LMU:H1B	20:A:7017:LMU:O3'	1.91	0.71
4:4:98:SER:CB	4:4:102:GLU:OE1	2.38	0.71
5:A:62:HIS:HB2	19:A:1785:CLA:HBA1	1.72	0.71
5:A:370:ILE:CG2	5:A:400:MET:HA	2.21	0.71
5:A:393:LEU:HD11	5:A:750:PHE:CE1	2.25	0.71
19:B:1741:CLA:HAA2	19:B:1741:CLA:H12	1.70	0.71
4:4:70:ILE:HG13	4:4:71:ASN:N	2.05	0.71
17:N:42:PHE:CD1	17:N:43:PRO:N	2.59	0.71
5:A:25:ASP:OD2	5:A:26:PRO:HD3	1.91	0.71
5:A:316:MET:HA	5:A:317:TYR:HD1	1.54	0.71
16:L:161:LEU:HD11	16:L:162:ASP:O	1.91	0.71
1:1:45:ILE:HG22	1:1:48:ARG:HD2	1.73	0.71
4:4:101:VAL:HG13	4:4:104:ARG:HH22	1.55	0.71
5:A:220:ARG:O	5:A:221:HIS:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:387:PHE:O	6:B:391:PRO:HD3	1.91	0.71
9:E:60:LYS:HG3	9:E:61:THR:N	2.04	0.71
9:E:85:ASP:O	9:E:86:GLU:HB3	1.90	0.71
10:F:140:ALA:O	10:F:144:LEU:HB3	1.90	0.71
3:3:97:PHE:HD2	3:3:98:ILE:N	1.88	0.71
3:3:94:ARG:CG	3:3:97:PHE:HZ	1.85	0.71
4:4:100:TYR:HA	4:4:103:ILE:CD1	2.20	0.71
19:4:1211:CLA:CBD	19:4:1211:CLA:HBA1	2.21	0.71
4:4:122:LYS:NZ	4:4:150:LYS:CD	2.52	0.71
19:A:1774:CLA:HBB2	19:A:1774:CLA:C10	2.21	0.71
5:A:545:HIS:CG	19:A:1792:CLA:HBB2	2.25	0.71
5:A:684:PHE:C	5:A:684:PHE:HD2	1.93	0.71
25:B:1783:SF4:FE1	25:B:1783:SF4:S3	1.82	0.71
16:L:164:PRO:CA	16:L:165:TYR:HD1	1.86	0.71
20:A:7039:LMU:H6'2	20:A:7039:LMU:C3'	2.17	0.71
7:C:31:TRP:O	7:C:33:GLY:N	2.23	0.71
15:K:51:ASP:HB3	15:K:52:PRO:HD3	1.70	0.71
5:A:218:TRP:O	5:A:222:GLN:HB2	1.90	0.71
6:B:530:THR:HG21	19:B:1755:CLA:HAC1	1.72	0.71
6:B:697:PRO:O	7:C:79:LEU:HD11	1.88	0.71
9:E:88:GLU:O	9:E:90:VAL:CA	2.39	0.71
17:N:61:LEU:HD11	17:N:63:ASP:CA	2.21	0.71
5:A:27:ILE:CB	5:A:28:LYS:HG2	2.21	0.71
16:L:164:PRO:CG	16:L:165:TYR:CE1	2.51	0.71
1:1:27:LEU:HD13	1:1:28:GLY:H	1.55	0.71
3:3:52:LYS:O	3:3:56:TYR:N	2.21	0.71
2:2:169:LEU:CD2	19:2:1215:CLA:CAB	2.63	0.71
10:F:153:ASN:C	10:F:153:ASN:ND2	2.41	0.71
20:A:7040:LMU:O3'	20:A:7040:LMU:C1B	2.38	0.71
10:F:151:ASP:OD2	10:F:154:PHE:CD1	2.44	0.71
12:H:42:THR:HG22	12:H:45:ALA:HB2	1.72	0.71
19:B:1749:CLA:OBD	19:B:1752:CLA:HBC3	1.89	0.71
19:B:1759:CLA:H62	24:B:1781:LMG:H182	1.73	0.71
5:A:714:LEU:HA	10:F:149:LEU:HD11	1.73	0.71
17:N:41:LYS:CB	17:N:42:PHE:CB	2.65	0.71
6:B:172:GLU:O	6:B:176:ASN:CB	2.39	0.71
7:C:26:LEU:N	7:C:43:PRO:HG3	2.05	0.71
6:B:692:ARG:HH22	6:B:694:ARG:HG2	1.54	0.71
5:A:464:ASN:HD22	5:A:464:ASN:N	1.86	0.71
19:A:1779:CLA:HBB2	23:A:1804:BCR:C35	2.21	0.71
6:B:310:PRO:HB2	6:B:311:PRO:CD	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:12:VAL:O	13:I:17:PRO:CD	2.37	0.71
4:4:70:ILE:O	4:4:73:PRO:HD3	1.91	0.71
17:N:41:LYS:HB2	17:N:42:PHE:CB	2.21	0.71
15:K:44:GLU:OE1	15:K:45:SER:C	2.29	0.71
4:4:171:ASN:C	4:4:173:THR:N	2.43	0.71
20:A:7013:LMU:H91	20:A:7049:LMU:C3'	2.21	0.71
8:D:113:HIS:NE2	8:D:118:VAL:CG1	2.54	0.71
5:A:349:ILE:CG2	5:A:349:ILE:O	2.39	0.71
6:B:98:GLN:C	6:B:100:ALA:H	1.93	0.71
10:F:95:GLY:O	10:F:99:TRP:HB2	1.91	0.71
19:A:1817:CLA:CBC	19:A:1817:CLA:HMC1	2.21	0.70
5:A:214:GLY:O	5:A:215:SER:HB3	1.91	0.70
5:A:723:ARG:NH1	5:A:723:ARG:HG2	2.04	0.70
7:C:63:LEU:CG	7:C:64:SER:H	2.04	0.70
19:H:1080:CLA:C3C	23:I:1032:BCR:HC22	2.17	0.70
4:4:69:ILE:O	4:4:70:ILE:C	2.29	0.70
17:N:63:ASP:N	17:N:64:ASP:CB	2.51	0.70
5:A:24:ARG:O	5:A:25:ASP:CG	2.30	0.70
18:R:30:UNK:O	18:R:32:UNK:O	2.08	0.70
4:4:58:MET:O	4:4:61:PRO:CD	2.39	0.70
19:A:1774:CLA:HBB2	19:A:1774:CLA:H8	1.72	0.70
19:A:1781:CLA:H43	19:A:1793:CLA:HBA1	1.73	0.70
23:A:1808:BCR:HC31	6:B:687:LEU:HD12	1.72	0.70
6:B:123:TRP:CZ3	19:B:1743:CLA:H191	2.25	0.70
6:B:310:PRO:CG	19:B:1753:CLA:HMA1	2.08	0.70
6:B:732:LYS:HD3	6:B:734:GLY:HA3	1.73	0.70
7:C:1:MET:CB	7:C:4:SER:OG	2.36	0.70
23:I:1032:BCR:H391	23:L:1169:BCR:H401	1.73	0.70
20:A:7016:LMU:C2	20:A:7016:LMU:C8	2.61	0.70
5:A:168:ALA:O	5:A:171:ALA:HB3	1.90	0.70
19:1:1188:CLA:HMC1	19:1:1188:CLA:HBC3	1.73	0.70
4:4:106:TRP:HD1	19:4:1196:CLA:O1D	1.75	0.70
6:B:137:THR:HA	6:B:140:ILE:CG1	2.20	0.70
6:B:167:TRP:HB2	11:G:41:MET:CE	2.21	0.70
6:B:463:ILE:O	6:B:464:GLN:HB3	1.91	0.70
6:B:545:LYS:HD3	6:B:546:LEU:H	1.56	0.70
1:1:25:ASP:HB3	1:1:26:PRO:CD	2.20	0.70
1:1:24:PHE:CG	6:B:314:ARG:NH2	2.59	0.70
10:F:22:LEU:O	10:F:25:LEU:N	2.23	0.70
20:A:7006:LMU:O5B	20:A:7006:LMU:H5'	1.88	0.70
21:B:8053:SUC:H3'	21:B:8053:SUC:C6	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:187:HIS:CE1	19:A:1767:CLA:C4D	2.73	0.70
19:A:1760:CLA:HBA2	19:A:1767:CLA:H62	1.74	0.70
5:A:217:SER:HG	23:A:1803:BCR:H17C	1.56	0.70
5:A:661:ALA:O	5:A:664:VAL:HG22	1.92	0.70
23:B:1780:BCR:C38	23:B:1780:BCR:H23C	2.21	0.70
6:B:53:GLN:C	6:B:55:ALA:H	1.95	0.70
9:E:42:GLU:HG2	9:E:43:SER:H	1.53	0.70
4:4:70:ILE:C	4:4:72:VAL:N	2.44	0.70
3:3:97:PHE:HD2	3:3:98:ILE:CG2	1.85	0.70
16:L:163:LEU:HD12	16:L:164:PRO:HG3	1.74	0.70
18:R:34:UNK:H	18:R:36:UNK:CA	2.00	0.70
2:2:110:TRP:HD1	2:2:113:ILE:CG2	2.04	0.70
3:3:106:TYR:O	3:3:108:ALA:HB2	1.91	0.70
19:R:1054:CLA:CHA	19:R:1054:CLA:CED	2.69	0.70
12:H:45:ALA:O	12:H:47:PHE:N	2.25	0.70
5:A:605:MET:HA	5:A:608:SER:OG	1.92	0.70
10:F:12:LYS:HG2	10:F:13:GLN:N	2.07	0.70
4:4:149:ALA:HB3	4:4:151:GLU:OE1	1.91	0.70
19:A:1760:CLA:C1	19:A:1767:CLA:H61	2.16	0.70
6:B:323:TYR:CE1	19:B:1754:CLA:HBC1	2.26	0.70
19:B:1768:CLA:H121	23:B:1779:BCR:H312	1.73	0.70
6:B:202:SER:HB3	6:B:270:LEU:HD11	1.74	0.70
6:B:471:THR:HG23	6:B:502:ASN:ND2	2.07	0.70
10:F:103:SER:C	10:F:105:LEU:H	1.95	0.70
3:3:92:TRP:O	3:3:94:ARG:C	2.29	0.70
16:L:165:TYR:C	16:L:166:TYR:O	2.30	0.70
3:3:64:TYR:HB3	19:3:1221:CLA:C4	2.21	0.70
3:3:157:ALA:C	3:3:158:TYR:CD2	2.64	0.70
15:K:43:ARG:CG	15:K:43:ARG:HH11	1.86	0.70
20:A:7042:LMU:H1B	20:A:7042:LMU:O3'	1.89	0.70
19:4:4014:CLA:HBC3	19:4:4014:CLA:HMC1	1.73	0.70
15:K:4:GLY:HA2	15:K:7:THR:HB	1.72	0.70
4:4:117:GLN:O	4:4:121:PHE:HE2	1.73	0.70
4:4:150:LYS:HG3	4:4:150:LYS:O	1.90	0.70
6:B:131:THR:O	6:B:135:LEU:N	2.24	0.70
6:B:317:ARG:HE	6:B:317:ARG:HA	1.54	0.70
11:G:27:GLN:O	11:G:28:ARG:HB3	1.90	0.70
4:4:69:ILE:CD1	4:4:175:LYS:HB2	2.08	0.70
20:A:7021:LMU:H22	20:A:7021:LMU:C6	2.14	0.70
20:2:1224:LMU:C1	20:2:1224:LMU:C7	2.69	0.70
15:K:16:THR:O	15:K:20:PHE:HB3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1814:CLA:C3B	6:B:589:TRP:CH2	2.74	0.70
6:B:732:LYS:HG2	6:B:733:PHE:O	1.91	0.70
17:N:45:ASN:ND2	17:N:54:LYS:CB	2.54	0.70
17:N:72:LYS:NZ	17:N:74:LYS:HE3	2.07	0.70
5:A:567:ARG:HH11	8:D:35:GLY:CA	2.04	0.70
20:A:7023:LMU:C9	20:A:7023:LMU:H41	2.22	0.70
5:A:527:VAL:CG1	5:A:528:ALA:N	2.55	0.70
4:4:124:TYR:HB2	4:4:143:PHE:CD1	2.25	0.70
4:4:124:TYR:HB3	4:4:143:PHE:CE1	2.26	0.70
5:A:187:HIS:CE1	19:A:1767:CLA:C1A	2.61	0.70
6:B:124:TRP:O	6:B:129:LEU:HB3	1.91	0.70
7:C:5:VAL:HG23	7:C:65:VAL:CG1	2.19	0.70
3:3:93:PHE:C	3:3:94:ARG:O	2.29	0.70
17:N:41:LYS:CB	17:N:42:PHE:CA	2.68	0.70
2:2:113:ILE:HG13	2:2:114:LEU:H	1.57	0.70
10:F:28:SER:O	10:F:29:LEU:C	2.29	0.70
8:D:102:ARG:HE	8:D:110:GLN:CB	2.03	0.70
14:J:31:ARG:HA	14:J:34:PRO:HA	1.72	0.70
12:H:58:ILE:HD11	16:L:97:MET:SD	2.31	0.70
3:3:163:PHE:O	3:3:164:PHE:HB2	1.91	0.70
23:A:1805:BCR:C31	23:A:1805:BCR:C8	2.69	0.70
6:B:58:PHE:HB3	6:B:146:SER:HB3	1.72	0.70
6:B:396:ARG:HH11	19:B:1759:CLA:HED2	1.57	0.70
19:B:1768:CLA:C16	23:B:1779:BCR:H313	2.20	0.70
6:B:596:TRP:CD1	6:B:623:TYR:HB2	2.26	0.70
7:C:7:ILE:CG2	7:C:65:VAL:HG21	2.21	0.70
9:E:45:TRP:HH2	9:E:78:SER:OG	1.73	0.70
19:H:1079:CLA:O2A	19:H:1079:CLA:HMA2	1.91	0.70
2:2:166:ASN:OD1	2:2:169:LEU:HD12	1.91	0.70
20:A:7013:LMU:H91	20:A:7049:LMU:C4'	2.21	0.70
19:1:1145:CLA:HMA1	19:1:1145:CLA:H61	1.73	0.70
20:A:7008:LMU:H6D	20:A:7008:LMU:C2	2.22	0.70
5:A:422:TYR:CD1	5:A:422:TYR:N	2.57	0.70
4:4:106:TRP:CD1	19:4:1196:CLA:O1D	2.44	0.70
19:A:1781:CLA:H72	19:A:1782:CLA:HED2	1.72	0.70
19:A:1800:CLA:HMC2	19:B:1770:CLA:H11	1.74	0.70
5:A:331:LEU:C	5:A:331:LEU:HD23	2.12	0.70
5:A:685:VAL:HG12	5:A:741:GLY:HA2	1.74	0.70
19:B:1769:CLA:CHA	19:B:1769:CLA:HBA1	2.20	0.70
6:B:654:HIS:CE1	19:B:1784:CLA:NB	2.60	0.70
10:F:151:ASP:HA	10:F:154:PHE:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:56:ASN:O	5:A:57:LEU:HB3	1.91	0.69
19:B:1753:CLA:C1A	19:B:1753:CLA:C4	2.60	0.69
23:B:1778:BCR:C39	10:F:90:PHE:HA	2.22	0.69
6:B:424:TRP:CZ2	19:B:1761:CLA:HAC1	2.26	0.69
6:B:16:PRO:HG3	7:C:74:THR:HB	1.74	0.69
10:F:93:ILE:O	10:F:96:TRP:CD1	2.41	0.69
11:G:28:ARG:CG	11:G:29:GLU:N	2.54	0.69
19:H:1079:CLA:O1A	19:H:1079:CLA:C4	2.39	0.69
5:A:27:ILE:HG22	5:A:28:LYS:HD3	1.44	0.69
20:2:1224:LMU:O5'	20:2:1224:LMU:C3	2.39	0.69
5:A:705:GLU:HA	5:A:708:VAL:HB	1.75	0.69
6:B:292:ARG:CZ	6:B:292:ARG:HA	2.21	0.69
6:B:295:PHE:N	6:B:295:PHE:HD2	1.90	0.69
6:B:295:PHE:N	6:B:295:PHE:CD2	2.60	0.69
6:B:421:HIS:CE1	19:B:1761:CLA:C4D	2.74	0.69
5:A:131:ILE:HD13	6:B:447:GLY:HA3	1.71	0.69
6:B:464:GLN:CD	6:B:469:LYS:HD3	2.13	0.69
13:I:7:LEU:CD1	23:I:1032:BCR:H333	2.15	0.69
20:A:7036:LMU:C2	20:A:7036:LMU:H82	2.21	0.69
4:4:106:TRP:CD2	19:4:1196:CLA:CED	2.72	0.69
5:A:281:LEU:HA	5:A:297:THR:O	1.92	0.69
6:B:120:VAL:CA	6:B:123:TRP:CD1	2.71	0.69
11:G:28:ARG:HG2	11:G:29:GLU:H	1.55	0.69
5:A:27:ILE:O	5:A:28:LYS:HD2	1.92	0.69
2:2:44:ASN:C	2:2:46:GLN:H	1.93	0.69
2:2:44:ASN:ND2	14:J:1:MET:HB2	2.08	0.69
4:4:147:LEU:CG	4:4:148:GLU:H	2.05	0.69
19:4:1206:CLA:CAA	19:4:1206:CLA:H12	2.20	0.69
20:A:7023:LMU:H2B	20:A:7023:LMU:C6B	2.22	0.69
14:J:11:ALA:HB1	14:J:12:PRO:CD	2.20	0.69
19:A:1763:CLA:HMB3	19:A:1764:CLA:HMB	1.73	0.69
19:A:1781:CLA:H52	19:A:1782:CLA:HED1	1.73	0.69
19:A:1787:CLA:H93	16:L:36:TYR:CE1	2.27	0.69
5:A:603:PHE:HZ	5:A:693:LEU:HD21	1.56	0.69
19:B:1764:CLA:C1D	19:B:1765:CLA:HBB2	2.21	0.69
19:B:1768:CLA:HBC1	10:F:83:PHE:HZ	1.53	0.69
6:B:437:TYR:HB3	6:B:616:LEU:CD2	2.22	0.69
4:4:147:LEU:HD22	4:4:148:GLU:HG3	1.75	0.69
20:A:7042:LMU:C3	20:A:7042:LMU:H6D	2.20	0.69
9:E:68:ARG:NE	9:E:68:ARG:O	2.24	0.69
4:4:163:PHE:O	4:4:166:PHE:HB3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:89:THR:N	4:4:90:LEU:HD22	2.08	0.69
19:A:1781:CLA:C5	19:A:1782:CLA:HED1	2.22	0.69
2:2:164:ILE:O	2:2:167:GLY:HA3	1.92	0.69
6:B:672:GLN:HE21	6:B:672:GLN:CA	1.92	0.69
2:2:205:PHE:C	2:2:205:PHE:CD1	2.66	0.69
20:A:7030:LMU:C4'	20:A:7030:LMU:O2B	2.40	0.69
6:B:224:PRO:HB3	6:B:227:THR:HB	1.74	0.69
5:A:259:TYR:CB	5:A:260:PRO:HD2	2.21	0.69
5:A:393:LEU:CD1	5:A:750:PHE:CE1	2.76	0.69
6:B:438:VAL:CG2	19:B:1763:CLA:HAC1	2.22	0.69
6:B:531:THR:O	6:B:535:VAL:HG12	1.93	0.69
2:2:129:LYS:C	2:2:131:THR:H	1.96	0.69
4:4:106:TRP:C	4:4:108:ASP:N	2.45	0.69
4:4:118:ASP:C	4:4:122:LYS:HA	2.12	0.69
19:A:1781:CLA:HBC2	19:A:1781:CLA:CHD	2.19	0.69
19:B:1756:CLA:C8	23:B:1777:BCR:H14C	2.23	0.69
19:B:1758:CLA:H43	23:B:1775:BCR:HC7	1.75	0.69
6:B:414:HIS:CD2	19:B:1760:CLA:HMA3	2.27	0.69
19:L:1168:CLA:HBC3	19:L:1168:CLA:CHD	2.14	0.69
5:A:472:ARG:HH22	16:L:74:LEU:HD21	1.58	0.69
1:1:179:THR:HG23	4:4:87:SER:HB3	1.72	0.69
12:H:25:GLY:HA3	12:H:27:ASP:N	2.08	0.69
6:B:305:LEU:HD22	19:B:1753:CLA:O1D	1.91	0.69
19:B:1762:CLA:HBB2	23:B:1778:BCR:H272	1.74	0.69
5:A:669:GLY:N	6:B:445:ALA:HA	2.07	0.69
5:A:205:HIS:CE1	19:A:1769:CLA:HMC2	2.28	0.69
19:A:1814:CLA:H11	6:B:616:LEU:CG	2.22	0.69
6:B:427:LEU:HD23	6:B:431:PHE:HZ	1.56	0.69
6:B:76:ALA:O	6:B:78:VAL:N	2.25	0.69
3:3:96:GLY:O	3:3:97:PHE:HB3	1.92	0.69
3:3:94:ARG:C	3:3:97:PHE:CE1	2.65	0.69
1:1:27:LEU:HD21	6:B:314:ARG:CG	2.22	0.69
19:2:2006:CLA:HAA1	19:2:2006:CLA:C2	2.22	0.69
20:A:7016:LMU:H31	20:A:7016:LMU:C1'	2.23	0.69
2:2:129:LYS:O	2:2:132:GLY:CA	2.41	0.69
19:1:1308:CLA:HMC1	19:1:1308:CLA:HBC2	1.73	0.69
6:B:20:ARG:HB3	6:B:20:ARG:HH11	1.57	0.69
10:F:61:LEU:HD23	10:F:69:PRO:HB2	1.73	0.69
5:A:107:GLU:CD	5:A:161:GLU:HG3	2.13	0.69
4:4:118:ASP:O	4:4:122:LYS:HA	1.93	0.69
4:4:42:GLN:OE1	4:4:120:ILE:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:747:TRP:CD2	23:A:1805:BCR:H401	2.28	0.69
5:A:304:LEU:HD22	19:A:1772:CLA:HBB2	1.75	0.69
6:B:167:TRP:HD1	11:G:41:MET:CE	2.06	0.69
11:G:28:ARG:HD2	11:G:33:LYS:HE2	1.75	0.69
11:G:45:GLU:O	11:G:46:ALA:C	2.29	0.69
4:4:194:VAL:HG12	4:4:195:GLN:CB	2.23	0.69
20:A:7042:LMU:H22	20:A:7042:LMU:H71	1.73	0.69
6:B:666:SER:HB3	6:B:671:TRP:NE1	2.08	0.69
8:D:86:LEU:HD13	8:D:90:LEU:HG	1.75	0.69
5:A:103:PHE:N	5:A:103:PHE:CD2	2.60	0.69
19:A:1795:CLA:OBD	10:F:105:LEU:HD11	1.93	0.69
5:A:353:SER:O	5:A:354:TRP:HB2	1.93	0.69
5:A:41:SER:O	5:A:44:ILE:HA	1.92	0.69
5:A:21:LEU:CD1	5:A:21:LEU:N	2.30	0.69
18:R:30:UNK:O	18:R:32:UNK:N	2.26	0.69
19:2:1213:CLA:H42	19:2:1213:CLA:C4C	2.21	0.69
16:L:77:THR:HG21	16:L:82:ALA:HB1	1.75	0.69
19:3:3011:CLA:HHD	19:3:3011:CLA:HBC2	1.75	0.69
4:4:128:ALA:HB1	4:4:141:LEU:CD2	2.23	0.68
5:A:126:ILE:HG12	19:A:1765:CLA:HMA3	1.76	0.68
19:A:1774:CLA:O1D	19:A:1774:CLA:H2A	1.92	0.68
5:A:244:LEU:HB2	5:A:247:GLU:HB2	1.75	0.68
5:A:308:ILE:HG22	5:A:309:LEU:N	2.07	0.68
5:A:358:LEU:HD11	5:A:413:HIS:CG	2.28	0.68
6:B:493:TRP:CZ2	19:B:1765:CLA:CBA	2.76	0.68
6:B:594:TRP:C	6:B:594:TRP:CD1	2.67	0.68
11:G:13:GLY:O	11:G:16:LEU:HG	1.93	0.68
6:B:525:LEU:HD22	6:B:525:LEU:O	1.92	0.68
6:B:278:LEU:HD12	19:B:1746:CLA:CMA	2.23	0.68
6:B:304:ILE:HD11	19:B:1749:CLA:HED3	1.73	0.68
2:2:137:TYR:CD1	2:2:138:PRO:HD2	2.28	0.68
20:A:7031:LMU:O6'	20:A:7031:LMU:H1B	1.93	0.68
19:A:1782:CLA:HMC1	19:A:1782:CLA:CBC	2.23	0.68
19:A:1789:CLA:HBC3	19:A:1789:CLA:CMC	2.23	0.68
5:A:581:CYS:CB	5:A:590:CYS:HA	2.16	0.68
5:A:737:HIS:HA	5:A:740:LEU:CD2	2.23	0.68
19:B:1744:CLA:HMB3	23:B:1776:BCR:H311	1.73	0.68
3:3:92:TRP:O	3:3:97:PHE:HD1	1.75	0.68
3:3:52:LYS:C	3:3:56:TYR:CD2	2.65	0.68
7:C:28:MET:HG2	7:C:38:GLN:HE21	1.58	0.68
8:D:69:ARG:O	8:D:70:GLU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1781:CLA:CBC	19:A:1781:CLA:HHD	2.16	0.68
19:A:1813:CLA:HAA1	19:B:1784:CLA:HBB2	1.75	0.68
5:A:663:GLN:HB3	5:A:752:ALA:O	1.93	0.68
19:B:1753:CLA:HBD	19:B:1753:CLA:HAA2	1.75	0.68
6:B:347:LEU:CD2	6:B:351:HIS:CE1	2.77	0.68
7:C:6:LYS:HB3	7:C:63:LEU:HD21	1.75	0.68
10:F:80:TRP:HE3	19:F:1157:CLA:HMC2	1.58	0.68
19:A:1789:CLA:H43	16:L:64:LEU:HD23	1.73	0.68
17:N:49:CYS:O	17:N:50:GLN:O	2.10	0.68
1:1:24:PHE:CB	6:B:314:ARG:NH2	2.35	0.68
2:2:59:ALA:HB1	2:2:172:LEU:HD22	1.74	0.68
20:R:1056:LMU:O6B	20:R:1056:LMU:H1B	1.93	0.68
6:B:468:GLY:O	6:B:470:THR:N	2.26	0.68
4:4:99:HIS:ND1	4:4:103:ILE:CD1	2.56	0.68
19:A:1763:CLA:C2B	23:A:1806:BCR:H331	2.23	0.68
5:A:438:HIS:CE1	5:A:442:ILE:HD11	2.29	0.68
5:A:96:MET:CE	19:A:1763:CLA:HBB2	2.23	0.68
19:B:1762:CLA:HBB2	23:B:1778:BCR:C26	2.23	0.68
6:B:623:TYR:O	6:B:624:LEU:HB2	1.91	0.68
5:A:555:ILE:HG22	6:B:670:TYR:HE2	1.56	0.68
9:E:87:VAL:C	9:E:89:GLU:H	1.97	0.68
17:N:70:GLU:C	17:N:72:LYS:N	2.46	0.68
2:2:161:THR:HB	2:2:165:LYS:HD2	1.75	0.68
2:2:168:ARG:HH11	2:2:168:ARG:HG2	1.59	0.68
7:C:49:VAL:HG22	7:C:50:GLY:H	1.59	0.68
2:2:187:GLY:O	2:2:189:ILE:HG12	1.93	0.68
4:4:121:PHE:CD1	4:4:128:ALA:HB3	2.29	0.68
5:A:690:LEU:CD2	6:B:661:PHE:HE1	2.06	0.68
6:B:560:ASP:HB2	7:C:66:ARG:NE	2.08	0.68
11:G:30:ASN:O	11:G:33:LYS:NZ	2.26	0.68
5:A:22:VAL:HB	5:A:24:ARG:CA	2.22	0.68
5:A:24:ARG:CZ	5:A:29:THR:HB	2.21	0.68
19:2:1223:CLA:H8	19:2:1223:CLA:C3	2.19	0.68
19:1:1145:CLA:H2	19:1:1145:CLA:CMA	2.24	0.68
12:H:49:LYS:O	12:H:51:GLY:N	2.26	0.68
19:A:1797:CLA:H102	19:A:1797:CLA:H51	1.76	0.68
6:B:212:PHE:HZ	19:B:1744:CLA:HAC1	1.59	0.68
19:B:1755:CLA:CBB	19:B:1769:CLA:HHB	2.24	0.68
19:B:1768:CLA:H161	23:B:1779:BCR:C31	2.22	0.68
6:B:560:ASP:OD1	7:C:52:LYS:NZ	2.26	0.68
4:4:147:LEU:HD22	4:4:148:GLU:CG	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7032:LMU:O2'	20:A:7032:LMU:H12	1.94	0.68
19:R:1054:CLA:C4D	19:R:1054:CLA:HED3	2.23	0.68
16:L:48:ASN:HD22	16:L:115:ALA:HB2	1.58	0.68
4:4:163:PHE:O	4:4:167:ILE:N	2.26	0.68
4:4:47:ASN:HB3	4:4:161:LEU:HD23	1.76	0.68
6:B:269:TRP:HE3	6:B:270:LEU:H	1.40	0.68
6:B:278:LEU:HD12	19:B:1746:CLA:HMA2	1.76	0.68
8:D:31:GLY:HA2	16:L:13:PRO:HB3	1.74	0.68
16:L:13:PRO:O	16:L:14:LEU:HB2	1.94	0.68
17:N:47:THR:HB	17:N:52:LEU:O	1.93	0.68
3:3:63:ARG:CZ	3:3:185:LYS:HG2	2.24	0.68
19:1:1142:CLA:CED	19:1:1143:CLA:CMB	2.67	0.68
20:A:7021:LMU:H6D	20:A:7021:LMU:H41	1.74	0.68
7:C:20:ALA:O	7:C:21:CYS:CB	2.39	0.68
12:H:53:LEU:HG	12:H:54:LEU:H	1.57	0.68
19:A:1781:CLA:HED3	19:A:1782:CLA:HMD1	1.74	0.68
5:A:207:LEU:HA	5:A:211:LEU:HG	1.75	0.68
5:A:207:LEU:HD21	5:A:314:GLY:HA2	1.75	0.68
5:A:665:ILE:O	6:B:621:ARG:HD3	1.93	0.68
6:B:598:HIS:HB3	6:B:602:TRP:CZ3	2.29	0.68
11:G:23:PHE:CD2	11:G:24:PHE:HB2	2.29	0.68
17:N:82:PHE:O	17:N:84:LYS:N	2.26	0.68
3:3:50:GLU:O	3:3:53:TRP:N	2.27	0.68
2:2:165:LYS:O	2:2:168:ARG:N	2.27	0.68
11:G:13:GLY:O	11:G:16:LEU:CB	2.42	0.68
11:G:7:VAL:CG2	11:G:8:ILE:H	2.07	0.68
15:K:38:LEU:CG	15:K:39:LYS:HD3	2.10	0.68
19:A:1760:CLA:H2A	19:A:1760:CLA:O2D	1.93	0.68
19:A:1763:CLA:CMB	23:A:1806:BCR:HC7	2.23	0.68
23:A:1809:BCR:C8	23:A:1809:BCR:H311	2.23	0.68
19:A:1817:CLA:HMC1	6:B:661:PHE:CB	2.23	0.68
5:A:85:GLN:O	5:A:89:ILE:HG13	1.93	0.68
6:B:732:LYS:C	6:B:733:PHE:O	2.29	0.68
7:C:5:VAL:HB	7:C:65:VAL:CG1	2.23	0.68
7:C:7:ILE:HG22	7:C:65:VAL:HG23	1.73	0.68
17:N:57:LYS:CG	17:N:58:VAL:N	2.35	0.68
5:A:21:LEU:C	5:A:22:VAL:O	2.30	0.68
16:L:163:LEU:HD12	16:L:165:TYR:CE1	2.28	0.68
1:1:25:ASP:HB3	1:1:26:PRO:HD2	1.75	0.68
7:C:17:CYS:C	7:C:58:CYS:HB2	2.14	0.68
20:A:7032:LMU:C3	20:A:7032:LMU:C1B	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:1222:CLA:H142	19:3:1222:CLA:H101	1.75	0.68
1:1:45:ILE:HA	1:1:48:ARG:HB2	1.76	0.68
6:B:533:ILE:HD11	6:B:575:ASP:O	1.93	0.68
7:C:74:THR:OG1	7:C:80:ALA:HB3	1.93	0.67
4:4:75:TRP:CG	19:4:1205:CLA:HMD3	2.29	0.67
15:K:27:ALA:HB3	15:K:28:PRO:CD	2.24	0.67
4:4:84:PHE:O	4:4:85:ALA:HB3	1.93	0.67
5:A:210:LEU:HD13	19:A:1769:CLA:HMB2	1.74	0.67
23:B:1778:BCR:H392	10:F:90:PHE:HA	1.75	0.67
6:B:212:PHE:CZ	19:B:1744:CLA:HAC1	2.28	0.67
6:B:615:TYR:HD1	6:B:615:TYR:H	1.42	0.67
11:G:33:LYS:NZ	11:G:33:LYS:HA	2.09	0.67
16:L:13:PRO:HG2	16:L:18:PRO:HB3	1.75	0.67
19:R:1054:CLA:HED3	19:R:1054:CLA:C1A	2.24	0.67
21:B:8059:SUC:O6	21:B:8059:SUC:H1	1.95	0.67
5:A:107:GLU:OE1	5:A:161:GLU:HG3	1.94	0.67
19:A:1781:CLA:HAA1	19:A:1781:CLA:HED2	1.74	0.67
19:A:1816:CLA:H93	19:A:1817:CLA:C9	2.17	0.67
6:B:546:LEU:HD11	6:B:567:THR:HG22	1.77	0.67
18:R:37:UNK:C	18:R:42:UNK:O	2.42	0.67
19:2:2006:CLA:CHD	19:2:2006:CLA:HBC2	2.24	0.67
2:2:98:GLU:CG	2:2:99:LEU:CD1	2.73	0.67
11:G:7:VAL:CG2	11:G:8:ILE:N	2.57	0.67
2:2:127:ASN:OD1	14:J:2:ARG:HA	1.94	0.67
4:4:144:ALA:HB3	4:4:148:GLU:O	1.93	0.67
19:A:1796:CLA:H43	19:A:1796:CLA:NC	2.09	0.67
5:A:713:LYS:HZ2	19:B:1761:CLA:C4	2.08	0.67
6:B:432:HIS:CE1	19:B:1762:CLA:NB	2.55	0.67
7:C:70:TRP:O	7:C:72:GLU:HB2	1.94	0.67
13:I:23:SER:O	13:I:26:LEU:HD23	1.95	0.67
4:4:70:ILE:HG13	4:4:71:ASN:H	1.60	0.67
19:2:1223:CLA:H3A	19:2:1223:CLA:CGA	2.23	0.67
7:C:44:ARG:HH22	8:D:127:ARG:NE	1.92	0.67
20:A:7037:LMU:C1	20:A:7037:LMU:H51	2.23	0.67
20:2:1224:LMU:O1'	20:2:1224:LMU:H72	1.94	0.67
14:J:31:ARG:NH2	19:J:1043:CLA:C4B	2.56	0.67
2:2:189:ILE:O	2:2:190:ASP:HB3	1.93	0.67
19:A:1781:CLA:C6	19:A:1782:CLA:HED1	2.25	0.67
5:A:615:HIS:CE1	19:A:1792:CLA:HBC3	2.30	0.67
19:A:1817:CLA:HBC3	6:B:661:PHE:HB3	1.76	0.67
5:A:365:LEU:HD23	19:A:1761:CLA:CED	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1783:SF4:S3	25:B:1783:SF4:S2	2.92	0.67
6:B:492:ILE:CD1	6:B:492:ILE:H	2.05	0.67
13:I:24:LEU:HD21	23:L:1169:BCR:H271	1.75	0.67
20:A:7042:LMU:C7	20:A:7042:LMU:H22	2.25	0.67
6:B:454:LEU:HD11	10:F:69:PRO:O	1.93	0.67
5:A:387:THR:CG2	5:A:523:VAL:HG11	2.25	0.67
5:A:387:THR:HG23	5:A:523:VAL:HG11	1.75	0.67
17:N:33:TYR:O	17:N:34:THR:HG22	1.95	0.67
4:4:106:TRP:CZ3	19:4:1198:CLA:HBC1	2.30	0.67
5:A:308:ILE:HD11	19:A:1772:CLA:H91	1.75	0.67
5:A:301:HIS:CD2	19:A:1772:CLA:O1D	2.47	0.67
4:4:37:LEU:HA	4:4:39:TRP:CG	2.29	0.67
2:2:113:ILE:HG13	2:2:114:LEU:N	2.10	0.67
11:G:13:GLY:O	11:G:16:LEU:CG	2.43	0.67
5:A:396:PHE:CE2	5:A:616:PHE:CG	2.83	0.67
4:4:122:LYS:HE2	4:4:150:LYS:CD	2.21	0.67
5:A:259:TYR:CE2	5:A:280:PHE:HA	2.30	0.67
5:A:308:ILE:O	5:A:312:ILE:N	2.24	0.67
5:A:98:PHE:HZ	19:A:1763:CLA:HMD3	1.59	0.67
6:B:648:TRP:CZ3	23:B:1780:BCR:H392	2.29	0.67
3:3:97:PHE:HD2	3:3:97:PHE:O	1.70	0.67
2:2:61:GLY:O	2:2:65:PRO:HG2	1.95	0.67
3:3:107:TRP:CD1	3:3:108:ALA:CA	2.77	0.67
20:A:7041:LMU:O6'	20:A:7041:LMU:H1B	1.94	0.67
8:D:102:ARG:NH1	8:D:104:PHE:CE1	2.63	0.67
6:B:160:LYS:HG3	6:B:161:TRP:H	1.59	0.67
1:1:183:ASP:OD2	1:1:184:PRO:HD3	1.94	0.67
4:4:106:TRP:HE3	19:4:1209:CLA:HMA1	1.59	0.67
4:4:122:LYS:CE	4:4:150:LYS:HD2	2.14	0.67
4:4:158:ARG:HA	4:4:161:LEU:HD12	1.77	0.67
5:A:195:TRP:CZ2	19:A:1766:CLA:CMA	2.76	0.67
5:A:370:ILE:HG23	5:A:403:GLY:CA	2.19	0.67
11:G:46:ALA:O	11:G:47:GLY:C	2.30	0.67
13:I:12:VAL:HG23	13:I:13:GLY:H	1.58	0.67
2:2:103:GLY:CA	19:2:1221:CLA:HBB2	2.24	0.67
3:3:173:GLU:CG	3:3:174:LYS:N	2.57	0.67
19:4:4014:CLA:CAB	20:A:7034:LMU:O3B	2.42	0.67
20:A:7030:LMU:O3'	20:A:7030:LMU:H3B	1.95	0.67
19:J:1043:CLA:O1A	19:J:1043:CLA:H152	1.95	0.67
6:B:456:GLU:HG2	10:F:70:HIS:HB3	1.77	0.67
20:A:7009:LMU:H22	20:A:7009:LMU:O2'	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:95:GLY:H	19:A:1763:CLA:HMC3	1.59	0.67
19:A:1796:CLA:H161	23:A:1805:BCR:HC22	1.76	0.67
6:B:275:HIS:HD1	19:B:1747:CLA:HMB1	1.59	0.67
7:C:55:GLU:O	7:C:57:ALA:N	2.20	0.67
9:E:53:VAL:HG12	9:E:54:ALA:H	1.60	0.67
10:F:96:TRP:CZ3	10:F:134:PHE:HB2	2.28	0.67
19:A:1789:CLA:C4	16:L:64:LEU:CD2	2.71	0.67
3:3:94:ARG:CB	3:3:97:PHE:CE1	2.61	0.67
19:2:1217:CLA:C7	19:2:1217:CLA:CBB	2.58	0.67
19:2:1223:CLA:C4A	19:2:1223:CLA:CBA	2.73	0.67
7:C:12:ILE:HB	7:C:38:GLN:O	1.95	0.67
16:L:58:LEU:HD21	16:L:153:TRP:CZ2	2.30	0.67
19:A:1788:CLA:C16	23:L:1169:BCR:C36	2.72	0.67
5:A:204:ASN:O	5:A:205:HIS:CB	2.42	0.67
5:A:708:VAL:HA	5:A:711:HIS:HD2	1.59	0.67
19:B:1737:CLA:HBA2	19:B:1737:CLA:HBD	1.77	0.67
6:B:187:SER:O	6:B:189:ALA:N	2.28	0.67
6:B:374:HIS:HB2	19:B:1757:CLA:C4B	2.23	0.67
9:E:39:LEU:H	9:E:40:ARG:CZ	2.08	0.67
13:I:7:LEU:HD12	23:I:1032:BCR:C33	2.17	0.67
19:L:1168:CLA:CBC	19:L:1168:CLA:CHD	2.73	0.67
16:L:30:SER:OG	16:L:32:LEU:HB2	1.94	0.67
17:N:62:SER:CB	17:N:66:ASP:CA	2.66	0.67
2:2:168:ARG:HH21	2:2:171:MET:CB	2.08	0.67
14:J:4:PHE:O	14:J:5:LYS:HB2	1.93	0.67
20:A:1812:LMU:O1'	20:A:1812:LMU:H52	1.95	0.67
5:A:119:SER:HB2	5:A:136:VAL:HG21	1.76	0.67
4:4:94:GLU:HB3	4:4:95:PHE:CD1	2.27	0.66
16:L:8:TYR:HE1	16:L:11:ILE:HG23	1.59	0.66
17:N:46:PHE:O	17:N:47:THR:HG23	1.95	0.66
3:3:63:ARG:NH1	3:3:185:LYS:O	2.28	0.66
10:F:53:PHE:C	10:F:55:ASN:H	1.97	0.66
15:K:7:THR:HA	15:K:10:ILE:HB	1.78	0.66
19:4:1199:CLA:H2A	19:4:1199:CLA:O2A	1.94	0.66
19:A:1762:CLA:H12	19:A:1762:CLA:HED2	1.77	0.66
19:B:1737:CLA:C12	19:B:1737:CLA:OBD	2.43	0.66
6:B:194:LEU:O	6:B:199:ILE:HG13	1.96	0.66
6:B:266:GLN:O	6:B:267:SER:CB	2.41	0.66
11:G:43:HIS:ND1	11:G:43:HIS:O	2.28	0.66
19:L:1168:CLA:HAA1	19:L:1168:CLA:O1D	1.96	0.66
19:4:1205:CLA:HED2	19:4:1205:CLA:CHA	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:50:GLN:HA	17:N:51:ASP:O	1.96	0.66
20:A:7005:LMU:C4	20:A:7005:LMU:O1'	2.43	0.66
4:4:122:LYS:HB2	4:4:143:PHE:CG	2.27	0.66
4:4:95:PHE:CE2	19:4:1210:CLA:C1C	2.78	0.66
19:A:1764:CLA:H111	23:A:1806:BCR:C11	2.25	0.66
5:A:451:ILE:CD1	19:A:1788:CLA:HED1	2.25	0.66
5:A:443:ILE:HD11	5:A:557:LEU:HG	1.77	0.66
5:A:713:LYS:NZ	19:B:1761:CLA:H41	2.10	0.66
6:B:350:GLN:OE1	19:B:1767:CLA:HBB2	1.95	0.66
16:L:66:GLY:N	16:L:67:PRO:HD2	2.10	0.66
3:3:94:ARG:CZ	3:3:98:ILE:CG2	2.73	0.66
16:L:163:LEU:CD1	16:L:165:TYR:CE1	2.78	0.66
3:3:47:GLY:O	3:3:49:ILE:N	2.27	0.66
3:3:106:TYR:CG	3:3:107:TRP:CD1	2.84	0.66
2:2:205:PHE:HD1	2:2:206:ALA:H	1.42	0.66
16:L:118:LEU:CD1	16:L:119:THR:H	2.07	0.66
19:A:1783:CLA:C10	23:A:1805:BCR:H372	2.25	0.66
5:A:700:TRP:CZ3	19:A:1815:CLA:O1D	2.48	0.66
5:A:398:HIS:CD2	19:A:1783:CLA:ND	2.64	0.66
6:B:167:TRP:CD1	11:G:41:MET:CE	2.78	0.66
23:B:1774:BCR:H343	11:G:21:PHE:CD1	2.30	0.66
6:B:596:TRP:NE1	6:B:623:TYR:HB2	2.10	0.66
6:B:707:LEU:O	6:B:710:LEU:HB3	1.94	0.66
18:R:38:UNK:C	18:R:39:UNK:O	2.42	0.66
15:K:79:LYS:HE3	15:K:84:LEU:C	2.13	0.66
19:1:1142:CLA:HED2	19:1:1143:CLA:CMB	2.26	0.66
5:A:527:VAL:CG1	5:A:528:ALA:H	2.08	0.66
19:4:1196:CLA:HHD	19:4:1196:CLA:CBC	2.21	0.66
5:A:210:LEU:HD13	19:A:1769:CLA:HHB	1.77	0.66
19:A:1800:CLA:H141	16:L:95:LEU:HD22	1.76	0.66
5:A:604:TRP:HE1	19:A:1817:CLA:C1D	2.07	0.66
23:B:1779:BCR:C27	23:B:1779:BCR:H403	2.20	0.66
9:E:88:GLU:O	9:E:90:VAL:N	2.28	0.66
4:4:75:TRP:CD1	19:4:1205:CLA:CHD	2.78	0.66
16:L:126:GLN:N	16:L:127:PRO:HD2	2.11	0.66
16:L:43:TYR:O	16:L:44:ARG:HB2	1.94	0.66
6:B:300:SER:HB3	11:G:52:LYS:CB	2.26	0.66
19:A:1776:CLA:HMD1	19:A:1777:CLA:HHD	1.77	0.66
5:A:401:TRP:O	5:A:405:PHE:HB2	1.95	0.66
17:N:63:ASP:CA	17:N:64:ASP:C	2.63	0.66
4:4:35:GLU:HB3	4:4:36:ASN:CB	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:98:GLU:HG3	2:2:99:LEU:CD1	2.25	0.66
6:B:331:HIS:CE1	6:B:392:ILE:HG21	2.30	0.66
5:A:621:GLN:HG2	5:A:637:ILE:HD12	1.77	0.66
6:B:729:THR:O	6:B:729:THR:HG22	1.96	0.66
6:B:689:ASN:OD1	6:B:689:ASN:N	2.29	0.66
5:A:744:ALA:HB2	23:A:1805:BCR:H391	0.79	0.66
6:B:424:TRP:HZ3	19:B:1769:CLA:HBC3	1.61	0.66
6:B:560:ASP:O	25:B:1783:SF4:S3	2.53	0.66
9:E:39:LEU:C	9:E:40:ARG:HD3	2.15	0.66
17:N:63:ASP:H	17:N:64:ASP:CA	2.08	0.66
4:4:172:VAL:O	4:4:173:THR:HG22	1.95	0.66
11:G:13:GLY:CA	11:G:16:LEU:HG	2.25	0.66
20:A:7032:LMU:H1B	20:A:7032:LMU:H31	1.77	0.66
5:A:631:GLN:HG3	5:A:631:GLN:O	1.96	0.66
5:A:133:ASN:ND2	5:A:142:GLY:HA2	2.11	0.66
19:B:1737:CLA:H151	19:B:1743:CLA:OBD	1.96	0.66
19:B:1737:CLA:H43	23:B:1775:BCR:H331	1.78	0.66
19:B:1765:CLA:CBB	23:B:1777:BCR:H281	2.26	0.66
19:A:1787:CLA:OBD	16:L:27:VAL:HB	1.96	0.66
17:N:83:TRP:O	17:N:83:TRP:HE3	1.77	0.66
5:A:25:ASP:OD2	5:A:26:PRO:N	2.29	0.66
19:3:1217:CLA:HAC1	19:3:1218:CLA:C7	2.25	0.66
4:4:144:ALA:C	4:4:145:PRO:O	2.29	0.66
20:A:7032:LMU:H2B	20:A:7032:LMU:H31	1.77	0.66
20:A:7005:LMU:H11	20:A:7005:LMU:O2'	1.95	0.66
10:F:94:ALA:HA	10:F:97:ILE:HG12	1.76	0.66
19:A:1777:CLA:CAD	19:A:1778:CLA:HMA1	2.26	0.66
5:A:201:SER:O	5:A:204:ASN:HB2	1.95	0.66
5:A:443:ILE:HG21	5:A:558:LYS:HB2	1.77	0.66
5:A:747:TRP:CE3	23:A:1805:BCR:H401	2.31	0.66
6:B:375:HIS:HE1	19:B:1758:CLA:NC	1.94	0.66
9:E:44:TYR:CG	9:E:73:ASN:HB2	2.31	0.66
5:A:24:ARG:NH1	5:A:28:LYS:O	2.29	0.66
19:2:1215:CLA:C2	19:2:1217:CLA:HMD3	2.21	0.66
20:A:7013:LMU:H51	20:A:7049:LMU:C1	2.25	0.66
5:A:103:PHE:HE1	19:A:1763:CLA:O1D	1.79	0.66
5:A:96:MET:HE2	19:A:1763:CLA:HBB2	1.78	0.66
5:A:375:HIS:CE1	19:A:1782:CLA:NC	2.64	0.66
5:A:239:PRO:HA	5:A:242:ILE:HD13	1.76	0.66
5:A:78:VAL:O	5:A:82:HIS:HB2	1.96	0.66
19:A:1765:CLA:HBB2	19:B:1763:CLA:CMD	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1773:PQN:H2M1	22:B:1773:PQN:H142	1.77	0.66
6:B:292:ARG:O	6:B:293:THR:OG1	2.14	0.66
13:I:12:VAL:HG21	19:I:1031:CLA:O1A	1.96	0.66
4:4:75:TRP:HD1	19:4:1205:CLA:CHD	2.09	0.66
17:N:59:PRO:HA	17:N:66:ASP:OD1	1.96	0.66
12:H:44:ALA:HB2	16:L:145:PHE:CE1	2.30	0.66
20:A:7023:LMU:H6'2	20:A:7023:LMU:H2B	1.78	0.66
4:4:154:ILE:CG1	4:4:155:ALA:H	2.08	0.65
4:4:160:MET:CE	19:4:1201:CLA:CAB	2.72	0.65
19:A:1763:CLA:HAA2	19:A:1765:CLA:CED	2.25	0.65
5:A:545:HIS:ND1	19:A:1792:CLA:HBB2	2.10	0.65
5:A:399:HIS:O	5:A:400:MET:HB2	1.94	0.65
6:B:38:THR:OG1	6:B:41:ARG:HB2	1.95	0.65
6:B:353:TYR:CD2	6:B:594:TRP:CZ3	2.83	0.65
19:A:1814:CLA:C1	6:B:616:LEU:HG	2.25	0.65
9:E:44:TYR:CD1	9:E:73:ASN:HB2	2.31	0.65
17:N:68:GLU:O	17:N:69:CYS:HB2	1.96	0.65
5:A:22:VAL:C	5:A:23:ASP:O	2.29	0.65
3:3:52:LYS:O	3:3:56:TYR:CG	2.49	0.65
17:N:11:LYS:HG2	17:N:12:THR:H	1.61	0.65
4:4:121:PHE:HZ	4:4:125:SER:O	1.79	0.65
4:4:149:ALA:HB3	4:4:151:GLU:CD	2.17	0.65
4:4:91:PHE:HD2	4:4:91:PHE:C	1.99	0.65
4:4:99:HIS:HE1	4:4:103:ILE:HD12	1.59	0.65
19:A:1787:CLA:H52	19:A:1801:CLA:CHB	2.25	0.65
19:B:1735:CLA:CBC	23:B:1778:BCR:H332	2.26	0.65
6:B:267:SER:HA	6:B:356:PRO:O	1.96	0.65
7:C:1:MET:CE	8:D:154:TYR:OH	2.43	0.65
7:C:2:SER:O	7:C:69:LEU:HB2	1.96	0.65
11:G:28:ARG:HA	19:G:1099:CLA:HMA3	1.77	0.65
4:4:73:PRO:O	4:4:74:LYS:CB	2.44	0.65
4:4:75:TRP:CZ3	4:4:76:TYR:HB3	2.30	0.65
3:3:92:TRP:O	3:3:95:THR:N	2.29	0.65
8:D:49:THR:HG22	8:D:99:GLN:HB3	1.78	0.65
3:3:163:PHE:C	3:3:163:PHE:HD1	1.99	0.65
10:F:116:GLN:C	10:F:118:GLU:H	2.00	0.65
19:A:1817:CLA:CMC	6:B:661:PHE:CB	2.74	0.65
5:A:217:SER:OG	23:A:1803:BCR:C16	2.44	0.65
6:B:91:ILE:HD12	6:B:104:PHE:CE2	2.31	0.65
8:D:31:GLY:HA3	16:L:23:LEU:HD21	1.77	0.65
17:N:57:LYS:O	17:N:60:PHE:CD1	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:1213:CLA:H41	19:2:1213:CLA:CHD	2.25	0.65
5:A:328:LYS:HE2	5:A:332:GLU:CG	2.26	0.65
20:R:1056:LMU:O6'	20:R:1056:LMU:H1'	1.96	0.65
19:J:1043:CLA:HED3	19:J:1043:CLA:CHA	2.26	0.65
20:A:7031:LMU:O2'	20:A:7031:LMU:H11	1.91	0.65
4:4:106:TRP:CG	19:4:1196:CLA:CED	2.68	0.65
19:A:1783:CLA:C17	23:A:1806:BCR:H15C	2.24	0.65
19:A:1787:CLA:H12	6:B:686:PRO:HG2	1.77	0.65
5:A:259:TYR:CD2	5:A:280:PHE:HA	2.32	0.65
5:A:401:TRP:HB3	19:A:1783:CLA:HMC3	1.77	0.65
5:A:599:PHE:CD2	5:A:735:VAL:HG21	2.31	0.65
9:E:83:ALA:O	9:E:86:GLU:CG	2.44	0.65
11:G:42:SER:OG	11:G:46:ALA:N	2.30	0.65
11:G:43:HIS:O	11:G:45:GLU:N	2.29	0.65
16:L:163:LEU:CD1	16:L:165:TYR:CD1	2.79	0.65
19:1:1190:CLA:CED	19:1:1190:CLA:C2A	2.73	0.65
2:2:171:MET:SD	2:2:172:LEU:HG	2.36	0.65
3:3:107:TRP:CD1	3:3:108:ALA:HA	2.32	0.65
20:A:7013:LMU:H91	20:A:7049:LMU:H4'	1.78	0.65
20:A:7037:LMU:H72	20:A:7037:LMU:C3	2.11	0.65
20:A:7041:LMU:H6'2	20:A:7042:LMU:H21	1.79	0.65
1:1:179:THR:CG2	4:4:87:SER:CB	2.71	0.65
19:A:1788:CLA:O1A	19:A:1800:CLA:H11	1.96	0.65
5:A:452:PHE:CE1	19:A:1793:CLA:CBB	2.67	0.65
6:B:65:LEU:HD22	6:B:124:TRP:CE3	2.31	0.65
6:B:415:LYS:HE3	6:B:539:LEU:O	1.96	0.65
7:C:74:THR:C	7:C:76:SER:N	2.47	0.65
10:F:2:ILE:HG22	10:F:3:ALA:N	2.11	0.65
16:L:36:TYR:OH	19:L:1167:CLA:HBA2	1.97	0.65
19:4:1205:CLA:H2A	19:4:1205:CLA:HED3	1.79	0.65
17:N:63:ASP:H	17:N:65:LEU:N	1.93	0.65
18:R:34:UNK:C	18:R:36:UNK:O	2.45	0.65
19:J:1043:CLA:HED3	19:J:1043:CLA:C1A	2.27	0.65
5:A:628:ILE:HG13	5:A:632:GLY:HA2	1.77	0.65
6:B:489:GLY:O	6:B:490:ARG:HG2	1.95	0.65
5:A:203:LEU:H	5:A:203:LEU:HD12	1.60	0.65
5:A:81:ALA:HB2	19:A:1760:CLA:HMA2	1.74	0.65
5:A:737:HIS:HA	5:A:740:LEU:HD23	1.78	0.65
5:A:80:SER:O	5:A:83:PHE:HB2	1.96	0.65
6:B:275:HIS:ND1	19:B:1747:CLA:HMB1	2.12	0.65
19:B:1768:CLA:H61	23:B:1779:BCR:H323	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:81:PRO:HG2	6:B:360:PHE:CD1	2.32	0.65
7:C:55:GLU:C	7:C:57:ALA:H	2.00	0.65
8:D:102:ARG:NH1	8:D:104:PHE:CD1	2.64	0.65
18:R:49:UNK:O	18:R:51:UNK:N	2.30	0.65
10:F:15:ALA:O	10:F:18:GLU:HB2	1.97	0.65
5:A:370:ILE:HD12	19:A:1781:CLA:O1D	1.96	0.65
5:A:393:LEU:HG	5:A:394:SER:H	1.62	0.65
5:A:432:LEU:HA	5:A:435:VAL:HG13	1.79	0.65
19:B:1752:CLA:O1A	11:G:54:TYR:OH	2.13	0.65
6:B:293:THR:C	6:B:294:ASN:ND2	2.50	0.65
5:A:709:TRP:CH2	6:B:417:ALA:HB2	2.31	0.65
6:B:602:TRP:O	6:B:604:GLY:N	2.24	0.65
3:3:94:ARG:NH1	3:3:97:PHE:CZ	2.63	0.65
17:N:80:ASN:OD1	17:N:82:PHE:HA	1.96	0.65
3:3:198:PHE:HA	3:3:201:ALA:CB	2.18	0.65
20:2:1224:LMU:C1	20:2:1224:LMU:C6	2.75	0.65
19:3:1222:CLA:CBC	19:3:1222:CLA:HMC1	2.26	0.65
6:B:167:TRP:HD1	11:G:41:MET:HE3	1.60	0.65
19:A:1788:CLA:H161	23:L:1169:BCR:H362	1.78	0.65
5:A:29:THR:O	5:A:29:THR:HG23	1.95	0.65
15:K:44:GLU:CD	15:K:45:SER:O	2.35	0.65
17:N:32:ALA:HB1	17:N:35:VAL:CG2	2.21	0.65
20:A:1810:LMU:O6'	20:A:1812:LMU:O3B	2.10	0.65
5:A:747:TRP:CD2	23:A:1805:BCR:C40	2.80	0.65
19:B:1750:CLA:NB	19:B:1750:CLA:H2	2.12	0.65
23:A:1805:BCR:HC31	23:B:1778:BCR:H17C	1.78	0.65
6:B:697:PRO:CB	19:B:1770:CLA:HBC3	2.27	0.65
17:N:60:PHE:CA	17:N:61:LEU:O	2.44	0.65
17:N:70:GLU:HB3	17:N:72:LYS:N	2.12	0.65
19:2:1213:CLA:H43	19:2:1213:CLA:CHD	2.23	0.65
12:H:32:TYR:OH	16:L:44:ARG:NE	2.25	0.65
5:A:129:GLN:O	5:A:130:GLU:HB2	1.94	0.65
19:A:1800:CLA:H201	16:L:64:LEU:HD21	1.77	0.65
19:A:1814:CLA:HMB3	19:B:1784:CLA:C18	2.26	0.65
5:A:691:MET:HB2	19:A:1815:CLA:C1C	2.27	0.65
5:A:693:LEU:HD21	5:A:735:VAL:H	1.62	0.65
23:B:1777:BCR:C23	23:B:1777:BCR:H382	2.24	0.65
19:A:1817:CLA:HMC1	6:B:661:PHE:HB2	1.74	0.65
19:A:1795:CLA:H43	10:F:121:ILE:HG21	1.79	0.65
10:F:2:ILE:HG22	10:F:3:ALA:H	1.62	0.65
4:4:37:LEU:O	4:4:39:TRP:CB	2.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1197:CLA:HAA2	19:1:1197:CLA:CGD	2.26	0.65
19:1:1143:CLA:HBC1	20:A:7001:LMU:C3B	2.27	0.65
20:A:7038:LMU:H101	20:A:7038:LMU:C6	2.26	0.65
6:B:454:LEU:CD1	10:F:69:PRO:O	2.45	0.65
12:H:53:LEU:CG	12:H:54:LEU:H	2.09	0.65
19:A:1772:CLA:HBA2	19:A:1772:CLA:C2	2.25	0.64
19:A:1790:CLA:OBD	19:A:1791:CLA:HAC1	1.97	0.64
5:A:355:HIS:ND1	5:A:416:ILE:CG2	2.60	0.64
19:B:1755:CLA:CBC	19:B:1755:CLA:CHD	2.73	0.64
19:B:1764:CLA:CGA	19:B:1765:CLA:HMB3	2.26	0.64
19:B:1768:CLA:HMA1	19:B:1769:CLA:HED1	1.78	0.64
18:R:34:UNK:N	18:R:36:UNK:C	2.57	0.64
8:D:78:ALA:CB	8:D:82:GLN:HE22	2.02	0.64
19:A:1789:CLA:H41	16:L:64:LEU:CD2	2.25	0.64
5:A:221:HIS:CE1	19:A:1770:CLA:C4A	2.81	0.64
6:B:273:VAL:O	6:B:277:HIS:HD2	1.80	0.64
16:L:99:LEU:CD1	23:L:1169:BCR:HC7	2.27	0.64
16:L:164:PRO:HB3	16:L:165:TYR:CD1	2.15	0.64
12:H:25:GLY:HA3	12:H:27:ASP:OD2	1.97	0.64
5:A:426:THR:HA	5:A:428:TYR:CE2	2.32	0.64
6:B:398:TYR:HD1	6:B:542:ARG:NH2	1.94	0.64
6:B:16:PRO:CG	7:C:74:THR:HB	2.28	0.64
16:L:10:VAL:O	16:L:10:VAL:HG22	1.97	0.64
19:4:1205:CLA:CED	19:4:1205:CLA:CHA	2.75	0.64
4:4:75:TRP:CD1	19:4:1205:CLA:HMD3	2.32	0.64
3:3:94:ARG:NH1	3:3:97:PHE:CG	2.65	0.64
17:N:63:ASP:N	17:N:65:LEU:N	2.46	0.64
4:4:40:PHE:O	4:4:43:ALA:HB3	1.98	0.64
12:H:19:GLY:O	12:H:20:GLN:HB2	1.98	0.64
19:J:1043:CLA:O1A	19:J:1043:CLA:C15	2.45	0.64
16:L:115:ALA:N	16:L:116:PRO:HD2	2.12	0.64
5:A:396:PHE:HE2	5:A:616:PHE:CB	2.10	0.64
6:B:154:TRP:HD1	6:B:158:GLN:HG2	1.61	0.64
5:A:207:LEU:HB2	19:A:1776:CLA:HBB2	1.79	0.64
5:A:553:VAL:H	5:A:556:LEU:HD12	1.62	0.64
5:A:54:ILE:O	5:A:58:HIS:CD2	2.50	0.64
5:A:90:PHE:CE1	19:A:1761:CLA:H91	2.32	0.64
5:A:98:PHE:O	5:A:99:HIS:HB2	1.96	0.64
19:B:1746:CLA:HED2	19:B:1746:CLA:HBA2	1.79	0.64
21:B:8055:SUC:H1'1	21:B:8055:SUC:O2	1.97	0.64
23:A:1805:BCR:H322	23:A:1806:BCR:H391	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1739:CLA:CMC	23:B:1780:BCR:H281	2.25	0.64
6:B:521:HIS:CE1	19:B:1768:CLA:NA	2.63	0.64
6:B:190:TRP:HE3	19:B:1744:CLA:HBB2	1.61	0.64
6:B:127:ILE:CD1	6:B:198:ALA:HB2	2.26	0.64
9:E:39:LEU:O	9:E:40:ARG:HD3	1.97	0.64
11:G:13:GLY:O	11:G:16:LEU:HB2	1.96	0.64
10:F:26:GLN:CA	10:F:26:GLN:OE1	2.39	0.64
8:D:102:ARG:NE	8:D:110:GLN:HB2	2.10	0.64
5:A:373:ALA:HB1	5:A:396:PHE:CD1	2.31	0.64
5:A:479:ASP:HA	5:A:536:THR:HG23	1.80	0.64
19:A:1770:CLA:HHC	23:A:1803:BCR:C17	2.13	0.64
23:A:1804:BCR:H23C	23:A:1804:BCR:C38	2.25	0.64
5:A:547:PHE:HE2	19:A:1817:CLA:O1A	1.81	0.64
19:B:1745:CLA:OBD	19:B:1745:CLA:O2D	2.12	0.64
17:N:72:LYS:HZ3	17:N:74:LYS:HE3	1.61	0.64
5:A:269:PHE:CD1	15:K:14:THR:HG21	2.32	0.64
2:2:95:PHE:HA	2:2:98:GLU:HG2	1.80	0.64
2:2:44:ASN:ND2	14:J:1:MET:SD	2.71	0.64
12:H:25:GLY:C	12:H:27:ASP:N	2.49	0.64
5:A:466:THR:O	5:A:470:LEU:HG	1.97	0.64
19:B:1768:CLA:C16	23:B:1779:BCR:C31	2.76	0.64
7:C:5:VAL:HB	7:C:65:VAL:CA	2.27	0.64
13:I:10:PRO:HA	13:I:14:LEU:HB2	1.79	0.64
19:1:1187:CLA:HBC3	19:1:1187:CLA:CMC	2.25	0.64
12:H:14:ILE:HG13	12:H:17:THR:OG1	1.97	0.64
6:B:160:LYS:HE3	6:B:161:TRP:CD2	2.33	0.64
20:A:7031:LMU:O2B	20:A:7031:LMU:H6E	1.97	0.64
19:A:1759:CLA:HMB1	19:A:1767:CLA:H18	1.80	0.64
19:A:1783:CLA:H43	19:A:1783:CLA:CBA	2.27	0.64
5:A:729:GLN:HE21	19:A:1796:CLA:HMD1	1.62	0.64
5:A:298:ASP:OD2	5:A:298:ASP:N	2.31	0.64
5:A:618:TRP:CZ2	5:A:655:ASP:HB2	2.32	0.64
23:B:1777:BCR:H321	23:B:1777:BCR:HC8	1.80	0.64
6:B:422:LEU:CD1	6:B:535:VAL:HG11	2.22	0.64
6:B:693:TRP:CD1	19:B:1770:CLA:C2D	2.80	0.64
10:F:83:PHE:O	10:F:87:GLY:CA	2.45	0.64
23:A:1808:BCR:H333	19:L:1167:CLA:C1C	2.28	0.64
16:L:64:LEU:HD22	16:L:91:LEU:HD22	1.80	0.64
4:4:38:ARG:HG3	4:4:39:TRP:H	1.63	0.64
18:R:34:UNK:N	18:R:36:UNK:O	2.30	0.64
10:F:23:LYS:HB2	10:F:24:LYS:NZ	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1148:CLA:O1A	19:1:1148:CLA:C2	2.45	0.64
6:B:5:ILE:CB	6:B:6:PRO:HD2	2.23	0.64
10:F:147:GLY:HA2	10:F:150:VAL:HB	1.80	0.64
5:A:103:PHE:N	5:A:103:PHE:HD2	1.95	0.64
19:A:1797:CLA:CGD	19:A:1797:CLA:HAA2	2.28	0.64
19:A:1783:CLA:H172	23:A:1806:BCR:H17C	1.79	0.64
19:B:1764:CLA:HMB3	19:B:1767:CLA:HED3	1.80	0.64
6:B:127:ILE:HG12	6:B:193:HIS:HE1	1.63	0.64
5:A:316:MET:CG	5:A:317:TYR:HD1	1.99	0.64
2:2:196:HIS:HE1	21:2:1225:SUC:O3	1.74	0.64
1:1:44:LEU:HD22	1:1:154:ALA:HB3	1.79	0.64
6:B:409:ALA:C	6:B:411:MET:H	2.01	0.64
1:1:184:PRO:CA	1:1:185:TRP:CD1	2.81	0.64
4:4:122:LYS:CD	4:4:150:LYS:HD2	2.14	0.64
19:H:1080:CLA:C3C	23:I:1032:BCR:HC21	2.27	0.64
16:L:66:GLY:HA3	19:L:1168:CLA:HHC	1.78	0.64
17:N:61:LEU:CD1	17:N:63:ASP:HB2	2.28	0.64
19:2:1215:CLA:H2	19:2:1217:CLA:CMD	2.23	0.64
2:2:44:ASN:C	2:2:46:GLN:N	2.51	0.64
8:D:126:GLY:C	8:D:127:ARG:HG2	2.17	0.64
2:2:79:TRP:CD1	2:2:81:THR:HG21	2.32	0.64
4:4:95:PHE:CD2	19:4:1210:CLA:C2C	2.79	0.63
19:A:1785:CLA:H101	19:A:1785:CLA:H152	1.80	0.63
19:A:1801:CLA:HED1	16:L:32:LEU:HD13	1.78	0.63
5:A:361:ASN:HD22	5:A:362:LEU:N	1.96	0.63
19:B:1736:CLA:HBC3	19:B:1759:CLA:H51	1.80	0.63
7:C:52:LYS:O	7:C:52:LYS:CG	2.46	0.63
9:E:86:GLU:CG	9:E:87:VAL:N	2.42	0.63
19:A:1800:CLA:C20	16:L:64:LEU:HD21	2.27	0.63
4:4:70:ILE:C	4:4:72:VAL:H	2.00	0.63
4:4:75:TRP:CD1	19:4:1205:CLA:C1D	2.80	0.63
11:G:16:LEU:HA	11:G:68:ILE:HG13	1.79	0.63
5:A:328:LYS:O	5:A:330:ILE:N	2.31	0.63
20:A:7042:LMU:H32	20:A:7042:LMU:C5'	2.28	0.63
6:B:341:LEU:O	6:B:345:THR:OG1	2.10	0.63
4:4:121:PHE:O	4:4:143:PHE:HD2	1.81	0.63
5:A:123:VAL:O	5:A:124:TRP:HB2	1.98	0.63
19:A:1779:CLA:CAB	23:A:1804:BCR:H351	2.28	0.63
19:A:1817:CLA:HMB3	19:B:1771:CLA:HMC3	1.80	0.63
5:A:606:TYR:O	5:A:610:SER:CB	2.46	0.63
6:B:304:ILE:HG22	19:B:1752:CLA:CGD	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1788:CLA:C16	23:L:1169:BCR:H362	2.28	0.63
4:4:171:ASN:C	4:4:173:THR:H	2.01	0.63
3:3:106:TYR:HB3	3:3:107:TRP:CD1	2.32	0.63
3:3:163:PHE:C	3:3:163:PHE:CD1	2.72	0.63
5:A:374:GLN:O	5:A:377:TYR:HD2	1.81	0.63
5:A:485:GLN:O	5:A:487:VAL:N	2.31	0.63
5:A:346:LEU:HD11	19:A:1779:CLA:CHD	2.29	0.63
7:C:62:PHE:HE2	9:E:42:GLU:OE1	1.78	0.63
2:2:97:VAL:HA	2:2:100:VAL:HG13	1.79	0.63
4:4:170:HIS:C	4:4:171:ASN:O	2.37	0.63
19:2:1223:CLA:CHD	19:2:1223:CLA:HBC3	2.28	0.63
6:B:456:GLU:OE1	10:F:70:HIS:ND1	2.30	0.63
6:B:426:SER:O	6:B:430:GLY:N	2.31	0.63
6:B:269:TRP:CB	6:B:497:TRP:HH2	2.03	0.63
8:D:31:GLY:HA2	16:L:13:PRO:CB	2.28	0.63
4:4:75:TRP:CD1	19:4:1205:CLA:C2D	2.82	0.63
19:1:1190:CLA:HMC3	19:1:1196:CLA:CAC	2.28	0.63
2:2:56:MET:SD	2:2:169:LEU:HA	2.38	0.63
4:4:192:THR:C	4:4:193:ILE:O	2.34	0.63
5:A:582:ASP:HB3	5:A:589:THR:HG22	1.80	0.63
19:A:1776:CLA:HAA2	19:A:1780:CLA:HBB2	1.78	0.63
5:A:257:GLN:O	5:A:258:LEU:HB2	1.98	0.63
6:B:510:LEU:HD22	6:B:510:LEU:H	1.62	0.63
5:A:680:LEU:CD2	6:B:617:MET:HB2	2.29	0.63
3:3:97:PHE:O	3:3:98:ILE:HG22	1.97	0.63
16:L:163:LEU:CD1	16:L:165:TYR:CD2	2.82	0.63
16:L:163:LEU:CD1	16:L:165:TYR:CZ	2.80	0.63
3:3:50:GLU:N	3:3:51:PRO:HD3	2.13	0.63
19:2:1217:CLA:O1D	19:2:1217:CLA:H2A	1.99	0.63
10:F:125:LEU:O	10:F:126:ALA:CB	2.46	0.63
7:C:31:TRP:CB	7:C:39:ILE:HG21	2.27	0.63
8:D:111:TYR:HD2	8:D:114:PRO:CB	2.10	0.63
4:4:103:ILE:HG13	19:4:1197:CLA:CMD	2.28	0.63
4:4:118:ASP:N	4:4:118:ASP:OD1	2.31	0.63
19:A:1773:CLA:HBC3	19:A:1773:CLA:HMC1	1.80	0.63
19:A:1776:CLA:CBC	19:A:1776:CLA:HMC1	2.28	0.63
5:A:458:PHE:CD2	19:A:1816:CLA:HMB2	2.33	0.63
5:A:361:ASN:HD21	19:A:1761:CLA:CED	2.11	0.63
5:A:706:SER:HB3	6:B:419:ILE:O	1.98	0.63
6:B:130:ARG:O	6:B:135:LEU:HD23	1.98	0.63
7:C:1:MET:N	7:C:3:HIS:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:1079:CLA:CGA	19:H:1079:CLA:C3A	2.76	0.63
13:I:24:LEU:C	13:I:26:LEU:N	2.50	0.63
19:A:1800:CLA:H92	23:L:1169:BCR:H321	1.78	0.63
6:B:404:ALA:C	6:B:406:ASN:N	2.51	0.63
8:D:47:VAL:HB	8:D:76:LYS:HA	1.81	0.63
3:3:180:LYS:HB2	3:3:181:LEU:HB2	1.81	0.63
10:F:20:GLN:CD	10:F:21:ALA:N	2.51	0.63
20:2:1224:LMU:H22	20:2:1224:LMU:C6	2.20	0.63
20:A:7034:LMU:C2B	20:A:7034:LMU:H5'	2.18	0.63
19:A:1774:CLA:O1A	19:A:1784:CLA:HMD1	1.99	0.63
19:A:1786:CLA:HMB2	19:A:1787:CLA:C1D	2.28	0.63
5:A:221:HIS:CE1	19:A:1770:CLA:NA	2.66	0.63
5:A:544:ILE:HD11	19:A:1813:CLA:H193	1.80	0.63
6:B:353:TYR:O	6:B:354:SER:OG	2.15	0.63
7:C:62:PHE:CE2	8:D:137:ILE:HB	2.34	0.63
6:B:545:LYS:CG	9:E:74:TYR:HE2	2.12	0.63
4:4:36:ASN:CB	4:4:39:TRP:CD2	2.81	0.63
19:2:2006:CLA:HBC2	19:2:2006:CLA:HHD	1.81	0.63
8:D:79:ARG:O	8:D:82:GLN:HB2	1.97	0.63
19:2:1213:CLA:O1A	19:2:1213:CLA:C4A	2.47	0.63
5:A:328:LYS:HE2	5:A:332:GLU:HG3	1.80	0.63
20:A:7042:LMU:H32	20:A:7042:LMU:O5'	1.99	0.63
2:2:43:TRP:C	2:2:45:VAL:H	2.01	0.63
4:4:122:LYS:HD3	4:4:150:LYS:CE	2.29	0.63
19:A:1764:CLA:HBB2	19:A:1765:CLA:C4D	2.29	0.63
19:A:1781:CLA:H2	19:A:1782:CLA:CED	2.28	0.63
6:B:141:PHE:HA	6:B:144:PHE:CD1	2.34	0.63
6:B:337:ALA:HA	19:B:1754:CLA:HAA1	1.81	0.63
10:F:76:ASP:O	10:F:78:ARG:N	2.32	0.63
11:G:48:ASP:H	11:G:49:THR:HG22	1.64	0.63
17:N:56:LYS:O	17:N:60:PHE:CD1	2.50	0.63
5:A:316:MET:CA	5:A:317:TYR:HD1	2.11	0.63
20:A:7020:LMU:C6'	20:A:7020:LMU:C5B	2.61	0.63
1:1:179:THR:HG21	4:4:87:SER:CA	2.27	0.63
5:A:464:ASN:HD22	5:A:464:ASN:H	1.45	0.63
6:B:14:GLN:H	6:B:14:GLN:HE21	1.47	0.63
19:A:1777:CLA:H2A	19:A:1777:CLA:O1D	1.99	0.63
19:A:1781:CLA:HED3	19:A:1782:CLA:CMD	2.28	0.63
5:A:368:LEU:CD1	19:A:1782:CLA:H61	2.28	0.63
5:A:39:HIS:O	5:A:40:PHE:HB3	1.98	0.63
6:B:174:ARG:HB2	19:B:1743:CLA:HBC3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1753:CLA:C15	19:B:1753:CLA:H102	2.22	0.63
19:B:1768:CLA:HMA2	19:B:1769:CLA:HED1	1.79	0.63
3:3:92:TRP:HB2	3:3:95:THR:OG1	1.98	0.63
5:A:24:ARG:HH12	5:A:29:THR:CB	2.12	0.63
4:4:39:TRP:O	4:4:40:PHE:HD1	1.72	0.63
2:2:103:GLY:HA2	19:2:1221:CLA:CBB	2.29	0.63
6:B:302:LYS:O	6:B:303:TYR:CB	2.41	0.63
20:A:7013:LMU:H5B	20:A:7049:LMU:H3B	1.81	0.63
20:A:7033:LMU:H3'	20:A:7033:LMU:O5B	1.98	0.63
5:A:514:THR:O	5:A:531:PRO:O	2.16	0.63
4:4:101:VAL:HG13	4:4:104:ARG:HH21	1.60	0.62
19:4:1196:CLA:OBD	19:4:1196:CLA:O2D	2.14	0.62
5:A:434:ARG:O	5:A:437:ARG:HB2	1.99	0.62
5:A:661:ALA:HA	5:A:664:VAL:HG13	1.81	0.62
19:B:1753:CLA:O2D	19:B:1753:CLA:C2A	2.47	0.62
22:B:1773:PQN:H291	24:B:1781:LMG:H201	1.80	0.62
6:B:711:VAL:HG22	24:B:1781:LMG:H391	1.80	0.62
6:B:711:VAL:HG12	6:B:711:VAL:O	1.96	0.62
6:B:732:LYS:CD	6:B:733:PHE:C	2.67	0.62
6:B:733:PHE:N	6:B:733:PHE:CD1	2.58	0.62
7:C:74:THR:HB	7:C:80:ALA:HB2	1.77	0.62
16:L:95:LEU:HD11	16:L:143:PHE:CZ	2.34	0.62
17:N:60:PHE:C	17:N:61:LEU:O	2.37	0.62
17:N:65:LEU:O	17:N:67:LEU:N	2.32	0.62
2:2:54:TRP:CE2	19:2:1221:CLA:O1D	2.52	0.62
8:D:111:TYR:CD2	8:D:114:PRO:HB3	2.33	0.62
5:A:636:HIS:C	5:A:638:THR:N	2.51	0.62
5:A:520:LEU:O	5:A:522:ALA:N	2.28	0.62
8:D:84:LEU:HD12	8:D:100:PHE:HZ	1.64	0.62
16:L:78:GLU:O	16:L:78:GLU:HG3	1.99	0.62
5:A:207:LEU:HD13	19:A:1776:CLA:HBB2	1.79	0.62
6:B:593:TYR:O	6:B:596:TRP:O	2.17	0.62
16:L:45:THR:HA	16:L:52:ARG:HH12	1.63	0.62
16:L:64:LEU:HA	16:L:67:PRO:CG	2.29	0.62
3:3:59:ILE:O	3:3:63:ARG:HG3	1.99	0.62
12:H:73:PRO:HG3	21:H:1082:SUC:C5'	2.09	0.62
20:A:7042:LMU:C2	20:A:7042:LMU:H71	2.28	0.62
5:A:527:VAL:HG12	5:A:528:ALA:N	2.14	0.62
4:4:81:GLU:O	4:4:82:GLU:CB	2.47	0.62
10:F:81:GLY:O	14:J:38:THR:HG23	1.98	0.62
19:4:1211:CLA:HBC3	19:4:1211:CLA:HHD	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1765:CLA:CBB	19:B:1763:CLA:CMD	2.77	0.62
5:A:708:VAL:HA	5:A:711:HIS:CD2	2.34	0.62
5:A:680:LEU:HD21	6:B:617:MET:HB2	1.81	0.62
2:2:211:LYS:HA	2:2:211:LYS:CE	2.28	0.62
5:A:173:VAL:HG23	5:A:174:PHE:HD1	1.64	0.62
5:A:385:LEU:O	5:A:386:ALA:CB	2.47	0.62
5:A:680:LEU:HD21	6:B:617:MET:HE3	1.80	0.62
6:B:493:TRP:CZ2	19:B:1765:CLA:CGA	2.82	0.62
6:B:178:HIS:C	6:B:180:SER:H	2.00	0.62
6:B:427:LEU:HB3	19:B:1762:CLA:HED1	1.81	0.62
11:G:44:PHE:CA	11:G:47:GLY:HA3	2.29	0.62
12:H:65:LEU:HD23	19:H:1079:CLA:H52	1.82	0.62
19:B:1771:CLA:H102	13:I:21:MET:SD	2.40	0.62
19:1:1197:CLA:HED2	19:1:1197:CLA:CAD	2.30	0.62
19:1:1142:CLA:HMD1	19:1:1143:CLA:C1A	2.29	0.62
7:C:29:ILE:CG2	8:D:126:GLY:HA2	2.29	0.62
19:A:1769:CLA:HBA1	19:A:1780:CLA:C4	2.28	0.62
5:A:229:ILE:O	5:A:229:ILE:HG22	1.98	0.62
5:A:237:VAL:HG21	5:A:242:ILE:HD12	1.81	0.62
5:A:453:LEU:HD13	5:A:547:PHE:HA	1.80	0.62
6:B:178:HIS:O	6:B:180:SER:N	2.32	0.62
6:B:293:THR:HG22	6:B:294:ASN:ND2	2.14	0.62
6:B:336:LEU:CD2	19:B:1754:CLA:HBB1	2.30	0.62
6:B:390:GLY:O	23:B:1777:BCR:HC42	2.00	0.62
23:A:1807:BCR:H321	19:H:1079:CLA:HMD3	1.82	0.62
16:L:95:LEU:HD13	23:L:1169:BCR:H312	1.81	0.62
3:3:94:ARG:O	3:3:95:THR:HG23	1.99	0.62
12:H:73:PRO:HD3	21:H:1082:SUC:C5'	2.28	0.62
2:2:210:PRO:O	2:2:211:LYS:HB2	1.99	0.62
10:F:24:LYS:C	10:F:26:GLN:N	2.49	0.62
20:A:7005:LMU:H41	20:A:7005:LMU:O1'	1.99	0.62
19:B:1766:CLA:O2A	19:B:1766:CLA:H3A	2.00	0.62
4:4:99:HIS:ND1	4:4:103:ILE:HD11	2.15	0.62
19:A:1779:CLA:C1D	23:A:1804:BCR:C19	2.77	0.62
5:A:286:GLY:C	5:A:287:LEU:HD22	2.19	0.62
6:B:203:ARG:HG2	6:B:204:GLY:H	1.65	0.62
6:B:269:TRP:CD1	6:B:497:TRP:CH2	2.87	0.62
23:I:1032:BCR:C29	23:L:1169:BCR:H281	2.30	0.62
3:3:93:PHE:HB2	3:3:94:ARG:O	2.00	0.62
17:N:62:SER:HA	17:N:64:ASP:HB3	1.82	0.62
4:4:36:ASN:O	4:4:39:TRP:CE3	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1190:CLA:CED	19:1:1190:CLA:CAA	2.73	0.62
12:H:23:VAL:O	12:H:23:VAL:CG1	2.47	0.62
11:G:60:SER:OG	11:G:63:PRO:HB2	1.99	0.62
6:B:715:VAL:O	6:B:719:PHE:N	2.31	0.62
6:B:503:GLU:HB3	6:B:507:SER:CB	2.30	0.62
6:B:689:ASN:O	6:B:691:ILE:N	2.31	0.62
19:1:1193:CLA:HAA2	19:1:1193:CLA:CGD	2.30	0.62
5:A:457:SER:O	5:A:544:ILE:HD13	1.99	0.62
6:B:58:PHE:HB2	6:B:146:SER:HB2	1.81	0.62
19:3:1217:CLA:HAC1	19:3:1218:CLA:H71	1.80	0.62
10:F:25:LEU:HD23	10:F:46:MET:HB3	1.78	0.62
20:A:7014:LMU:C1	20:A:7014:LMU:H62	2.24	0.62
10:F:42:ILE:C	10:F:43:LYS:HE3	2.20	0.62
5:A:193:LEU:HA	5:A:196:PHE:CE2	2.34	0.62
6:B:44:GLN:OE1	6:B:163:PRO:HB2	1.99	0.62
6:B:82:PHE:O	6:B:84:VAL:N	2.32	0.62
4:4:142:ASN:CA	4:4:150:LYS:HZ1	2.13	0.62
19:A:1763:CLA:C3B	23:A:1806:BCR:H333	2.29	0.62
19:A:1770:CLA:CHC	23:A:1803:BCR:H19C	2.26	0.62
5:A:340:GLY:O	5:A:343:HIS:N	2.32	0.62
5:A:58:HIS:CE1	19:A:1759:CLA:C4D	2.82	0.62
19:B:1742:CLA:H11	19:B:1742:CLA:H61	1.82	0.62
19:B:1761:CLA:HMC2	19:B:1769:CLA:HBC2	1.80	0.62
5:A:131:ILE:HG12	6:B:445:ALA:O	1.99	0.62
6:B:73:ASN:HB3	6:B:76:ALA:HB3	1.79	0.62
17:N:49:CYS:C	17:N:51:ASP:O	2.38	0.62
17:N:72:LYS:N	17:N:72:LYS:HD3	2.13	0.62
18:R:34:UNK:CB	18:R:35:UNK:C	2.77	0.62
2:2:98:GLU:HG3	2:2:99:LEU:CG	2.29	0.62
19:3:1221:CLA:C19	19:3:1221:CLA:H152	2.29	0.62
19:1:1308:CLA:CGD	19:1:1308:CLA:CGA	2.77	0.62
19:4:1199:CLA:H2	19:4:1199:CLA:HED1	1.82	0.62
19:B:1738:CLA:C4	24:B:1781:LMG:H321	2.30	0.62
7:C:1:MET:HB3	7:C:4:SER:HG	1.63	0.62
15:K:31:ASN:H	15:K:32:ARG:HH11	1.48	0.62
19:L:1167:CLA:HAC1	23:L:1169:BCR:H322	1.80	0.62
4:4:72:VAL:O	4:4:73:PRO:O	2.17	0.62
3:3:97:PHE:O	3:3:98:ILE:HG23	2.00	0.62
20:2:1224:LMU:H21	20:2:1224:LMU:C6'	2.24	0.62
11:G:67:ASN:HA	11:G:70:ASP:OD2	1.99	0.62
5:A:217:SER:CA	23:A:1803:BCR:H351	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:370:ILE:CD1	19:A:1781:CLA:O1D	2.48	0.62
5:A:707:ILE:C	5:A:711:HIS:CD2	2.73	0.62
5:A:710:ALA:CB	19:B:1735:CLA:HED2	2.30	0.62
5:A:64:PHE:HZ	5:A:77:LYS:CE	2.12	0.62
23:B:1779:BCR:H333	19:F:1156:CLA:HHB	1.81	0.62
6:B:464:GLN:OE1	6:B:469:LYS:HD3	1.99	0.62
9:E:35:LYS:NZ	9:E:89:GLU:OE2	2.33	0.62
23:I:1032:BCR:H322	23:I:1032:BCR:C4	2.30	0.62
3:3:94:ARG:NH1	3:3:98:ILE:CG2	2.63	0.62
5:A:490:GLN:HG2	16:L:166:TYR:CE1	2.35	0.62
16:L:163:LEU:CD1	16:L:165:TYR:CG	2.83	0.62
3:3:74:ALA:CA	19:3:1216:CLA:C2D	2.75	0.62
4:4:145:PRO:O	4:4:147:LEU:CA	2.47	0.62
19:I:1192:CLA:H61	19:I:1192:CLA:H122	1.82	0.62
6:B:694:ARG:HE	16:L:105:ALA:HA	1.64	0.62
17:N:34:THR:OG1	17:N:36:GLU:HB3	1.99	0.62
3:3:62:GLY:HA2	3:3:65:ALA:HB3	1.82	0.62
4:4:98:SER:HB2	4:4:102:GLU:OE1	1.99	0.61
19:A:1780:CLA:OBD	19:A:1780:CLA:H92	2.00	0.61
5:A:340:GLY:O	5:A:343:HIS:CB	2.47	0.61
5:A:454:GLY:N	5:A:457:SER:HB3	2.07	0.61
6:B:130:ARG:HG2	6:B:130:ARG:HH11	1.64	0.61
6:B:282:PHE:O	6:B:286:ILE:HG13	1.99	0.61
6:B:310:PRO:CB	6:B:311:PRO:CD	2.78	0.61
6:B:355:LEU:HD21	19:B:1756:CLA:HMC2	1.82	0.61
5:A:131:ILE:HD13	6:B:447:GLY:CA	2.30	0.61
17:N:62:SER:CB	17:N:66:ASP:CG	2.67	0.61
2:2:50:VAL:O	2:2:54:TRP:CD1	2.43	0.61
2:2:93:THR:O	2:2:97:VAL:HG22	1.99	0.61
19:3:1221:CLA:O1D	19:3:1221:CLA:C2A	2.47	0.61
20:A:7023:LMU:H41	20:A:7023:LMU:H92	1.82	0.61
16:L:113:SER:O	16:L:116:PRO:HD2	2.00	0.61
8:D:48:ILE:HB	8:D:100:PHE:HB3	1.82	0.61
1:1:140:LEU:H	1:1:140:LEU:HD23	1.65	0.61
19:A:1781:CLA:CAA	19:A:1781:CLA:HED2	2.30	0.61
19:A:1774:CLA:CGA	19:A:1784:CLA:CMD	2.77	0.61
5:A:95:GLY:HA3	19:A:1763:CLA:C1C	2.30	0.61
3:3:52:LYS:CA	3:3:55:ALA:HB3	2.30	0.61
3:3:104:TYR:HB2	3:3:106:TYR:H	1.64	0.61
8:D:113:HIS:CD2	8:D:118:VAL:HG21	2.36	0.61
5:A:425:THR:HG1	5:A:428:TYR:HE1	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7004:LMU:O6'	20:A:7004:LMU:H11	1.99	0.61
5:A:91:LEU:O	19:A:1763:CLA:CMC	2.48	0.61
5:A:467:MET:HA	5:A:470:LEU:HB2	1.83	0.61
6:B:190:TRP:HE3	19:B:1744:CLA:CBB	2.12	0.61
6:B:57:ILE:HG12	19:B:1738:CLA:HMC2	1.80	0.61
6:B:294:ASN:CB	11:G:36:PRO:HD2	2.27	0.61
17:N:61:LEU:CG	17:N:62:SER:N	2.61	0.61
4:4:38:ARG:CG	4:4:39:TRP:H	2.10	0.61
2:2:63:PHE:HD2	2:2:172:LEU:HD21	1.64	0.61
11:G:16:LEU:HD12	11:G:17:PHE:CE2	2.36	0.61
11:G:68:ILE:H	11:G:68:ILE:HD12	1.66	0.61
5:A:197:GLN:NE2	5:A:351:THR:HB	2.15	0.61
20:2:1224:LMU:C2B	20:2:1224:LMU:C6'	2.78	0.61
17:N:32:ALA:CB	17:N:35:VAL:HG22	2.23	0.61
5:A:88:ILE:HG22	5:A:89:ILE:N	2.16	0.61
6:B:167:TRP:HB2	11:G:41:MET:HE3	1.80	0.61
6:B:290:MET:HA	19:B:1751:CLA:CAC	2.30	0.61
19:B:1751:CLA:HHD	19:B:1751:CLA:CBC	2.20	0.61
6:B:175:LEU:O	6:B:179:LEU:HG	2.00	0.61
6:B:437:TYR:HB3	6:B:616:LEU:HD23	1.81	0.61
16:L:9:GLN:C	16:L:11:ILE:H	2.03	0.61
4:4:30:LEU:CB	20:4:1212:LMU:H121	2.30	0.61
4:4:33:ASP:HB3	4:4:34:PRO:HD3	1.82	0.61
4:4:193:ILE:H	4:4:193:ILE:HD12	1.66	0.61
12:H:21:TRP:H	12:H:22:ASP:CB	2.13	0.61
19:2:1212:CLA:CGA	19:2:1212:CLA:H42	2.31	0.61
5:A:519:ASP:C	5:A:520:LEU:HG	2.19	0.61
20:A:7006:LMU:C2'	20:A:7006:LMU:H22	2.31	0.61
5:A:445:HIS:O	5:A:446:LEU:CB	2.48	0.61
20:A:7026:LMU:H2B	20:A:7026:LMU:H6'2	1.82	0.61
4:4:95:PHE:HZ	19:4:1210:CLA:C4C	2.10	0.61
4:4:142:ASN:C	4:4:150:LYS:HZ1	2.01	0.61
19:A:1765:CLA:HBD	19:A:1765:CLA:HBA2	1.81	0.61
19:A:1776:CLA:C3C	19:A:1782:CLA:H172	2.31	0.61
19:B:1768:CLA:HMA1	19:B:1769:CLA:CED	2.31	0.61
7:C:1:MET:H1	7:C:3:HIS:C	1.96	0.61
4:4:76:TYR:CD1	4:4:76:TYR:O	2.54	0.61
1:1:27:LEU:CG	6:B:314:ARG:NH1	2.63	0.61
6:B:247:THR:HG23	6:B:250:ALA:HB3	1.83	0.61
10:F:22:LEU:H	10:F:22:LEU:CD1	2.09	0.61
10:F:22:LEU:O	10:F:25:LEU:CB	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:173:GLU:HG2	3:3:174:LYS:N	2.08	0.61
9:E:68:ARG:NH2	9:E:69:PHE:HA	2.15	0.61
6:B:8:PHE:O	6:B:35:ASP:CB	2.49	0.61
19:1:1193:CLA:HBA2	19:1:1193:CLA:HMA3	1.80	0.61
5:A:720:THR:HG22	5:A:720:THR:O	2.01	0.61
19:4:1196:CLA:HBC2	19:4:1196:CLA:CHD	2.21	0.61
4:4:121:PHE:C	4:4:122:LYS:HD2	2.20	0.61
5:A:452:PHE:CD1	19:A:1793:CLA:HBB2	2.32	0.61
5:A:223:VAL:HG23	5:A:227:LEU:HD13	1.83	0.61
5:A:281:LEU:HG	5:A:282:THR:H	1.65	0.61
6:B:29:HIS:CG	19:B:1737:CLA:CBB	2.83	0.61
9:E:72:VAL:O	9:E:73:ASN:CB	2.48	0.61
17:N:47:THR:CB	17:N:52:LEU:O	2.49	0.61
19:2:1223:CLA:C8	19:2:1223:CLA:H41	2.23	0.61
7:C:39:ILE:HG12	7:C:40:ALA:N	2.06	0.61
2:2:203:THR:O	2:2:204:ILE:HG23	1.99	0.61
20:R:1056:LMU:O5B	20:R:1056:LMU:H6D	2.00	0.61
10:F:42:ILE:CG1	10:F:43:LYS:H	2.06	0.61
9:E:69:PHE:CD2	9:E:71:LYS:HG2	2.35	0.61
17:N:18:ASP:HB2	17:N:22:LEU:CG	2.27	0.61
21:B:8056:SUC:H1	21:B:8056:SUC:H5'	1.81	0.61
19:1:1189:CLA:CBD	19:1:1189:CLA:HBA2	2.29	0.61
4:4:101:VAL:O	4:4:104:ARG:CZ	2.49	0.61
4:4:122:LYS:HB3	4:4:143:PHE:HB3	1.77	0.61
19:A:1796:CLA:H62	19:A:1815:CLA:H193	1.83	0.61
5:A:545:HIS:CE1	5:A:612:VAL:HG22	2.36	0.61
19:B:1755:CLA:HED2	19:B:1756:CLA:HMD1	1.83	0.61
19:B:1758:CLA:OBD	19:B:1758:CLA:O1D	2.12	0.61
19:B:1762:CLA:HBB2	23:B:1778:BCR:C27	2.31	0.61
5:A:668:TYR:CE2	6:B:617:MET:SD	2.94	0.61
6:B:16:PRO:HG3	7:C:74:THR:CB	2.30	0.61
17:N:57:LYS:O	17:N:60:PHE:C	2.39	0.61
2:2:70:LYS:CG	2:2:73:ILE:HG13	2.26	0.61
19:1:1142:CLA:CMD	19:1:1143:CLA:C1A	2.79	0.61
10:F:24:LYS:O	10:F:27:ALA:HB2	2.01	0.61
5:A:154:ARG:HG3	5:A:383:PRO:HB2	1.83	0.61
5:A:631:GLN:O	20:A:1810:LMU:H6E	2.01	0.61
5:A:527:VAL:HG13	5:A:528:ALA:H	1.65	0.61
4:4:121:PHE:O	4:4:122:LYS:HB2	2.01	0.61
19:A:1760:CLA:HBB2	19:A:1762:CLA:C4D	2.30	0.61
19:A:1763:CLA:CGA	19:A:1765:CLA:H12	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1783:CLA:C20	23:A:1806:BCR:C17	2.68	0.61
5:A:701:GLN:OE1	9:E:74:TYR:CE1	2.54	0.61
19:B:1735:CLA:HBB2	19:B:1735:CLA:H122	1.83	0.61
19:B:1753:CLA:HAA2	19:B:1753:CLA:CBD	2.30	0.61
8:D:39:LYS:HD2	8:D:42:VAL:HG13	1.81	0.61
17:N:72:LYS:CB	17:N:74:LYS:N	2.43	0.61
20:A:7023:LMU:C2B	20:A:7023:LMU:C6B	2.75	0.61
5:A:412:ALA:HA	5:A:598:VAL:HG21	1.83	0.61
5:A:478:SER:HB3	5:A:644:GLN:OE1	2.01	0.61
19:A:1781:CLA:C7	19:A:1782:CLA:CED	2.70	0.61
19:A:1814:CLA:CED	19:B:1784:CLA:H2	2.30	0.61
5:A:40:PHE:CE1	5:A:53:TRP:CD1	2.82	0.61
6:B:289:LEU:O	19:B:1751:CLA:HMC1	2.01	0.61
6:B:317:ARG:NE	6:B:317:ARG:CA	2.60	0.61
6:B:557:PHE:CD1	6:B:571:SER:HB3	2.35	0.61
7:C:55:GLU:C	7:C:57:ALA:N	2.53	0.61
5:A:701:GLN:OE1	9:E:74:TYR:HE1	1.83	0.61
19:1:1146:CLA:H2A	19:1:1146:CLA:O1A	1.99	0.61
5:A:588:GLY:H	6:B:668:ARG:NH1	1.97	0.61
3:3:106:TYR:CD1	3:3:107:TRP:N	2.68	0.61
5:A:150:PHE:H	5:A:153:TRP:HE3	1.49	0.61
19:1:1149:CLA:CBC	19:1:1149:CLA:HMC1	2.24	0.61
6:B:517:PHE:HD2	6:B:517:PHE:O	1.82	0.61
4:4:58:MET:O	4:4:59:LEU:C	2.39	0.61
19:R:1054:CLA:H2A	19:R:1054:CLA:O1A	2.00	0.61
19:A:1788:CLA:HAA1	23:A:1808:BCR:C13	2.31	0.61
19:A:1796:CLA:H192	14:J:19:PHE:CD2	2.36	0.61
5:A:229:ILE:CG2	5:A:229:ILE:O	2.49	0.61
5:A:360:ILE:O	5:A:361:ASN:CB	2.48	0.61
6:B:280:ILE:HD13	19:B:1748:CLA:HBB2	1.83	0.61
6:B:510:LEU:HD21	19:B:1767:CLA:HHD	1.82	0.61
7:C:5:VAL:HB	7:C:65:VAL:HG22	1.82	0.61
2:2:60:ALA:HA	2:2:63:PHE:CE2	2.35	0.61
16:L:158:MET:CG	16:L:159:TYR:H	2.14	0.61
14:J:10:VAL:CG1	14:J:11:ALA:N	2.64	0.61
6:B:409:ALA:O	6:B:411:MET:N	2.26	0.61
19:A:1760:CLA:CBA	19:A:1767:CLA:H62	2.31	0.60
5:A:309:LEU:O	5:A:310:PHE:HB2	2.01	0.60
5:A:604:TRP:O	5:A:607:ASN:N	2.32	0.60
5:A:678:PHE:O	5:A:680:LEU:N	2.33	0.60
6:B:196:HIS:CE1	19:B:1745:CLA:HED2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1768:CLA:C15	23:B:1779:BCR:H313	2.28	0.60
6:B:556:SER:C	6:B:558:PRO:CD	2.69	0.60
4:4:71:ASN:O	4:4:72:VAL:C	2.39	0.60
3:3:97:PHE:CE2	3:3:98:ILE:CD1	2.33	0.60
17:N:80:ASN:C	17:N:82:PHE:H	2.03	0.60
4:4:36:ASN:OD1	4:4:39:TRP:CG	2.54	0.60
17:N:4:GLU:OE2	17:N:5:GLU:CB	2.47	0.60
8:D:46:TYR:HE1	8:D:80:LYS:HE2	1.64	0.60
21:B:8059:SUC:C3	21:B:8059:SUC:O2'	2.49	0.60
2:2:36:SER:O	2:2:37:ASP:HB2	2.01	0.60
19:A:1768:CLA:C3D	19:A:1769:CLA:HMC3	2.31	0.60
19:A:1788:CLA:H11	19:A:1800:CLA:H43	1.83	0.60
5:A:472:ARG:O	5:A:474:GLN:N	2.34	0.60
5:A:492:ILE:HD11	19:A:1792:CLA:O1D	2.00	0.60
6:B:551:LYS:CG	6:B:552:ASP:H	2.14	0.60
7:C:1:MET:N	7:C:4:SER:CA	2.54	0.60
23:B:1779:BCR:HC32	19:F:1156:CLA:CMA	2.31	0.60
11:G:44:PHE:CA	11:G:47:GLY:CA	2.78	0.60
4:4:194:VAL:HG12	4:4:195:GLN:HB2	1.83	0.60
12:H:72:ALA:HA	21:H:1082:SUC:H6'2	1.82	0.60
19:1:1143:CLA:CAC	20:A:7001:LMU:C3B	2.79	0.60
14:J:22:LEU:O	14:J:25:LEU:N	2.34	0.60
20:A:7021:LMU:H41	20:A:7021:LMU:C6'	2.31	0.60
10:F:46:MET:O	10:F:49:THR:N	2.34	0.60
12:H:47:PHE:CD2	16:L:141:GLY:HA2	2.35	0.60
5:A:396:PHE:HE2	5:A:616:PHE:CG	2.18	0.60
19:A:1790:CLA:C3D	19:A:1791:CLA:HAC1	2.31	0.60
5:A:353:SER:HB2	5:A:356:ALA:HB3	1.82	0.60
5:A:364:MET:O	5:A:368:LEU:N	2.33	0.60
19:B:1768:CLA:H121	23:B:1779:BCR:H311	1.81	0.60
18:R:34:UNK:H	18:R:36:UNK:CB	2.10	0.60
20:A:7013:LMU:H3O2	20:A:7049:LMU:H6'	1.48	0.60
10:F:7:PRO:HB3	10:F:60:GLY:O	2.00	0.60
6:B:143:LEU:C	6:B:145:LEU:H	2.04	0.60
6:B:282:PHE:CZ	19:B:1746:CLA:C1	2.79	0.60
6:B:288:GLY:O	6:B:289:LEU:HB2	2.01	0.60
6:B:347:LEU:HD21	6:B:351:HIS:HE1	1.66	0.60
6:B:732:LYS:CA	6:B:733:PHE:O	2.49	0.60
9:E:88:GLU:O	9:E:90:VAL:CB	2.49	0.60
15:K:79:LYS:CD	15:K:84:LEU:O	2.48	0.60
7:C:12:ILE:CB	7:C:39:ILE:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:7025:LMU:H41	20:A:7025:LMU:O2'	2.01	0.60
4:4:99:HIS:HE1	4:4:103:ILE:CD1	2.10	0.60
4:4:121:PHE:CD2	4:4:122:LYS:O	2.54	0.60
5:A:618:TRP:CZ2	5:A:655:ASP:CB	2.84	0.60
5:A:707:ILE:O	5:A:711:HIS:CD2	2.55	0.60
10:F:23:LYS:HB2	10:F:24:LYS:HZ1	1.65	0.60
20:A:7013:LMU:O3'	20:A:7049:LMU:O6'	2.19	0.60
17:N:29:PHE:CE1	17:N:32:ALA:HB3	2.36	0.60
20:A:7043:LMU:C6	20:A:7043:LMU:H102	2.27	0.60
16:L:160:VAL:O	16:L:160:VAL:HG22	2.00	0.60
6:B:450:GLU:O	6:B:452:GLN:N	2.27	0.60
4:4:104:ARG:NH1	4:4:105:ARG:HB3	2.10	0.60
4:4:169:GLN:NE2	19:4:1199:CLA:CHD	2.61	0.60
19:A:1815:CLA:H93	6:B:431:PHE:HD1	1.66	0.60
5:A:187:HIS:CD2	19:A:1767:CLA:C4C	2.85	0.60
5:A:660:GLN:O	5:A:661:ALA:CB	2.48	0.60
6:B:144:PHE:CD2	6:B:144:PHE:O	2.54	0.60
6:B:51:PHE:CD1	19:B:1743:CLA:HED1	2.37	0.60
6:B:276:HIS:HB2	19:B:1747:CLA:C1B	2.31	0.60
6:B:732:LYS:HZ3	6:B:732:LYS:HB2	1.66	0.60
6:B:696:LYS:HG2	7:C:80:ALA:CA	2.31	0.60
13:I:8:PHE:CD1	19:I:1031:CLA:H12	2.36	0.60
17:N:65:LEU:HD23	17:N:65:LEU:C	2.22	0.60
16:L:163:LEU:CD1	16:L:165:TYR:CE2	2.84	0.60
12:H:45:ALA:HB3	12:H:46:PRO:CD	2.31	0.60
8:D:28:ILE:HG12	8:D:67:ILE:CG1	2.31	0.60
5:A:500:PRO:HB3	5:A:506:GLY:HA2	1.84	0.60
19:1:1193:CLA:HBC3	19:1:1193:CLA:HMC1	1.82	0.60
12:H:67:TYR:O	12:H:70:ALA:O	2.20	0.60
19:A:1767:CLA:HMC1	19:A:1767:CLA:HBC3	1.84	0.60
19:A:1787:CLA:HBB2	19:A:1793:CLA:H192	1.83	0.60
19:A:1815:CLA:H93	6:B:431:PHE:CD1	2.37	0.60
5:A:281:LEU:CD1	19:A:1772:CLA:H2A	2.32	0.60
5:A:679:PHE:CE2	5:A:683:HIS:HD2	2.19	0.60
5:A:697:ARG:HD3	6:B:566:GLY:O	1.99	0.60
5:A:713:LYS:NZ	19:B:1761:CLA:H43	2.15	0.60
6:B:467:HIS:NE2	19:B:1764:CLA:C1A	2.65	0.60
17:N:55:GLN:O	17:N:56:LYS:HG3	2.00	0.60
10:F:102:ARG:HG2	10:F:106:ILE:CD1	2.19	0.60
20:2:1224:LMU:C2	20:2:1224:LMU:H62	2.32	0.60
4:4:121:PHE:CZ	4:4:125:SER:O	2.53	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1773:CLA:H52	19:A:1790:CLA:HBA1	1.83	0.60
5:A:76:ARG:O	5:A:186:TYR:HD2	1.84	0.60
5:A:370:ILE:HG22	5:A:400:MET:CA	2.29	0.60
5:A:705:GLU:CB	6:B:545:LYS:HZ2	2.14	0.60
6:B:396:ARG:NH1	19:B:1759:CLA:HED2	2.17	0.60
7:C:73:THR:HG1	7:C:76:SER:HB3	1.65	0.60
9:E:44:TYR:HB3	9:E:45:TRP:CE3	2.36	0.60
4:4:34:PRO:HG3	4:4:35:GLU:OE1	2.01	0.60
1:1:23:GLY:HA3	19:1:1198:CLA:C3C	2.32	0.60
19:2:1213:CLA:C4C	19:2:1213:CLA:H43	2.30	0.60
2:2:103:GLY:CA	19:2:1221:CLA:CBB	2.79	0.60
19:4:1206:CLA:C15	19:4:1206:CLA:C19	2.66	0.60
19:4:1206:CLA:C1	19:4:1206:CLA:CAA	2.80	0.60
14:J:10:VAL:HG13	14:J:11:ALA:H	1.66	0.60
9:E:51:SER:HB3	9:E:68:ARG:NH1	2.16	0.60
5:A:586:ARG:H	7:C:49:VAL:HG22	1.66	0.60
15:K:27:ALA:CB	15:K:28:PRO:CD	2.79	0.60
8:D:94:TYR:O	8:D:95:LYS:CG	2.49	0.60
17:N:11:LYS:HG2	17:N:12:THR:N	2.17	0.60
6:B:98:GLN:O	6:B:100:ALA:N	2.35	0.60
5:A:620:MET:HG3	5:A:625:TRP:CE2	2.37	0.60
3:3:141:GLN:HG2	3:3:142:TYR:N	2.16	0.60
5:A:227:LEU:HD23	5:A:231:GLN:HE22	1.66	0.60
19:B:1747:CLA:HBD	19:B:1756:CLA:CBB	2.32	0.60
19:B:1738:CLA:HBB2	19:B:1758:CLA:HHC	1.82	0.60
6:B:280:ILE:HA	6:B:283:LEU:HD12	1.84	0.60
7:C:73:THR:OG1	7:C:76:SER:CB	2.46	0.60
9:E:40:ARG:CB	9:E:42:GLU:OE2	2.50	0.60
11:G:28:ARG:HH21	11:G:29:GLU:N	1.98	0.60
3:3:181:LEU:HD13	3:3:184:VAL:HG21	1.82	0.60
5:A:249:ILE:O	5:A:251:ASN:N	2.34	0.60
16:L:158:MET:SD	16:L:159:TYR:N	2.75	0.60
20:A:7041:LMU:O2'	20:A:7041:LMU:H5'	2.01	0.60
20:2:1224:LMU:H22	20:2:1224:LMU:H62	1.83	0.60
1:1:61:GLU:HG2	1:1:61:GLU:O	2.02	0.60
4:4:169:GLN:CD	19:4:1199:CLA:HAC2	2.22	0.60
5:A:113:PRO:C	5:A:115:HIS:H	2.04	0.60
5:A:301:HIS:HE2	19:A:1772:CLA:CHA	2.15	0.60
5:A:578:ARG:HA	5:A:595:TRP:HB2	1.83	0.60
5:A:669:GLY:H	6:B:445:ALA:CA	2.08	0.60
5:A:81:ALA:CB	19:A:1761:CLA:HBB2	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:390:GLY:N	6:B:391:PRO:CD	2.65	0.60
23:B:1778:BCR:H23C	10:F:90:PHE:CD1	2.36	0.60
2:2:171:MET:SD	2:2:171:MET:C	2.80	0.60
2:2:125:PHE:O	2:2:126:PRO:C	2.40	0.60
10:F:126:ALA:O	10:F:128:SER:N	2.35	0.60
12:H:44:ALA:CB	16:L:145:PHE:CD1	2.62	0.60
11:G:62:ASP:HB2	11:G:63:PRO:HD3	1.84	0.60
5:A:585:GLY:O	5:A:589:THR:OG1	2.20	0.60
10:F:17:ARG:HE	10:F:17:ARG:HA	1.66	0.60
1:1:183:ASP:OD1	1:1:184:PRO:HD2	1.98	0.59
19:A:1815:CLA:HMD3	6:B:578:LEU:CD2	2.18	0.59
4:4:73:PRO:O	4:4:74:LYS:HB2	2.02	0.59
17:N:61:LEU:CD1	17:N:63:ASP:C	2.56	0.59
17:N:79:SER:CA	17:N:80:ASN:O	2.45	0.59
4:4:37:LEU:O	4:4:39:TRP:HD1	1.82	0.59
19:3:1221:CLA:H193	19:3:1221:CLA:C15	2.31	0.59
3:3:194:ILE:HD11	19:3:1213:CLA:HMC2	1.83	0.59
19:A:1782:CLA:HBB2	19:A:1790:CLA:HMA2	0.64	0.59
19:A:1800:CLA:H152	23:A:1808:BCR:H352	1.83	0.59
19:A:1800:CLA:H203	19:L:1167:CLA:HBB2	1.84	0.59
23:A:1805:BCR:C31	19:A:1815:CLA:H142	2.28	0.59
5:A:735:VAL:O	5:A:739:LEU:HG	2.01	0.59
6:B:131:THR:HB	6:B:134:ASP:CB	2.19	0.59
6:B:290:MET:HA	19:B:1751:CLA:HAC2	1.84	0.59
19:B:1752:CLA:CBB	19:B:1752:CLA:H72	2.25	0.59
19:B:1755:CLA:H12	19:B:1769:CLA:CED	2.32	0.59
19:B:1756:CLA:H41	19:B:1756:CLA:H72	1.84	0.59
19:B:1768:CLA:CMA	19:B:1769:CLA:CED	2.80	0.59
4:4:34:PRO:CB	4:4:35:GLU:HB2	2.32	0.59
15:K:44:GLU:O	15:K:46:GLY:C	2.40	0.59
8:D:75:LEU:HD21	16:L:19:PHE:CE2	2.37	0.59
2:2:162:LYS:C	2:2:162:LYS:HD3	2.22	0.59
10:F:24:LYS:O	10:F:27:ALA:CB	2.50	0.59
2:2:182:ILE:O	2:2:204:ILE:O	2.19	0.59
2:2:191:ASN:HB3	21:2:1225:SUC:C6	2.33	0.59
21:B:8059:SUC:O2	21:B:8059:SUC:H1'2	2.02	0.59
6:B:154:TRP:CD1	6:B:158:GLN:HG2	2.37	0.59
21:B:8055:SUC:C1'	21:B:8055:SUC:O2	2.50	0.59
4:4:122:LYS:CB	4:4:143:PHE:CG	2.85	0.59
19:A:1759:CLA:CGA	19:A:1796:CLA:H2	2.33	0.59
5:A:218:TRP:HD1	5:A:303:HIS:HD1	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:370:ILE:CG2	5:A:403:GLY:HA3	2.26	0.59
5:A:679:PHE:O	5:A:683:HIS:HB2	2.03	0.59
6:B:310:PRO:CB	6:B:311:PRO:HD2	2.31	0.59
6:B:732:LYS:CG	6:B:733:PHE:C	2.69	0.59
13:I:26:LEU:HD13	13:I:30:LYS:HB3	1.83	0.59
17:N:63:ASP:H	17:N:64:ASP:C	2.05	0.59
19:2:1213:CLA:C4	19:2:1213:CLA:NC	2.65	0.59
19:1:1146:CLA:O1A	19:1:1146:CLA:C2A	2.49	0.59
11:G:68:ILE:HG23	11:G:72:LEU:CD1	2.26	0.59
2:2:182:ILE:HG23	2:2:205:PHE:HB2	1.83	0.59
5:A:141:ARG:HH21	5:A:141:ARG:CG	2.11	0.59
5:A:47:GLY:O	10:F:115:THR:HB	2.02	0.59
2:2:143:PHE:HD1	2:2:144:ASP:N	2.00	0.59
20:A:1811:LMU:O5B	20:A:1811:LMU:H5'	2.01	0.59
5:A:451:ILE:HD12	19:A:1788:CLA:CED	2.24	0.59
6:B:622:ASP:HA	6:B:626:LEU:HB3	1.82	0.59
9:E:34:SER:O	9:E:35:LYS:HB3	2.02	0.59
16:L:40:LEU:HB3	16:L:41:PRO:CD	2.33	0.59
1:1:24:PHE:HD2	6:B:314:ARG:CZ	2.13	0.59
6:B:98:GLN:C	6:B:100:ALA:N	2.56	0.59
2:2:208:PHE:CG	2:2:209:THR:N	2.70	0.59
4:4:160:MET:HA	4:4:163:PHE:HB2	1.83	0.59
5:A:217:SER:HG	23:A:1803:BCR:H15C	1.67	0.59
23:A:1805:BCR:H313	19:A:1815:CLA:H142	1.84	0.59
5:A:681:GLY:HA2	5:A:684:PHE:HB3	1.84	0.59
19:B:1741:CLA:H43	19:B:1741:CLA:HAA2	1.85	0.59
19:B:1755:CLA:HBB2	19:B:1769:CLA:HBB	1.84	0.59
23:B:1780:BCR:HC8	23:B:1780:BCR:C33	2.32	0.59
6:B:464:GLN:HA	6:B:467:HIS:HB2	1.83	0.59
7:C:66:ARG:NH2	7:C:66:ARG:HG2	1.99	0.59
11:G:43:HIS:HB2	11:G:44:PHE:HD1	1.59	0.59
19:4:1205:CLA:CED	19:4:1205:CLA:C1A	2.81	0.59
17:N:70:GLU:O	17:N:72:LYS:CD	2.48	0.59
4:4:33:ASP:CB	4:4:34:PRO:CD	2.75	0.59
19:2:1213:CLA:H42	19:2:1213:CLA:NC	2.18	0.59
8:D:125:PRO:HG2	8:D:127:ARG:HD3	1.83	0.59
20:2:1224:LMU:O6'	20:2:1224:LMU:H2B	2.03	0.59
19:A:1816:CLA:O2A	6:B:651:LEU:HB3	2.03	0.59
5:A:603:PHE:CE2	6:B:665:ILE:HG21	2.37	0.59
6:B:190:TRP:CA	19:B:1744:CLA:HBB2	2.31	0.59
6:B:212:PHE:CE1	19:B:1744:CLA:HHD	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:175:LEU:HD11	19:B:1749:CLA:HMA1	1.85	0.59
6:B:188:LEU:O	6:B:191:ALA:N	2.35	0.59
6:B:292:ARG:NH2	6:B:297:ILE:HG13	2.18	0.59
13:I:12:VAL:HG21	19:I:1031:CLA:HBA1	1.85	0.59
4:4:73:PRO:HB2	4:4:75:TRP:HB2	1.83	0.59
15:K:83:VAL:O	15:K:84:LEU:C	2.39	0.59
11:G:68:ILE:O	11:G:72:LEU:HB2	2.03	0.59
8:D:86:LEU:CD1	8:D:90:LEU:HG	2.33	0.59
6:B:529:THR:HA	6:B:532:LEU:HD23	1.84	0.59
19:A:1760:CLA:H12	19:A:1767:CLA:H92	1.84	0.59
19:A:1796:CLA:H71	19:A:1815:CLA:H171	1.84	0.59
5:A:472:ARG:N	5:A:473:PRO:CD	2.64	0.59
6:B:141:PHE:HD2	6:B:144:PHE:CE1	2.21	0.59
6:B:193:HIS:HB2	19:B:1744:CLA:CHC	2.33	0.59
13:I:20:ALA:O	13:I:24:LEU:HB3	2.03	0.59
3:3:180:LYS:CB	3:3:181:LEU:HB2	2.33	0.59
2:2:124:ILE:CB	2:2:129:LYS:HB3	2.32	0.59
19:2:1223:CLA:C8	19:2:1223:CLA:C4	2.78	0.59
19:2:1223:CLA:CED	19:2:1223:CLA:OBD	2.51	0.59
14:J:10:VAL:HG13	14:J:11:ALA:N	2.17	0.59
10:F:151:ASP:C	10:F:154:PHE:HB3	2.23	0.59
1:1:184:PRO:HB2	19:1:1199:CLA:O1D	2.02	0.59
4:4:123:GLN:O	4:4:143:PHE:CG	2.55	0.59
19:A:1814:CLA:CED	19:A:1814:CLA:CAD	2.80	0.59
19:B:1756:CLA:H8	23:B:1777:BCR:H14C	1.84	0.59
6:B:595:HIS:HD2	6:B:623:TYR:OH	1.86	0.59
7:C:1:MET:HE1	8:D:154:TYR:OH	2.03	0.59
16:L:99:LEU:O	16:L:102:TYR:N	2.34	0.59
3:3:199:VAL:HG22	19:3:1215:CLA:C4C	2.32	0.59
2:2:195:ALA:HB1	2:2:197:LEU:HG	1.84	0.59
6:B:378:ILE:HG22	6:B:379:ALA:H	1.67	0.59
6:B:224:PRO:CB	6:B:227:THR:HB	2.32	0.59
4:4:101:VAL:O	4:4:104:ARG:HB3	2.02	0.59
23:A:1805:BCR:H353	19:A:1814:CLA:H41	1.85	0.59
6:B:568:CYS:O	6:B:570:ILE:N	2.35	0.59
2:2:43:TRP:C	2:2:45:VAL:N	2.56	0.59
3:3:194:ILE:HG23	3:3:197:TYR:OH	2.02	0.59
19:A:1764:CLA:HMC3	19:A:1765:CLA:HHD	1.83	0.59
19:A:1797:CLA:C12	19:A:1797:CLA:C7	2.66	0.59
19:A:1800:CLA:HMB2	19:L:1167:CLA:HBC1	1.85	0.59
5:A:207:LEU:HA	5:A:211:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:361:ASN:O	5:A:365:LEU:N	2.35	0.59
5:A:665:ILE:HB	6:B:621:ARG:HB2	1.83	0.59
19:A:1765:CLA:HBB2	19:B:1763:CLA:HMD2	1.82	0.59
6:B:79:GLN:O	6:B:80:ASP:HB3	2.01	0.59
17:N:49:CYS:O	17:N:51:ASP:O	2.21	0.59
2:2:163:GLU:HG2	19:2:1217:CLA:C2C	2.33	0.59
21:B:8059:SUC:O2'	21:B:8059:SUC:C2	2.50	0.59
5:A:158:ILE:O	5:A:243:PRO:HG2	2.02	0.58
19:A:1796:CLA:NC	19:A:1796:CLA:C4	2.66	0.58
5:A:544:ILE:O	5:A:548:THR:OG1	2.14	0.58
5:A:645:SER:HB3	6:B:637:PRO:CG	2.27	0.58
5:A:713:LYS:HZ1	19:B:1761:CLA:H41	1.68	0.58
5:A:679:PHE:HE1	5:A:749:PHE:HB2	1.68	0.58
19:B:1735:CLA:NC	19:B:1735:CLA:H52	2.18	0.58
6:B:424:TRP:CZ3	19:B:1769:CLA:HBC3	2.38	0.58
5:A:25:ASP:CG	5:A:26:PRO:CA	2.64	0.58
1:1:25:ASP:CB	1:1:26:PRO:CD	2.81	0.58
19:2:1213:CLA:CBC	19:2:1213:CLA:CHD	2.73	0.58
20:A:7038:LMU:C10	20:A:7038:LMU:C6	2.80	0.58
6:B:692:ARG:NH2	6:B:694:ARG:HG2	2.18	0.58
5:A:373:ALA:HB1	5:A:396:PHE:HD1	1.68	0.58
4:4:123:GLN:HG2	4:4:124:TYR:N	2.18	0.58
19:A:1817:CLA:HMC1	19:A:1817:CLA:HBC3	1.85	0.58
5:A:232:PHE:CZ	5:A:242:ILE:HG22	2.38	0.58
5:A:555:ILE:HG23	19:A:1817:CLA:OBD	2.03	0.58
5:A:81:ALA:CB	19:A:1760:CLA:HMA3	2.31	0.58
19:B:1741:CLA:H12	19:B:1741:CLA:CAA	2.29	0.58
6:B:444:LEU:O	6:B:445:ALA:HB3	2.02	0.58
19:A:1815:CLA:CMD	6:B:578:LEU:HD23	2.19	0.58
9:E:65:VAL:HG13	9:E:82:TYR:O	2.02	0.58
4:4:36:ASN:ND2	4:4:39:TRP:CE2	2.72	0.58
18:R:39:UNK:N	18:R:42:UNK:CB	2.65	0.58
19:1:1190:CLA:HED3	19:1:1190:CLA:C2A	2.32	0.58
15:K:42:ALA:O	15:K:43:ARG:CB	2.50	0.58
8:D:118:VAL:CG1	8:D:119:TYR:N	2.66	0.58
6:B:15:ASP:O	6:B:20:ARG:HG2	2.04	0.58
12:H:41:GLU:OE2	12:H:42:THR:OG1	2.20	0.58
4:4:104:ARG:HE	4:4:105:ARG:N	2.00	0.58
19:A:1774:CLA:H42	19:A:1774:CLA:O2A	2.03	0.58
19:A:1783:CLA:C7	23:A:1805:BCR:C37	2.81	0.58
5:A:459:GLY:O	5:A:462:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1753:CLA:H43	19:B:1753:CLA:CAA	2.29	0.58
6:B:67:HIS:O	6:B:68:VAL:HG23	2.02	0.58
8:D:31:GLY:CA	16:L:13:PRO:HB3	2.33	0.58
2:2:60:ALA:HA	2:2:63:PHE:CD2	2.39	0.58
3:3:157:ALA:O	3:3:158:TYR:HB2	2.02	0.58
7:C:12:ILE:HD12	7:C:12:ILE:N	2.18	0.58
16:L:122:GLY:O	16:L:124:LYS:N	2.36	0.58
6:B:160:LYS:HE3	6:B:161:TRP:CE2	2.39	0.58
5:A:692:PHE:CZ	19:A:1796:CLA:HBC3	2.38	0.58
19:A:1800:CLA:H112	19:A:1800:CLA:C6	2.32	0.58
5:A:281:LEU:HD13	19:A:1772:CLA:H2A	1.85	0.58
5:A:42:ARG:C	5:A:44:ILE:H	2.06	0.58
5:A:708:VAL:CA	5:A:711:HIS:HD2	2.17	0.58
11:G:34:GLN:O	11:G:35:VAL:C	2.42	0.58
11:G:42:SER:OG	11:G:46:ALA:CA	2.50	0.58
10:F:22:LEU:O	10:F:24:LYS:N	2.36	0.58
19:1:1189:CLA:CED	19:1:1189:CLA:CAD	2.81	0.58
5:A:373:ALA:O	5:A:396:PHE:CD1	2.57	0.58
16:L:58:LEU:HD11	16:L:153:TRP:HZ2	1.68	0.58
16:L:107:PHE:HB2	16:L:109:GLU:OE1	2.02	0.58
4:4:47:ASN:HB3	4:4:161:LEU:CD2	2.34	0.58
4:4:88:SER:O	4:4:90:LEU:HA	2.03	0.58
5:A:114:THR:CG2	5:A:115:HIS:CE1	2.84	0.58
19:A:1776:CLA:CBA	19:A:1780:CLA:HBB2	2.34	0.58
5:A:229:ILE:CG1	5:A:243:PRO:HB3	2.33	0.58
5:A:74:ILE:O	5:A:78:VAL:HG13	2.04	0.58
5:A:558:LYS:HZ1	6:B:674:LEU:HB3	1.68	0.58
19:A:1789:CLA:CMD	6:B:95:HIS:HD2	2.17	0.58
9:E:85:ASP:O	9:E:86:GLU:CB	2.52	0.58
16:L:40:LEU:HB3	16:L:41:PRO:HD3	1.84	0.58
16:L:56:VAL:HA	19:L:1167:CLA:HED1	1.80	0.58
4:4:72:VAL:O	4:4:72:VAL:HG13	2.03	0.58
11:G:88:THR:OG1	11:G:92:GLY:HA3	2.04	0.58
3:3:52:LYS:N	3:3:55:ALA:HB3	2.19	0.58
2:2:74:LEU:O	2:2:75:ASN:ND2	2.36	0.58
12:H:16:ASN:HD22	12:H:19:GLY:HA2	1.68	0.58
15:K:42:ALA:C	15:K:43:ARG:HD3	2.23	0.58
20:A:7032:LMU:H6'2	20:A:7032:LMU:H22	1.85	0.58
4:4:61:PRO:HB3	4:4:67:ILE:O	2.04	0.58
5:A:389:TYR:HE1	5:A:625:TRP:CD1	2.22	0.58
1:1:184:PRO:O	1:1:185:TRP:CD2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1774:CLA:H71	19:A:1774:CLA:CBB	2.33	0.58
19:A:1815:CLA:H2	19:A:1815:CLA:HMA1	1.85	0.58
5:A:618:TRP:CH2	5:A:655:ASP:HB2	2.39	0.58
6:B:197:VAL:O	6:B:197:VAL:HG12	2.03	0.58
6:B:203:ARG:H	6:B:270:LEU:HD11	1.68	0.58
6:B:284:PHE:CE1	19:B:1749:CLA:HHC	2.39	0.58
6:B:569:ASP:HB3	6:B:574:ASP:HB3	1.86	0.58
1:I:27:LEU:HD12	6:B:314:ARG:NH1	2.16	0.58
19:2:1213:CLA:HBD	19:2:1217:CLA:HMA3	1.85	0.58
6:B:247:THR:C	6:B:250:ALA:HB2	2.24	0.58
8:D:111:TYR:CD2	8:D:114:PRO:CB	2.86	0.58
8:D:60:MET:SD	8:D:61:PRO:HD2	2.43	0.58
6:B:633:ASN:ND2	6:B:636:THR:HB	2.19	0.58
17:N:24:THR:O	17:N:26:GLY:N	2.36	0.58
19:4:1198:CLA:C2A	19:4:1198:CLA:CGD	2.81	0.58
23:A:1803:BCR:H341	23:A:1803:BCR:C12	2.32	0.58
19:A:1817:CLA:HHB	19:A:1817:CLA:C4	2.29	0.58
5:A:255:LEU:CD1	5:A:280:PHE:HZ	2.15	0.58
5:A:607:ASN:HD21	19:A:1813:CLA:H42	1.68	0.58
6:B:269:TRP:HD1	6:B:497:TRP:CH2	2.22	0.58
11:G:92:GLY:O	11:G:93:TYR:C	2.41	0.58
19:1:1145:CLA:C2	19:1:1145:CLA:CMA	2.81	0.58
18:R:3:UNK:O	18:R:4:UNK:CB	2.51	0.58
19:H:1081:CLA:HAA2	19:H:1081:CLA:HED2	1.86	0.58
4:4:106:TRP:CH2	19:4:1198:CLA:HBC1	2.38	0.58
5:A:122:VAL:HA	5:A:133:ASN:HD21	1.68	0.58
5:A:708:VAL:O	5:A:711:HIS:HB2	2.04	0.58
5:A:733:VAL:HG11	19:A:1796:CLA:C1D	2.33	0.58
6:B:127:ILE:CD1	6:B:193:HIS:CE1	2.87	0.58
6:B:351:HIS:NE2	19:B:1756:CLA:NC	2.52	0.58
6:B:493:TRP:CH2	19:B:1765:CLA:HBA1	2.38	0.58
6:B:438:VAL:HG22	19:B:1763:CLA:HMC3	1.85	0.58
6:B:577:TYR:HE2	6:B:578:LEU:HD12	1.68	0.58
19:A:1816:CLA:H62	6:B:648:TRP:CZ2	2.39	0.58
16:L:10:VAL:O	16:L:10:VAL:CG2	2.52	0.58
5:A:21:LEU:HB2	5:A:22:VAL:O	2.04	0.58
5:A:21:LEU:HD13	5:A:21:LEU:O	2.03	0.58
12:H:72:ALA:HA	21:H:1082:SUC:C6'	2.33	0.58
10:F:123:VAL:HB	10:F:126:ALA:C	2.24	0.58
5:A:513:LEU:HB3	5:A:529:LEU:HD13	1.85	0.58
4:4:90:LEU:HD22	4:4:90:LEU:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:281:LEU:O	5:A:282:THR:C	2.42	0.58
19:B:1760:CLA:HMB2	19:B:1761:CLA:CHB	2.34	0.58
19:B:1761:CLA:HHD	19:B:1761:CLA:HBC2	1.80	0.58
6:B:266:GLN:HE21	6:B:363:GLN:HG2	1.69	0.58
20:A:7016:LMU:C9	20:A:7016:LMU:H32	2.34	0.58
20:A:7016:LMU:C3	20:A:7016:LMU:H81	2.34	0.58
10:F:21:ALA:O	10:F:22:LEU:C	2.42	0.58
9:E:48:ASN:ND2	9:E:71:LYS:NZ	2.51	0.58
2:2:79:TRP:CG	2:2:79:TRP:O	2.57	0.58
4:4:90:LEU:H	4:4:90:LEU:CD2	2.16	0.58
19:A:1769:CLA:HMA2	19:A:1769:CLA:C2	2.33	0.58
5:A:310:PHE:HE2	19:A:1774:CLA:HMC3	1.69	0.58
22:A:1802:PQN:H142	23:B:1778:BCR:HC22	1.84	0.58
5:A:413:HIS:ND1	5:A:416:ILE:HD12	2.19	0.58
19:B:1755:CLA:H11	19:B:1769:CLA:CAD	2.33	0.58
19:B:1768:CLA:HHB	19:B:1769:CLA:OBD	2.04	0.58
19:B:1764:CLA:HBB2	23:B:1777:BCR:C38	2.34	0.58
9:E:39:LEU:HA	9:E:46:PHE:CE1	2.38	0.58
16:L:25:THR:HB	16:L:26:PRO:CD	2.34	0.58
17:N:65:LEU:HD23	17:N:66:ASP:O	2.03	0.58
19:2:1213:CLA:O1A	19:2:1213:CLA:H2	2.04	0.58
10:F:46:MET:O	10:F:48:LYS:N	2.37	0.58
5:A:141:ARG:HG3	5:A:141:ARG:NH2	2.10	0.58
5:A:415:ALA:HB2	5:A:560:VAL:HG12	1.85	0.58
19:1:1192:CLA:CBC	19:1:1192:CLA:CHD	2.82	0.58
21:3:1223:SUC:O2'	21:3:1223:SUC:C5	2.51	0.58
6:B:156:HIS:O	6:B:163:PRO:HB3	2.04	0.58
19:A:1783:CLA:C7	23:A:1805:BCR:H372	2.33	0.57
23:A:1803:BCR:C40	23:A:1803:BCR:C23	2.82	0.57
5:A:431:LEU:O	5:A:435:VAL:HG12	2.04	0.57
5:A:397:THR:HB	5:A:613:ILE:HG12	1.85	0.57
6:B:122:GLN:O	6:B:126:THR:OG1	2.13	0.57
19:B:1765:CLA:HHD	19:B:1765:CLA:HBC2	1.85	0.57
6:B:510:LEU:CD2	6:B:510:LEU:H	2.16	0.57
19:H:1079:CLA:HBC2	19:H:1079:CLA:HHD	1.86	0.57
16:L:63:LEU:HD22	16:L:64:LEU:N	2.17	0.57
2:2:72:GLY:C	2:2:74:LEU:H	2.04	0.57
2:2:54:TRP:HZ2	2:2:109:ARG:HB3	1.69	0.57
19:1:1146:CLA:CMA	19:1:1146:CLA:O1A	2.52	0.57
4:4:147:LEU:CD2	4:4:148:GLU:CG	2.76	0.57
19:1:1149:CLA:HBC2	19:1:1149:CLA:CMC	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1145:CLA:HMA1	19:1:1145:CLA:C2	2.33	0.57
12:H:67:TYR:C	12:H:67:TYR:HD1	2.08	0.57
10:F:33:ALA:HA	10:F:36:SER:HB2	1.85	0.57
16:L:135:GLY:HA2	16:L:138:LYS:HE2	1.86	0.57
5:A:365:LEU:HD22	19:A:1761:CLA:HED3	1.83	0.57
6:B:167:TRP:CZ2	19:B:1741:CLA:HMA1	2.39	0.57
6:B:277:HIS:HE1	19:B:1748:CLA:NC	2.02	0.57
6:B:29:HIS:HB2	19:B:1759:CLA:HBA1	1.86	0.57
19:B:1769:CLA:C2A	19:B:1769:CLA:O1D	2.52	0.57
6:B:382:ILE:CG2	6:B:383:MET:N	2.51	0.57
6:B:594:TRP:C	6:B:594:TRP:HD1	2.08	0.57
23:I:1032:BCR:H291	23:L:1169:BCR:H281	1.86	0.57
4:4:36:ASN:ND2	4:4:39:TRP:CZ2	2.72	0.57
2:2:211:LYS:HG2	3:3:113:LEU:CD1	2.23	0.57
20:A:7005:LMU:C5	20:A:7005:LMU:O1'	2.51	0.57
3:3:162:PRO:HG2	3:3:164:PHE:CD1	2.40	0.57
15:K:55:PHE:CD1	15:K:55:PHE:N	2.72	0.57
19:A:1763:CLA:HHB	19:A:1764:CLA:HMB3	1.86	0.57
5:A:229:ILE:HG12	5:A:243:PRO:HB3	1.85	0.57
5:A:508:THR:O	5:A:509:ALA:CB	2.53	0.57
6:B:152:ALA:O	6:B:153:GLY:C	2.42	0.57
19:A:1817:CLA:HBC1	6:B:665:ILE:HD12	1.86	0.57
3:3:92:TRP:HA	3:3:95:THR:OG1	1.98	0.57
2:2:128:ASN:CG	2:2:130:LEU:HB2	2.24	0.57
20:A:7032:LMU:C3	20:A:7032:LMU:H1B	2.32	0.57
6:B:172:GLU:HG3	6:B:301:ILE:HG13	1.85	0.57
19:A:1781:CLA:CBC	19:A:1781:CLA:CHD	2.81	0.57
19:A:1786:CLA:HMB2	19:A:1787:CLA:C2D	2.33	0.57
19:A:1779:CLA:C1D	23:A:1804:BCR:H19C	2.33	0.57
23:B:1778:BCR:C37	10:F:93:ILE:HG22	2.35	0.57
6:B:183:PHE:HE1	19:B:1743:CLA:H71	1.69	0.57
6:B:693:TRP:HD1	19:B:1770:CLA:C1D	2.17	0.57
6:B:76:ALA:O	6:B:79:GLN:N	2.38	0.57
11:G:26:PHE:HB2	11:G:27:GLN:NE2	2.14	0.57
11:G:40:GLY:C	11:G:41:MET:SD	2.83	0.57
13:I:11:LEU:CD1	23:I:1032:BCR:C10	2.67	0.57
17:N:61:LEU:HD12	17:N:62:SER:N	2.19	0.57
17:N:74:LYS:O	17:N:75:TYR:C	2.41	0.57
17:N:76:LYS:O	17:N:77:CYS:O	2.21	0.57
17:N:84:LYS:C	17:N:85:TRP:HD1	2.08	0.57
3:3:205:GLY:N	5:A:252:ARG:NH2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:98:GLU:HG2	2:2:99:LEU:CD1	2.34	0.57
21:B:8056:SUC:H3'	21:B:8056:SUC:HO2	1.69	0.57
4:4:116:ASN:O	4:4:123:GLN:HG3	2.04	0.57
19:A:1762:CLA:CED	19:A:1762:CLA:HBA2	2.34	0.57
19:A:1815:CLA:H3A	19:A:1815:CLA:CGA	2.34	0.57
5:A:331:LEU:HD21	5:A:343:HIS:C	2.12	0.57
5:A:53:TRP:HA	5:A:56:ASN:CB	2.34	0.57
6:B:22:TRP:CE2	19:B:1770:CLA:HMB1	2.39	0.57
19:B:1771:CLA:C19	13:I:21:MET:HB3	2.34	0.57
6:B:418:ILE:O	6:B:422:LEU:HD12	2.04	0.57
6:B:576:PHE:CE2	19:B:1759:CLA:HAC1	2.39	0.57
6:B:329:SER:O	6:B:330:ILE:HG22	2.03	0.57
5:A:109:TRP:HA	5:A:116:ILE:HG13	1.86	0.57
4:4:58:MET:O	4:4:60:LEU:N	2.37	0.57
8:D:102:ARG:HH21	8:D:110:GLN:HB2	1.70	0.57
19:R:1054:CLA:HBD	19:R:1054:CLA:HBA2	1.87	0.57
5:A:733:VAL:HG11	19:A:1796:CLA:C2D	2.34	0.57
5:A:547:PHE:CE2	19:A:1817:CLA:O1A	2.56	0.57
5:A:382:TYR:CE2	19:A:1784:CLA:HED3	2.39	0.57
5:A:54:ILE:O	5:A:58:HIS:HD2	1.87	0.57
5:A:690:LEU:HD21	5:A:738:TYR:HE1	1.69	0.57
6:B:120:VAL:CA	6:B:123:TRP:HD1	2.14	0.57
19:B:1738:CLA:H71	24:B:1781:LMG:H381	1.85	0.57
12:H:20:GLN:CB	12:H:22:ASP:CB	2.68	0.57
2:2:128:ASN:ND2	14:J:3:ASP:HB3	2.19	0.57
20:2:1224:LMU:H2B	20:2:1224:LMU:C6'	2.35	0.57
20:A:7027:LMU:O2'	20:A:7027:LMU:C1	2.51	0.57
17:N:34:THR:C	17:N:36:GLU:H	2.07	0.57
18:R:43:UNK:O	18:R:44:UNK:C	2.50	0.57
4:4:122:LYS:HD3	4:4:142:ASN:O	2.04	0.57
4:4:93:ILE:O	4:4:94:GLU:C	2.42	0.57
19:A:1760:CLA:H12	19:A:1767:CLA:C6	2.20	0.57
19:A:1763:CLA:HMB2	23:A:1806:BCR:HC7	1.86	0.57
19:A:1800:CLA:H112	19:A:1800:CLA:H61	1.86	0.57
6:B:77:TRP:CZ2	6:B:122:GLN:NE2	2.73	0.57
19:B:1771:CLA:H2	22:B:1773:PQN:H251	1.86	0.57
6:B:347:LEU:CD2	6:B:351:HIS:HE1	2.16	0.57
4:4:70:ILE:O	4:4:72:VAL:N	2.37	0.57
2:2:126:PRO:HG2	2:2:129:LYS:H	1.70	0.57
5:A:109:TRP:CH2	5:A:154:ARG:HD3	2.39	0.57
20:2:1224:LMU:H31	20:2:1224:LMU:H72	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:187:GLY:O	2:2:188:PRO:C	2.42	0.57
4:4:106:TRP:CD1	19:4:1196:CLA:CGD	2.88	0.57
19:B:1747:CLA:H52	19:B:1756:CLA:CMB	2.31	0.57
6:B:560:ASP:CG	7:C:52:LYS:HZ3	2.08	0.57
15:K:46:GLY:C	15:K:47:LEU:CG	2.74	0.57
2:2:127:ASN:O	2:2:128:ASN:HB2	2.03	0.57
5:A:112:ASP:O	5:A:116:ILE:HG12	2.05	0.57
5:A:426:THR:HA	5:A:428:TYR:CZ	2.40	0.57
10:F:151:ASP:CA	10:F:154:PHE:HB3	2.34	0.57
6:B:408:LEU:O	6:B:411:MET:HB3	2.04	0.57
3:3:190:ALA:O	19:3:1213:CLA:HMC1	2.05	0.57
11:G:64:VAL:O	11:G:64:VAL:HG12	2.04	0.57
4:4:91:PHE:CG	4:4:92:VAL:N	2.73	0.57
5:A:101:ALA:O	5:A:104:SER:HA	2.05	0.57
19:A:1760:CLA:HBB2	19:A:1762:CLA:CAD	2.34	0.57
19:A:1813:CLA:HMB3	19:A:1814:CLA:CAD	2.35	0.57
5:A:699:TYR:HD1	5:A:700:TRP:CD1	2.23	0.57
19:B:1747:CLA:HBD	19:B:1756:CLA:HBB2	1.87	0.57
19:A:1789:CLA:CGD	16:L:73:PRO:HA	2.35	0.57
17:N:70:GLU:OE2	17:N:72:LYS:O	2.23	0.57
1:1:28:GLY:HA2	19:1:1198:CLA:C3C	2.35	0.57
8:D:45:PHE:C	8:D:46:TYR:HD2	2.08	0.57
2:2:54:TRP:HZ2	2:2:109:ARG:CD	2.13	0.57
15:K:42:ALA:O	15:K:43:ARG:HG2	2.05	0.57
20:2:1224:LMU:H12	20:2:1224:LMU:H72	1.76	0.57
5:A:105:ASN:HB2	5:A:140:PHE:HZ	1.70	0.57
1:1:105:ILE:O	1:1:108:VAL:HG12	2.05	0.57
18:R:27:UNK:O	18:R:29:UNK:N	2.31	0.57
4:4:121:PHE:O	4:4:143:PHE:CD2	2.58	0.57
4:4:128:ALA:HB3	4:4:143:PHE:HE2	1.65	0.57
4:4:93:ILE:HG22	4:4:94:GLU:N	2.19	0.57
19:A:1790:CLA:HMC1	19:A:1790:CLA:HBC3	1.87	0.57
5:A:402:ILE:C	5:A:404:GLY:H	2.08	0.57
6:B:347:LEU:HD13	6:B:351:HIS:HD1	1.70	0.57
6:B:414:HIS:O	6:B:414:HIS:CG	2.58	0.57
6:B:693:TRP:CD1	19:B:1770:CLA:C1D	2.88	0.57
7:C:77:MET:O	7:C:79:LEU:N	2.34	0.57
9:E:80:ASN:HB3	9:E:82:TYR:CE2	2.40	0.57
6:B:167:TRP:HB2	11:G:41:MET:HE2	1.86	0.57
16:L:25:THR:HB	16:L:26:PRO:HD2	1.87	0.57
17:N:42:PHE:H	17:N:43:PRO:CD	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:75:LEU:HD21	16:L:19:PHE:CD2	2.39	0.57
2:2:100:VAL:CG2	2:2:101:PHE:N	2.67	0.57
19:3:1217:CLA:CBA	19:3:1217:CLA:CB	2.83	0.57
6:B:20:ARG:CB	6:B:20:ARG:HH11	2.17	0.57
15:K:69:ILE:HA	15:K:72:VAL:CG1	2.33	0.57
6:B:221:GLY:C	6:B:223:GLY:H	2.08	0.57
15:K:55:PHE:N	15:K:55:PHE:HD1	2.03	0.57
4:4:169:GLN:CG	19:4:1199:CLA:CAC	2.82	0.56
19:A:1787:CLA:O1A	6:B:686:PRO:HD3	2.05	0.56
5:A:364:MET:O	5:A:368:LEU:HB2	2.04	0.56
5:A:132:LEU:HD11	5:A:674:ALA:HB2	1.86	0.56
6:B:127:ILE:CD1	6:B:193:HIS:HE1	2.18	0.56
6:B:576:PHE:HE2	19:B:1759:CLA:HAC1	1.70	0.56
6:B:414:HIS:HD2	19:B:1760:CLA:HMA3	1.68	0.56
6:B:284:PHE:O	6:B:288:GLY:N	2.31	0.56
11:G:44:PHE:N	11:G:47:GLY:H	2.02	0.56
4:4:73:PRO:HG2	19:4:1205:CLA:HMD2	1.87	0.56
17:N:42:PHE:O	17:N:43:PRO:C	2.43	0.56
6:B:406:ASN:HD22	6:B:406:ASN:C	2.09	0.56
2:2:116:PRO:HB2	2:2:136:GLY:CA	2.35	0.56
8:D:86:LEU:C	8:D:90:LEU:HB3	2.26	0.56
5:A:439:ARG:NH1	5:A:565:SER:O	2.37	0.56
4:4:102:GLU:OE2	19:4:1209:CLA:CHC	2.53	0.56
4:4:104:ARG:HA	4:4:107:GLN:HE21	1.69	0.56
23:A:1809:BCR:HC8	23:A:1809:BCR:H321	1.87	0.56
5:A:700:TRP:HZ3	19:A:1815:CLA:O1D	1.87	0.56
5:A:207:LEU:HD12	5:A:310:PHE:CD1	2.38	0.56
5:A:402:ILE:CD1	19:A:1784:CLA:HBB2	2.35	0.56
5:A:40:PHE:CZ	5:A:56:ASN:HB3	2.41	0.56
5:A:711:HIS:HB3	5:A:717:ALA:CB	2.32	0.56
19:B:1745:CLA:HMA1	23:B:1776:BCR:H372	1.87	0.56
6:B:196:HIS:CE1	19:B:1745:CLA:ND	2.73	0.56
6:B:299:HIS:HE1	19:B:1752:CLA:HMD1	1.70	0.56
6:B:632:ILE:C	6:B:634:GLY:H	2.08	0.56
7:C:60:THR:CG2	7:C:63:LEU:O	2.53	0.56
4:4:73:PRO:CB	4:4:75:TRP:HB2	2.34	0.56
19:1:1142:CLA:HMD1	19:1:1143:CLA:C4A	2.35	0.56
14:J:18:TRP:CH2	14:J:22:LEU:HD22	2.40	0.56
16:L:124:LYS:O	16:L:126:GLN:N	2.35	0.56
19:J:1043:CLA:O1A	19:J:1043:CLA:C14	2.52	0.56
5:A:389:TYR:CE1	5:A:625:TRP:CD1	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:91:LEU:O	10:F:94:ALA:O	2.23	0.56
10:F:37:ALA:N	10:F:38:PRO:HD3	2.20	0.56
4:4:104:ARG:NE	4:4:105:ARG:N	2.53	0.56
4:4:128:ALA:C	4:4:130:GLU:H	2.08	0.56
4:4:140:PRO:O	4:4:141:LEU:HB2	2.04	0.56
4:4:93:ILE:O	4:4:95:PHE:N	2.39	0.56
6:B:70:TRP:HB3	6:B:136:TYR:OH	2.03	0.56
19:B:1755:CLA:H72	19:B:1769:CLA:C3D	2.35	0.56
19:A:1783:CLA:H111	23:A:1806:BCR:H353	1.87	0.56
5:A:553:VAL:O	5:A:557:LEU:HB2	2.05	0.56
6:B:34:HIS:O	6:B:36:ASP:N	2.37	0.56
6:B:710:LEU:C	6:B:712:HIS:N	2.58	0.56
9:E:44:TYR:CE1	9:E:73:ASN:HA	2.40	0.56
16:L:9:GLN:HG3	16:L:10:VAL:H	1.71	0.56
4:4:71:ASN:O	4:4:73:PRO:N	2.38	0.56
16:L:163:LEU:HB3	16:L:164:PRO:HD3	1.57	0.56
4:4:36:ASN:OD1	4:4:39:TRP:CD2	2.59	0.56
15:K:46:GLY:O	15:K:47:LEU:HB2	2.03	0.56
2:2:164:ILE:O	2:2:167:GLY:CA	2.53	0.56
20:A:7001:LMU:C8	20:A:7001:LMU:H42	2.21	0.56
12:H:14:ILE:O	12:H:16:ASN:N	2.37	0.56
10:F:52:ARG:NH1	10:F:55:ASN:OD1	2.36	0.56
19:B:1766:CLA:CHD	19:B:1766:CLA:HBC3	2.33	0.56
19:3:1222:CLA:H2A	19:3:1222:CLA:O2D	2.05	0.56
16:L:124:LYS:NZ	16:L:124:LYS:HB2	2.19	0.56
16:L:161:LEU:C	16:L:161:LEU:HD12	2.26	0.56
19:3:3011:CLA:CHD	19:3:3011:CLA:HBC2	2.35	0.56
5:A:625:TRP:HB3	5:A:637:ILE:HD11	1.87	0.56
6:B:482:ASN:OD1	6:B:485:ALA:HB2	2.04	0.56
5:A:174:PHE:O	5:A:175:ALA:HB2	2.04	0.56
19:B:1760:CLA:CMA	19:B:1761:CLA:O1A	2.54	0.56
7:C:7:ILE:O	7:C:8:TYR:C	2.42	0.56
7:C:1:MET:HE2	8:D:154:TYR:OH	2.06	0.56
17:N:49:CYS:O	17:N:50:GLN:C	2.44	0.56
17:N:57:LYS:N	17:N:60:PHE:O	2.38	0.56
5:A:249:ILE:C	5:A:251:ASN:H	2.09	0.56
3:3:74:ALA:CA	19:3:1216:CLA:C3D	2.67	0.56
2:2:90:ASP:HB3	2:2:94:LEU:HB2	1.87	0.56
10:F:20:GLN:O	10:F:21:ALA:CB	2.54	0.56
15:K:1:ASP:CA	15:K:5:SER:HB3	2.27	0.56
1:1:48:ARG:O	1:1:52:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:105:ASN:HB2	5:A:140:PHE:CZ	2.41	0.56
5:A:392:GLN:HA	5:A:395:LEU:HD23	1.88	0.56
5:A:66:SER:O	5:A:67:HIS:HB2	2.05	0.56
19:A:1787:CLA:HBB2	19:A:1793:CLA:C20	2.35	0.56
19:A:1783:CLA:H71	23:A:1805:BCR:H372	1.87	0.56
5:A:58:HIS:CE1	19:A:1759:CLA:C1D	2.89	0.56
5:A:79:PHE:HE2	5:A:185:HIS:CE1	2.24	0.56
19:B:1739:CLA:H142	19:B:1739:CLA:H102	1.86	0.56
19:A:1815:CLA:H11	6:B:431:PHE:CE1	2.41	0.56
17:N:63:ASP:N	17:N:64:ASP:C	2.59	0.56
4:4:35:GLU:CB	4:4:36:ASN:HB3	2.28	0.56
15:K:44:GLU:C	15:K:46:GLY:HA2	2.25	0.56
8:D:44:GLU:CB	8:D:46:TYR:HE2	2.08	0.56
5:A:109:TRP:HH2	5:A:154:ARG:HD3	1.70	0.56
8:D:58:PHE:HD2	8:D:59:GLU:H	1.52	0.56
15:K:72:VAL:HG13	15:K:73:GLY:N	2.20	0.56
4:4:81:GLU:O	4:4:82:GLU:HG2	2.06	0.56
6:B:154:TRP:CD1	6:B:158:GLN:CG	2.89	0.56
1:1:115:GLU:HG3	1:1:116:LYS:H	1.71	0.56
1:1:111:GLN:HE21	1:1:111:GLN:HA	1.71	0.56
19:A:1762:CLA:HBA2	19:A:1762:CLA:HED2	1.86	0.56
5:A:302:HIS:HB2	19:A:1773:CLA:CHB	2.35	0.56
19:A:1787:CLA:HMB1	19:A:1800:CLA:HAA2	1.86	0.56
5:A:42:ARG:C	5:A:44:ILE:N	2.59	0.56
5:A:680:LEU:HB3	19:A:1814:CLA:C2	2.36	0.56
19:B:1746:CLA:CBA	19:B:1746:CLA:HED2	2.36	0.56
6:B:278:LEU:O	6:B:281:ALA:N	2.38	0.56
6:B:388:ALA:C	6:B:391:PRO:CD	2.73	0.56
6:B:577:TYR:CE2	6:B:578:LEU:HD12	2.41	0.56
19:2:1215:CLA:HBC2	19:2:1215:CLA:HMC1	1.87	0.56
7:C:28:MET:HB3	8:D:122:LYS:O	2.06	0.56
2:2:203:THR:C	2:2:204:ILE:HG12	2.25	0.56
20:A:7025:LMU:O6B	20:A:7025:LMU:H6D	2.06	0.56
16:L:48:ASN:HB2	16:L:50:LEU:HD22	1.88	0.56
3:3:194:ILE:HA	3:3:197:TYR:CE1	2.40	0.56
5:A:711:HIS:CE1	19:A:1795:CLA:HAC1	2.40	0.56
19:B:1749:CLA:OBD	19:B:1752:CLA:CBC	2.52	0.56
9:E:36:VAL:CG2	9:E:52:VAL:HG22	2.35	0.56
9:E:44:TYR:CZ	9:E:73:ASN:HA	2.41	0.56
19:2:1217:CLA:C9	19:2:1217:CLA:H41	2.29	0.56
20:A:7022:LMU:H1B	20:A:7022:LMU:O2'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:3011:CLA:O2A	19:3:3011:CLA:HMA2	2.06	0.56
5:A:377:TYR:CD1	5:A:616:PHE:HE1	2.24	0.56
6:B:496:GLY:O	6:B:499:ASN:HB2	2.06	0.56
5:A:310:PHE:H	5:A:313:ALA:HB3	1.71	0.56
5:A:462:ILE:HG21	19:A:1789:CLA:CMC	2.36	0.56
5:A:491:TRP:CD1	5:A:492:ILE:HG23	2.41	0.56
5:A:698:GLY:CA	6:B:570:ILE:HG21	2.36	0.56
6:B:120:VAL:HA	6:B:123:TRP:HE1	1.71	0.56
19:B:1756:CLA:H71	23:B:1777:BCR:H14C	1.87	0.56
5:A:699:TYR:O	6:B:536:LYS:NZ	2.38	0.56
6:B:558:PRO:HG2	6:B:703:VAL:CB	2.21	0.56
11:G:24:PHE:CE1	11:G:27:GLN:O	2.59	0.56
13:I:22:ALA:O	13:I:23:SER:C	2.43	0.56
17:N:38:GLY:HA3	17:N:46:PHE:CD1	2.41	0.56
18:R:38:UNK:O	18:R:42:UNK:CB	2.53	0.56
8:D:75:LEU:HD21	16:L:19:PHE:CZ	2.41	0.56
21:B:8052:SUC:O4'	21:B:8052:SUC:H1	2.05	0.56
2:2:191:ASN:CB	21:2:1225:SUC:C6	2.84	0.56
12:H:25:GLY:C	12:H:27:ASP:H	1.93	0.56
20:A:1812:LMU:H52	20:A:1812:LMU:C1	2.36	0.56
19:A:1782:CLA:H101	19:A:1782:CLA:H143	1.88	0.56
5:A:401:TRP:HD1	19:A:1783:CLA:CHC	2.18	0.56
5:A:448:TRP:CD1	19:A:1788:CLA:CED	2.89	0.56
5:A:455:PHE:HD1	19:A:1788:CLA:CMA	2.19	0.56
7:C:5:VAL:HB	7:C:65:VAL:CG2	2.36	0.56
11:G:28:ARG:NH2	11:G:29:GLU:O	2.39	0.56
17:N:61:LEU:O	17:N:62:SER:HB2	2.05	0.56
17:N:76:LYS:HG3	17:N:77:CYS:N	2.12	0.56
18:R:38:UNK:C	18:R:42:UNK:CB	2.83	0.56
8:D:79:ARG:H	8:D:82:GLN:NE2	2.04	0.56
2:2:129:LYS:HA	2:2:131:THR:HG23	1.86	0.56
19:1:1143:CLA:HBC1	20:A:7001:LMU:O3B	2.04	0.56
19:3:3011:CLA:C1	19:3:3011:CLA:HMA2	2.36	0.56
5:A:641:ASN:HD22	5:A:641:ASN:H	1.54	0.56
21:3:1223:SUC:H1'1	21:3:1223:SUC:H6'2	1.88	0.56
16:L:48:ASN:HB3	16:L:49:PRO:CD	2.36	0.56
6:B:213:LEU:HD12	6:B:214:ASP:N	2.21	0.56
8:D:48:ILE:HG22	8:D:83:CYS:HB2	1.86	0.56
12:H:67:TYR:CD1	12:H:67:TYR:C	2.80	0.56
10:F:17:ARG:HA	10:F:17:ARG:NE	2.20	0.56
17:N:25:THR:CG2	17:N:26:GLY:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:475:ASP:HA	6:B:480:SER:HA	1.88	0.56
6:B:49:SER:O	6:B:52:GLY:N	2.39	0.56
5:A:124:TRP:HD1	19:A:1765:CLA:HED2	1.71	0.56
23:A:1809:BCR:HC8	23:A:1809:BCR:H311	1.87	0.56
5:A:672:LEU:HD23	5:A:672:LEU:H	1.71	0.56
19:B:1768:CLA:CGA	19:B:1768:CLA:C1A	2.84	0.56
6:B:305:LEU:O	6:B:306:GLU:C	2.44	0.56
6:B:731:GLY:O	6:B:732:LYS:HB2	2.04	0.56
9:E:63:TYR:HA	9:E:83:ALA:HB2	1.88	0.56
23:I:1032:BCR:H311	23:I:1032:BCR:C8	2.35	0.56
3:3:97:PHE:CE2	3:3:98:ILE:HG21	2.35	0.56
3:3:49:ILE:HA	3:3:51:PRO:HD2	1.88	0.56
4:4:84:PHE:O	4:4:85:ALA:CB	2.54	0.56
4:4:106:TRP:CE3	19:4:1209:CLA:HMA1	2.40	0.55
5:A:32:GLU:OE2	19:A:1767:CLA:HMA2	2.06	0.55
19:A:1777:CLA:C1C	19:A:1777:CLA:H52	2.36	0.55
23:A:1808:BCR:C33	19:L:1167:CLA:NB	2.44	0.55
5:A:578:ARG:O	5:A:579:PHE:CD1	2.59	0.55
6:B:55:ALA:HB1	6:B:150:LEU:CD1	2.37	0.55
6:B:649:MET:O	6:B:653:GLY:N	2.38	0.55
9:E:73:ASN:C	9:E:73:ASN:HD22	2.08	0.55
13:I:11:LEU:HG	23:I:1032:BCR:HC7	1.85	0.55
19:A:1789:CLA:O1D	16:L:73:PRO:HA	2.04	0.55
3:3:48:PHE:CD2	3:3:49:ILE:CG2	2.69	0.55
2:2:171:MET:HE3	2:2:175:MET:HB2	1.87	0.55
8:D:113:HIS:N	8:D:114:PRO:CD	2.69	0.55
1:1:149:LYS:HB3	19:1:1192:CLA:CMC	2.35	0.55
17:N:1:GLY:O	17:N:2:VAL:CG1	2.53	0.55
16:L:128:ASP:CG	16:L:129:GLN:N	2.59	0.55
12:H:63:SER:O	12:H:67:TYR:CB	2.54	0.55
6:B:681:ALA:O	6:B:684:ARG:N	2.30	0.55
5:A:123:VAL:HG22	5:A:133:ASN:OD1	2.06	0.55
5:A:81:ALA:CA	19:A:1760:CLA:HMA1	2.35	0.55
19:A:1800:CLA:C9	23:L:1169:BCR:H321	2.36	0.55
5:A:214:GLY:O	5:A:215:SER:CB	2.53	0.55
19:B:1753:CLA:CMC	19:B:1753:CLA:HBC3	2.32	0.55
19:B:1768:CLA:C6	23:B:1779:BCR:H323	2.36	0.55
6:B:645:VAL:HG11	19:B:1739:CLA:HAC1	1.88	0.55
6:B:646:TRP:O	6:B:649:MET:HB2	2.06	0.55
9:E:87:VAL:C	9:E:89:GLU:N	2.57	0.55
10:F:103:SER:C	10:F:105:LEU:N	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:I:1032:BCR:C39	23:L:1169:BCR:H401	2.35	0.55
8:D:75:LEU:HD22	8:D:76:LYS:H	1.70	0.55
3:3:201:ALA:C	3:3:202:LEU:HD22	2.27	0.55
6:B:666:SER:CB	6:B:671:TRP:HE1	2.14	0.55
13:I:2:ILE:HG12	13:I:3:ASN:ND2	2.21	0.55
8:D:48:ILE:CG2	8:D:83:CYS:HB2	2.37	0.55
5:A:478:SER:C	5:A:480:THR:H	2.10	0.55
5:A:436:LEU:O	5:A:439:ARG:HB3	2.05	0.55
1:1:185:TRP:CH2	19:1:1199:CLA:H2	2.41	0.55
5:A:144:GLN:CG	5:A:145:ILE:H	2.19	0.55
19:A:1783:CLA:H72	23:A:1805:BCR:H371	1.87	0.55
19:A:1790:CLA:H2A	19:A:1790:CLA:O1D	2.05	0.55
5:A:472:ARG:HG2	6:B:97:GLY:HA3	1.88	0.55
19:B:1751:CLA:CHD	19:B:1751:CLA:CBC	2.83	0.55
5:A:709:TRP:CZ3	6:B:417:ALA:HA	2.42	0.55
6:B:559:CYS:HB2	6:B:702:ILE:HD12	1.87	0.55
6:B:670:TYR:C	6:B:670:TYR:CD1	2.80	0.55
19:1:1142:CLA:OBD	19:1:1143:CLA:CHB	2.55	0.55
5:A:230:ASN:HA	5:A:233:LEU:HB2	1.88	0.55
20:A:7036:LMU:H11	20:A:7036:LMU:H92	1.87	0.55
5:A:103:PHE:HE1	19:A:1763:CLA:CGD	2.19	0.55
19:A:1788:CLA:C14	19:A:1788:CLA:H101	2.36	0.55
5:A:255:LEU:HD11	5:A:280:PHE:HZ	1.71	0.55
5:A:88:ILE:HG22	5:A:89:ILE:H	1.72	0.55
6:B:167:TRP:CZ2	19:B:1743:CLA:HAC2	2.41	0.55
6:B:195:VAL:HA	6:B:199:ILE:HG13	1.89	0.55
6:B:17:THR:HA	6:B:696:LYS:H	1.71	0.55
4:4:73:PRO:O	4:4:74:LYS:CG	2.54	0.55
16:L:165:TYR:CG	16:L:165:TYR:O	2.58	0.55
9:E:69:PHE:HD2	9:E:71:LYS:HG2	1.72	0.55
5:A:586:ARG:H	7:C:49:VAL:CG2	2.18	0.55
5:A:514:THR:HB	5:A:532:ILE:CG2	2.37	0.55
5:A:479:ASP:OD2	5:A:536:THR:HG23	2.05	0.55
18:R:26:UNK:O	18:R:27:UNK:C	2.55	0.55
5:A:132:LEU:HD23	6:B:446:PHE:HE1	1.72	0.55
19:A:1764:CLA:HBB2	19:A:1765:CLA:C3D	2.36	0.55
6:B:50:HIS:HA	6:B:53:GLN:HB2	1.89	0.55
6:B:573:TRP:O	6:B:577:TYR:N	2.31	0.55
7:C:62:PHE:CE1	9:E:42:GLU:HB2	2.41	0.55
3:3:50:GLU:H	3:3:51:PRO:HD3	1.71	0.55
5:A:269:PHE:HE1	15:K:14:THR:CG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:102:ILE:HD11	19:2:1222:CLA:HMD1	1.87	0.55
12:H:21:TRP:H	12:H:22:ASP:HB3	1.72	0.55
10:F:22:LEU:C	10:F:24:LYS:H	2.09	0.55
20:2:1224:LMU:O5'	20:2:1224:LMU:C2	2.53	0.55
10:F:131:PHE:O	10:F:133:GLY:N	2.40	0.55
20:A:7034:LMU:O2B	20:A:7034:LMU:H6D	2.06	0.55
18:R:8:UNK:CB	19:R:1054:CLA:CED	2.84	0.55
6:B:529:THR:O	6:B:533:ILE:HG22	2.07	0.55
12:H:36:GLN:O	12:H:36:GLN:HG2	2.05	0.55
4:4:107:GLN:O	19:4:1196:CLA:HMA1	2.04	0.55
19:A:1789:CLA:HBC2	19:H:1079:CLA:HBC1	1.88	0.55
5:A:393:LEU:HG	5:A:394:SER:N	2.21	0.55
5:A:432:LEU:C	5:A:434:ARG:N	2.59	0.55
6:B:197:VAL:O	6:B:198:ALA:HB2	2.06	0.55
6:B:203:ARG:HB3	6:B:270:LEU:HD12	1.87	0.55
7:C:55:GLU:HG3	7:C:60:THR:HG22	1.88	0.55
4:4:71:ASN:C	4:4:73:PRO:HD3	2.27	0.55
17:N:73:ASP:O	17:N:75:TYR:N	2.39	0.55
17:N:4:GLU:O	17:N:4:GLU:HG3	2.06	0.55
2:2:59:ALA:CB	2:2:172:LEU:HD22	2.36	0.55
19:3:1221:CLA:CBC	19:3:1221:CLA:CHD	2.77	0.55
20:A:7020:LMU:H5B	20:A:7020:LMU:O6'	2.06	0.55
2:2:44:ASN:HD21	14:J:1:MET:HB2	1.70	0.55
3:3:202:LEU:HB3	3:3:204:THR:HG23	1.87	0.55
5:A:464:ASN:O	5:A:468:SER:N	2.39	0.55
5:A:396:PHE:O	5:A:396:PHE:CG	2.58	0.55
7:C:35:LYS:C	7:C:37:LYS:H	2.08	0.55
4:4:105:ARG:HG3	4:4:105:ARG:O	2.05	0.55
4:4:160:MET:HE1	19:4:1201:CLA:CAB	2.34	0.55
4:4:95:PHE:HD1	4:4:95:PHE:H	1.51	0.55
19:A:1813:CLA:HMB3	19:A:1814:CLA:HMD1	1.89	0.55
5:A:707:ILE:C	5:A:711:HIS:HD2	2.10	0.55
6:B:124:TRP:C	6:B:124:TRP:CD1	2.79	0.55
6:B:132:ASN:HA	6:B:135:LEU:HG	1.88	0.55
6:B:174:ARG:CB	19:B:1743:CLA:CBC	2.79	0.55
6:B:424:TRP:CE2	19:B:1761:CLA:HAC1	2.42	0.55
6:B:544:SER:O	6:B:546:LEU:N	2.39	0.55
17:N:54:LYS:HB3	17:N:57:LYS:CE	2.37	0.55
17:N:65:LEU:O	17:N:66:ASP:C	2.44	0.55
19:3:1218:CLA:CHD	19:3:1218:CLA:HBC3	2.31	0.55
14:J:9:SER:O	14:J:10:VAL:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:188:PRO:HB2	2:2:189:ILE:HD13	1.88	0.55
5:A:308:ILE:HG21	19:A:1772:CLA:HMC2	1.87	0.55
19:B:1755:CLA:HBA1	19:B:1756:CLA:HED3	1.88	0.55
6:B:292:ARG:NH2	6:B:297:ILE:H	2.04	0.55
3:3:199:VAL:HG22	19:3:1215:CLA:C3C	2.36	0.55
17:N:67:LEU:HB2	17:N:68:GLU:CB	2.37	0.55
5:A:25:ASP:HA	5:A:27:ILE:N	2.22	0.55
11:G:93:TYR:HA	11:G:94:ASP:CG	2.26	0.55
20:2:1224:LMU:O5'	20:2:1224:LMU:H32	2.07	0.55
19:1:1145:CLA:CGA	19:1:1145:CLA:C3A	2.85	0.55
16:L:161:LEU:HD12	16:L:162:ASP:C	2.26	0.55
18:R:27:UNK:C	18:R:29:UNK:H	2.14	0.55
1:1:182:ALA:O	1:1:183:ASP:O	2.24	0.55
4:4:121:PHE:HB2	4:4:128:ALA:HB3	1.89	0.55
5:A:372:VAL:HG22	19:A:1774:CLA:C4	2.37	0.55
19:A:1762:CLA:O1A	19:A:1785:CLA:HMB2	2.06	0.55
19:A:1816:CLA:CBB	19:A:1817:CLA:CHB	2.84	0.55
5:A:225:VAL:O	5:A:229:ILE:HB	2.07	0.55
5:A:98:PHE:O	5:A:99:HIS:CB	2.54	0.55
19:B:1758:CLA:H101	23:B:1776:BCR:H343	1.89	0.55
23:B:1776:BCR:H331	23:B:1776:BCR:HC8	1.87	0.55
6:B:304:ILE:HD11	19:B:1749:CLA:HED2	1.87	0.55
6:B:535:VAL:HG22	6:B:539:LEU:HD23	1.89	0.55
18:R:38:UNK:C	18:R:42:UNK:C	2.85	0.55
19:2:1222:CLA:CBC	19:2:1222:CLA:HMC1	2.35	0.55
19:1:1197:CLA:CAD	19:1:1197:CLA:CED	2.84	0.55
19:1:1197:CLA:OBD	19:1:1197:CLA:HED2	2.07	0.55
19:3:1218:CLA:O2D	19:3:1218:CLA:H2A	2.06	0.55
19:1:1308:CLA:CMA	19:2:1223:CLA:HED2	2.32	0.55
7:C:11:CYS:SG	7:C:12:ILE:N	2.79	0.55
8:D:122:LYS:NZ	8:D:124:ASN:OD1	2.40	0.55
5:A:425:THR:O	5:A:428:TYR:CE1	2.60	0.55
8:D:60:MET:HG3	8:D:61:PRO:O	2.07	0.55
18:R:8:UNK:CB	19:R:1054:CLA:O2D	2.55	0.55
8:D:64:GLY:O	8:D:65:ALA:CB	2.55	0.55
1:1:167:ALA:C	1:1:169:PRO:HD3	2.27	0.55
6:B:31:PHE:O	6:B:37:ILE:HG21	2.06	0.55
11:G:83:TYR:O	11:G:83:TYR:CG	2.59	0.55
4:4:101:VAL:O	4:4:104:ARG:NH2	2.40	0.55
19:A:1764:CLA:HAA2	19:A:1783:CLA:HED3	1.89	0.55
5:A:281:LEU:O	5:A:283:PHE:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:584:PRO:HG3	6:B:559:CYS:SG	2.46	0.55
19:B:1739:CLA:CGA	19:B:1739:CLA:C1A	2.85	0.55
19:B:1749:CLA:HBB2	19:B:1754:CLA:H41	1.88	0.55
19:B:1759:CLA:HMD2	24:B:1781:LMG:H341	1.89	0.55
6:B:187:SER:O	6:B:188:LEU:C	2.43	0.55
6:B:291:TYR:CE1	19:B:1749:CLA:HED1	2.42	0.55
6:B:646:TRP:CH2	6:B:726:ILE:HG21	2.42	0.55
11:G:43:HIS:CB	11:G:44:PHE:CD1	2.76	0.55
20:A:7032:LMU:O1'	20:A:7032:LMU:H1B	2.07	0.55
20:A:7023:LMU:O6'	20:A:7023:LMU:H1'	2.07	0.55
10:F:58:LYS:O	10:F:60:GLY:N	2.40	0.55
5:A:284:ARG:HA	5:A:284:ARG:NH1	2.21	0.55
5:A:284:ARG:HH22	5:A:507:ALA:C	2.10	0.55
17:N:33:TYR:O	17:N:34:THR:CG2	2.55	0.55
6:B:261:PHE:CZ	6:B:500:ALA:HB2	2.42	0.55
5:A:418:MET:O	5:A:564:ARG:HD2	2.06	0.55
11:G:78:GLY:O	11:G:79:HIS:ND1	2.40	0.55
4:4:158:ARG:HA	4:4:161:LEU:CD1	2.36	0.54
4:4:52:MET:CE	4:4:156:ASN:HB2	2.37	0.54
4:4:99:HIS:ND1	4:4:99:HIS:C	2.59	0.54
5:A:79:PHE:CE2	5:A:185:HIS:CE1	2.95	0.54
5:A:362:LEU:CB	5:A:410:ALA:HB2	2.35	0.54
19:B:1750:CLA:HBB2	11:G:18:LEU:HD13	1.88	0.54
6:B:29:HIS:CD2	19:B:1737:CLA:CBB	2.90	0.54
2:2:129:LYS:C	2:2:131:THR:N	2.60	0.54
15:K:39:LYS:N	15:K:39:LYS:HD2	2.21	0.54
3:3:158:TYR:OH	19:3:1214:CLA:C2B	2.54	0.54
6:B:232:LEU:HD21	6:B:235:GLN:OE1	2.08	0.54
5:A:394:SER:HB2	19:A:1783:CLA:CMA	2.30	0.54
5:A:462:ILE:CD1	19:A:1816:CLA:H72	2.37	0.54
6:B:124:TRP:CG	6:B:129:LEU:HD13	2.42	0.54
6:B:292:ARG:HH22	6:B:297:ILE:HG13	1.72	0.54
16:L:36:TYR:O	16:L:37:LEU:HB3	2.06	0.54
3:3:98:ILE:C	17:N:63:ASP:O	2.45	0.54
17:N:62:SER:HB2	17:N:66:ASP:OD1	2.07	0.54
3:3:56:TYR:HD1	3:3:185:LYS:HZ1	1.52	0.54
21:H:1082:SUC:O2	21:H:1082:SUC:H5	2.06	0.54
12:H:21:TRP:H	12:H:22:ASP:HA	1.68	0.54
4:4:147:LEU:HD22	4:4:148:GLU:N	2.22	0.54
20:2:1224:LMU:C3	20:2:1224:LMU:H72	2.37	0.54
19:4:4014:CLA:CED	19:4:4014:CLA:HBA1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:81:GLU:O	4:4:82:GLU:CG	2.55	0.54
2:2:79:TRP:CD1	2:2:81:THR:CG2	2.91	0.54
3:3:134:LYS:O	3:3:135:PRO:C	2.45	0.54
4:4:160:MET:CE	4:4:163:PHE:CD2	2.89	0.54
5:A:406:LEU:HD11	19:A:1762:CLA:HMB3	1.90	0.54
19:A:1765:CLA:H51	23:A:1806:BCR:H10C	1.90	0.54
5:A:401:TRP:CB	19:A:1783:CLA:HMC3	2.38	0.54
5:A:581:CYS:HB2	5:A:590:CYS:O	2.07	0.54
6:B:292:ARG:HH22	19:B:1750:CLA:HED1	1.72	0.54
6:B:561:GLY:HA3	7:C:52:LYS:CB	2.38	0.54
9:E:36:VAL:C	9:E:49:VAL:HG13	2.28	0.54
9:E:45:TRP:CZ3	9:E:78:SER:OG	2.61	0.54
19:A:1800:CLA:C19	16:L:60:HIS:HD1	2.19	0.54
17:N:61:LEU:HG	17:N:64:ASP:HB2	1.89	0.54
7:C:44:ARG:HH21	8:D:127:ARG:CB	2.09	0.54
20:A:7010:LMU:O3'	20:A:7010:LMU:H1B	2.08	0.54
6:B:393:PHE:CD2	6:B:397:ASP:OD1	2.53	0.54
2:2:41:LEU:O	2:2:43:TRP:N	2.41	0.54
4:4:103:ILE:CG1	19:4:1197:CLA:HMD1	2.35	0.54
5:A:157:GLY:O	5:A:158:ILE:HB	2.07	0.54
19:A:1763:CLA:HBA2	19:A:1765:CLA:C1	2.36	0.54
5:A:747:TRP:CE3	23:A:1805:BCR:C40	2.90	0.54
19:A:1817:CLA:HED3	19:A:1817:CLA:HBA2	1.89	0.54
5:A:612:VAL:O	5:A:615:HIS:HB3	2.07	0.54
5:A:714:LEU:HD13	23:B:1779:BCR:H393	1.89	0.54
6:B:178:HIS:HE1	19:B:1743:CLA:NC	2.05	0.54
6:B:282:PHE:HE2	19:B:1746:CLA:H3A	1.72	0.54
9:E:41:ARG:HG3	9:E:46:PHE:CZ	2.42	0.54
19:3:1221:CLA:HBB1	19:3:1221:CLA:HHC	1.88	0.54
19:2:1223:CLA:C3A	19:2:1223:CLA:CGA	2.86	0.54
6:B:228:GLY:HA3	11:G:8:ILE:HB	1.88	0.54
3:3:66:MET:HG2	3:3:195:LEU:HD11	1.88	0.54
5:A:176:GLY:O	5:A:180:PHE:HB2	2.08	0.54
21:B:8061:SUC:H1'2	21:B:8061:SUC:O5	2.07	0.54
5:A:158:ILE:HG23	5:A:163:GLN:NE2	2.23	0.54
19:A:1773:CLA:H51	19:A:1782:CLA:HMB1	1.89	0.54
5:A:361:ASN:HD22	5:A:361:ASN:C	2.11	0.54
5:A:678:PHE:O	5:A:681:GLY:O	2.25	0.54
6:B:124:TRP:CZ2	6:B:135:LEU:HD22	2.43	0.54
6:B:412:LEU:O	6:B:415:LYS:HB3	2.07	0.54
6:B:555:TYR:O	6:B:571:SER:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:94:ARG:HH12	3:3:98:ILE:CG2	2.19	0.54
17:N:38:GLY:HA3	17:N:46:PHE:HD1	1.72	0.54
17:N:48:GLY:CA	17:N:49:CYS:SG	2.96	0.54
5:A:22:VAL:HB	5:A:24:ARG:N	2.22	0.54
1:1:29:LEU:O	1:1:31:GLU:N	2.41	0.54
19:2:1223:CLA:C3A	19:2:1223:CLA:O1A	2.44	0.54
3:3:156:PRO:O	3:3:157:ALA:C	2.46	0.54
6:B:664:LEU:C	6:B:667:TRP:CZ3	2.77	0.54
19:B:1766:CLA:HBC2	19:B:1766:CLA:CHD	2.32	0.54
10:F:40:LEU:HA	10:F:42:ILE:CG1	2.34	0.54
16:L:123:ARG:HB3	16:L:126:GLN:CG	2.37	0.54
2:2:85:GLN:OE1	2:2:86:GLU:N	2.41	0.54
4:4:81:GLU:O	4:4:82:GLU:HB3	2.06	0.54
6:B:409:ALA:C	6:B:411:MET:N	2.60	0.54
2:2:143:PHE:CD1	2:2:144:ASP:N	2.76	0.54
4:4:107:GLN:HA	19:4:1196:CLA:H2A	1.90	0.54
4:4:93:ILE:O	4:4:96:ILE:HD12	2.08	0.54
19:A:1781:CLA:O1A	19:A:1781:CLA:C2	2.52	0.54
5:A:213:LEU:O	5:A:217:SER:HB2	2.07	0.54
5:A:308:ILE:CG2	5:A:309:LEU:N	2.70	0.54
5:A:664:VAL:HG11	5:A:749:PHE:HA	1.88	0.54
5:A:697:ARG:NH1	5:A:724:ALA:HB3	2.22	0.54
6:B:421:HIS:NE2	19:B:1761:CLA:C1D	2.69	0.54
6:B:732:LYS:HD3	6:B:734:GLY:CA	2.33	0.54
10:F:78:ARG:O	10:F:80:TRP:HD1	1.90	0.54
19:B:1768:CLA:CBC	10:F:83:PHE:HZ	2.20	0.54
2:2:203:THR:C	2:2:204:ILE:CG1	2.76	0.54
4:4:117:GLN:O	4:4:122:LYS:O	2.24	0.54
5:A:207:LEU:HB3	19:A:1776:CLA:HBB2	1.89	0.54
19:A:1781:CLA:HBA2	19:A:1794:CLA:CED	2.32	0.54
5:A:740:LEU:HD13	19:A:1796:CLA:HMA1	1.89	0.54
5:A:295:TRP:HB2	5:A:298:ASP:OD2	2.08	0.54
5:A:472:ARG:HH22	16:L:74:LEU:CD2	2.21	0.54
6:B:438:VAL:HG21	19:B:1763:CLA:HMC1	1.88	0.54
6:B:519:VAL:HG11	6:B:593:TYR:HB2	1.89	0.54
7:C:6:LYS:HE2	8:D:137:ILE:HG12	1.90	0.54
9:E:53:VAL:O	9:E:55:VAL:N	2.40	0.54
11:G:48:ASP:N	11:G:48:ASP:OD2	2.41	0.54
6:B:231:ASN:OD1	11:G:5:SER:HB2	2.08	0.54
17:N:62:SER:CA	17:N:66:ASP:H	2.21	0.54
17:N:66:ASP:O	17:N:67:LEU:CG	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:39:TRP:CA	4:4:40:PHE:HD1	2.19	0.54
3:3:53:TRP:HA	3:3:56:TYR:HD2	1.73	0.54
10:F:42:ILE:CG1	10:F:43:LYS:N	2.66	0.54
5:A:425:THR:OG1	5:A:428:TYR:HE1	1.91	0.54
8:D:102:ARG:NH2	8:D:109:VAL:O	2.40	0.54
20:A:7011:LMU:H42	20:A:7011:LMU:O1'	2.08	0.54
6:B:289:LEU:O	19:B:1751:CLA:HAC1	2.08	0.54
6:B:707:LEU:HD11	6:B:711:VAL:HG21	1.90	0.54
7:C:1:MET:N	7:C:4:SER:N	2.42	0.54
10:F:144:LEU:CD1	10:F:149:LEU:HD13	2.37	0.54
11:G:30:ASN:HD22	11:G:30:ASN:C	2.10	0.54
11:G:43:HIS:HE1	11:G:45:GLU:HG2	1.72	0.54
19:H:1080:CLA:CAC	23:I:1032:BCR:C2	2.86	0.54
4:4:33:ASP:CB	4:4:34:PRO:HD3	2.37	0.54
20:A:7042:LMU:H5'	20:A:7042:LMU:C2B	2.37	0.54
4:4:62:GLU:C	4:4:65:THR:HG22	2.28	0.54
5:A:393:LEU:HD11	5:A:750:PHE:CD1	2.42	0.54
5:A:88:ILE:CG2	5:A:89:ILE:N	2.70	0.54
19:B:1738:CLA:C19	19:B:1757:CLA:H141	2.38	0.54
6:B:724:PHE:CD1	19:B:1784:CLA:HMD1	2.43	0.54
6:B:463:ILE:O	6:B:464:GLN:CB	2.54	0.54
6:B:654:HIS:HE1	19:B:1784:CLA:NB	2.05	0.54
9:E:52:VAL:C	9:E:53:VAL:HG23	2.26	0.54
9:E:36:VAL:HG22	9:E:52:VAL:CG2	2.38	0.54
10:F:104:TYR:O	10:F:104:TYR:CD2	2.60	0.54
16:L:52:ARG:O	16:L:56:VAL:HG23	2.08	0.54
16:L:96:SER:OG	16:L:143:PHE:HD2	1.91	0.54
3:3:106:TYR:HB3	3:3:107:TRP:HD1	1.71	0.54
6:B:171:ALA:O	6:B:172:GLU:HB2	2.08	0.54
4:4:90:LEU:CD2	4:4:90:LEU:N	2.71	0.54
5:A:114:THR:O	5:A:525:ASN:ND2	2.41	0.54
19:A:1781:CLA:HAA2	19:A:1782:CLA:CAD	2.38	0.54
5:A:281:LEU:HD22	19:A:1772:CLA:HMA3	1.90	0.54
5:A:491:TRP:HE1	19:A:1792:CLA:C1	2.21	0.54
6:B:557:PHE:N	6:B:558:PRO:HD2	2.18	0.54
6:B:294:ASN:OD1	11:G:38:GLN:N	2.41	0.54
8:D:27:PRO:O	16:L:19:PHE:HZ	1.91	0.54
20:A:7020:LMU:H3B	20:A:7020:LMU:O6'	2.08	0.54
2:2:174:VAL:O	2:2:178:TRP:HD1	1.85	0.54
19:1:1148:CLA:H2A	19:1:1148:CLA:O2D	2.06	0.54
19:4:4014:CLA:CBA	19:4:4014:CLA:O2D	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:425:THR:O	5:A:427:ARG:NE	2.40	0.54
19:J:1043:CLA:HAA1	19:J:1043:CLA:H143	1.90	0.54
16:L:54:VAL:O	16:L:58:LEU:HB2	2.07	0.54
5:A:439:ARG:HG2	5:A:562:PHE:CE2	2.42	0.54
5:A:263:ALA:O	5:A:264:GLU:HG3	2.08	0.54
4:4:95:PHE:CZ	19:4:1210:CLA:C1C	2.91	0.53
5:A:158:ILE:HG23	5:A:163:GLN:HE22	1.73	0.53
19:A:1781:CLA:O2A	19:A:1794:CLA:O2D	2.26	0.53
23:A:1807:BCR:C4	19:A:1817:CLA:H142	2.37	0.53
23:B:1775:BCR:HC8	23:B:1775:BCR:H331	1.91	0.53
22:A:1802:PQN:C13	23:B:1778:BCR:H322	2.38	0.53
5:A:653:LEU:HD23	19:B:1784:CLA:HBC2	1.89	0.53
6:B:458:ILE:HG13	6:B:459:PHE:N	2.22	0.53
7:C:74:THR:C	7:C:76:SER:H	2.11	0.53
15:K:46:GLY:C	15:K:47:LEU:HG	2.28	0.53
3:3:49:ILE:HG13	3:3:52:LYS:HB2	1.90	0.53
20:A:7009:LMU:H3'	20:A:7009:LMU:O5B	2.07	0.53
4:4:119:PRO:CG	19:4:1208:CLA:C2D	2.73	0.53
4:4:44:GLU:O	4:4:46:VAL:N	2.41	0.53
19:A:1782:CLA:CGD	19:A:1782:CLA:HBA1	2.38	0.53
19:A:1789:CLA:H171	19:A:1793:CLA:C20	2.38	0.53
5:A:466:THR:CG2	19:B:1740:CLA:CHC	2.74	0.53
5:A:704:ILE:HA	5:A:707:ILE:HG13	1.89	0.53
5:A:558:LYS:NZ	6:B:674:LEU:HD23	2.22	0.53
6:B:70:TRP:NE1	6:B:71:GLN:OE1	2.41	0.53
6:B:560:ASP:HB2	7:C:66:ARG:HE	1.71	0.53
9:E:37:LYS:HB2	9:E:49:VAL:HG22	1.90	0.53
16:L:14:LEU:CD2	16:L:21:GLY:O	2.57	0.53
16:L:163:LEU:CD1	16:L:163:LEU:C	2.75	0.53
8:D:46:TYR:CD2	8:D:46:TYR:N	2.76	0.53
19:1:1143:CLA:C3A	19:1:1143:CLA:CGA	2.84	0.53
15:K:43:ARG:CG	15:K:43:ARG:NH1	2.52	0.53
20:A:7021:LMU:C2	20:A:7021:LMU:H62	2.21	0.53
5:A:233:LEU:O	5:A:235:ALA:N	2.36	0.53
20:A:7023:LMU:H82	20:A:7023:LMU:C3	2.36	0.53
4:4:115:VAL:HG13	4:4:116:ASN:H	1.72	0.53
4:4:118:ASP:OD2	19:4:1200:CLA:HMA1	2.08	0.53
19:4:1201:CLA:C2	19:4:1201:CLA:O1A	2.54	0.53
19:A:1765:CLA:CBD	19:A:1765:CLA:HBA2	2.38	0.53
19:A:1788:CLA:H52	23:B:1780:BCR:C34	2.36	0.53
5:A:216:LEU:HD12	23:A:1803:BCR:C35	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1771:CLA:CBB	23:A:1803:BCR:H352	2.38	0.53
19:A:1813:CLA:HBB2	19:A:1814:CLA:HED1	1.91	0.53
5:A:79:PHE:HE2	5:A:185:HIS:CD2	2.22	0.53
5:A:207:LEU:HA	5:A:211:LEU:CG	2.38	0.53
5:A:246:HIS:O	5:A:248:PHE:CD2	2.56	0.53
5:A:497:ALA:HA	5:A:510:SER:OG	2.08	0.53
9:E:44:TYR:CD2	9:E:45:TRP:HE3	2.25	0.53
17:N:75:TYR:C	17:N:76:LYS:O	2.44	0.53
6:B:406:ASN:ND2	6:B:406:ASN:C	2.62	0.53
2:2:98:GLU:OE2	19:2:1222:CLA:ND	2.40	0.53
4:4:147:LEU:CG	4:4:148:GLU:N	2.70	0.53
19:B:1766:CLA:O1D	19:B:1766:CLA:C2A	2.53	0.53
10:F:153:ASN:ND2	10:F:153:ASN:O	2.41	0.53
20:A:7033:LMU:C5B	20:A:7033:LMU:H3'	2.37	0.53
20:A:7025:LMU:O6B	20:A:7025:LMU:C6'	2.57	0.53
8:D:28:ILE:CG2	8:D:67:ILE:HG13	2.37	0.53
1:1:136:ASP:HB2	1:1:140:LEU:HB3	1.89	0.53
6:B:475:ASP:CA	6:B:480:SER:HA	2.38	0.53
5:A:462:ILE:CG2	19:A:1789:CLA:HMC3	2.38	0.53
23:A:1807:BCR:H272	23:I:1032:BCR:H352	1.89	0.53
19:B:1762:CLA:H51	23:B:1779:BCR:C40	2.38	0.53
5:A:698:GLY:HA3	6:B:570:ILE:HG21	1.91	0.53
6:B:574:ASP:OD2	6:B:706:ARG:NE	2.42	0.53
19:H:1080:CLA:CHD	23:I:1032:BCR:HC22	2.38	0.53
16:L:41:PRO:HG3	16:L:52:ARG:HD3	1.91	0.53
17:N:59:PRO:CA	17:N:66:ASP:OD1	2.57	0.53
17:N:80:ASN:O	17:N:82:PHE:HD2	1.92	0.53
2:2:128:ASN:ND2	14:J:4:PHE:H	2.06	0.53
20:A:7023:LMU:C9	20:A:7023:LMU:C4	2.86	0.53
16:L:124:LYS:C	16:L:126:GLN:N	2.61	0.53
4:4:150:LYS:HG2	4:4:150:LYS:O	2.05	0.53
5:A:123:VAL:HB	5:A:129:GLN:OE1	2.09	0.53
19:A:1788:CLA:HAA1	23:A:1808:BCR:C14	2.39	0.53
5:A:472:ARG:O	5:A:474:GLN:HG3	2.09	0.53
19:B:1756:CLA:H122	23:B:1777:BCR:H14C	1.91	0.53
6:B:696:LYS:HD2	7:C:81:TYR:HA	1.90	0.53
6:B:724:PHE:CE1	19:B:1784:CLA:HMD1	2.43	0.53
7:C:5:VAL:CB	7:C:65:VAL:HG22	2.37	0.53
9:E:87:VAL:O	9:E:87:VAL:HG12	2.07	0.53
18:R:30:UNK:C	18:R:32:UNK:N	2.72	0.53
2:2:68:LEU:O	2:2:70:LYS:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:22:LEU:HB3	10:F:23:LYS:NZ	2.24	0.53
6:B:20:ARG:CG	6:B:20:ARG:HH11	2.21	0.53
6:B:117:TYR:O	6:B:367:THR:HG23	2.09	0.53
19:4:1199:CLA:H2	19:4:1199:CLA:CED	2.39	0.53
19:A:1765:CLA:CHA	19:A:1765:CLA:HBA2	2.37	0.53
5:A:281:LEU:CD1	19:A:1772:CLA:HED2	2.39	0.53
5:A:578:ARG:NH1	5:A:578:ARG:HB2	2.23	0.53
5:A:581:CYS:CB	5:A:590:CYS:O	2.56	0.53
6:B:189:ALA:HB1	19:B:1758:CLA:H203	1.90	0.53
19:B:1765:CLA:CMB	23:B:1777:BCR:H391	2.38	0.53
6:B:615:TYR:HD1	6:B:615:TYR:N	2.06	0.53
1:1:27:LEU:HD12	1:1:28:GLY:H	1.72	0.53
3:3:56:TYR:O	3:3:60:ILE:HD12	2.07	0.53
8:D:124:ASN:CB	8:D:125:PRO:CD	2.85	0.53
20:A:7033:LMU:H6'2	20:A:7033:LMU:O2'	2.09	0.53
20:A:7033:LMU:C3'	20:A:7033:LMU:O5B	2.56	0.53
8:D:94:TYR:O	8:D:95:LYS:CB	2.57	0.53
4:4:168:ILE:HG13	4:4:168:ILE:O	2.09	0.53
19:A:1790:CLA:CAD	19:A:1791:CLA:HAC1	2.37	0.53
5:A:648:THR:CG2	5:A:651:GLY:H	2.16	0.53
6:B:143:LEU:C	6:B:145:LEU:N	2.61	0.53
6:B:334:LEU:CB	19:B:1737:CLA:HMD3	2.36	0.53
6:B:293:THR:O	6:B:294:ASN:ND2	2.41	0.53
6:B:310:PRO:HB2	6:B:311:PRO:HD2	1.91	0.53
8:D:31:GLY:HA3	16:L:23:LEU:CD2	2.39	0.53
19:B:1768:CLA:CBC	10:F:83:PHE:CZ	2.83	0.53
13:I:19:VAL:O	13:I:23:SER:N	2.42	0.53
6:B:25:ILE:HG22	23:L:1169:BCR:H282	1.89	0.53
17:N:66:ASP:C	17:N:67:LEU:HD12	2.29	0.53
7:C:59:PRO:HB3	7:C:61:ASP:OD1	2.08	0.53
2:2:51:HIS:HA	2:2:54:TRP:HB2	1.91	0.53
19:1:1142:CLA:HMD3	19:1:1143:CLA:ND	2.23	0.53
5:A:118:PRO:HB3	5:A:150:PHE:CE2	2.43	0.53
11:G:60:SER:CA	11:G:63:PRO:HD2	2.31	0.53
20:A:7040:LMU:C1B	20:A:7040:LMU:H3O2	2.22	0.53
20:A:7038:LMU:H62	20:A:7038:LMU:C10	2.38	0.53
6:B:224:PRO:O	6:B:226:LEU:N	2.42	0.53
6:B:44:GLN:CD	6:B:163:PRO:HB2	2.29	0.53
12:H:63:SER:O	12:H:67:TYR:HB2	2.08	0.53
4:4:98:SER:O	4:4:102:GLU:HG3	2.09	0.53
4:4:169:GLN:HE22	19:4:1199:CLA:HHD	1.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:158:ARG:O	4:4:159:LEU:C	2.46	0.53
5:A:124:TRP:HA	5:A:124:TRP:CE3	2.44	0.53
19:A:1760:CLA:HBA2	19:A:1767:CLA:C6	2.38	0.53
19:A:1776:CLA:C2C	19:A:1782:CLA:C17	2.86	0.53
5:A:378:SER:HG	5:A:512:SER:HG	1.55	0.53
5:A:397:THR:HB	5:A:613:ILE:HD11	1.91	0.53
3:3:92:TRP:CA	3:3:95:THR:HG21	2.20	0.53
17:N:70:GLU:CB	17:N:72:LYS:H	2.18	0.53
5:A:25:ASP:HA	5:A:26:PRO:C	2.29	0.53
5:A:26:PRO:HB2	5:A:27:ILE:HB	1.90	0.53
4:4:40:PHE:CD2	4:4:43:ALA:HB2	2.43	0.53
8:D:124:ASN:HB3	8:D:125:PRO:CD	2.33	0.53
2:2:203:THR:O	2:2:204:ILE:HG12	2.09	0.53
5:A:392:GLN:O	5:A:392:GLN:CG	2.57	0.53
19:4:4007:CLA:HBC2	19:4:4007:CLA:HHD	1.90	0.53
19:4:1201:CLA:CGA	19:4:1201:CLA:HMA2	2.39	0.53
4:4:129:GLY:C	4:4:131:VAL:N	2.61	0.53
4:4:164:LEU:O	4:4:165:GLY:C	2.46	0.53
4:4:97:LEU:O	4:4:98:SER:C	2.47	0.53
5:A:174:PHE:O	5:A:175:ALA:CB	2.56	0.53
5:A:185:HIS:O	5:A:188:LYS:N	2.42	0.53
5:A:368:LEU:HD21	19:A:1774:CLA:H91	1.90	0.53
5:A:435:VAL:HA	5:A:438:HIS:CE1	2.44	0.53
5:A:46:LYS:HG3	5:A:48:PRO:HB2	1.91	0.53
22:B:1773:PQN:H192	23:B:1780:BCR:C10	2.33	0.53
6:B:708:VAL:O	6:B:710:LEU:O	2.27	0.53
9:E:35:LYS:CE	9:E:89:GLU:OE2	2.57	0.53
11:G:33:LYS:CA	11:G:33:LYS:HE3	2.27	0.53
3:3:80:LYS:HB2	19:3:1215:CLA:C3D	2.39	0.53
7:C:17:CYS:SG	7:C:18:VAL:N	2.81	0.53
3:3:64:TYR:CB	19:3:1221:CLA:H42	2.36	0.53
20:A:7039:LMU:C6B	20:A:7039:LMU:C3'	2.84	0.53
20:A:7030:LMU:C2	20:A:7030:LMU:O5'	2.55	0.53
6:B:715:VAL:O	6:B:719:PHE:HB2	2.09	0.53
18:R:5:UNK:O	18:R:6:UNK:CB	2.57	0.53
5:A:448:TRP:CD1	19:A:1788:CLA:HED2	2.43	0.53
5:A:114:THR:HG1	5:A:525:ASN:HB2	1.74	0.53
5:A:697:ARG:C	5:A:699:TYR:H	2.13	0.53
5:A:703:LEU:O	5:A:707:ILE:HG12	2.09	0.53
5:A:87:SER:O	5:A:88:ILE:HB	2.08	0.53
19:B:1751:CLA:HBA2	19:B:1752:CLA:O1A	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:713:LYS:HZ1	19:B:1761:CLA:C4	2.21	0.53
2:2:163:GLU:HG2	19:2:1217:CLA:C3C	2.38	0.53
2:2:110:TRP:CD2	19:2:1221:CLA:HED1	2.44	0.53
19:3:1217:CLA:CBC	19:3:1217:CLA:CMC	2.85	0.53
19:2:1212:CLA:H2A	19:2:1212:CLA:CGD	2.39	0.53
19:J:1043:CLA:H2	19:J:1043:CLA:C16	2.39	0.53
3:3:208:PRO:HB3	3:3:210:GLN:CD	2.29	0.53
10:F:147:GLY:C	10:F:150:VAL:HB	2.30	0.53
18:R:26:UNK:O	18:R:28:UNK:CB	2.57	0.53
5:A:132:LEU:HD11	5:A:674:ALA:CB	2.39	0.52
5:A:455:PHE:HD1	19:A:1788:CLA:HMA2	1.73	0.52
6:B:141:PHE:O	6:B:143:LEU:N	2.42	0.52
5:A:710:ALA:HB1	19:B:1735:CLA:HED2	1.91	0.52
8:D:37:LEU:O	8:D:39:LYS:N	2.42	0.52
19:B:1736:CLA:C4C	23:I:1032:BCR:H401	2.39	0.52
16:L:62:PHE:HB2	16:L:154:ALA:HB2	1.90	0.52
3:3:132:TRP:CZ3	3:3:155:GLU:OE1	2.57	0.52
4:4:37:LEU:HA	4:4:39:TRP:CD1	2.44	0.52
19:2:2006:CLA:CAD	19:2:2006:CLA:HED3	2.38	0.52
5:A:316:MET:HA	5:A:317:TYR:CD1	2.39	0.52
6:B:664:LEU:O	6:B:667:TRP:CZ3	2.61	0.52
8:D:41:GLN:HG3	16:L:125:LYS:HZ2	1.73	0.52
12:H:25:GLY:CA	12:H:27:ASP:N	2.66	0.52
20:A:7006:LMU:H2'	20:A:7006:LMU:H22	1.91	0.52
4:4:127:PRO:O	4:4:129:GLY:N	2.35	0.52
4:4:142:ASN:HA	4:4:150:LYS:HZ1	1.72	0.52
19:A:1776:CLA:CAA	19:A:1780:CLA:HBB2	2.39	0.52
5:A:338:PHE:O	5:A:339:THR:O	2.27	0.52
5:A:651:GLY:O	5:A:655:ASP:N	2.42	0.52
6:B:132:ASN:OD1	6:B:132:ASN:C	2.48	0.52
6:B:140:ILE:N	6:B:140:ILE:HD13	2.18	0.52
22:B:1773:PQN:C16	23:B:1780:BCR:H333	2.08	0.52
5:A:696:GLY:HA3	6:B:569:ASP:HB2	1.92	0.52
8:D:39:LYS:NZ	8:D:43:GLU:OE2	2.41	0.52
13:I:14:LEU:C	13:I:17:PRO:HD2	2.29	0.52
3:3:92:TRP:O	3:3:97:PHE:CD1	2.59	0.52
1:1:27:LEU:HD11	6:B:314:ARG:NE	2.17	0.52
15:K:44:GLU:C	15:K:44:GLU:OE1	2.47	0.52
2:2:54:TRP:NE1	19:2:1221:CLA:O1D	2.42	0.52
19:1:1191:CLA:CAB	19:1:1197:CLA:CHD	2.88	0.52
6:B:247:THR:CG2	6:B:250:ALA:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1192:CLA:HHD	19:1:1192:CLA:HBC3	1.88	0.52
5:A:408:VAL:HG21	5:A:602:LEU:HG	1.90	0.52
5:A:309:LEU:O	5:A:310:PHE:CB	2.56	0.52
5:A:443:ILE:HG12	5:A:558:LYS:HB2	1.91	0.52
5:A:662:SER:HA	5:A:665:ILE:HD11	1.92	0.52
6:B:50:HIS:HB3	19:B:1737:CLA:CHB	2.39	0.52
19:B:1738:CLA:H41	24:B:1781:LMG:H321	1.90	0.52
19:B:1737:CLA:HMC3	19:B:1759:CLA:H3A	1.89	0.52
6:B:53:GLN:C	6:B:55:ALA:N	2.63	0.52
6:B:597:LYS:O	6:B:598:HIS:HB2	2.09	0.52
6:B:628:SER:O	6:B:631:LEU:HD23	2.10	0.52
6:B:87:ILE:O	6:B:121:TYR:HE2	1.91	0.52
19:L:1167:CLA:HBC3	19:L:1167:CLA:HMC1	1.91	0.52
17:N:61:LEU:HD12	17:N:62:SER:C	2.30	0.52
17:N:42:PHE:H	17:N:43:PRO:HD2	1.74	0.52
12:H:25:GLY:CA	12:H:27:ASP:OD2	2.56	0.52
21:B:8056:SUC:C5'	21:B:8056:SUC:H1	2.39	0.52
3:3:194:ILE:CD1	19:3:1213:CLA:HMC2	2.38	0.52
5:A:571:ASP:OD2	8:D:88:THR:HG21	2.09	0.52
4:4:183:GLN:HG2	4:4:183:GLN:O	2.09	0.52
19:4:1198:CLA:O1D	19:4:1198:CLA:H2A	2.09	0.52
5:A:661:ALA:O	5:A:665:ILE:HG13	2.08	0.52
5:A:680:LEU:HD21	6:B:617:MET:CE	2.40	0.52
19:B:1764:CLA:C1D	19:B:1765:CLA:CBB	2.87	0.52
9:E:61:THR:HG22	9:E:62:ARG:N	2.20	0.52
11:G:19:GLY:O	11:G:22:VAL:N	2.43	0.52
16:L:46:ALA:HB2	16:L:52:ARG:NH2	2.24	0.52
16:L:63:LEU:O	16:L:64:LEU:C	2.47	0.52
19:4:1205:CLA:CBA	19:4:1205:CLA:CBD	2.85	0.52
19:4:1205:CLA:C2A	19:4:1205:CLA:HED3	2.38	0.52
3:3:74:ALA:HA	19:3:1216:CLA:C1D	2.39	0.52
8:D:101:TYR:CD1	8:D:114:PRO:HD3	2.44	0.52
19:1:1193:CLA:HBA2	19:1:1193:CLA:CMA	2.40	0.52
6:B:475:ASP:HA	6:B:480:SER:O	2.09	0.52
12:H:75:ASP:CG	12:H:77:LEU:HG	2.29	0.52
4:4:104:ARG:HA	4:4:107:GLN:CB	2.38	0.52
4:4:118:ASP:HA	4:4:122:LYS:CA	2.39	0.52
4:4:161:LEU:O	4:4:162:ALA:CB	2.57	0.52
19:A:1783:CLA:C1A	19:A:1783:CLA:CGA	2.88	0.52
5:A:312:ILE:O	5:A:313:ALA:CB	2.57	0.52
5:A:701:GLN:O	5:A:704:ILE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1749:CLA:HBD	19:B:1749:CLA:HBA1	1.92	0.52
19:B:1767:CLA:OBD	19:B:1767:CLA:O2D	2.27	0.52
19:B:1771:CLA:H151	16:L:98:CYS:SG	2.49	0.52
6:B:398:TYR:CD1	6:B:542:ARG:NH2	2.77	0.52
5:A:25:ASP:OD2	5:A:25:ASP:C	2.46	0.52
18:R:41:UNK:CA	18:R:42:UNK:CB	2.88	0.52
3:3:60:ILE:HA	3:3:63:ARG:HD2	1.92	0.52
2:2:168:ARG:NE	2:2:168:ARG:HA	2.24	0.52
20:A:7013:LMU:H92	20:A:7049:LMU:O3'	2.08	0.52
4:4:136:GLY:O	4:4:137:ILE:HB	2.09	0.52
19:A:1770:CLA:C2D	19:A:1798:CLA:HBC3	2.40	0.52
23:A:1807:BCR:HC42	19:A:1817:CLA:H142	1.92	0.52
5:A:205:HIS:ND1	19:A:1769:CLA:HMC2	2.24	0.52
19:B:1754:CLA:C8	19:B:1756:CLA:H43	2.39	0.52
6:B:437:TYR:CG	6:B:616:LEU:HD22	2.44	0.52
6:B:630:GLN:HE21	6:B:731:GLY:HA3	1.75	0.52
16:L:95:LEU:HA	16:L:98:CYS:CB	2.39	0.52
17:N:80:ASN:C	17:N:82:PHE:N	2.63	0.52
3:3:49:ILE:CG1	3:3:52:LYS:HB2	2.39	0.52
2:2:50:VAL:CG1	2:2:50:VAL:O	2.58	0.52
20:A:7042:LMU:C1	20:A:7042:LMU:H71	2.40	0.52
8:D:28:ILE:HG21	8:D:67:ILE:HG13	1.91	0.52
8:D:69:ARG:O	8:D:70:GLU:CB	2.57	0.52
19:A:1764:CLA:CMB	19:A:1765:CLA:H11	2.37	0.52
19:A:1776:CLA:C1C	19:A:1782:CLA:H171	2.40	0.52
5:A:42:ARG:HA	5:A:44:ILE:HG12	1.92	0.52
6:B:124:TRP:CD1	6:B:129:LEU:HD13	2.45	0.52
19:B:1746:CLA:CHD	19:B:1746:CLA:CBC	2.88	0.52
6:B:175:LEU:HA	6:B:178:HIS:HB2	1.91	0.52
19:B:1764:CLA:HMC3	19:B:1767:CLA:H2	1.92	0.52
9:E:90:VAL:C	9:E:92:ALA:N	2.61	0.52
8:D:32:SER:N	16:L:23:LEU:HG	2.19	0.52
12:H:65:LEU:HD11	16:L:90:GLY:HA2	1.92	0.52
19:4:1205:CLA:C1A	19:4:1205:CLA:HED3	2.39	0.52
19:3:1221:CLA:CBB	19:3:1221:CLA:CHC	2.82	0.52
5:A:137:GLY:C	5:A:139:GLY:H	2.12	0.52
21:2:1225:SUC:C2	21:2:1225:SUC:O2'	2.57	0.52
19:2:1212:CLA:NA	19:2:1212:CLA:O1A	2.43	0.52
8:D:96:ILE:O	8:D:97:LYS:HB2	2.08	0.52
4:4:104:ARG:CA	4:4:107:GLN:HB2	2.39	0.52
5:A:368:LEU:CD2	19:A:1774:CLA:H91	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1813:CLA:H192	19:A:1816:CLA:C2B	2.40	0.52
5:A:157:GLY:HA2	5:A:229:ILE:HG21	1.91	0.52
5:A:302:HIS:HE1	19:A:1774:CLA:CHB	2.23	0.52
5:A:307:ALA:O	5:A:308:ILE:C	2.49	0.52
5:A:449:VAL:HG22	19:A:1794:CLA:HMC3	1.92	0.52
5:A:750:PHE:O	5:A:752:ALA:N	2.42	0.52
19:B:1753:CLA:HMD2	19:B:1754:CLA:CAB	2.37	0.52
19:B:1758:CLA:H62	23:B:1776:BCR:H321	1.91	0.52
6:B:438:VAL:CG2	19:B:1763:CLA:CMC	2.81	0.52
6:B:557:PHE:HE2	7:C:66:ARG:NE	2.05	0.52
6:B:595:HIS:CE1	6:B:599:ILE:HD11	2.45	0.52
6:B:625:TRP:HE3	6:B:626:LEU:N	2.08	0.52
6:B:674:LEU:HD12	6:B:674:LEU:C	2.30	0.52
6:B:707:LEU:CD1	6:B:711:VAL:HG21	2.40	0.52
9:E:39:LEU:H	9:E:40:ARG:HH11	1.54	0.52
17:N:63:ASP:HA	17:N:64:ASP:C	2.29	0.52
4:4:36:ASN:O	4:4:39:TRP:CG	2.62	0.52
3:3:47:GLY:C	3:3:49:ILE:H	2.10	0.52
6:B:633:ASN:ND2	6:B:636:THR:CB	2.72	0.52
5:A:370:ILE:HD13	19:A:1781:CLA:CAD	2.40	0.52
19:A:1787:CLA:H92	19:A:1801:CLA:H2	1.92	0.52
5:A:177:LEU:C	5:A:179:LEU:H	2.13	0.52
5:A:223:VAL:O	5:A:228:PRO:HD3	2.09	0.52
5:A:64:PHE:HE2	19:A:1761:CLA:HMC1	1.75	0.52
19:A:1795:CLA:H41	19:B:1735:CLA:H202	1.92	0.52
19:B:1737:CLA:H43	23:B:1775:BCR:C33	2.39	0.52
6:B:194:LEU:O	6:B:198:ALA:HB3	2.10	0.52
6:B:199:ILE:HG22	6:B:203:ARG:CZ	2.40	0.52
6:B:442:VAL:HG21	19:B:1763:CLA:CAC	2.33	0.52
10:F:80:TRP:CE3	19:F:1157:CLA:HMC2	2.43	0.52
19:4:1205:CLA:CBA	19:4:1205:CLA:O1D	2.53	0.52
14:J:26:LEU:HA	14:J:29:ILE:HG22	1.91	0.52
1:1:179:THR:HG21	4:4:87:SER:O	2.10	0.52
5:A:261:SER:O	5:A:262:PHE:CD2	2.63	0.52
6:B:322:LEU:O	6:B:326:ILE:HG22	2.10	0.52
5:A:68:THR:C	5:A:70:ASP:H	2.13	0.52
4:4:122:LYS:HB2	4:4:143:PHE:HB2	1.81	0.52
5:A:81:ALA:HB1	19:A:1760:CLA:HMA3	1.89	0.52
5:A:370:ILE:CD1	19:A:1781:CLA:CAD	2.88	0.52
5:A:44:ILE:O	5:A:45:ALA:C	2.48	0.52
5:A:591:GLN:OE1	5:A:600:LEU:HD21	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:684:PHE:HB2	19:A:1814:CLA:HAA1	1.91	0.52
6:B:135:LEU:HD12	6:B:135:LEU:O	2.10	0.52
19:B:1758:CLA:C14	23:B:1776:BCR:H10C	2.32	0.52
19:A:1814:CLA:HED1	19:B:1784:CLA:H61	1.92	0.52
6:B:295:PHE:O	11:G:33:LYS:HB2	2.09	0.52
6:B:391:PRO:HB3	6:B:538:ALA:CA	2.32	0.52
6:B:586:THR:C	6:B:588:GLY:N	2.61	0.52
10:F:73:VAL:HG11	10:F:83:PHE:HB2	1.90	0.52
16:L:8:TYR:CE1	16:L:11:ILE:HG23	2.42	0.52
3:3:92:TRP:O	3:3:95:THR:OG1	2.28	0.52
17:N:70:GLU:CD	17:N:72:LYS:O	2.48	0.52
7:C:14:CYS:C	7:C:17:CYS:SG	2.87	0.52
2:2:54:TRP:CZ2	2:2:109:ARG:CG	2.93	0.52
14:J:2:ARG:HH12	14:J:8:LEU:CD1	2.17	0.52
3:3:104:TYR:CB	3:3:106:TYR:H	2.22	0.52
20:A:7034:LMU:O2B	20:A:7034:LMU:C5'	2.58	0.52
20:A:7034:LMU:C2	20:A:7034:LMU:O2'	2.55	0.52
9:E:69:PHE:HD2	9:E:71:LYS:H	1.54	0.52
19:J:1043:CLA:O2D	19:J:1043:CLA:H2A	2.10	0.52
20:A:7038:LMU:H1B	20:A:7038:LMU:C6'	2.40	0.52
6:B:369:ALA:O	6:B:725:LEU:CD1	2.57	0.52
5:A:539:PHE:HD2	5:A:539:PHE:O	1.93	0.52
19:A:1817:CLA:H111	23:B:1780:BCR:C35	2.40	0.51
5:A:281:LEU:HB2	5:A:301:HIS:HD2	1.74	0.51
5:A:475:ASP:HB3	19:A:1789:CLA:HED3	1.91	0.51
5:A:92:TRP:O	5:A:93:LEU:HB2	2.10	0.51
19:B:1735:CLA:H52	19:B:1735:CLA:C4C	2.40	0.51
19:B:1751:CLA:HMA3	19:B:1752:CLA:C4D	2.40	0.51
6:B:528:HIS:HE1	19:B:1769:CLA:NB	2.07	0.51
6:B:615:TYR:CD1	6:B:615:TYR:N	2.77	0.51
17:N:61:LEU:HD21	17:N:63:ASP:O	2.09	0.51
4:4:30:LEU:O	4:4:32:GLU:N	2.43	0.51
20:A:7003:LMU:H3B	21:B:8054:SUC:O4'	2.10	0.51
5:A:629:ASN:HD21	5:A:633:VAL:CG2	2.22	0.51
5:A:374:GLN:O	5:A:377:TYR:CD2	2.63	0.51
3:3:153:SER:OG	3:3:154:GLY:N	2.43	0.51
4:4:103:ILE:O	4:4:107:GLN:HB2	2.10	0.51
4:4:52:MET:HE1	4:4:156:ASN:HB2	1.92	0.51
5:A:165:TYR:O	5:A:165:TYR:CD2	2.63	0.51
19:A:1762:CLA:H51	19:A:1785:CLA:C4C	2.40	0.51
19:A:1817:CLA:H111	23:B:1780:BCR:H351	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:130:ARG:CG	6:B:130:ARG:HH11	2.22	0.51
6:B:451:LYS:HD2	19:B:1763:CLA:O2D	2.10	0.51
6:B:652:PHE:O	6:B:656:VAL:HG23	2.09	0.51
6:B:542:ARG:HH12	8:D:141:VAL:HA	1.75	0.51
5:A:28:LYS:CB	5:A:28:LYS:HZ2	2.10	0.51
16:L:163:LEU:O	16:L:165:TYR:HB3	2.09	0.51
8:D:117:GLY:O	8:D:118:VAL:CG2	2.48	0.51
6:B:587:ILE:CG2	6:B:587:ILE:O	2.58	0.51
5:A:464:ASN:H	5:A:464:ASN:ND2	2.08	0.51
23:A:1803:BCR:C8	23:A:1803:BCR:H311	2.12	0.51
5:A:492:ILE:HA	5:A:495:THR:HG23	1.91	0.51
5:A:701:GLN:NE2	5:A:724:ALA:H	2.08	0.51
19:B:1742:CLA:CAC	19:B:1743:CLA:CBB	2.52	0.51
19:B:1751:CLA:HMA3	19:B:1752:CLA:C3D	2.40	0.51
19:B:1738:CLA:CBB	19:B:1758:CLA:HHC	2.40	0.51
6:B:74:PHE:C	6:B:76:ALA:H	2.13	0.51
10:F:72:ILE:HG22	10:F:73:VAL:N	2.25	0.51
19:H:1080:CLA:O1D	19:H:1080:CLA:H2A	2.09	0.51
17:N:62:SER:HB3	17:N:66:ASP:N	2.23	0.51
1:1:29:LEU:O	1:1:33:PRO:HD3	2.10	0.51
15:K:47:LEU:HB3	15:K:48:GLN:HB2	1.91	0.51
3:3:106:TYR:CB	3:3:107:TRP:CD1	2.92	0.51
12:H:27:ASP:C	12:H:29:PRO:HD3	2.28	0.51
5:A:536:THR:HA	5:A:539:PHE:CB	2.40	0.51
5:A:164:LEU:HA	5:A:167:THR:HG23	1.91	0.51
19:A:1791:CLA:O1A	19:A:1791:CLA:H3A	2.11	0.51
23:A:1807:BCR:H392	19:I:1031:CLA:H142	1.93	0.51
5:A:397:THR:HB	5:A:613:ILE:CD1	2.41	0.51
5:A:708:VAL:N	5:A:711:HIS:HD2	2.09	0.51
6:B:438:VAL:O	6:B:441:ASP:N	2.42	0.51
6:B:538:ALA:O	6:B:540:ASP:N	2.43	0.51
6:B:551:LYS:O	6:B:553:PHE:CD2	2.64	0.51
7:C:52:LYS:C	7:C:54:CYS:N	2.62	0.51
17:N:50:GLN:HA	17:N:51:ASP:C	2.31	0.51
15:K:44:GLU:C	15:K:47:LEU:HG	2.27	0.51
5:A:588:GLY:HA3	6:B:668:ARG:HB3	1.92	0.51
6:B:715:VAL:HA	6:B:718:ILE:HG22	1.92	0.51
6:B:694:ARG:HE	16:L:105:ALA:CB	2.23	0.51
6:B:429:LEU:HB3	6:B:525:LEU:HB2	1.91	0.51
18:R:4:UNK:O	18:R:5:UNK:CB	2.59	0.51
1:1:182:ALA:O	1:1:183:ASP:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:144:GLN:HG3	5:A:145:ILE:H	1.75	0.51
19:A:1814:CLA:H101	19:A:1814:CLA:H152	1.92	0.51
5:A:385:LEU:O	5:A:386:ALA:HB3	2.10	0.51
5:A:462:ILE:HD11	19:A:1816:CLA:C5	2.29	0.51
5:A:555:ILE:HG22	6:B:670:TYR:CZ	2.45	0.51
19:B:1755:CLA:O1A	19:B:1769:CLA:HED2	2.10	0.51
6:B:580:VAL:CG1	6:B:710:LEU:HD21	2.41	0.51
16:L:69:VAL:HG11	16:L:84:GLY:N	2.25	0.51
17:N:62:SER:O	17:N:63:ASP:CB	2.58	0.51
3:3:157:ALA:O	3:3:158:TYR:CD2	2.63	0.51
14:J:2:ARG:NH1	14:J:8:LEU:HB2	2.25	0.51
7:C:12:ILE:HD13	7:C:39:ILE:HG13	1.93	0.51
19:1:1145:CLA:H3A	19:1:1145:CLA:CGA	2.34	0.51
1:1:89:VAL:HB	1:1:90:PRO:CD	2.32	0.51
19:2:1212:CLA:O1A	19:2:1212:CLA:C4A	2.58	0.51
13:I:2:ILE:HG12	13:I:3:ASN:CG	2.31	0.51
7:C:30:PRO:HB3	7:C:37:LYS:O	2.10	0.51
4:4:121:PHE:O	4:4:122:LYS:CB	2.58	0.51
4:4:164:LEU:O	4:4:167:ILE:N	2.44	0.51
19:A:1763:CLA:HAA2	19:A:1765:CLA:HED1	1.93	0.51
19:A:1795:CLA:HED1	19:B:1735:CLA:H18	1.93	0.51
19:A:1817:CLA:HBC2	19:A:1817:CLA:HMC1	1.92	0.51
5:A:472:ARG:N	5:A:473:PRO:HD2	2.24	0.51
19:B:1770:CLA:HMC1	19:B:1770:CLA:HBC2	1.93	0.51
6:B:388:ALA:O	6:B:391:PRO:HD2	2.10	0.51
6:B:555:TYR:CD2	6:B:573:TRP:HB2	2.44	0.51
6:B:592:PHE:HA	6:B:721:TYR:OH	2.11	0.51
15:K:32:ARG:HA	15:K:32:ARG:NE	2.25	0.51
17:N:79:SER:CA	17:N:80:ASN:C	2.74	0.51
4:4:34:PRO:HA	4:4:35:GLU:CD	2.31	0.51
15:K:44:GLU:CG	15:K:45:SER:N	2.30	0.51
2:2:55:ALA:CB	2:2:56:MET:HE1	2.39	0.51
2:2:124:ILE:CG2	2:2:129:LYS:HB3	2.40	0.51
6:B:228:GLY:HA3	11:G:8:ILE:HD13	1.93	0.51
20:A:7009:LMU:H5'	20:A:7009:LMU:O2B	2.10	0.51
6:B:479:SER:O	6:B:481:THR:N	2.38	0.51
3:3:116:PHE:O	3:3:120:LEU:HB2	2.10	0.51
6:B:40:GLY:HA2	6:B:165:VAL:HG23	1.91	0.51
5:A:114:THR:CG2	5:A:115:HIS:ND1	2.71	0.51
5:A:210:LEU:HD12	19:A:1769:CLA:HMB2	1.93	0.51
5:A:302:HIS:HB2	19:A:1773:CLA:C1B	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:438:HIS:HB2	5:A:441:ALA:HB3	1.91	0.51
19:B:1754:CLA:HMA2	19:B:1754:CLA:H61	1.91	0.51
19:B:1762:CLA:H51	23:B:1779:BCR:H401	1.93	0.51
6:B:710:LEU:C	6:B:712:HIS:H	2.13	0.51
7:C:70:TRP:O	7:C:72:GLU:CB	2.59	0.51
23:I:1032:BCR:H292	23:L:1169:BCR:H281	1.92	0.51
3:3:97:PHE:C	3:3:98:ILE:HG23	2.30	0.51
8:D:36:LEU:HB2	16:L:19:PHE:O	2.10	0.51
8:D:78:ALA:O	8:D:79:ARG:NH1	2.37	0.51
3:3:63:ARG:NH2	3:3:189:LEU:HD23	2.19	0.51
11:G:17:PHE:O	11:G:20:ARG:CB	2.54	0.51
6:B:378:ILE:CA	6:B:381:PHE:HB2	2.41	0.51
2:2:81:THR:O	2:2:83:GLY:N	2.44	0.51
12:H:74:GLN:OE1	12:H:74:GLN:O	2.29	0.51
5:A:122:VAL:HG22	5:A:142:GLY:HA2	1.92	0.51
19:A:1788:CLA:HED1	19:A:1800:CLA:O1A	2.11	0.51
5:A:462:ILE:CG2	19:A:1789:CLA:CMC	2.89	0.51
5:A:732:ALA:HB1	19:A:1796:CLA:HED2	1.93	0.51
5:A:243:PRO:O	5:A:244:LEU:O	2.28	0.51
6:B:124:TRP:HD1	6:B:124:TRP:O	1.94	0.51
6:B:70:TRP:HB3	6:B:136:TYR:HH	1.76	0.51
19:B:1750:CLA:HMA1	11:G:21:PHE:CG	2.46	0.51
6:B:175:LEU:HD11	19:B:1749:CLA:CMA	2.41	0.51
6:B:400:PRO:HD2	8:D:143:PRO:HD3	1.92	0.51
6:B:655:LEU:CD2	19:B:1771:CLA:CBB	2.89	0.51
13:I:10:PRO:O	13:I:15:LEU:N	2.35	0.51
17:N:47:THR:OG1	17:N:52:LEU:O	2.29	0.51
4:4:32:GLU:HA	4:4:32:GLU:OE2	2.10	0.51
8:D:75:LEU:HD21	16:L:19:PHE:CG	2.45	0.51
20:A:7005:LMU:O2B	20:A:7005:LMU:H5B	2.10	0.51
20:A:7043:LMU:C11	20:A:7043:LMU:H71	2.41	0.51
20:A:7034:LMU:O2B	20:A:7034:LMU:C4'	2.59	0.51
5:A:624:VAL:O	5:A:636:HIS:CD2	2.64	0.51
5:A:520:LEU:HD22	20:A:1810:LMU:O1'	2.10	0.51
1:1:141:GLU:O	1:1:143:LEU:O	2.29	0.51
6:B:63:GLY:HA2	6:B:66:PHE:HB3	1.93	0.51
19:A:1764:CLA:H43	23:A:1805:BCR:H383	1.93	0.51
19:A:1772:CLA:CBA	19:A:1772:CLA:H2	2.33	0.51
22:A:1802:PQN:H272	22:A:1802:PQN:H241	1.93	0.51
19:A:1817:CLA:CMB	19:A:1817:CLA:H41	2.41	0.51
5:A:258:LEU:O	5:A:280:PHE:CE1	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:86:LEU:HD22	5:A:86:LEU:H	1.76	0.51
5:A:713:LYS:CE	19:B:1761:CLA:H43	2.41	0.51
6:B:353:TYR:C	6:B:355:LEU:H	2.13	0.51
12:H:65:LEU:HD23	19:H:1079:CLA:C5	2.41	0.51
13:I:12:VAL:CG2	19:I:1031:CLA:O1A	2.59	0.51
16:L:33:ILE:HD11	16:L:36:TYR:HD1	1.75	0.51
19:4:1205:CLA:CBA	19:4:1205:CLA:HBD	2.41	0.51
17:N:50:GLN:OE1	17:N:51:ASP:HA	2.10	0.51
17:N:80:ASN:O	17:N:82:PHE:N	2.32	0.51
3:3:182:LYS:O	3:3:185:LYS:HB3	2.11	0.51
19:1:1146:CLA:CMC	19:1:1146:CLA:HBC2	2.37	0.51
5:A:327:ILE:O	5:A:328:LYS:O	2.29	0.51
6:B:503:GLU:HB3	6:B:507:SER:HB2	1.92	0.51
16:L:5:LYS:HA	16:L:5:LYS:HE2	1.93	0.51
19:A:1781:CLA:HAA2	19:A:1782:CLA:OBD	2.12	0.51
19:A:1797:CLA:CHD	19:A:1797:CLA:HBC2	2.31	0.51
19:A:1816:CLA:C9	19:A:1817:CLA:C9	2.86	0.51
19:B:1735:CLA:HBC3	23:B:1778:BCR:H332	1.92	0.51
6:B:354:SER:O	6:B:355:LEU:HD13	2.11	0.51
6:B:464:GLN:HG3	6:B:469:LYS:HD3	1.93	0.51
7:C:69:LEU:HD23	7:C:70:TRP:N	2.26	0.51
16:L:102:TYR:C	16:L:104:ILE:H	2.14	0.51
8:D:46:TYR:HD1	8:D:80:LYS:HB3	1.75	0.51
10:F:53:PHE:C	10:F:55:ASN:N	2.62	0.51
19:2:1212:CLA:O2A	19:2:1212:CLA:H42	2.10	0.51
5:A:598:VAL:HG12	5:A:598:VAL:O	2.11	0.51
6:B:378:ILE:HA	6:B:381:PHE:HB2	1.92	0.51
1:1:42:SER:HA	1:1:45:ILE:HG12	1.92	0.51
6:B:320:LYS:O	6:B:322:LEU:N	2.44	0.51
6:B:166:SER:C	6:B:168:PHE:H	2.14	0.51
10:F:92:TYR:C	10:F:92:TYR:CD2	2.84	0.51
8:D:93:LYS:HB3	8:D:93:LYS:NZ	2.26	0.51
5:A:160:SER:HB2	5:A:163:GLN:OE1	2.11	0.50
19:A:1817:CLA:HMC1	6:B:661:PHE:HB3	1.92	0.50
5:A:210:LEU:N	5:A:213:LEU:H	2.09	0.50
5:A:309:LEU:HA	5:A:312:ILE:O	2.11	0.50
5:A:711:HIS:CB	5:A:717:ALA:HB2	2.35	0.50
19:B:1768:CLA:C6	23:B:1779:BCR:C32	2.89	0.50
6:B:551:LYS:HG2	6:B:552:ASP:H	1.76	0.50
6:B:696:LYS:NZ	8:D:39:LYS:HE3	2.25	0.50
6:B:77:TRP:CE2	6:B:81:PRO:HB3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:32:ARG:HH22	9:E:53:VAL:HA	1.76	0.50
17:N:61:LEU:HD11	17:N:63:ASP:CB	2.40	0.50
8:D:36:LEU:HD21	8:D:45:PHE:CZ	2.45	0.50
2:2:170:ALA:O	2:2:171:MET:C	2.48	0.50
2:2:50:VAL:O	2:2:50:VAL:HG12	2.10	0.50
20:A:7013:LMU:O6B	20:A:7013:LMU:C1B	2.54	0.50
5:A:141:ARG:HD3	10:F:39:ALA:HA	1.92	0.50
5:A:514:THR:HB	5:A:532:ILE:HG23	1.93	0.50
21:B:8060:SUC:H5	21:B:8060:SUC:HO1'	1.76	0.50
10:F:116:GLN:C	10:F:118:GLU:N	2.64	0.50
5:A:446:LEU:CD1	5:A:554:LEU:HA	2.42	0.50
19:4:1199:CLA:HAA1	19:F:1157:CLA:C4	2.36	0.50
19:A:1777:CLA:HBC3	19:A:1779:CLA:HED1	1.92	0.50
19:A:1789:CLA:H171	19:A:1793:CLA:H202	1.93	0.50
23:A:1806:BCR:C23	23:A:1806:BCR:C39	2.77	0.50
5:A:746:THR:HG1	19:A:1813:CLA:CGD	2.24	0.50
5:A:552:THR:O	5:A:553:VAL:HB	2.11	0.50
5:A:700:TRP:CZ2	22:A:1802:PQN:H2M3	2.47	0.50
6:B:55:ALA:HB1	6:B:150:LEU:HD12	1.93	0.50
7:C:7:ILE:O	7:C:60:THR:HA	2.11	0.50
9:E:40:ARG:NE	9:E:86:GLU:CD	2.60	0.50
16:L:33:ILE:CD1	16:L:36:TYR:HD1	2.25	0.50
17:N:51:ASP:O	17:N:52:LEU:HD22	2.11	0.50
15:K:44:GLU:OE1	15:K:45:SER:O	2.29	0.50
19:2:1213:CLA:OBD	19:2:1213:CLA:O2D	2.30	0.50
3:3:157:ALA:O	3:3:158:TYR:CB	2.59	0.50
14:J:15:SER:HA	14:J:18:TRP:HB3	1.93	0.50
10:F:125:LEU:HD11	14:J:18:TRP:CZ3	2.45	0.50
2:2:128:ASN:HD21	14:J:4:PHE:H	1.58	0.50
5:A:149:PHE:O	5:A:150:PHE:HB2	2.10	0.50
18:R:49:UNK:O	18:R:51:UNK:CB	2.58	0.50
16:L:128:ASP:OD2	16:L:129:GLN:N	2.41	0.50
19:1:1193:CLA:H43	19:1:1193:CLA:CGA	2.41	0.50
5:A:262:PHE:O	5:A:264:GLU:N	2.44	0.50
6:B:92:TRP:O	6:B:92:TRP:CD1	2.64	0.50
5:A:157:GLY:HA2	5:A:229:ILE:CG2	2.41	0.50
19:A:1773:CLA:H12	19:A:1773:CLA:C4A	2.42	0.50
5:A:725:LEU:HD21	19:A:1796:CLA:HMD3	1.93	0.50
5:A:733:VAL:HG21	19:A:1796:CLA:HMD3	1.93	0.50
6:B:75:GLU:HB2	6:B:132:ASN:HD22	1.76	0.50
19:A:1788:CLA:H191	22:B:1773:PQN:H303	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1805:BCR:C3	23:B:1778:BCR:H17C	2.41	0.50
6:B:527:LEU:HD12	19:B:1755:CLA:C1D	2.42	0.50
9:E:73:ASN:C	9:E:73:ASN:ND2	2.64	0.50
11:G:45:GLU:C	11:G:47:GLY:N	2.54	0.50
17:N:48:GLY:HA3	17:N:49:CYS:SG	2.51	0.50
17:N:45:ASN:ND2	17:N:54:LYS:HB2	2.26	0.50
17:N:61:LEU:HD12	17:N:63:ASP:HB2	1.93	0.50
2:2:57:LEU:HD23	2:2:58:GLY:N	2.26	0.50
20:A:7016:LMU:C3	20:A:7016:LMU:C8	2.89	0.50
14:J:2:ARG:HB3	14:J:7:TYR:CZ	2.45	0.50
18:R:47:UNK:O	18:R:48:UNK:O	2.30	0.50
15:K:4:GLY:HA2	15:K:7:THR:CB	2.41	0.50
6:B:694:ARG:HE	16:L:105:ALA:CA	2.24	0.50
20:A:7026:LMU:C6B	20:A:7026:LMU:H2B	2.41	0.50
5:A:478:SER:HB3	5:A:644:GLN:CD	2.31	0.50
2:2:154:GLN:OE1	2:2:154:GLN:HA	2.11	0.50
4:4:46:VAL:HG21	4:4:105:ARG:NH1	2.26	0.50
4:4:114:SER:O	4:4:117:GLN:N	2.44	0.50
5:A:475:ASP:HB3	19:A:1789:CLA:CED	2.41	0.50
19:A:1783:CLA:C17	23:A:1806:BCR:H17C	2.40	0.50
5:A:188:LYS:O	5:A:190:ALA:N	2.45	0.50
5:A:360:ILE:O	5:A:361:ASN:HB3	2.11	0.50
5:A:390:ALA:HB1	5:A:754:ILE:HD13	1.93	0.50
5:A:44:ILE:O	5:A:46:LYS:HA	2.11	0.50
19:B:1758:CLA:H62	23:B:1776:BCR:C32	2.42	0.50
6:B:127:ILE:CG1	6:B:193:HIS:HE1	2.24	0.50
6:B:558:PRO:O	6:B:559:CYS:HB3	2.12	0.50
8:D:29:PHE:O	8:D:30:ALA:HB3	2.12	0.50
18:R:34:UNK:C	18:R:36:UNK:N	2.75	0.50
15:K:44:GLU:OE2	15:K:45:SER:O	2.29	0.50
3:3:182:LYS:O	3:3:182:LYS:HG2	2.12	0.50
2:2:106:GLU:O	19:2:1221:CLA:HMA3	2.10	0.50
3:3:109:ASP:O	3:3:110:SER:O	2.28	0.50
11:G:68:ILE:HG22	11:G:72:LEU:HD13	1.91	0.50
10:F:22:LEU:N	10:F:22:LEU:HD12	2.10	0.50
10:F:26:GLN:O	10:F:28:SER:N	2.44	0.50
20:A:7036:LMU:C7	20:A:7036:LMU:C3	2.85	0.50
20:A:7043:LMU:C7	20:A:7043:LMU:C11	2.88	0.50
5:A:592:VAL:O	5:A:597:HIS:CD2	2.65	0.50
20:A:7009:LMU:C4B	20:A:7009:LMU:O1B	2.56	0.50
5:A:96:MET:HE1	19:A:1763:CLA:HBB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1782:CLA:CBB	19:A:1790:CLA:C3A	2.90	0.50
5:A:58:HIS:HE1	19:A:1759:CLA:C4D	2.20	0.50
19:B:1738:CLA:H43	24:B:1781:LMG:H321	1.93	0.50
19:B:1741:CLA:HED2	19:B:1741:CLA:O2A	2.11	0.50
19:B:1756:CLA:C7	23:B:1777:BCR:H14C	2.42	0.50
22:B:1773:PQN:H192	23:B:1780:BCR:C8	2.41	0.50
6:B:338:LEU:O	6:B:339:ALA:HB3	2.11	0.50
6:B:440:ASN:ND2	6:B:453:ILE:O	2.45	0.50
6:B:558:PRO:HB3	6:B:706:ARG:HH21	1.75	0.50
6:B:594:TRP:HD1	6:B:595:HIS:HB2	1.77	0.50
7:C:60:THR:HG23	7:C:63:LEU:O	2.11	0.50
9:E:88:GLU:O	9:E:90:VAL:HB	2.11	0.50
11:G:37:GLU:OE2	11:G:42:SER:N	2.44	0.50
19:A:1796:CLA:C19	14:J:19:PHE:CD2	2.94	0.50
4:4:76:TYR:CD1	4:4:76:TYR:C	2.83	0.50
16:L:163:LEU:C	16:L:163:LEU:HD13	2.31	0.50
18:R:34:UNK:O	18:R:36:UNK:O	2.29	0.50
15:K:47:LEU:O	15:K:48:GLN:OE1	2.30	0.50
19:2:1217:CLA:H93	19:2:1217:CLA:C4	2.32	0.50
2:2:163:GLU:OE1	2:2:163:GLU:HA	2.10	0.50
2:2:98:GLU:CG	2:2:99:LEU:HD12	2.41	0.50
19:3:1218:CLA:O2D	19:3:1218:CLA:HBA1	2.11	0.50
8:D:116:ASP:HB3	8:D:127:ARG:HH12	1.76	0.50
5:A:583:GLY:O	5:A:589:THR:HB	2.11	0.50
19:1:1189:CLA:HBD	19:1:1189:CLA:CAA	2.41	0.50
12:H:45:ALA:HB3	12:H:46:PRO:HD3	1.92	0.50
5:A:445:HIS:O	5:A:446:LEU:HB2	2.11	0.50
2:2:37:ASP:OD2	3:3:41:ASP:CG	2.50	0.50
14:J:36:ALA:O	14:J:37:LEU:HB2	2.11	0.50
16:L:17:ASP:OD1	16:L:17:ASP:O	2.29	0.50
4:4:114:SER:O	4:4:117:GLN:HG3	2.12	0.50
19:4:1198:CLA:CAA	19:4:1198:CLA:CED	2.78	0.50
19:A:1785:CLA:C10	19:A:1785:CLA:H152	2.41	0.50
19:A:1787:CLA:H141	19:A:1801:CLA:H93	1.93	0.50
19:A:1783:CLA:C11	23:A:1806:BCR:H353	2.40	0.50
19:A:1814:CLA:HED1	19:B:1784:CLA:H2	1.93	0.50
5:A:223:VAL:HA	5:A:227:LEU:HB2	1.94	0.50
5:A:707:ILE:HG22	5:A:711:HIS:CD2	2.45	0.50
19:B:1739:CLA:H42	19:B:1739:CLA:C4C	2.42	0.50
6:B:54:LEU:HD11	19:B:1743:CLA:HBA2	1.94	0.50
6:B:30:ASP:O	6:B:34:HIS:HD2	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:439:HIS:CD2	6:B:453:ILE:HG22	2.47	0.50
6:B:75:GLU:CB	6:B:132:ASN:HD22	2.24	0.50
10:F:80:TRP:HB3	19:F:1157:CLA:HHC	1.93	0.50
16:L:63:LEU:CD2	16:L:64:LEU:H	2.22	0.50
4:4:69:ILE:O	4:4:71:ASN:N	2.45	0.50
17:N:83:TRP:O	17:N:83:TRP:CE3	2.63	0.50
18:R:38:UNK:O	18:R:39:UNK:O	2.29	0.50
2:2:162:LYS:O	2:2:162:LYS:HD3	2.12	0.50
2:2:203:THR:CG2	2:2:204:ILE:N	2.73	0.50
19:1:1148:CLA:C1	19:1:1148:CLA:CGD	2.88	0.50
4:4:97:LEU:C	4:4:99:HIS:N	2.60	0.50
19:A:1763:CLA:HMB1	23:A:1806:BCR:HC7	1.91	0.50
19:A:1759:CLA:HBA2	19:A:1796:CLA:H2	1.93	0.50
5:A:555:ILE:CG2	19:A:1817:CLA:OBD	2.60	0.50
5:A:131:ILE:CG2	6:B:446:PHE:HA	2.36	0.50
6:B:353:TYR:CD1	6:B:594:TRP:HZ3	2.30	0.50
6:B:91:ILE:CD1	6:B:104:PHE:CE2	2.95	0.50
11:G:28:ARG:HG3	11:G:29:GLU:CG	2.41	0.50
17:N:54:LYS:HB3	17:N:57:LYS:HB2	1.94	0.50
17:N:80:ASN:OD1	17:N:82:PHE:CA	2.60	0.50
17:N:80:ASN:OD1	17:N:82:PHE:N	2.45	0.50
4:4:40:PHE:HA	4:4:43:ALA:H	1.75	0.50
4:4:192:THR:CG2	4:4:193:ILE:N	2.75	0.50
20:A:7006:LMU:C5B	20:A:7006:LMU:H3'	2.42	0.50
18:R:43:UNK:O	18:R:44:UNK:O	2.29	0.50
15:K:35:THR:HG23	15:K:36:ALA:H	1.77	0.50
19:4:1196:CLA:O1D	19:4:1196:CLA:H2A	2.12	0.50
4:4:142:ASN:N	4:4:150:LYS:NZ	2.56	0.50
19:A:1798:CLA:H92	23:A:1809:BCR:H361	1.94	0.50
5:A:59:ALA:O	5:A:61:ALA:N	2.44	0.50
6:B:119:GLY:O	6:B:121:TYR:N	2.45	0.50
6:B:196:HIS:NE2	19:B:1745:CLA:ND	2.60	0.50
19:B:1738:CLA:H191	19:B:1757:CLA:H141	1.93	0.50
6:B:193:HIS:CD2	19:B:1744:CLA:NB	2.80	0.50
6:B:492:ILE:HD13	6:B:492:ILE:N	2.17	0.50
6:B:594:TRP:CD2	6:B:598:HIS:CE1	3.00	0.50
5:A:24:ARG:O	5:A:25:ASP:OD1	2.30	0.50
2:2:97:VAL:CA	2:2:100:VAL:HG13	2.41	0.50
16:L:148:VAL:O	16:L:149:SER:CB	2.54	0.50
8:D:58:PHE:CD2	8:D:59:GLU:N	2.80	0.50
5:A:49:ASP:HB2	5:A:720:THR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:755:ILE:O	5:A:756:ALA:HB3	2.12	0.50
4:4:127:PRO:HB2	4:4:143:PHE:CE1	2.47	0.50
4:4:92:VAL:HG12	4:4:93:ILE:N	2.27	0.50
19:A:1779:CLA:CAB	23:A:1804:BCR:C35	2.90	0.50
5:A:209:GLY:C	5:A:213:LEU:HB2	2.32	0.50
6:B:124:TRP:CD1	6:B:124:TRP:O	2.64	0.50
19:B:1753:CLA:CBC	19:B:1753:CLA:HMC1	2.35	0.50
6:B:385:GLY:N	19:B:1759:CLA:HBC3	2.27	0.50
19:B:1737:CLA:HAC1	19:B:1759:CLA:HMA1	1.94	0.50
6:B:202:SER:CB	6:B:270:LEU:HD21	2.42	0.50
16:L:163:LEU:HD11	16:L:165:TYR:CE1	2.45	0.50
1:1:27:LEU:HG	6:B:314:ARG:NH1	2.26	0.50
2:2:171:MET:CE	2:2:175:MET:HB2	2.42	0.50
3:3:106:TYR:CD2	3:3:107:TRP:CG	2.99	0.50
10:F:50:LYS:C	10:F:52:ARG:N	2.65	0.50
5:A:638:THR:OG1	5:A:641:ASN:ND2	2.44	0.50
16:L:135:GLY:O	16:L:138:LYS:HG2	2.12	0.50
6:B:681:ALA:O	6:B:682:HIS:C	2.50	0.50
19:A:1766:CLA:HBB2	19:A:1769:CLA:HMA3	1.92	0.49
19:A:1788:CLA:H152	23:L:1169:BCR:C36	2.42	0.49
5:A:335:LYS:HE3	5:A:341:GLN:HB2	1.93	0.49
5:A:44:ILE:O	5:A:46:LYS:CA	2.60	0.49
5:A:599:PHE:CD1	5:A:600:LEU:HD23	2.35	0.49
5:A:618:TRP:CD1	5:A:618:TRP:O	2.64	0.49
5:A:651:GLY:O	5:A:655:ASP:HB2	2.12	0.49
5:A:683:HIS:O	19:A:1814:CLA:HAA2	2.11	0.49
5:A:711:HIS:NE2	19:A:1795:CLA:CAC	2.74	0.49
5:A:98:PHE:HD1	5:A:99:HIS:HD2	1.58	0.49
19:B:1757:CLA:CGA	19:B:1757:CLA:H3A	2.38	0.49
6:B:299:HIS:NE2	6:B:304:ILE:HG21	2.27	0.49
6:B:438:VAL:O	6:B:442:VAL:N	2.44	0.49
6:B:595:HIS:CD2	6:B:623:TYR:OH	2.65	0.49
19:F:1156:CLA:O1D	19:F:1156:CLA:H2A	2.12	0.49
17:N:84:LYS:C	17:N:85:TRP:CD1	2.85	0.49
6:B:321:GLY:O	6:B:325:THR:HG22	2.11	0.49
2:2:98:GLU:HG2	2:2:99:LEU:HD12	1.93	0.49
3:3:158:TYR:CB	3:3:159:PRO:HD2	2.22	0.49
10:F:123:VAL:HB	10:F:126:ALA:O	2.12	0.49
16:L:48:ASN:CB	16:L:49:PRO:HD2	2.39	0.49
6:B:454:LEU:N	6:B:454:LEU:HD12	2.27	0.49
5:A:464:ASN:ND2	5:A:464:ASN:N	2.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:475:ASP:O	6:B:479:SER:OG	2.30	0.49
19:A:1777:CLA:C2D	19:A:1778:CLA:HMB3	2.42	0.49
5:A:736:THR:HG21	19:A:1785:CLA:H91	1.94	0.49
5:A:308:ILE:HG13	19:A:1772:CLA:CBB	2.43	0.49
5:A:690:LEU:HD23	5:A:693:LEU:HD12	1.93	0.49
19:B:1765:CLA:HBB1	23:B:1777:BCR:C28	2.39	0.49
6:B:334:LEU:CA	19:B:1737:CLA:HMD3	2.42	0.49
6:B:583:MET:HA	19:B:1755:CLA:HBC1	1.93	0.49
7:C:65:VAL:HG12	7:C:66:ARG:N	2.26	0.49
4:4:36:ASN:C	4:4:39:TRP:CG	2.86	0.49
18:R:37:UNK:O	18:R:42:UNK:O	2.30	0.49
15:K:44:GLU:O	15:K:46:GLY:O	2.30	0.49
8:D:36:LEU:HD12	8:D:78:ALA:H	1.77	0.49
2:2:103:GLY:O	2:2:104:TRP:C	2.49	0.49
2:2:128:ASN:CG	14:J:3:ASP:HB3	2.31	0.49
20:A:7005:LMU:C4	20:A:7005:LMU:H81	2.42	0.49
12:H:25:GLY:HA3	12:H:27:ASP:CG	2.32	0.49
20:A:7031:LMU:H4'	20:A:7031:LMU:O2B	2.12	0.49
4:4:82:GLU:O	4:4:83:TYR:HD1	1.95	0.49
6:B:242:HIS:O	6:B:243:LEU:HG	2.12	0.49
5:A:182:GLY:HA3	19:A:1767:CLA:HAC1	1.94	0.49
5:A:207:LEU:CD1	19:A:1776:CLA:HBB2	2.42	0.49
5:A:398:HIS:HD2	19:A:1783:CLA:ND	2.10	0.49
19:A:1793:CLA:H11	19:A:1793:CLA:ND	2.26	0.49
19:B:1735:CLA:H61	23:B:1778:BCR:H12C	1.94	0.49
6:B:292:ARG:NE	6:B:297:ILE:O	2.45	0.49
6:B:305:LEU:O	6:B:308:HIS:N	2.28	0.49
6:B:309:ILE:HG22	6:B:319:HIS:CD2	2.48	0.49
6:B:382:ILE:O	6:B:385:GLY:N	2.43	0.49
6:B:459:PHE:O	6:B:463:ILE:HD13	2.12	0.49
6:B:542:ARG:NH2	8:D:143:PRO:HG3	2.27	0.49
8:D:50:TRP:N	8:D:50:TRP:CD1	2.80	0.49
19:2:1212:CLA:O2A	19:2:1212:CLA:C4	2.60	0.49
5:A:636:HIS:O	5:A:638:THR:N	2.45	0.49
5:A:582:ASP:HB3	5:A:589:THR:CG2	2.41	0.49
6:B:607:SER:HA	6:B:610:ASN:ND2	2.27	0.49
6:B:357:ALA:O	6:B:358:TYR:CD1	2.65	0.49
4:4:98:SER:OG	4:4:102:GLU:OE1	2.28	0.49
5:A:442:ILE:CG2	19:A:1786:CLA:HMC3	2.37	0.49
19:A:1796:CLA:HBA2	19:A:1796:CLA:C4A	2.35	0.49
5:A:258:LEU:O	5:A:259:TYR:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:312:ILE:O	5:A:313:ALA:HB2	2.12	0.49
5:A:435:VAL:HA	5:A:438:HIS:HE1	1.77	0.49
5:A:443:ILE:HD13	5:A:561:LEU:HD12	1.95	0.49
5:A:56:ASN:O	5:A:57:LEU:CB	2.56	0.49
5:A:63:ASP:HA	19:A:1785:CLA:HED2	1.94	0.49
6:B:535:VAL:HG13	6:B:536:LYS:N	2.28	0.49
6:B:53:GLN:HA	6:B:53:GLN:OE1	2.04	0.49
6:B:596:TRP:O	6:B:597:LYS:CB	2.60	0.49
6:B:616:LEU:O	6:B:619:TRP:HB2	2.12	0.49
7:C:1:MET:HB3	7:C:4:SER:CB	2.37	0.49
19:F:1157:CLA:CAD	19:F:1157:CLA:HED2	2.41	0.49
11:G:44:PHE:C	11:G:47:GLY:N	2.65	0.49
4:4:175:LYS:O	4:4:175:LYS:HD2	2.12	0.49
6:B:325:THR:HG21	6:B:403:ASN:HD21	1.77	0.49
19:1:1308:CLA:CBA	19:1:1308:CLA:CBD	2.78	0.49
10:F:125:LEU:O	10:F:126:ALA:HB2	2.12	0.49
12:H:37:SER:HB3	16:L:51:LEU:HG	1.94	0.49
6:B:376:GLN:OE1	6:B:376:GLN:HA	2.12	0.49
5:A:625:TRP:CB	5:A:637:ILE:HD11	2.43	0.49
18:R:27:UNK:C	18:R:29:UNK:N	2.73	0.49
19:A:1774:CLA:C4	19:A:1774:CLA:O2A	2.58	0.49
23:A:1805:BCR:H323	23:A:1806:BCR:H391	1.93	0.49
5:A:746:THR:O	5:A:750:PHE:N	2.40	0.49
19:B:1755:CLA:C1	19:B:1769:CLA:HED2	2.43	0.49
6:B:527:LEU:HD13	6:B:586:THR:HG21	1.94	0.49
6:B:646:TRP:CZ2	6:B:726:ILE:HG21	2.47	0.49
6:B:662:MET:HE2	22:B:1773:PQN:H2M3	1.94	0.49
7:C:1:MET:HA	7:C:2:SER:C	2.33	0.49
9:E:58:ASP:OD1	9:E:58:ASP:N	2.39	0.49
19:G:1099:CLA:H2A	19:G:1099:CLA:O1D	2.12	0.49
2:2:57:LEU:O	2:2:60:ALA:CB	2.61	0.49
4:4:195:GLN:HA	4:4:195:GLN:OE1	2.13	0.49
1:1:142:GLU:OE1	19:1:1187:CLA:C2D	2.60	0.49
19:1:1142:CLA:HED1	19:1:1143:CLA:CMB	2.37	0.49
20:A:7020:LMU:H6E	20:A:7020:LMU:C6B	2.42	0.49
19:3:1218:CLA:HHD	19:3:1218:CLA:CBC	2.34	0.49
6:B:376:GLN:HB3	6:B:587:ILE:HD12	1.94	0.49
1:1:136:ASP:O	1:1:138:LYS:N	2.46	0.49
18:R:6:UNK:CB	18:R:10:UNK:CB	2.90	0.49
3:3:133:ALA:O	3:3:134:LYS:HB2	2.12	0.49
2:2:192:LEU:HG	2:2:193:PHE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:170:GLY:C	5:A:173:VAL:HG22	2.33	0.49
19:A:1785:CLA:H122	19:A:1796:CLA:HMA2	1.94	0.49
19:A:1783:CLA:H171	23:A:1806:BCR:H351	1.94	0.49
5:A:369:THR:HG21	5:A:402:ILE:CG2	2.43	0.49
5:A:679:PHE:O	5:A:683:HIS:CB	2.60	0.49
5:A:83:PHE:HA	5:A:86:LEU:HD23	1.94	0.49
19:B:1743:CLA:H192	19:B:1748:CLA:OBD	2.13	0.49
19:B:1768:CLA:C12	23:B:1779:BCR:H311	2.43	0.49
6:B:436:LEU:O	6:B:437:TYR:HB2	2.13	0.49
10:F:83:PHE:O	10:F:87:GLY:N	2.46	0.49
19:A:1778:CLA:HAA1	15:K:32:ARG:CZ	2.43	0.49
5:A:24:ARG:O	5:A:25:ASP:O	2.30	0.49
18:R:36:UNK:C	18:R:38:UNK:CB	2.90	0.49
17:N:5:GLU:O	17:N:5:GLU:OE1	2.30	0.49
8:D:75:LEU:HD21	16:L:19:PHE:CE1	2.47	0.49
1:I:144:LYS:HE3	19:1:1187:CLA:CGD	2.41	0.49
15:K:38:LEU:HG	15:K:39:LYS:HD2	1.87	0.49
14:J:20:GLY:O	14:J:21:SER:HB2	2.11	0.49
14:J:26:LEU:H	14:J:28:GLU:H	1.60	0.49
6:B:247:THR:HB	6:B:248:GLN:OE1	2.12	0.49
17:N:27:ALA:O	17:N:28:ASN:O	2.30	0.49
19:A:1763:CLA:HBA2	19:A:1763:CLA:H3A	1.50	0.49
5:A:225:VAL:HG12	5:A:248:PHE:CD1	2.48	0.49
5:A:281:LEU:HD12	19:A:1772:CLA:HED2	1.95	0.49
5:A:331:LEU:CD2	5:A:331:LEU:C	2.80	0.49
5:A:382:TYR:HB2	5:A:385:LEU:HD11	1.94	0.49
19:B:1755:CLA:C2B	23:B:1777:BCR:H352	2.42	0.49
6:B:363:GLN:HA	6:B:365:PHE:CE1	2.47	0.49
7:C:8:TYR:HB2	7:C:41:SER:OG	2.13	0.49
17:N:62:SER:CA	17:N:64:ASP:HB3	2.42	0.49
17:N:39:SER:OG	17:N:41:LYS:CA	2.58	0.49
3:3:74:ALA:CB	3:3:75:PRO:HD3	2.26	0.49
19:R:1055:CLA:H92	20:R:1056:LMU:O4'	2.12	0.49
20:A:7043:LMU:H112	20:A:7043:LMU:H71	1.93	0.49
3:3:129:PHE:O	3:3:129:PHE:CD1	2.66	0.49
1:1:184:PRO:O	1:1:185:TRP:CE2	2.66	0.49
19:4:1198:CLA:O1A	19:4:1198:CLA:C2	2.59	0.49
19:4:1201:CLA:CMA	19:4:1201:CLA:CBA	2.70	0.49
5:A:83:PHE:CE2	5:A:185:HIS:CD2	3.01	0.49
5:A:207:LEU:HB3	19:A:1776:CLA:CBB	2.43	0.49
5:A:78:VAL:O	5:A:82:HIS:CD2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:256:THR:HG22	6:B:271:THR:OG1	2.12	0.49
7:C:1:MET:CB	7:C:4:SER:CB	2.91	0.49
9:E:89:GLU:O	9:E:90:VAL:HB	2.13	0.49
19:F:1157:CLA:OBD	19:F:1157:CLA:HED2	2.12	0.49
13:I:8:PHE:CZ	19:I:1031:CLA:H43	2.48	0.49
17:N:45:ASN:HB2	17:N:54:LYS:CB	2.42	0.49
17:N:58:VAL:C	17:N:60:PHE:H	2.16	0.49
17:N:70:GLU:O	17:N:72:LYS:CE	2.61	0.49
5:A:22:VAL:CG1	5:A:24:ARG:HA	2.42	0.49
19:3:1221:CLA:HHC	19:3:1221:CLA:CBB	2.43	0.49
5:A:327:ILE:O	5:A:328:LYS:C	2.50	0.49
10:F:130:LEU:CG	10:F:131:PHE:H	2.09	0.49
2:2:188:PRO:O	2:2:189:ILE:C	2.50	0.49
16:L:97:MET:HA	16:L:100:THR:HG23	1.95	0.49
5:A:536:THR:HA	5:A:539:PHE:HB3	1.95	0.49
4:4:107:GLN:C	19:4:1196:CLA:HMA2	2.22	0.49
4:4:107:GLN:HA	19:4:1196:CLA:C2A	2.42	0.49
5:A:146:THR:HA	5:A:391:THR:HG23	1.95	0.49
19:A:1771:CLA:HAA1	19:A:1771:CLA:CED	2.43	0.49
19:A:1774:CLA:CBB	19:A:1774:CLA:C10	2.90	0.49
5:A:549:ILE:O	5:A:552:THR:O	2.31	0.49
5:A:96:MET:N	5:A:98:PHE:O	2.46	0.49
6:B:354:SER:OG	19:B:1756:CLA:HBC3	2.13	0.49
19:B:1760:CLA:HMB2	19:B:1761:CLA:C4A	2.43	0.49
5:A:713:LYS:HE3	19:B:1761:CLA:H43	1.94	0.49
19:B:1771:CLA:HED1	24:B:1781:LMG:C21	2.43	0.49
6:B:304:ILE:CD1	19:B:1749:CLA:HED3	2.41	0.49
6:B:340:SER:O	6:B:344:ILE:HG13	2.13	0.49
6:B:407:VAL:HG23	19:B:1760:CLA:HMD3	1.95	0.49
6:B:60:TRP:CD1	19:B:1738:CLA:HBC1	2.48	0.49
19:A:1800:CLA:H201	16:L:64:LEU:CD2	2.41	0.49
2:2:64:ILE:HD13	19:2:1213:CLA:HMB1	1.95	0.49
9:E:69:PHE:CD2	9:E:70:ALA:N	2.80	0.49
16:L:50:LEU:HG	16:L:51:LEU:HD23	1.95	0.49
5:A:193:LEU:O	5:A:194:ALA:C	2.50	0.49
5:A:536:THR:O	5:A:537:ALA:HB3	2.13	0.49
6:B:481:THR:O	6:B:482:ASN:HB2	2.13	0.49
1:1:184:PRO:N	1:1:185:TRP:CD1	2.81	0.49
19:4:1199:CLA:CBC	19:4:1199:CLA:CMC	2.78	0.49
19:4:1211:CLA:HBC3	19:4:1211:CLA:CHD	2.42	0.49
5:A:205:HIS:CG	19:A:1769:CLA:HMC2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1743:CLA:H41	19:B:1748:CLA:CBC	2.43	0.49
6:B:693:TRP:CD1	19:B:1770:CLA:HMD3	2.48	0.49
19:B:1751:CLA:HMD2	23:B:1774:BCR:C32	2.43	0.49
6:B:255:LEU:HA	6:B:271:THR:HB	1.95	0.49
7:C:52:LYS:NZ	7:C:64:SER:OG	2.33	0.49
8:D:31:GLY:O	8:D:32:SER:CB	2.61	0.49
2:2:166:ASN:OD1	2:2:169:LEU:CD1	2.58	0.49
2:2:120:ASN:OD1	2:2:120:ASN:N	2.45	0.49
2:2:127:ASN:OD1	14:J:7:TYR:CD2	2.65	0.49
5:A:100:GLY:HA3	5:A:153:TRP:CZ3	2.48	0.49
19:1:1148:CLA:HBC3	19:1:1148:CLA:HHD	1.95	0.49
19:1:1193:CLA:HAA2	19:1:1193:CLA:CBD	2.43	0.49
20:A:7011:LMU:C4	20:A:7011:LMU:O1'	2.58	0.49
4:4:104:ARG:HA	4:4:107:GLN:NE2	2.28	0.48
4:4:116:ASN:HB3	4:4:118:ASP:OD1	2.13	0.48
5:A:221:HIS:NE2	19:A:1770:CLA:NA	2.61	0.48
19:A:1815:CLA:HBC2	19:A:1815:CLA:HMC1	1.95	0.48
5:A:711:HIS:O	5:A:716:VAL:HG22	2.14	0.48
6:B:291:TYR:HE1	19:B:1749:CLA:HED1	1.78	0.48
19:B:1760:CLA:HBA2	19:B:1760:CLA:H3A	1.48	0.48
6:B:336:LEU:HD21	19:B:1754:CLA:HBB1	1.94	0.48
6:B:400:PRO:HG2	8:D:141:VAL:C	2.34	0.48
16:L:101:MET:SD	16:L:104:ILE:HG12	2.53	0.48
17:N:45:ASN:HD21	17:N:54:LYS:HD3	1.68	0.48
8:D:40:ALA:HA	8:D:44:GLU:O	2.13	0.48
8:D:75:LEU:HD21	16:L:19:PHE:CD1	2.48	0.48
2:2:98:GLU:CG	2:2:99:LEU:HD11	2.42	0.48
14:J:26:LEU:C	14:J:26:LEU:HD23	2.33	0.48
17:N:35:VAL:HG12	17:N:37:PHE:CE1	2.48	0.48
19:4:4014:CLA:HBB2	20:A:7034:LMU:O3B	2.08	0.48
5:A:107:GLU:OE1	5:A:161:GLU:CG	2.59	0.48
17:N:27:ALA:O	17:N:28:ASN:C	2.51	0.48
8:D:152:GLN:HA	8:D:153:PRO:HD2	1.69	0.48
19:A:1760:CLA:H2A	19:A:1760:CLA:CED	2.43	0.48
19:A:1788:CLA:H143	19:A:1788:CLA:H101	1.93	0.48
6:B:145:LEU:HA	6:B:148:ILE:HD12	1.95	0.48
6:B:462:TRP:HZ3	19:B:1764:CLA:CBC	2.26	0.48
6:B:356:PRO:HB2	6:B:361:ILE:CG2	2.44	0.48
6:B:68:VAL:O	6:B:69:ALA:CB	2.60	0.48
11:G:33:LYS:O	11:G:34:GLN:O	2.31	0.48
13:I:9:VAL:H	13:I:10:PRO:CD	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:69:ILE:CG2	4:4:70:ILE:N	2.47	0.48
10:F:123:VAL:O	10:F:126:ALA:N	2.46	0.48
6:B:664:LEU:O	6:B:667:TRP:HZ3	1.96	0.48
2:2:191:ASN:HD21	2:2:194:ALA:HA	1.78	0.48
6:B:216:LEU:HD22	6:B:218:TYR:H	1.77	0.48
20:A:7031:LMU:O2B	20:A:7031:LMU:C6'	2.61	0.48
19:A:1781:CLA:HAA1	19:A:1781:CLA:HBD	1.94	0.48
19:A:1776:CLA:C2C	19:A:1782:CLA:H171	2.43	0.48
19:A:1801:CLA:HED1	16:L:32:LEU:CD1	2.43	0.48
5:A:40:PHE:CE1	5:A:53:TRP:HD1	2.19	0.48
5:A:83:PHE:HE2	5:A:185:HIS:CD2	2.31	0.48
6:B:102:GLU:O	6:B:103:ALA:C	2.51	0.48
6:B:336:LEU:HD22	19:B:1754:CLA:HBB1	1.95	0.48
6:B:550:LYS:CG	6:B:550:LYS:O	2.60	0.48
9:E:41:ARG:HG3	9:E:46:PHE:CE1	2.48	0.48
16:L:95:LEU:O	16:L:99:LEU:HD13	2.13	0.48
17:N:62:SER:CB	17:N:66:ASP:HA	2.37	0.48
16:L:163:LEU:HD12	16:L:165:TYR:CG	2.46	0.48
2:2:168:ARG:NH1	2:2:168:ARG:HG2	2.28	0.48
11:G:13:GLY:HA2	11:G:16:LEU:CG	2.35	0.48
10:F:47:GLU:CG	10:F:51:LYS:HE3	2.28	0.48
7:C:12:ILE:HG21	7:C:39:ILE:C	2.34	0.48
11:G:58:LEU:HD12	11:G:59:LYS:HE3	1.95	0.48
5:A:583:GLY:O	5:A:585:GLY:N	2.47	0.48
10:F:151:ASP:O	10:F:154:PHE:CB	2.56	0.48
19:1:1189:CLA:C2	19:1:1189:CLA:O1A	2.61	0.48
5:A:350:LEU:HA	5:A:350:LEU:HD23	1.66	0.48
19:A:1774:CLA:OBD	19:A:1784:CLA:H43	2.13	0.48
19:B:1762:CLA:HMB3	19:B:1763:CLA:HBB2	1.96	0.48
23:B:1774:BCR:H343	11:G:21:PHE:CE1	2.48	0.48
6:B:464:GLN:CG	6:B:469:LYS:HD3	2.42	0.48
6:B:528:HIS:CE1	19:B:1769:CLA:NB	2.81	0.48
6:B:536:LYS:O	6:B:537:GLY:C	2.51	0.48
9:E:52:VAL:HG12	9:E:53:VAL:N	2.16	0.48
9:E:58:ASP:OD2	9:E:60:LYS:NZ	2.38	0.48
4:4:174:GLY:C	4:4:175:LYS:HG3	2.23	0.48
4:4:36:ASN:OD1	4:4:39:TRP:CD1	2.67	0.48
18:R:38:UNK:O	18:R:39:UNK:C	2.61	0.48
2:2:167:GLY:O	2:2:169:LEU:N	2.47	0.48
7:C:11:CYS:C	7:C:13:GLY:H	2.17	0.48
2:2:178:TRP:O	2:2:182:ILE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:179:THR:OG1	4:4:87:SER:OG	2.16	0.48
19:2:1212:CLA:C2A	19:2:1212:CLA:CGD	2.91	0.48
20:A:7010:LMU:H2O1	20:A:7010:LMU:H3'	1.74	0.48
6:B:166:SER:O	6:B:168:PHE:N	2.44	0.48
11:G:57:LEU:O	11:G:61:ASN:OD1	2.31	0.48
19:A:1816:CLA:NB	19:A:1817:CLA:HBB2	2.29	0.48
5:A:341:GLN:HB3	5:A:434:ARG:NH1	2.28	0.48
6:B:48:ALA:HB3	6:B:157:LEU:HD22	1.93	0.48
19:B:1741:CLA:HAA2	19:B:1741:CLA:C1	2.42	0.48
6:B:182:LEU:HA	19:B:1743:CLA:HMB2	1.94	0.48
6:B:192:GLY:HA2	19:B:1745:CLA:HMC3	1.94	0.48
6:B:428:PHE:HA	19:B:1762:CLA:O1D	2.14	0.48
5:A:723:ARG:NH2	9:E:73:ASN:O	2.45	0.48
11:G:18:LEU:C	11:G:21:PHE:H	2.17	0.48
5:A:24:ARG:NH1	5:A:29:THR:CA	2.64	0.48
2:2:54:TRP:NE1	2:2:109:ARG:HD2	2.29	0.48
11:G:7:VAL:HG23	11:G:8:ILE:N	2.28	0.48
3:3:157:ALA:O	3:3:158:TYR:HD2	1.94	0.48
20:A:7037:LMU:H61	20:A:7037:LMU:H11	1.96	0.48
8:D:61:PRO:HD3	8:D:86:LEU:HD21	1.96	0.48
8:D:87:GLY:N	8:D:90:LEU:HB3	2.29	0.48
5:A:468:SER:HB2	5:A:476:MET:SD	2.54	0.48
16:L:5:LYS:N	16:L:6:PRO:HD3	2.28	0.48
5:A:603:PHE:CZ	5:A:735:VAL:HG22	2.49	0.48
19:B:1736:CLA:H3A	19:B:1736:CLA:HBA2	1.61	0.48
6:B:190:TRP:CD2	19:B:1748:CLA:HMD3	2.48	0.48
7:C:81:TYR:CD1	7:C:81:TYR:N	2.82	0.48
11:G:19:GLY:C	11:G:21:PHE:H	2.15	0.48
4:4:193:ILE:HG21	14:J:42:PHE:HD1	1.79	0.48
2:2:97:VAL:HG23	2:2:98:GLU:H	1.79	0.48
5:A:151:GLN:HA	5:A:154:ARG:HG2	1.95	0.48
20:A:7041:LMU:H111	20:A:7041:LMU:H82	1.76	0.48
1:1:89:VAL:HG12	11:G:77:ILE:HG21	1.96	0.48
6:B:715:VAL:HG23	6:B:719:PHE:HD2	1.75	0.48
12:H:37:SER:C	12:H:39:PHE:H	2.15	0.48
6:B:154:TRP:CD1	6:B:154:TRP:C	2.86	0.48
19:4:4007:CLA:C6	19:4:4007:CLA:C1	2.91	0.48
5:A:359:SER:OG	5:A:414:ALA:HB2	2.14	0.48
4:4:128:ALA:O	4:4:130:GLU:HG2	2.14	0.48
5:A:132:LEU:HD13	5:A:671:SER:O	2.14	0.48
5:A:202:MET:HB3	19:A:1780:CLA:HMD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:210:LEU:HB2	19:A:1769:CLA:HMB2	1.96	0.48
5:A:257:GLN:O	5:A:258:LEU:CB	2.62	0.48
5:A:309:LEU:HD23	5:A:309:LEU:C	2.34	0.48
5:A:370:ILE:HD11	19:A:1781:CLA:C3D	2.43	0.48
5:A:685:VAL:HG12	5:A:741:GLY:CA	2.42	0.48
19:B:1736:CLA:HBC3	19:B:1759:CLA:H41	1.94	0.48
10:F:2:ILE:HD11	10:F:76:ASP:OD2	2.13	0.48
4:4:36:ASN:O	4:4:39:TRP:HE3	1.93	0.48
15:K:47:LEU:O	15:K:48:GLN:CB	2.59	0.48
5:A:567:ARG:NH2	8:D:82:GLN:OE1	2.44	0.48
2:2:51:HIS:C	2:2:54:TRP:HB2	2.34	0.48
10:F:123:VAL:HG13	14:J:7:TYR:H	1.77	0.48
15:K:42:ALA:C	15:K:43:ARG:CD	2.80	0.48
20:A:7043:LMU:C6	20:A:7043:LMU:C10	2.80	0.48
20:A:7034:LMU:C2B	20:A:7034:LMU:C5'	2.87	0.48
17:N:18:ASP:HB2	17:N:22:LEU:CD1	2.44	0.48
5:A:502:THR:C	5:A:504:ALA:N	2.67	0.48
19:A:1759:CLA:CBA	19:A:1796:CLA:H2	2.43	0.48
5:A:216:LEU:HD12	23:A:1803:BCR:H353	1.93	0.48
5:A:458:PHE:CD2	19:A:1816:CLA:CMB	2.96	0.48
5:A:40:PHE:HZ	5:A:56:ASN:HB3	1.77	0.48
19:B:1749:CLA:H61	19:B:1749:CLA:H41	1.63	0.48
19:B:1760:CLA:HED2	19:B:1760:CLA:HAA1	1.96	0.48
19:B:1771:CLA:H51	22:B:1773:PQN:H251	1.95	0.48
6:B:433:THR:O	6:B:436:LEU:O	2.31	0.48
8:D:139:LYS:NZ	9:E:41:ARG:NH1	2.62	0.48
17:N:50:GLN:C	17:N:51:ASP:O	2.52	0.48
17:N:58:VAL:C	17:N:60:PHE:N	2.67	0.48
20:A:7005:LMU:O2'	20:A:7005:LMU:C1	2.61	0.48
12:H:53:LEU:O	12:H:54:LEU:HB3	2.13	0.48
21:B:8059:SUC:C1	21:B:8059:SUC:O6	2.60	0.48
12:H:36:GLN:HE22	19:H:1081:CLA:CAD	2.26	0.48
6:B:478:LEU:O	6:B:479:SER:HB3	2.13	0.48
11:G:96:SER:C	11:G:98:PHE:H	2.16	0.48
22:A:1802:PQN:H212	22:A:1802:PQN:H243	1.77	0.48
19:A:1779:CLA:HBC1	23:A:1804:BCR:C39	2.44	0.48
5:A:202:MET:HG3	19:A:1769:CLA:HBC2	1.95	0.48
5:A:622:SER:OG	5:A:642:PHE:HB2	2.14	0.48
6:B:170:ASN:O	6:B:323:TYR:OH	2.29	0.48
19:B:1752:CLA:HBA2	19:B:1752:CLA:H3A	1.48	0.48
6:B:420:SER:O	6:B:424:TRP:N	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:1735:CLA:H191	10:F:104:TYR:CG	2.48	0.48
10:F:62:LEU:CG	10:F:72:ILE:HD13	2.41	0.48
16:L:99:LEU:O	16:L:136:TRP:HZ3	1.96	0.48
16:L:68:PHE:HD1	16:L:68:PHE:H	1.60	0.48
8:D:75:LEU:HD11	16:L:19:PHE:CD1	2.49	0.48
2:2:96:ILE:O	2:2:100:VAL:HG13	2.14	0.48
5:A:154:ARG:HH21	5:A:233:LEU:HD13	1.78	0.48
20:A:7037:LMU:H4B	20:A:7037:LMU:H1B	1.47	0.48
20:A:7032:LMU:H81	20:A:7032:LMU:H52	1.51	0.48
5:A:172:LEU:O	5:A:175:ALA:O	2.32	0.48
23:A:1808:BCR:H332	19:L:1167:CLA:C2B	2.42	0.48
5:A:746:THR:OG1	19:A:1813:CLA:O1D	2.32	0.48
5:A:361:ASN:ND2	5:A:361:ASN:C	2.67	0.48
5:A:38:GLY:O	5:A:39:HIS:HB3	2.14	0.48
5:A:431:LEU:O	5:A:435:VAL:CG1	2.62	0.48
5:A:660:GLN:HE21	5:A:660:GLN:H	1.61	0.48
19:B:1738:CLA:H161	19:B:1738:CLA:H91	1.95	0.48
6:B:697:PRO:HB3	19:B:1770:CLA:CBC	2.41	0.48
9:E:73:ASN:ND2	9:E:78:SER:HB2	2.29	0.48
5:A:22:VAL:HG23	5:A:23:ASP:HA	1.70	0.48
3:3:181:LEU:HD13	3:3:184:VAL:CG2	2.44	0.48
2:2:68:LEU:O	2:2:69:THR:C	2.52	0.48
2:2:73:ILE:H	2:2:73:ILE:CD1	2.18	0.48
4:4:144:ALA:CB	4:4:148:GLU:O	2.61	0.48
20:A:7041:LMU:C5'	20:A:7041:LMU:O2'	2.61	0.48
20:A:7027:LMU:C6B	20:A:7027:LMU:H2B	2.44	0.48
11:G:85:ILE:O	11:G:86:LEU:HB2	2.14	0.48
19:A:1774:CLA:CAB	19:A:1774:CLA:H101	2.44	0.47
5:A:240:LYS:H	5:A:243:PRO:HD3	1.78	0.47
5:A:369:THR:O	5:A:372:VAL:HG23	2.14	0.47
5:A:379:MET:SD	5:A:511:THR:O	2.71	0.47
5:A:723:ARG:HH11	5:A:723:ARG:HG3	1.75	0.47
5:A:734:GLY:O	5:A:736:THR:N	2.47	0.47
6:B:185:VAL:HG22	6:B:188:LEU:HD23	1.96	0.47
6:B:30:ASP:OD2	6:B:396:ARG:NH1	2.38	0.47
16:L:30:SER:C	16:L:32:LEU:N	2.68	0.47
19:A:1789:CLA:HAA2	16:L:71:ALA:O	2.14	0.47
3:3:93:PHE:N	3:3:94:ARG:O	2.46	0.47
17:N:7:LEU:O	17:N:8:GLU:HB2	2.14	0.47
4:4:192:THR:HG21	4:4:195:GLN:CA	2.44	0.47
2:2:102:ILE:HG22	2:2:106:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:113:HIS:HD2	8:D:118:VAL:HG21	1.77	0.47
20:A:7034:LMU:H1B	20:A:7034:LMU:H5'	1.31	0.47
5:A:506:GLY:O	5:A:507:ALA:HB3	2.14	0.47
17:N:25:THR:HG22	17:N:26:GLY:H	1.79	0.47
2:2:148:TRP:O	2:2:150:SER:N	2.47	0.47
19:4:1198:CLA:HAA2	19:4:1198:CLA:O2D	2.11	0.47
4:4:142:ASN:O	4:4:143:PHE:CD2	2.66	0.47
19:A:1774:CLA:CBB	19:A:1774:CLA:H101	2.44	0.47
19:A:1783:CLA:H172	23:A:1806:BCR:C17	2.43	0.47
5:A:684:PHE:CD2	5:A:685:VAL:N	2.74	0.47
19:B:1756:CLA:H41	19:B:1756:CLA:C7	2.44	0.47
19:B:1771:CLA:H192	13:I:21:MET:HB3	1.96	0.47
6:B:442:VAL:O	6:B:446:PHE:HB2	2.14	0.47
17:N:51:ASP:C	17:N:52:LEU:HD22	2.34	0.47
18:R:38:UNK:O	18:R:42:UNK:O	2.32	0.47
15:K:44:GLU:O	15:K:47:LEU:CD1	2.62	0.47
19:1:1190:CLA:CMC	19:1:1196:CLA:CAC	2.91	0.47
12:H:14:ILE:O	12:H:14:ILE:HD13	2.14	0.47
10:F:23:LYS:C	10:F:24:LYS:CE	2.77	0.47
20:A:7032:LMU:H5B	20:A:7032:LMU:H3'	1.96	0.47
8:D:118:VAL:HG12	8:D:119:TYR:N	2.29	0.47
9:E:50:GLY:HA3	9:E:69:PHE:HB2	1.96	0.47
11:G:60:SER:HG	11:G:63:PRO:HB2	1.76	0.47
16:L:112:PRO:O	16:L:113:SER:HB3	2.14	0.47
6:B:373:THR:O	6:B:377:TYR:N	2.36	0.47
10:F:95:GLY:O	10:F:99:TRP:CB	2.62	0.47
5:A:569:ILE:HB	5:A:572:LYS:HG3	1.96	0.47
6:B:498:LEU:HD12	6:B:498:LEU:O	2.14	0.47
4:4:154:ILE:O	4:4:157:GLY:HA3	2.14	0.47
5:A:182:GLY:C	19:A:1767:CLA:HAC1	2.35	0.47
19:A:1789:CLA:H111	19:A:1789:CLA:H91	1.58	0.47
19:A:1798:CLA:H11	19:A:1798:CLA:H52	1.64	0.47
5:A:211:LEU:O	5:A:214:GLY:O	2.33	0.47
5:A:331:LEU:CD2	5:A:343:HIS:C	2.77	0.47
5:A:369:THR:HG21	5:A:402:ILE:HG22	1.95	0.47
19:B:1742:CLA:C3C	19:B:1743:CLA:HBB2	2.41	0.47
6:B:334:LEU:O	6:B:334:LEU:CG	2.60	0.47
6:B:420:SER:H	6:B:422:LEU:H	1.62	0.47
12:H:66:THR:HA	12:H:69:SER:OG	2.13	0.47
17:N:61:LEU:CD1	17:N:63:ASP:CB	2.92	0.47
17:N:41:LYS:HG3	17:N:42:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1190:CLA:CBC	19:1:1190:CLA:CMC	2.84	0.47
19:2:1215:CLA:H42	19:2:1217:CLA:CMD	2.42	0.47
2:2:51:HIS:O	2:2:54:TRP:HB2	2.14	0.47
19:1:1145:CLA:HMA2	19:1:1145:CLA:H61	1.90	0.47
6:B:509:PHE:CD2	6:B:509:PHE:N	2.80	0.47
21:B:8062:SUC:C6'	21:B:8062:SUC:H1'2	2.44	0.47
1:1:184:PRO:O	1:1:185:TRP:NE1	2.48	0.47
4:4:126:LEU:HD23	4:4:127:PRO:CG	2.44	0.47
19:A:1767:CLA:H171	19:A:1767:CLA:H141	1.96	0.47
23:A:1805:BCR:H312	19:A:1815:CLA:H143	1.90	0.47
5:A:227:LEU:O	5:A:231:GLN:HB2	2.14	0.47
5:A:362:LEU:HD11	19:A:1785:CLA:CBB	2.33	0.47
6:B:22:TRP:CZ2	19:B:1770:CLA:HMB1	2.50	0.47
6:B:186:SER:C	6:B:187:SER:O	2.52	0.47
6:B:309:ILE:HD12	6:B:312:GLY:HA3	1.96	0.47
19:A:1787:CLA:H93	16:L:36:TYR:HE1	1.78	0.47
5:A:328:LYS:CE	5:A:332:GLU:CG	2.80	0.47
3:3:195:LEU:HA	3:3:198:PHE:HB2	1.96	0.47
20:A:7034:LMU:O2B	20:A:7034:LMU:C6'	2.61	0.47
9:E:48:ASN:ND2	9:E:71:LYS:HZ2	2.11	0.47
20:A:7006:LMU:C5'	20:A:7006:LMU:O5B	2.58	0.47
5:A:396:PHE:CE2	5:A:616:PHE:CB	2.96	0.47
1:1:121:LYS:HG3	1:1:122:LYS:HG2	1.96	0.47
1:1:18:ALA:N	1:1:19:PRO:HD2	2.28	0.47
19:4:1201:CLA:CGD	19:4:1201:CLA:CAA	2.81	0.47
5:A:103:PHE:H	5:A:103:PHE:HD2	1.59	0.47
19:A:1765:CLA:H51	23:A:1806:BCR:C10	2.43	0.47
19:A:1765:CLA:HBB2	19:B:1763:CLA:HMD1	1.94	0.47
19:A:1783:CLA:H18	19:A:1783:CLA:H122	1.96	0.47
19:A:1783:CLA:O1D	19:A:1783:CLA:H2A	2.14	0.47
19:A:1789:CLA:H141	19:A:1789:CLA:H161	1.71	0.47
5:A:42:ARG:O	5:A:44:ILE:HG13	2.15	0.47
5:A:697:ARG:C	5:A:699:TYR:N	2.67	0.47
5:A:693:LEU:HD11	5:A:738:TYR:CD1	2.50	0.47
6:B:427:LEU:HB3	19:B:1762:CLA:CED	2.44	0.47
6:B:419:ILE:C	6:B:420:SER:OG	2.53	0.47
6:B:462:TRP:CZ3	19:B:1764:CLA:CBC	2.98	0.47
9:E:40:ARG:N	9:E:46:PHE:HE1	2.12	0.47
11:G:30:ASN:ND2	11:G:34:GLN:H	2.13	0.47
16:L:33:ILE:O	16:L:36:TYR:N	2.47	0.47
17:N:54:LYS:CB	17:N:57:LYS:NZ	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:19:ARG:NE	8:D:121:GLU:OE2	2.48	0.47
2:2:205:PHE:O	2:2:206:ALA:CB	2.62	0.47
19:3:3011:CLA:CMA	19:3:3011:CLA:CGA	2.91	0.47
10:F:12:LYS:HG2	10:F:13:GLN:H	1.76	0.47
1:1:115:GLU:O	1:1:116:LYS:HB2	2.14	0.47
1:1:85:LEU:HD13	1:1:85:LEU:H	1.78	0.47
4:4:159:LEU:O	4:4:163:PHE:HB2	2.15	0.47
19:A:1760:CLA:HBC3	19:A:1760:CLA:HHD	1.95	0.47
19:A:1801:CLA:H41	19:A:1801:CLA:H62	1.56	0.47
5:A:207:LEU:CB	19:A:1776:CLA:CBB	2.90	0.47
5:A:237:VAL:CG2	5:A:242:ILE:HD12	2.44	0.47
5:A:87:SER:OG	5:A:179:LEU:HB2	2.14	0.47
19:B:1756:CLA:H8	23:B:1777:BCR:C12	2.41	0.47
23:B:1776:BCR:H23C	23:B:1776:BCR:H382	1.97	0.47
6:B:272:ASP:C	6:B:274:ALA:H	2.18	0.47
6:B:387:PHE:HE2	19:B:1755:CLA:HHC	1.79	0.47
6:B:492:ILE:O	6:B:493:TRP:HB2	2.14	0.47
6:B:711:VAL:O	6:B:711:VAL:CG1	2.62	0.47
16:L:14:LEU:HD22	16:L:21:GLY:O	2.14	0.47
4:4:75:TRP:CD1	19:4:1205:CLA:CMD	2.98	0.47
6:B:668:ARG:NH2	6:B:672:GLN:OE1	2.48	0.47
2:2:128:ASN:O	2:2:130:LEU:CD1	2.60	0.47
10:F:124:PRO:O	10:F:125:LEU:HB2	2.14	0.47
20:A:7036:LMU:O5B	20:A:7036:LMU:C6'	2.62	0.47
16:L:124:LYS:HZ2	16:L:124:LYS:HB2	1.80	0.47
4:4:126:LEU:HD23	4:4:127:PRO:HG3	1.96	0.47
4:4:124:TYR:HD1	4:4:127:PRO:HG2	1.80	0.47
4:4:128:ALA:HB3	4:4:143:PHE:CE2	2.38	0.47
4:4:99:HIS:CE1	4:4:103:ILE:HD13	2.44	0.47
5:A:157:GLY:O	5:A:248:PHE:CE1	2.68	0.47
5:A:162:LEU:C	5:A:165:TYR:HB3	2.35	0.47
19:A:1774:CLA:H121	19:A:1774:CLA:H8	1.74	0.47
19:A:1800:CLA:HMC3	19:B:1770:CLA:C1D	2.45	0.47
19:A:1787:CLA:C9	19:A:1801:CLA:H2	2.44	0.47
6:B:124:TRP:HE1	6:B:129:LEU:HD22	1.73	0.47
19:B:1755:CLA:CED	19:B:1756:CLA:OBD	2.63	0.47
6:B:596:TRP:O	6:B:597:LYS:HB3	2.13	0.47
4:4:169:GLN:OE1	19:4:1199:CLA:HHD	2.15	0.47
19:A:1783:CLA:H43	19:A:1783:CLA:CGA	2.44	0.47
19:A:1788:CLA:HMA1	23:A:1807:BCR:HC31	1.96	0.47
23:A:1805:BCR:H17C	19:A:1814:CLA:H172	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:365:LEU:O	5:A:369:THR:HG23	2.15	0.47
5:A:744:ALA:HA	5:A:747:TRP:HB3	1.95	0.47
19:B:1742:CLA:H61	19:B:1742:CLA:C1	2.43	0.47
19:B:1758:CLA:H142	23:B:1776:BCR:C10	2.33	0.47
19:B:1765:CLA:HBC2	19:B:1765:CLA:CHD	2.45	0.47
6:B:203:ARG:HB3	6:B:270:LEU:CD1	2.44	0.47
5:A:128:GLY:HA3	6:B:446:PHE:CD2	2.49	0.47
6:B:608:GLN:O	6:B:612:SER:HB3	2.15	0.47
6:B:80:ASP:HA	6:B:81:PRO:HD3	1.55	0.47
6:B:696:LYS:HG2	7:C:80:ALA:C	2.35	0.47
16:L:66:GLY:N	16:L:67:PRO:CD	2.78	0.47
17:N:41:LYS:HG3	17:N:42:PHE:CG	2.47	0.47
8:D:46:TYR:HE1	8:D:80:LYS:CE	2.28	0.47
3:3:52:LYS:C	3:3:56:TYR:HD2	2.10	0.47
3:3:59:ILE:HB	3:3:63:ARG:HH21	1.79	0.47
2:2:161:THR:HB	2:2:165:LYS:HB2	1.97	0.47
2:2:63:PHE:CD1	2:2:64:ILE:N	2.83	0.47
12:H:73:PRO:CD	21:H:1082:SUC:H5'	2.43	0.47
11:G:16:LEU:CA	11:G:68:ILE:HG13	2.45	0.47
19:4:1206:CLA:H18	19:4:1206:CLA:ND	2.29	0.47
20:A:7042:LMU:H52	20:A:7042:LMU:H81	1.48	0.47
19:1:1145:CLA:C6	19:1:1145:CLA:HMA1	2.43	0.47
19:3:3011:CLA:HMA2	19:3:3011:CLA:CGA	2.45	0.47
4:4:60:LEU:HG	4:4:61:PRO:CD	2.36	0.47
6:B:714:SER:O	6:B:718:ILE:HG22	2.15	0.47
19:1:1192:CLA:H121	19:1:1192:CLA:HBC3	1.96	0.47
21:B:8059:SUC:HO2	21:B:8059:SUC:H1'2	1.78	0.47
21:B:8055:SUC:O2	21:B:8055:SUC:C2'	2.63	0.47
3:3:141:GLN:O	3:3:142:TYR:HB2	2.14	0.47
16:L:5:LYS:N	16:L:6:PRO:CD	2.78	0.47
19:1:1505:CLA:C10	19:1:1505:CLA:H41	2.45	0.47
5:A:337:PRO:HG2	19:A:1799:CLA:C3B	2.44	0.47
19:4:1198:CLA:H2A	19:4:1198:CLA:CGD	2.45	0.47
5:A:127:VAL:CG1	14:J:30:ASN:ND2	2.78	0.47
19:A:1768:CLA:C4D	19:A:1769:CLA:HMC3	2.45	0.47
19:A:1776:CLA:C4C	19:A:1782:CLA:H172	2.44	0.47
19:A:1779:CLA:HBB2	23:A:1804:BCR:H353	1.96	0.47
19:A:1793:CLA:H171	19:A:1801:CLA:CBB	2.45	0.47
19:A:1815:CLA:H2	19:A:1815:CLA:CMA	2.44	0.47
5:A:347:TYR:HE1	5:A:417:PHE:HZ	1.61	0.47
5:A:362:LEU:HB3	5:A:406:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:393:LEU:HD21	5:A:754:ILE:HG12	1.95	0.47
5:A:466:THR:O	5:A:470:LEU:CG	2.62	0.47
5:A:401:TRP:CZ3	5:A:609:ILE:HB	2.49	0.47
6:B:493:TRP:NE1	19:B:1746:CLA:HAC2	2.27	0.47
6:B:421:HIS:CE1	19:B:1761:CLA:CHA	2.98	0.47
9:E:85:ASP:OD1	9:E:85:ASP:O	2.32	0.47
13:I:12:VAL:HG21	19:I:1031:CLA:CGA	2.43	0.47
3:3:94:ARG:CA	3:3:97:PHE:CD1	2.80	0.47
17:N:5:GLU:HA	17:N:6:TYR:CD2	2.50	0.47
2:2:64:ILE:CG2	2:2:65:PRO:HD3	2.44	0.47
14:J:22:LEU:O	14:J:23:ALA:C	2.53	0.47
14:J:2:ARG:NH1	14:J:8:LEU:HD13	2.21	0.47
5:A:592:VAL:HG23	5:A:593:SER:N	2.30	0.47
2:2:86:GLU:HA	2:2:86:GLU:OE2	2.15	0.47
6:B:575:ASP:O	6:B:579:ALA:N	2.44	0.47
19:A:1797:CLA:CAA	19:A:1797:CLA:O2D	2.58	0.47
5:A:211:LEU:HB3	5:A:310:PHE:CD2	2.50	0.47
5:A:390:ALA:HA	5:A:393:LEU:HD23	1.97	0.47
5:A:681:GLY:C	5:A:683:HIS:H	2.16	0.47
5:A:711:HIS:NE2	19:A:1795:CLA:HAC1	2.30	0.47
6:B:53:GLN:HE21	19:B:1736:CLA:HBB1	1.78	0.47
8:D:39:LYS:HG3	8:D:43:GLU:HG2	1.96	0.47
10:F:104:TYR:HD2	10:F:104:TYR:C	2.18	0.47
16:L:40:LEU:CB	16:L:41:PRO:CD	2.90	0.47
3:3:97:PHE:CE2	3:3:98:ILE:CG1	2.97	0.47
17:N:46:PHE:O	17:N:47:THR:OG1	2.33	0.47
15:K:46:GLY:O	15:K:47:LEU:HG	2.12	0.47
5:A:567:ARG:NH2	5:A:567:ARG:HB3	2.30	0.47
3:3:63:ARG:NH1	3:3:189:LEU:H	2.13	0.47
3:3:189:LEU:C	3:3:191:MET:H	2.18	0.47
2:2:49:LEU:CB	19:2:1215:CLA:HAC2	2.45	0.47
19:1:1308:CLA:H12	19:1:1308:CLA:O1D	2.15	0.47
8:D:99:GLN:OE1	8:D:101:TYR:OH	2.33	0.47
4:4:62:GLU:O	4:4:65:THR:HG22	2.14	0.47
6:B:216:LEU:O	6:B:218:TYR:N	2.48	0.47
6:B:224:PRO:HB3	6:B:227:THR:CB	2.43	0.47
6:B:486:LEU:HB2	6:B:489:GLY:O	2.14	0.47
3:3:171:LYS:HE3	3:3:171:LYS:N	2.29	0.47
4:4:88:SER:HB3	4:4:89:THR:HG22	1.96	0.47
19:A:1764:CLA:H2A	19:A:1764:CLA:O2D	2.15	0.47
19:A:1800:CLA:C1A	19:A:1800:CLA:CGA	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:457:SER:OG	5:A:544:ILE:HA	2.15	0.47
5:A:508:THR:O	5:A:509:ALA:HB3	2.15	0.47
5:A:697:ARG:CD	6:B:566:GLY:O	2.63	0.47
19:B:1736:CLA:CHD	23:I:1032:BCR:H401	2.44	0.47
6:B:29:HIS:CD2	19:B:1737:CLA:HBB1	2.50	0.47
19:B:1747:CLA:CBD	19:B:1756:CLA:CBB	2.89	0.47
19:B:1754:CLA:HMB2	19:B:1756:CLA:H92	1.97	0.47
6:B:427:LEU:C	19:B:1762:CLA:HED2	2.36	0.47
19:B:1771:CLA:CHD	22:B:1773:PQN:H18	2.44	0.47
6:B:29:HIS:CE1	19:B:1759:CLA:H43	2.49	0.47
6:B:546:LEU:HD12	6:B:570:ILE:HD13	1.97	0.47
10:F:104:TYR:C	10:F:104:TYR:CD2	2.89	0.47
3:3:80:LYS:HD3	3:3:105:ASN:HB3	1.91	0.47
2:2:165:LYS:C	2:2:167:GLY:N	2.67	0.47
10:F:123:VAL:HG13	14:J:7:TYR:HB2	1.96	0.47
5:A:328:LYS:HE2	5:A:332:GLU:CD	2.35	0.47
20:2:1224:LMU:C3	20:2:1224:LMU:C7	2.91	0.47
9:E:69:PHE:CG	9:E:70:ALA:N	2.82	0.47
6:B:211:ASN:CB	6:B:214:ASP:HB3	2.42	0.47
8:D:70:GLU:HB3	8:D:71:GLY:H	1.48	0.47
17:N:28:ASN:HA	17:N:30:ALA:H	1.79	0.47
19:4:1201:CLA:HAA2	19:4:1201:CLA:O1D	2.14	0.46
5:A:127:VAL:CG2	19:A:1765:CLA:CBB	2.94	0.46
19:A:1774:CLA:C4D	19:A:1784:CLA:H72	2.45	0.46
19:A:1797:CLA:H41	19:A:1797:CLA:H62	1.55	0.46
19:A:1817:CLA:CAD	6:B:670:TYR:OH	2.63	0.46
19:B:1769:CLA:CHA	19:B:1769:CLA:CBA	2.91	0.46
19:B:1742:CLA:HMC1	23:B:1775:BCR:H373	1.97	0.46
6:B:431:PHE:CD2	19:B:1762:CLA:CMA	2.98	0.46
9:E:52:VAL:CG1	9:E:53:VAL:H	2.15	0.46
9:E:88:GLU:O	9:E:89:GLU:C	2.53	0.46
19:H:1079:CLA:HBC2	19:H:1079:CLA:CHD	2.45	0.46
23:I:1032:BCR:HC42	23:I:1032:BCR:H322	1.96	0.46
17:N:61:LEU:HG	17:N:62:SER:N	2.29	0.46
12:H:14:ILE:HD11	12:H:17:THR:H	1.80	0.46
7:C:28:MET:HA	7:C:38:GLN:HB2	1.97	0.46
19:2:1212:CLA:H3A	19:2:1212:CLA:HBA2	1.62	0.46
17:N:18:ASP:HB3	17:N:22:LEU:HG	1.93	0.46
3:3:127:ARG:C	3:3:129:PHE:H	2.18	0.46
5:A:159:THR:O	5:A:160:SER:CB	2.64	0.46
5:A:206:HIS:O	5:A:211:LEU:HD23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:595:TRP:HE3	5:A:596:ASP:OD2	1.98	0.46
6:B:50:HIS:CA	6:B:53:GLN:HB2	2.44	0.46
6:B:658:ALA:O	6:B:661:PHE:HD2	1.98	0.46
6:B:732:LYS:HG3	6:B:732:LYS:HZ2	1.50	0.46
16:L:25:THR:O	16:L:28:THR:HB	2.15	0.46
19:3:1221:CLA:HBD	19:3:1221:CLA:HAA1	1.97	0.46
5:A:568:LEU:O	5:A:586:ARG:HD3	2.15	0.46
1:1:160:GLY:CA	19:1:1189:CLA:HBB2	2.44	0.46
3:3:164:PHE:O	3:3:165:ASN:C	2.53	0.46
5:A:389:TYR:CD1	5:A:625:TRP:CG	3.03	0.46
2:2:209:THR:HG23	2:2:209:THR:O	2.14	0.46
4:4:109:ILE:HG22	4:4:120:ILE:HG23	1.96	0.46
19:4:1198:CLA:H3A	19:4:1198:CLA:HBA2	1.09	0.46
19:4:1200:CLA:HED3	19:4:1211:CLA:C1	2.45	0.46
4:4:128:ALA:CA	4:4:143:PHE:CZ	2.98	0.46
5:A:156:SER:O	5:A:158:ILE:N	2.49	0.46
19:A:1765:CLA:CHA	19:A:1765:CLA:CBA	2.92	0.46
19:A:1795:CLA:HBA1	19:A:1795:CLA:H3A	1.64	0.46
5:A:358:LEU:O	5:A:361:ASN:HB3	2.14	0.46
5:A:75:SER:HB3	5:A:354:TRP:CZ2	2.50	0.46
19:B:1739:CLA:H141	19:B:1757:CLA:H91	1.97	0.46
6:B:293:THR:C	6:B:294:ASN:CG	2.74	0.46
6:B:436:LEU:O	6:B:437:TYR:CB	2.63	0.46
6:B:471:THR:CG2	6:B:502:ASN:ND2	2.78	0.46
7:C:81:TYR:HD1	7:C:81:TYR:N	2.14	0.46
19:A:1800:CLA:HMB2	19:L:1167:CLA:CBC	2.45	0.46
4:4:73:PRO:O	4:4:74:LYS:HG3	2.14	0.46
17:N:45:ASN:C	17:N:46:PHE:O	2.52	0.46
3:3:180:LYS:C	3:3:182:LYS:H	2.18	0.46
3:3:56:TYR:HD1	3:3:185:LYS:CE	2.29	0.46
5:A:253:ASP:O	5:A:256:ALA:HB3	2.14	0.46
1:1:50:ALA:O	1:1:54:VAL:HG23	2.15	0.46
19:1:1145:CLA:HBA1	19:1:1145:CLA:H3A	1.79	0.46
9:E:56:ASP:HB2	9:E:64:PRO:CB	2.32	0.46
19:2:1212:CLA:O1A	19:2:1212:CLA:C1A	2.63	0.46
5:A:574:ASN:OD1	5:A:574:ASN:N	2.48	0.46
12:H:57:LEU:O	12:H:57:LEU:HD13	2.14	0.46
5:A:127:VAL:HG12	14:J:30:ASN:ND2	2.30	0.46
19:A:1794:CLA:CMC	19:A:1794:CLA:HBC3	2.42	0.46
5:A:614:PHE:HE1	19:A:1813:CLA:H62	1.80	0.46
6:B:127:ILE:O	6:B:128:GLY:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:130:ARG:NH1	6:B:130:ARG:CG	2.78	0.46
19:B:1756:CLA:C10	23:B:1777:BCR:H14C	2.45	0.46
19:B:1759:CLA:HMC1	19:B:1759:CLA:HBC3	1.96	0.46
6:B:439:HIS:HB2	19:B:1763:CLA:C1C	2.45	0.46
23:B:1780:BCR:H331	23:B:1780:BCR:C8	2.46	0.46
6:B:545:LYS:HG2	6:B:546:LEU:N	2.30	0.46
6:B:553:PHE:O	6:B:555:TYR:N	2.49	0.46
16:L:46:ALA:CB	16:L:52:ARG:NH2	2.78	0.46
16:L:68:PHE:CD1	16:L:68:PHE:N	2.84	0.46
19:2:1217:CLA:HBA1	20:A:7003:LMU:H51	1.97	0.46
4:4:192:THR:HG21	4:4:195:GLN:HA	1.98	0.46
20:A:7042:LMU:C5'	20:A:7042:LMU:O2B	2.55	0.46
19:3:1222:CLA:O1A	19:3:1222:CLA:CMA	2.63	0.46
10:F:40:LEU:HD12	10:F:42:ILE:HD11	1.97	0.46
6:B:15:ASP:O	6:B:20:ARG:CG	2.63	0.46
20:A:7038:LMU:H101	20:A:7038:LMU:H61	1.97	0.46
21:B:8055:SUC:O1'	21:B:8055:SUC:O3'	2.33	0.46
1:1:34:ALA:O	1:1:38:ARG:N	2.39	0.46
19:A:1767:CLA:C4A	19:A:1767:CLA:CBA	2.93	0.46
19:A:1774:CLA:H2	19:A:1774:CLA:HMB2	1.96	0.46
19:A:1776:CLA:H43	19:A:1779:CLA:H2	1.96	0.46
19:A:1776:CLA:HMC1	19:A:1776:CLA:HBC2	1.96	0.46
19:A:1813:CLA:C1A	19:B:1784:CLA:HBB2	2.46	0.46
5:A:378:SER:OG	19:A:1782:CLA:HBC2	2.16	0.46
19:B:1737:CLA:CAB	19:B:1738:CLA:HBA2	2.46	0.46
19:B:1739:CLA:HMC2	23:B:1780:BCR:C28	2.34	0.46
6:B:197:VAL:O	6:B:198:ALA:CB	2.63	0.46
6:B:308:HIS:HD1	6:B:309:ILE:N	2.12	0.46
6:B:362:ALA:C	6:B:364:ASP:H	2.19	0.46
6:B:395:ILE:HD13	6:B:555:TYR:H	1.80	0.46
7:C:79:LEU:CD2	7:C:81:TYR:C	2.83	0.46
9:E:44:TYR:HD2	9:E:45:TRP:HE3	1.62	0.46
17:N:81:VAL:O	17:N:82:PHE:C	2.53	0.46
7:C:14:CYS:O	7:C:14:CYS:SG	2.73	0.46
19:4:1206:CLA:C15	19:4:1206:CLA:H193	2.35	0.46
10:F:44:ALA:C	10:F:46:MET:N	2.69	0.46
10:F:46:MET:C	10:F:50:LYS:HB2	2.36	0.46
5:A:149:PHE:C	5:A:151:GLN:N	2.67	0.46
4:4:125:SER:HB3	4:4:126:LEU:H	1.43	0.46
5:A:187:HIS:CE1	19:A:1767:CLA:CHA	2.95	0.46
5:A:356:ALA:O	5:A:360:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:370:ILE:CD1	19:A:1781:CLA:C3D	2.94	0.46
5:A:662:SER:O	5:A:666:GLN:HB2	2.15	0.46
5:A:72:GLU:HB2	5:A:73:GLU:H	1.57	0.46
6:B:311:PRO:HD3	19:B:1772:CLA:C3C	2.46	0.46
6:B:231:ASN:O	6:B:233:TYR:N	2.48	0.46
6:B:233:TYR:HB3	6:B:254:ILE:O	2.16	0.46
6:B:180:SER:CB	6:B:288:GLY:HA3	2.38	0.46
6:B:309:ILE:HD11	6:B:313:GLY:H	1.80	0.46
6:B:350:GLN:HG3	6:B:372:TYR:HE1	1.80	0.46
6:B:54:LEU:HD11	19:B:1743:CLA:CBA	2.46	0.46
7:C:62:PHE:CD1	9:E:42:GLU:HB2	2.51	0.46
19:4:1199:CLA:HAA1	19:F:1157:CLA:H12	1.97	0.46
19:F:1157:CLA:HBD	19:F:1157:CLA:HAA2	1.97	0.46
18:R:38:UNK:O	18:R:42:UNK:C	2.64	0.46
3:3:56:TYR:HD1	3:3:185:LYS:NZ	2.12	0.46
2:2:73:ILE:N	2:2:73:ILE:HD12	2.24	0.46
20:A:7025:LMU:H92	20:A:7025:LMU:H62	1.62	0.46
16:L:118:LEU:HD12	16:L:119:THR:N	2.21	0.46
6:B:377:TYR:O	6:B:378:ILE:HB	2.16	0.46
4:4:142:ASN:O	4:4:143:PHE:CB	2.63	0.46
19:A:1774:CLA:CGA	19:A:1784:CLA:HMD1	2.43	0.46
19:A:1817:CLA:H41	19:A:1817:CLA:HMB2	1.96	0.46
6:B:138:GLY:H	6:B:140:ILE:HG12	1.79	0.46
6:B:48:ALA:HB1	6:B:157:LEU:HD22	1.95	0.46
19:B:1739:CLA:HMB3	19:I:1031:CLA:HMA1	1.96	0.46
19:B:1753:CLA:C9	19:B:1753:CLA:HBB2	2.46	0.46
19:B:1755:CLA:CGA	19:B:1769:CLA:HAA1	2.46	0.46
6:B:183:PHE:HB3	6:B:284:PHE:HD2	1.81	0.46
6:B:50:HIS:HB2	6:B:53:GLN:HB2	1.98	0.46
6:B:594:TRP:CD1	6:B:595:HIS:N	2.84	0.46
6:B:625:TRP:CE3	6:B:626:LEU:N	2.83	0.46
6:B:721:TYR:HA	6:B:724:PHE:HB3	1.97	0.46
9:E:53:VAL:HG12	9:E:54:ALA:N	2.30	0.46
10:F:96:TRP:CZ2	19:F:1155:CLA:C3B	2.99	0.46
23:A:1808:BCR:HC8	19:L:1167:CLA:HHC	1.97	0.46
17:N:46:PHE:O	17:N:47:THR:CG2	2.63	0.46
17:N:59:PRO:CB	17:N:75:TYR:CE1	2.96	0.46
3:3:132:TRP:HZ3	3:3:155:GLU:CD	1.82	0.46
4:4:33:ASP:O	4:4:34:PRO:O	2.32	0.46
6:B:672:GLN:HE22	6:B:698:VAL:HA	1.81	0.46
4:4:144:ALA:HB3	4:4:147:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:1149:CLA:O1D	19:1:1149:CLA:CBA	2.64	0.46
20:R:1056:LMU:O5B	20:R:1056:LMU:C5'	2.60	0.46
3:3:165:ASN:HA	3:3:165:ASN:HD22	1.59	0.46
5:A:392:GLN:HG2	5:A:392:GLN:O	2.14	0.46
5:A:293:GLY:O	5:A:294:LEU:HB3	2.15	0.46
5:A:686:TRP:O	5:A:689:SER:OG	2.28	0.46
4:4:165:GLY:O	4:4:169:GLN:CG	2.59	0.46
19:A:1774:CLA:HBA2	19:A:1774:CLA:H3A	1.34	0.46
23:A:1809:BCR:H341	23:A:1809:BCR:H11C	1.64	0.46
5:A:680:LEU:HB3	19:A:1814:CLA:C1	2.45	0.46
19:A:1814:CLA:C3D	19:A:1814:CLA:HED2	2.46	0.46
5:A:656:PHE:O	5:A:659:ALA:N	2.48	0.46
6:B:174:ARG:HH12	19:B:1754:CLA:HMD2	1.80	0.46
6:B:348:VAL:HG12	6:B:349:ALA:N	2.30	0.46
6:B:17:THR:HA	6:B:696:LYS:N	2.31	0.46
11:G:44:PHE:O	11:G:47:GLY:CA	2.28	0.46
12:H:65:LEU:O	19:H:1079:CLA:H52	2.16	0.46
15:K:31:ASN:H	15:K:32:ARG:NH1	2.12	0.46
16:L:64:LEU:CA	16:L:67:PRO:HG2	2.45	0.46
4:4:75:TRP:CD2	4:4:76:TYR:N	2.84	0.46
3:3:97:PHE:HE2	3:3:98:ILE:HD13	0.49	0.46
2:2:129:LYS:O	2:2:132:GLY:HA3	2.14	0.46
2:2:54:TRP:CB	19:2:1221:CLA:OBD	2.64	0.46
19:3:1221:CLA:HBB1	19:3:1221:CLA:CHC	2.45	0.46
5:A:118:PRO:HB3	5:A:150:PHE:CD2	2.50	0.46
20:A:7030:LMU:H21	20:A:7030:LMU:C6'	2.45	0.46
8:D:90:LEU:HD13	8:D:90:LEU:O	2.16	0.46
15:K:24:PHE:HB3	15:K:52:PRO:CG	2.43	0.46
20:A:7009:LMU:H1B	20:A:7009:LMU:O1'	2.16	0.46
8:D:48:ILE:CB	8:D:100:PHE:HB3	2.45	0.46
4:4:101:VAL:O	4:4:104:ARG:HD3	2.15	0.46
19:A:1776:CLA:HBC3	19:A:1776:CLA:HMC1	1.96	0.46
23:A:1805:BCR:H11C	23:A:1805:BCR:H341	1.69	0.46
5:A:207:LEU:O	5:A:310:PHE:CB	2.58	0.46
5:A:242:ILE:HG12	5:A:243:PRO:CG	2.45	0.46
6:B:124:TRP:C	6:B:124:TRP:HD1	2.18	0.46
6:B:271:THR:OG1	6:B:272:ASP:N	2.49	0.46
11:G:33:LYS:HZ2	11:G:33:LYS:HA	1.79	0.46
16:L:66:GLY:C	19:L:1168:CLA:HMC3	2.36	0.46
4:4:38:ARG:HH11	4:4:38:ARG:CG	2.28	0.46
17:N:4:GLU:O	17:N:4:GLU:CG	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:36:LEU:HB3	16:L:20:ILE:HG13	1.97	0.46
2:2:49:LEU:HB3	19:2:1215:CLA:HAC2	1.98	0.46
20:A:7016:LMU:C4	20:A:7016:LMU:O6'	2.64	0.46
20:A:7032:LMU:C3	20:A:7032:LMU:O5B	2.59	0.46
19:1:1145:CLA:HMC1	19:1:1145:CLA:CBC	2.39	0.46
6:B:378:ILE:HG22	6:B:379:ALA:N	2.31	0.46
3:3:162:PRO:HG2	3:3:164:PHE:CG	2.51	0.46
5:A:389:TYR:CE1	5:A:625:TRP:CG	3.03	0.46
4:4:142:ASN:O	4:4:143:PHE:CG	2.68	0.46
4:4:142:ASN:C	4:4:143:PHE:CG	2.89	0.46
4:4:93:ILE:C	4:4:96:ILE:HD12	2.35	0.46
19:A:1766:CLA:CBB	19:A:1769:CLA:HMA3	2.46	0.46
19:A:1761:CLA:HMC3	19:A:1785:CLA:HMA1	1.97	0.46
19:A:1796:CLA:H192	14:J:19:PHE:HD2	1.78	0.46
23:A:1806:BCR:C23	23:A:1806:BCR:H393	2.08	0.46
5:A:207:LEU:CD2	5:A:314:GLY:HA2	2.43	0.46
6:B:29:HIS:CB	19:B:1759:CLA:HBA1	2.46	0.46
19:B:1755:CLA:CAD	19:B:1767:CLA:CBB	2.94	0.46
6:B:545:LYS:CD	6:B:546:LEU:H	2.26	0.46
5:A:654:ARG:HH21	6:B:637:PRO:HD2	1.80	0.46
7:C:66:ARG:NH2	7:C:66:ARG:CG	2.74	0.46
6:B:167:TRP:CB	11:G:41:MET:HE3	2.45	0.46
3:3:97:PHE:CD2	3:3:98:ILE:N	2.73	0.46
4:4:36:ASN:O	4:4:38:ARG:NH1	2.49	0.46
5:A:567:ARG:HH11	8:D:35:GLY:N	2.13	0.46
3:3:188:ARG:HA	3:3:191:MET:HB2	1.97	0.46
19:2:1213:CLA:HBA2	19:2:1213:CLA:H3A	1.34	0.46
2:2:93:THR:HA	2:2:96:ILE:HG12	1.99	0.46
10:F:24:LYS:CA	10:F:26:GLN:H	2.29	0.46
2:2:205:PHE:CD1	2:2:206:ALA:CA	2.99	0.46
20:A:7042:LMU:H61	20:A:7042:LMU:H31	1.39	0.46
5:A:594:ALA:O	5:A:598:VAL:HG23	2.16	0.46
8:D:102:ARG:NH2	8:D:110:GLN:HB2	2.29	0.46
1:1:44:LEU:O	1:1:48:ARG:HG3	2.16	0.46
10:F:11:SER:OG	10:F:14:PHE:HB3	2.16	0.46
4:4:42:GLN:NE2	4:4:119:PRO:HB2	2.31	0.45
4:4:98:SER:C	4:4:102:GLU:OE1	2.54	0.45
5:A:132:LEU:HD23	6:B:446:PHE:CE1	2.51	0.45
5:A:145:ILE:HG22	5:A:147:SER:H	1.80	0.45
19:A:1797:CLA:CHD	19:A:1797:CLA:HBC3	2.32	0.45
23:A:1808:BCR:C23	23:A:1808:BCR:C38	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1813:CLA:CBB	19:A:1814:CLA:HED1	2.46	0.45
5:A:334:HIS:HB3	19:A:1777:CLA:CMA	2.46	0.45
5:A:353:SER:O	5:A:354:TRP:CB	2.64	0.45
5:A:538:ASP:O	5:A:542:HIS:HB2	2.16	0.45
5:A:603:PHE:HZ	5:A:693:LEU:CD2	2.25	0.45
6:B:122:GLN:HG3	6:B:361:ILE:CG1	2.43	0.45
19:B:1746:CLA:CHD	19:B:1746:CLA:HBC2	2.37	0.45
19:B:1755:CLA:HED1	19:B:1756:CLA:HMD2	1.98	0.45
6:B:292:ARG:NH2	19:B:1750:CLA:HED1	2.31	0.45
6:B:53:GLN:O	6:B:54:LEU:HB2	2.16	0.45
6:B:560:ASP:CG	6:B:561:GLY:N	2.69	0.45
19:L:1167:CLA:HBA1	19:L:1167:CLA:CHA	2.47	0.45
12:H:73:PRO:CD	21:H:1082:SUC:C5'	2.93	0.45
2:2:97:VAL:HA	2:2:100:VAL:CG1	2.46	0.45
1:1:144:LYS:NZ	19:1:1187:CLA:CGD	2.79	0.45
3:3:66:MET:CE	3:3:69:ALA:HB3	2.46	0.45
20:A:7039:LMU:H82	20:A:7039:LMU:H112	1.53	0.45
19:3:1222:CLA:H41	19:3:1222:CLA:H61	1.61	0.45
5:A:374:GLN:O	5:A:376:MET:N	2.49	0.45
5:A:291:THR:O	5:A:293:GLY:N	2.42	0.45
5:A:308:ILE:HD13	19:A:1772:CLA:H91	1.94	0.45
19:A:1763:CLA:C4B	23:A:1806:BCR:H333	2.46	0.45
5:A:347:TYR:CE1	5:A:417:PHE:HZ	2.33	0.45
5:A:618:TRP:HB2	5:A:656:PHE:CE1	2.51	0.45
6:B:120:VAL:HG22	6:B:123:TRP:HE1	1.82	0.45
19:B:1735:CLA:H71	19:B:1735:CLA:HMC2	1.98	0.45
19:B:1739:CLA:H42	19:B:1739:CLA:CHD	2.46	0.45
19:B:1762:CLA:HBA1	19:B:1762:CLA:HBD	1.98	0.45
19:B:1762:CLA:HBC1	19:B:1768:CLA:H151	1.97	0.45
19:B:1764:CLA:O2A	19:B:1765:CLA:CMB	2.51	0.45
23:B:1779:BCR:H24C	23:B:1779:BCR:H371	1.72	0.45
6:B:592:PHE:CZ	19:B:1784:CLA:H62	2.52	0.45
6:B:353:TYR:HB2	6:B:594:TRP:HH2	1.81	0.45
6:B:621:ARG:HB3	6:B:621:ARG:HE	1.60	0.45
7:C:60:THR:HG21	7:C:64:SER:HB3	1.97	0.45
11:G:31:MET:O	11:G:34:GLN:N	2.38	0.45
19:H:1079:CLA:HMB3	13:I:14:LEU:HD12	1.99	0.45
18:R:39:UNK:C	18:R:42:UNK:CB	2.92	0.45
2:2:168:ARG:HH21	2:2:171:MET:CG	2.29	0.45
2:2:205:PHE:CE1	2:2:206:ALA:HA	2.51	0.45
2:2:189:ILE:HD13	2:2:189:ILE:N	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:520:LEU:HD13	20:A:1810:LMU:O2'	2.16	0.45
5:A:284:ARG:HH12	5:A:507:ALA:HB1	1.81	0.45
8:D:21:ASP:HB3	8:D:22:PRO:HD3	1.98	0.45
3:3:58:GLU:HG2	19:3:1220:CLA:C1D	2.46	0.45
6:B:543:GLY:HA3	6:B:548:PRO:O	2.16	0.45
5:A:185:HIS:O	5:A:187:HIS:N	2.49	0.45
5:A:354:TRP:O	5:A:358:LEU:N	2.49	0.45
6:B:58:PHE:CE2	6:B:145:LEU:HD12	2.51	0.45
6:B:346:SER:O	6:B:350:GLN:N	2.47	0.45
6:B:459:PHE:CD2	19:B:1768:CLA:C2D	3.00	0.45
6:B:551:LYS:O	6:B:553:PHE:CE2	2.69	0.45
6:B:662:MET:HG2	22:B:1773:PQN:O1	2.17	0.45
7:C:73:THR:HB	7:C:74:THR:H	1.37	0.45
6:B:294:ASN:HB2	11:G:38:GLN:NE2	2.17	0.45
19:A:1788:CLA:C16	23:L:1169:BCR:H361	2.37	0.45
17:N:61:LEU:HG	17:N:62:SER:H	1.81	0.45
4:4:36:ASN:C	4:4:36:ASN:OD1	2.55	0.45
20:A:7020:LMU:O2'	20:A:7020:LMU:H5'	2.16	0.45
3:3:106:TYR:O	3:3:107:TRP:C	2.54	0.45
6:B:247:THR:HG23	6:B:250:ALA:CB	2.46	0.45
10:F:44:ALA:HB1	10:F:48:LYS:HB3	1.97	0.45
20:A:7042:LMU:C3	20:A:7042:LMU:O5'	2.63	0.45
8:D:41:GLN:HG3	16:L:125:LYS:NZ	2.31	0.45
19:4:4014:CLA:O1A	19:4:4014:CLA:O2D	2.33	0.45
19:4:4014:CLA:HAA2	19:4:4014:CLA:O2D	2.17	0.45
2:2:79:TRP:O	2:2:79:TRP:CD2	2.69	0.45
19:1:1199:CLA:HMC1	19:4:1198:CLA:CMB	2.42	0.45
1:1:183:ASP:HB3	1:1:185:TRP:HE1	1.81	0.45
5:A:126:ILE:O	5:A:129:GLN:HB2	2.15	0.45
5:A:95:GLY:HA3	19:A:1763:CLA:CHC	2.46	0.45
6:B:323:TYR:HE1	19:B:1754:CLA:HBC1	1.78	0.45
6:B:355:LEU:CD2	19:B:1756:CLA:HMC2	2.46	0.45
6:B:74:PHE:C	6:B:76:ALA:N	2.69	0.45
19:H:1080:CLA:C2C	23:I:1032:BCR:HC21	2.47	0.45
5:A:21:LEU:HA	5:A:22:VAL:O	2.15	0.45
2:2:56:MET:O	2:2:57:LEU:C	2.55	0.45
6:B:667:TRP:O	6:B:669:GLY:N	2.49	0.45
4:4:58:MET:O	4:4:61:PRO:HD3	2.13	0.45
21:B:8059:SUC:O2	21:B:8059:SUC:C2'	2.63	0.45
8:D:131:GLY:O	8:D:132:LEU:HB2	2.15	0.45
5:A:431:LEU:HD22	19:A:1779:CLA:HMC3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1800:CLA:H152	23:A:1808:BCR:C35	2.47	0.45
5:A:258:LEU:HG	5:A:280:PHE:CD1	2.51	0.45
5:A:497:ALA:O	5:A:498:LEU:HB2	2.17	0.45
5:A:618:TRP:CZ2	5:A:655:ASP:HB3	2.52	0.45
5:A:655:ASP:O	5:A:660:GLN:NE2	2.49	0.45
5:A:749:PHE:CG	19:A:1813:CLA:HMD1	2.51	0.45
19:B:1753:CLA:H12	19:B:1753:CLA:HAA1	1.99	0.45
19:B:1755:CLA:H11	19:B:1769:CLA:CBD	2.45	0.45
6:B:375:HIS:CE1	19:B:1758:CLA:NC	2.82	0.45
19:B:1764:CLA:H3A	19:B:1764:CLA:HBA2	1.40	0.45
19:B:1764:CLA:NC	19:B:1765:CLA:CBB	2.79	0.45
19:B:1769:CLA:O1A	19:B:1769:CLA:C4A	2.64	0.45
19:B:1768:CLA:C12	23:B:1779:BCR:C31	2.92	0.45
9:E:43:SER:CB	9:E:82:TYR:HE1	2.26	0.45
11:G:19:GLY:N	11:G:21:PHE:H	2.15	0.45
16:L:65:VAL:HG11	16:L:154:ALA:HB1	1.98	0.45
19:A:1789:CLA:C3	16:L:67:PRO:HB2	2.46	0.45
4:4:30:LEU:O	4:4:32:GLU:CD	2.55	0.45
4:4:38:ARG:HG3	4:4:39:TRP:CA	2.43	0.45
20:A:7016:LMU:H91	20:A:7016:LMU:H32	1.98	0.45
2:2:126:PRO:HG2	2:2:129:LYS:N	2.31	0.45
16:L:108:LYS:O	16:L:132:SER:CB	2.45	0.45
19:1:1148:CLA:O2D	19:1:1148:CLA:H2	2.16	0.45
20:A:7010:LMU:H22	20:A:7010:LMU:H51	1.67	0.45
8:D:87:GLY:H	8:D:90:LEU:H	1.64	0.45
10:F:63:CYS:CA	10:F:69:PRO:HA	2.43	0.45
4:4:119:PRO:C	4:4:121:PHE:H	2.18	0.45
5:A:170:GLY:O	5:A:173:VAL:CG2	2.59	0.45
19:A:1764:CLA:ND	19:A:1783:CLA:H42	2.32	0.45
23:A:1809:BCR:C31	23:A:1809:BCR:C8	2.92	0.45
5:A:471:GLY:O	5:A:472:ARG:HG2	2.16	0.45
5:A:64:PHE:CZ	5:A:77:LYS:HE2	2.50	0.45
19:B:1739:CLA:CMC	23:B:1780:BCR:C28	2.92	0.45
19:B:1755:CLA:HBA2	19:B:1755:CLA:H3A	1.59	0.45
6:B:557:PHE:CE2	7:C:66:ARG:NE	2.85	0.45
9:E:73:ASN:ND2	9:E:75:ALA:H	2.15	0.45
10:F:62:LEU:HG	10:F:72:ILE:CD1	2.42	0.45
4:4:68:GLY:C	4:4:71:ASN:HB2	2.35	0.45
20:A:7016:LMU:C3	20:A:7016:LMU:O6'	2.65	0.45
5:A:97:TYR:HA	5:A:153:TRP:HZ2	1.82	0.45
2:2:205:PHE:O	2:2:206:ALA:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:216:LEU:HD21	6:B:221:GLY:CA	2.41	0.45
5:A:499:ALA:N	5:A:500:PRO:CD	2.79	0.45
6:B:224:PRO:HA	6:B:227:THR:OG1	2.16	0.45
20:A:7026:LMU:C1B	20:A:7026:LMU:O6B	2.64	0.45
8:D:34:GLY:HA3	8:D:62:THR:HB	1.97	0.45
6:B:262:HIS:O	6:B:265:THR:O	2.35	0.45
19:A:1778:CLA:HAA1	15:K:32:ARG:NE	2.32	0.45
5:A:358:LEU:HD11	5:A:413:HIS:CB	2.47	0.45
5:A:388:ASP:O	5:A:390:ALA:N	2.50	0.45
5:A:733:VAL:HG12	5:A:737:HIS:CE1	2.51	0.45
19:B:1747:CLA:C3D	19:B:1756:CLA:HBB2	2.47	0.45
6:B:655:LEU:HD21	19:B:1771:CLA:HBB1	1.99	0.45
6:B:287:GLY:O	6:B:290:MET:HB2	2.16	0.45
6:B:535:VAL:CG2	6:B:539:LEU:HD23	2.47	0.45
6:B:570:ILE:O	6:B:570:ILE:HG13	2.17	0.45
7:C:7:ILE:C	7:C:8:TYR:O	2.54	0.45
4:4:76:TYR:HB2	19:4:1205:CLA:O2D	2.17	0.45
5:A:25:ASP:CA	5:A:27:ILE:N	2.78	0.45
5:A:490:GLN:HG2	16:L:166:TYR:HE1	1.76	0.45
4:4:36:ASN:HB2	4:4:39:TRP:CH2	2.42	0.45
4:4:37:LEU:O	4:4:39:TRP:CG	2.70	0.45
2:2:110:TRP:CD2	19:2:1221:CLA:CED	3.00	0.45
2:2:51:HIS:CB	19:2:1221:CLA:OBD	2.63	0.45
10:F:124:PRO:C	10:F:126:ALA:H	2.20	0.45
20:A:7013:LMU:H112	20:A:7049:LMU:O5B	2.17	0.45
2:2:196:HIS:CE1	21:2:1225:SUC:HO3	2.28	0.45
20:A:7032:LMU:C3	20:A:7032:LMU:H2B	2.46	0.45
19:4:4014:CLA:HAA2	19:4:4014:CLA:CGD	2.47	0.45
19:4:4014:CLA:HED1	19:4:4014:CLA:HBA1	1.99	0.45
5:A:636:HIS:C	5:A:638:THR:H	2.19	0.45
12:H:39:PHE:O	12:H:40:PHE:CD1	2.69	0.45
5:A:630:ASP:C	5:A:632:GLY:N	2.70	0.45
6:B:587:ILE:HA	6:B:587:ILE:HD13	1.76	0.45
5:A:539:PHE:HE2	5:A:543:HIS:CE1	2.34	0.45
6:B:232:LEU:HA	6:B:232:LEU:HD22	1.69	0.45
4:4:100:TYR:CA	4:4:103:ILE:HG12	2.42	0.45
19:A:1762:CLA:H51	19:A:1785:CLA:NC	2.32	0.45
5:A:398:HIS:HD2	19:A:1783:CLA:NC	2.15	0.45
19:B:1756:CLA:H122	23:B:1777:BCR:C13	2.46	0.45
6:B:29:HIS:O	19:B:1759:CLA:HAA2	2.16	0.45
6:B:323:TYR:CD1	19:B:1754:CLA:HBC1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:553:PHE:O	6:B:554:GLY:C	2.54	0.45
6:B:655:LEU:HD21	19:B:1771:CLA:CBB	2.46	0.45
6:B:704:GLN:HG3	24:B:1781:LMG:H132	1.99	0.45
3:3:94:ARG:NH1	3:3:98:ILE:HG23	2.30	0.45
17:N:47:THR:O	17:N:48:GLY:C	2.56	0.45
17:N:48:GLY:HA3	17:N:49:CYS:CB	2.47	0.45
17:N:61:LEU:CG	17:N:62:SER:H	2.29	0.45
19:2:1213:CLA:O1A	19:2:1213:CLA:C2	2.64	0.45
1:1:51:MET:SD	1:1:54:VAL:HB	2.57	0.45
3:3:111:TYR:HB2	3:3:112:THR:H	1.68	0.45
21:2:1225:SUC:H2	21:2:1225:SUC:O2'	2.17	0.45
20:A:7032:LMU:O5B	20:A:7032:LMU:C3'	2.49	0.45
2:2:118:CYS:O	2:2:119:VAL:CG1	2.52	0.45
6:B:160:LYS:NZ	6:B:160:LYS:HB2	2.29	0.45
5:A:284:ARG:NH1	5:A:507:ALA:HB1	2.30	0.45
5:A:363:ALA:O	5:A:367:SER:CB	2.65	0.45
5:A:34:TRP:O	5:A:35:ALA:CB	2.65	0.45
20:A:7019:LMU:H32	20:A:7019:LMU:O2'	2.16	0.45
4:4:123:GLN:CG	4:4:124:TYR:N	2.80	0.45
4:4:94:GLU:CB	4:4:95:PHE:HD1	2.26	0.45
19:A:1764:CLA:ND	19:A:1783:CLA:C4	2.80	0.45
19:A:1788:CLA:O1A	19:A:1800:CLA:C1	2.62	0.45
23:A:1808:BCR:C8	23:A:1808:BCR:C33	2.86	0.45
5:A:207:LEU:HA	5:A:211:LEU:CB	2.45	0.45
5:A:388:ASP:OD1	5:A:391:THR:HB	2.17	0.45
5:A:654:ARG:HA	6:B:632:ILE:CD1	2.44	0.45
5:A:731:ARG:O	5:A:735:VAL:HG23	2.15	0.45
6:B:190:TRP:CE3	19:B:1744:CLA:HBB2	2.47	0.45
19:B:1753:CLA:C4	19:B:1753:CLA:HAA1	2.31	0.45
19:B:1768:CLA:C9	19:B:1769:CLA:HAC1	2.47	0.45
6:B:558:PRO:CB	6:B:703:VAL:HB	2.47	0.45
6:B:618:GLY:HA2	6:B:621:ARG:HB3	1.98	0.45
6:B:655:LEU:HD22	19:B:1771:CLA:CBB	2.46	0.45
7:C:62:PHE:CE2	9:E:42:GLU:CD	2.87	0.45
9:E:36:VAL:HG22	9:E:52:VAL:HG22	1.98	0.45
10:F:96:TRP:CE3	10:F:134:PHE:N	2.85	0.45
13:I:7:LEU:HB2	23:I:1032:BCR:H333	1.98	0.45
17:N:62:SER:C	17:N:66:ASP:H	2.20	0.45
17:N:59:PRO:C	17:N:66:ASP:OD1	2.55	0.45
19:1:1143:CLA:CBC	20:A:7001:LMU:C3B	2.93	0.45
19:4:1206:CLA:HAA2	19:4:1206:CLA:HBD	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:20:GLN:HG2	10:F:24:LYS:HD2	1.99	0.45
20:A:7013:LMU:H3O2	20:A:7013:LMU:C1B	2.30	0.45
11:G:58:LEU:O	11:G:60:SER:N	2.48	0.45
5:A:428:TYR:CD1	8:D:57:ILE:HG12	2.52	0.45
20:A:7009:LMU:H1B	20:A:7009:LMU:C1'	2.47	0.45
18:R:24:UNK:O	18:R:27:UNK:CB	2.65	0.45
6:B:31:PHE:O	6:B:32:GLU:C	2.55	0.45
1:1:34:ALA:HB3	1:1:137:PRO:CB	2.47	0.45
10:F:113:LYS:HA	10:F:114:PRO:HD3	1.68	0.45
6:B:673:GLU:O	6:B:676:GLU:HB2	2.17	0.45
2:2:181:HIS:CE1	19:2:1214:CLA:ND	2.85	0.45
19:4:1198:CLA:CAA	19:4:1198:CLA:CGD	2.94	0.45
19:A:1765:CLA:HMC1	19:A:1765:CLA:HBC3	1.99	0.45
19:A:1789:CLA:H43	16:L:64:LEU:CD2	2.42	0.45
5:A:435:VAL:O	5:A:438:HIS:ND1	2.44	0.45
5:A:607:ASN:HD22	5:A:607:ASN:HA	1.65	0.45
6:B:29:HIS:HB3	19:B:1737:CLA:HBB2	1.98	0.45
6:B:272:ASP:HB3	19:B:1747:CLA:HMA1	1.99	0.45
6:B:36:ASP:O	6:B:41:ARG:NE	2.50	0.45
6:B:594:TRP:HD1	6:B:595:HIS:N	2.15	0.45
7:C:5:VAL:CG1	7:C:65:VAL:HG13	2.41	0.45
8:D:140:ASN:HA	8:D:142:SER:OG	2.16	0.45
19:B:1771:CLA:C19	13:I:21:MET:CB	2.94	0.45
17:N:57:LYS:HE2	17:N:57:LYS:HB2	1.44	0.45
18:R:38:UNK:C	18:R:42:UNK:CA	2.94	0.45
3:3:49:ILE:CG1	3:3:52:LYS:CB	2.94	0.45
20:A:7013:LMU:H22	20:A:7013:LMU:O5'	2.16	0.45
10:F:131:PHE:C	10:F:133:GLY:N	2.69	0.45
17:N:2:VAL:HG23	17:N:2:VAL:O	2.17	0.45
12:H:45:ALA:C	12:H:48:THR:H	2.12	0.45
20:A:7027:LMU:H31	20:A:7027:LMU:H62	1.53	0.45
17:N:34:THR:C	17:N:36:GLU:N	2.71	0.45
2:2:43:TRP:O	2:2:45:VAL:N	2.50	0.45
6:B:450:GLU:C	6:B:452:GLN:H	2.16	0.45
19:4:4007:CLA:HBC2	19:4:4007:CLA:CHD	2.47	0.45
8:D:132:LEU:HD12	8:D:136:SER:OG	2.17	0.45
5:A:440:ASP:HA	6:B:677:THR:HB	1.98	0.45
19:4:1200:CLA:CBC	19:4:1200:CLA:CMC	2.89	0.44
5:A:113:PRO:C	5:A:115:HIS:N	2.71	0.44
5:A:146:THR:H	19:A:1764:CLA:HMD1	1.81	0.44
5:A:143:ILE:HG12	19:A:1764:CLA:HBC2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1765:CLA:HBB1	6:B:446:PHE:HE2	1.82	0.44
19:A:1790:CLA:O1A	19:A:1791:CLA:HBC3	2.17	0.44
5:A:733:VAL:HG13	19:A:1796:CLA:C3D	2.47	0.44
5:A:360:ILE:HD13	23:A:1804:BCR:C37	2.43	0.44
5:A:648:THR:O	5:A:649:ILE:HG22	2.16	0.44
19:B:1745:CLA:O1D	19:B:1745:CLA:H2A	2.17	0.44
6:B:389:HIS:HE1	19:B:1759:CLA:NC	2.15	0.44
6:B:444:LEU:O	6:B:445:ALA:CB	2.65	0.44
6:B:458:ILE:HG13	6:B:459:PHE:CD1	2.53	0.44
6:B:602:TRP:C	6:B:604:GLY:H	2.17	0.44
6:B:732:LYS:HZ3	6:B:732:LYS:CB	2.16	0.44
9:E:38:ILE:HB	9:E:46:PHE:O	2.18	0.44
10:F:144:LEU:HD12	10:F:149:LEU:HD13	1.99	0.44
19:B:1762:CLA:NB	10:F:90:PHE:CE1	2.85	0.44
19:H:1079:CLA:H41	16:L:87:ALA:HB2	1.98	0.44
17:N:57:LYS:O	17:N:60:PHE:N	2.49	0.44
1:1:27:LEU:O	1:1:31:GLU:HB2	2.16	0.44
15:K:44:GLU:OE1	15:K:45:SER:CA	2.62	0.44
5:A:249:ILE:C	5:A:251:ASN:N	2.71	0.44
2:2:167:GLY:O	2:2:168:ARG:C	2.55	0.44
2:2:51:HIS:CA	2:2:54:TRP:HB2	2.47	0.44
12:H:19:GLY:O	12:H:20:GLN:CB	2.63	0.44
11:G:16:LEU:CD2	11:G:68:ILE:HG21	2.47	0.44
4:4:58:MET:SD	4:4:59:LEU:HA	2.56	0.44
20:A:7033:LMU:H1B	20:A:7033:LMU:H5'	1.59	0.44
6:B:217:PRO:HB2	6:B:218:TYR:HD1	1.82	0.44
11:G:79:HIS:NE2	11:G:82:ALA:HB2	2.33	0.44
19:A:1783:CLA:HAA1	19:A:1783:CLA:HBD	1.98	0.44
5:A:369:THR:HG22	19:A:1784:CLA:HMC1	1.99	0.44
5:A:362:LEU:CD1	19:A:1785:CLA:HBB2	2.34	0.44
5:A:723:ARG:O	19:A:1795:CLA:CBB	2.66	0.44
5:A:209:GLY:HA3	5:A:213:LEU:HD12	1.99	0.44
5:A:157:GLY:O	5:A:248:PHE:HE1	2.00	0.44
5:A:258:LEU:HG	5:A:280:PHE:CE1	2.52	0.44
19:B:1756:CLA:H71	23:B:1777:BCR:C14	2.47	0.44
19:4:1199:CLA:CAA	19:F:1157:CLA:H42	2.40	0.44
16:L:23:LEU:O	16:L:25:THR:N	2.50	0.44
16:L:67:PRO:O	16:L:71:ALA:HB3	2.18	0.44
16:L:163:LEU:HD12	16:L:164:PRO:CA	2.44	0.44
2:2:63:PHE:HE2	2:2:168:ARG:CD	2.30	0.44
3:3:74:ALA:N	19:3:1216:CLA:C2D	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:102:ILE:HD13	2:2:102:ILE:N	2.32	0.44
4:4:144:ALA:O	4:4:147:LEU:O	2.35	0.44
7:C:29:ILE:CG2	8:D:126:GLY:CA	2.95	0.44
20:A:7005:LMU:H51	20:A:7005:LMU:H22	1.85	0.44
20:2:1224:LMU:H1'	20:2:1224:LMU:H4'	1.46	0.44
16:L:123:ARG:HB3	16:L:126:GLN:HG3	1.97	0.44
12:H:55:LYS:O	12:H:56:PHE:HB2	2.18	0.44
4:4:139:ASN:HA	4:4:139:ASN:HD22	1.62	0.44
5:A:126:ILE:O	5:A:126:ILE:HD12	2.17	0.44
19:A:1774:CLA:ND	19:A:1784:CLA:H72	2.32	0.44
19:A:1783:CLA:H191	19:A:1814:CLA:H13	1.98	0.44
5:A:309:LEU:HD21	19:A:1776:CLA:HMC3	1.99	0.44
5:A:462:ILE:HG21	19:A:1789:CLA:HMC1	1.99	0.44
5:A:473:PRO:C	5:A:475:ASP:N	2.71	0.44
6:B:467:HIS:NE2	19:B:1764:CLA:CHA	2.80	0.44
6:B:290:MET:HG2	6:B:290:MET:O	2.16	0.44
6:B:362:ALA:O	6:B:363:GLN:CG	2.61	0.44
6:B:390:GLY:HA3	23:B:1777:BCR:HC22	1.98	0.44
5:A:558:LYS:HZ2	6:B:674:LEU:HB3	1.80	0.44
8:D:139:LYS:HZ3	9:E:41:ARG:NH1	2.16	0.44
13:I:28:VAL:O	13:I:29:GLU:CD	2.56	0.44
8:D:33:THR:HG23	16:L:23:LEU:HD12	1.98	0.44
16:L:65:VAL:O	16:L:69:VAL:N	2.51	0.44
17:N:62:SER:O	17:N:63:ASP:HB2	2.17	0.44
19:2:2006:CLA:CAA	19:2:2006:CLA:C2	2.94	0.44
10:F:50:LYS:O	10:F:52:ARG:C	2.56	0.44
7:C:39:ILE:HG23	7:C:40:ALA:N	2.31	0.44
1:1:179:THR:HB	1:1:180:HIS:H	1.49	0.44
8:D:28:ILE:O	8:D:66:ALA:HB3	2.18	0.44
8:D:28:ILE:HG13	8:D:66:ALA:HB1	1.98	0.44
6:B:221:GLY:C	6:B:223:GLY:N	2.71	0.44
20:A:1810:LMU:H51	20:A:1810:LMU:H22	1.77	0.44
6:B:454:LEU:HD13	10:F:69:PRO:O	2.18	0.44
1:1:168:TYR:N	1:1:169:PRO:HD3	2.32	0.44
6:B:326:ILE:O	6:B:326:ILE:HG12	2.17	0.44
15:K:3:ILE:HD13	15:K:3:ILE:O	2.17	0.44
19:A:1817:CLA:CBA	19:A:1817:CLA:HED3	2.48	0.44
19:A:1817:CLA:C3A	19:A:1817:CLA:O2A	2.61	0.44
6:B:356:PRO:HB2	6:B:361:ILE:HG22	2.00	0.44
6:B:447:GLY:O	6:B:449:PRO:HD3	2.18	0.44
8:D:30:ALA:O	16:L:18:PRO:CB	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:65:VAL:HG23	16:L:66:GLY:H	1.82	0.44
5:A:24:ARG:C	5:A:25:ASP:CG	2.76	0.44
5:A:22:VAL:CA	5:A:24:ARG:HA	2.48	0.44
5:A:22:VAL:HG12	5:A:24:ARG:HA	1.99	0.44
3:3:50:GLU:OE1	3:3:54:LEU:HB2	2.17	0.44
2:2:57:LEU:C	2:2:57:LEU:HD23	2.37	0.44
1:1:56:GLY:HA3	19:1:1191:CLA:C4D	2.48	0.44
3:3:112:THR:HG1	3:3:113:LEU:H	1.57	0.44
11:G:10:LEU:HD23	11:G:13:GLY:HA3	2.00	0.44
11:G:13:GLY:C	11:G:16:LEU:HG	2.37	0.44
2:2:120:ASN:CG	14:J:5:LYS:HD2	2.38	0.44
15:K:43:ARG:HA	15:K:43:ARG:HD2	1.48	0.44
10:F:22:LEU:HA	10:F:25:LEU:HD13	1.99	0.44
6:B:172:GLU:C	6:B:176:ASN:HB2	2.37	0.44
5:A:349:ILE:HD13	5:A:422:TYR:HB3	1.99	0.44
12:H:50:ARG:NH1	12:H:53:LEU:C	2.67	0.44
20:A:7006:LMU:H5B	20:A:7006:LMU:H3'	1.99	0.44
10:F:116:GLN:HE21	10:F:116:GLN:HB2	1.60	0.44
5:A:81:ALA:HA	19:A:1760:CLA:HMA1	1.97	0.44
19:A:1777:CLA:HBA2	19:A:1777:CLA:H3A	1.75	0.44
19:A:1783:CLA:H72	23:A:1805:BCR:C37	2.45	0.44
19:A:1789:CLA:H62	19:A:1789:CLA:H92	1.73	0.44
5:A:260:PRO:HG3	5:A:277:TYR:CZ	2.52	0.44
5:A:277:TYR:HD2	5:A:279:ASP:H	1.64	0.44
23:B:1775:BCR:H24C	23:B:1775:BCR:H371	1.58	0.44
23:B:1780:BCR:C33	23:B:1780:BCR:C8	2.93	0.44
6:B:188:LEU:HG	6:B:189:ALA:N	2.32	0.44
6:B:202:SER:HB3	6:B:270:LEU:HD21	1.99	0.44
6:B:202:SER:O	6:B:245:GLY:CA	2.50	0.44
6:B:257:ILE:HA	6:B:272:ASP:OD2	2.17	0.44
6:B:395:ILE:HG22	6:B:551:LYS:HG3	2.00	0.44
6:B:545:LYS:CG	6:B:546:LEU:N	2.79	0.44
6:B:568:CYS:HB3	6:B:569:ASP:H	1.65	0.44
6:B:573:TRP:O	6:B:576:PHE:HB3	2.18	0.44
4:4:75:TRP:HD1	19:4:1205:CLA:HHD	1.80	0.44
17:N:58:VAL:O	17:N:60:PHE:N	2.51	0.44
17:N:67:LEU:CA	17:N:68:GLU:HG2	2.47	0.44
4:4:32:GLU:O	4:4:33:ASP:OD1	2.35	0.44
4:4:36:ASN:CA	4:4:39:TRP:CE3	3.01	0.44
20:A:7016:LMU:C5	20:A:7016:LMU:O6'	2.60	0.44
19:1:1142:CLA:HAA2	19:1:1142:CLA:HBD	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:ASN:CG	14:J:3:ASP:CB	2.85	0.44
5:A:230:ASN:HD22	5:A:230:ASN:C	2.21	0.44
7:C:28:MET:HB2	8:D:121:GLU:HA	1.98	0.44
19:1:1148:CLA:CED	19:1:1148:CLA:H72	2.47	0.44
19:1:1145:CLA:HMA3	19:1:1145:CLA:H61	1.91	0.44
20:A:7030:LMU:H31	20:A:7030:LMU:H61	1.52	0.44
5:A:631:GLN:HG2	5:A:633:VAL:HG13	1.98	0.44
3:3:164:PHE:HA	3:3:164:PHE:HD1	1.71	0.44
12:H:77:LEU:HB3	12:H:78:PRO:CD	2.47	0.44
5:A:420:ARG:HG2	5:A:421:ASP:N	2.31	0.44
4:4:115:VAL:HG13	4:4:116:ASN:N	2.32	0.44
22:A:1802:PQN:H261	22:A:1802:PQN:H293	1.87	0.44
19:A:1817:CLA:H162	19:A:1817:CLA:H202	1.72	0.44
5:A:222:GLN:O	5:A:227:LEU:HD12	2.18	0.44
5:A:335:LYS:CG	5:A:336:GLY:N	2.67	0.44
5:A:59:ALA:C	5:A:61:ALA:H	2.21	0.44
5:A:73:GLU:O	5:A:74:ILE:C	2.56	0.44
19:B:1758:CLA:H3A	19:B:1758:CLA:HBA2	1.52	0.44
6:B:700:LEU:N	22:B:1773:PQN:O4	2.34	0.44
6:B:22:TRP:HE1	19:B:1770:CLA:HBB2	1.75	0.44
6:B:361:ILE:C	6:B:362:ALA:O	2.56	0.44
6:B:365:PHE:HB3	6:B:602:TRP:CZ2	2.53	0.44
16:L:68:PHE:N	16:L:68:PHE:HD1	2.14	0.44
17:N:54:LYS:HA	17:N:54:LYS:HD2	1.32	0.44
17:N:4:GLU:C	17:N:4:GLU:OE2	2.56	0.44
19:1:1142:CLA:HMD3	19:1:1143:CLA:NA	2.31	0.44
19:1:1308:CLA:H2A	19:1:1308:CLA:O1D	2.18	0.44
6:B:517:PHE:CG	6:B:517:PHE:O	2.69	0.44
19:2:1212:CLA:CHD	19:2:1212:CLA:CBC	2.88	0.44
20:A:7025:LMU:O2'	20:A:7025:LMU:H21	2.18	0.44
8:D:83:CYS:O	8:D:83:CYS:SG	2.75	0.44
5:A:419:VAL:HG21	5:A:577:PHE:HB2	2.00	0.44
20:L:1170:LMU:H82	20:L:1170:LMU:H52	1.81	0.44
19:4:1196:CLA:CBC	19:4:1196:CLA:CHD	2.85	0.44
4:4:143:PHE:N	4:4:150:LYS:HE2	2.33	0.44
4:4:142:ASN:HA	4:4:150:LYS:NZ	2.21	0.44
5:A:212:GLY:C	5:A:214:GLY:H	2.20	0.44
5:A:509:ALA:O	5:A:510:SER:OG	2.25	0.44
5:A:64:PHE:HZ	5:A:77:LYS:HE2	1.79	0.44
6:B:174:ARG:HH12	19:B:1754:CLA:CMD	2.27	0.44
23:B:1774:BCR:H15C	23:B:1774:BCR:H351	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:230:TRP:CE3	19:B:1746:CLA:HAA2	2.52	0.44
6:B:387:PHE:O	6:B:391:PRO:HG3	2.17	0.44
6:B:527:LEU:O	19:B:1769:CLA:HMA3	2.17	0.44
7:C:73:THR:N	7:C:76:SER:OG	2.50	0.44
4:4:40:PHE:CD1	4:4:40:PHE:N	2.77	0.44
19:2:1217:CLA:H112	19:2:1217:CLA:H142	1.67	0.44
2:2:164:ILE:O	2:2:168:ARG:NH1	2.50	0.44
21:B:8054:SUC:H3'	21:B:8054:SUC:H1	1.58	0.44
19:3:1218:CLA:H41	19:3:1218:CLA:C9	2.44	0.44
5:A:148:GLY:C	5:A:149:PHE:O	2.54	0.44
20:A:7023:LMU:O6'	20:A:7023:LMU:C1'	2.65	0.44
19:3:3011:CLA:H72	19:3:3011:CLA:H112	1.28	0.44
6:B:715:VAL:O	6:B:716:GLY:C	2.56	0.44
5:A:34:TRP:O	5:A:35:ALA:HB3	2.18	0.44
4:4:86:SER:O	4:4:88:SER:N	2.49	0.44
19:A:1789:CLA:HBA1	19:A:1789:CLA:H3A	1.45	0.44
19:A:1800:CLA:HMC3	19:B:1770:CLA:ND	2.32	0.44
23:A:1803:BCR:C31	23:A:1803:BCR:C8	2.80	0.44
5:A:239:PRO:CA	5:A:242:ILE:HD11	2.43	0.44
5:A:274:TRP:NE1	5:A:277:TYR:CE2	2.86	0.44
5:A:430:ASP:H	5:A:433:ASP:CG	2.21	0.44
6:B:597:LYS:HG2	19:B:1767:CLA:HBC1	2.00	0.44
19:A:1813:CLA:HBB1	6:B:624:LEU:HD11	2.00	0.44
19:G:1099:CLA:H52	19:G:1099:CLA:H12	1.75	0.44
19:H:1079:CLA:HBB2	13:I:13:GLY:C	2.37	0.44
19:A:1800:CLA:H201	16:L:64:LEU:CG	2.48	0.44
19:A:1800:CLA:H202	16:L:64:LEU:HD21	2.00	0.44
4:4:69:ILE:CG1	4:4:175:LYS:HB2	2.48	0.44
17:N:62:SER:CB	17:N:66:ASP:OD1	2.65	0.44
2:2:100:VAL:HG22	2:2:101:PHE:N	2.32	0.44
19:1:1187:CLA:HMA2	19:1:1187:CLA:HBA1	1.99	0.44
11:G:12:THR:HG22	11:G:72:LEU:CD1	2.46	0.44
19:J:1043:CLA:CED	19:J:1043:CLA:CHA	2.94	0.44
19:J:1043:CLA:HBA2	19:J:1043:CLA:H3A	1.25	0.44
2:2:137:TYR:CD1	2:2:138:PRO:CD	3.00	0.44
4:4:81:GLU:HA	4:4:81:GLU:OE2	2.18	0.44
4:4:104:ARG:HE	4:4:105:ARG:CA	2.31	0.44
19:A:1779:CLA:CHD	23:A:1804:BCR:C20	2.95	0.44
5:A:462:ILE:HG21	19:A:1789:CLA:HMC3	1.98	0.44
23:A:1808:BCR:H383	23:A:1808:BCR:H23C	1.99	0.44
5:A:308:ILE:HD12	19:A:1772:CLA:HHC	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:41:SER:O	5:A:44:ILE:CA	2.61	0.44
5:A:430:ASP:O	5:A:432:LEU:N	2.51	0.44
5:A:472:ARG:HG3	6:B:97:GLY:HA2	1.99	0.44
5:A:701:GLN:NE2	5:A:701:GLN:HA	2.33	0.44
6:B:144:PHE:HD2	6:B:144:PHE:O	1.98	0.44
6:B:193:HIS:HD2	19:B:1744:CLA:NC	2.16	0.44
19:B:1737:CLA:H71	19:B:1754:CLA:O1A	2.17	0.44
8:D:139:LYS:HG2	8:D:141:VAL:HG22	2.00	0.44
9:E:43:SER:HB2	9:E:82:TYR:CE1	2.39	0.44
11:G:32:ALA:O	11:G:33:LYS:C	2.56	0.44
19:H:1079:CLA:HBA1	19:H:1079:CLA:H3A	1.59	0.44
19:A:1787:CLA:H42	16:L:33:ILE:HG12	2.00	0.44
16:L:69:VAL:HG11	16:L:84:GLY:H	1.83	0.44
3:3:50:GLU:OE2	3:3:54:LEU:HD13	2.17	0.44
15:K:14:THR:O	15:K:18:MET:HG2	2.17	0.44
19:1:1308:CLA:H2A	19:1:1308:CLA:O2A	2.18	0.44
11:G:8:ILE:CG1	11:G:8:ILE:O	2.63	0.44
10:F:24:LYS:C	10:F:26:GLN:H	2.20	0.44
2:2:206:ALA:O	2:2:207:ALA:CB	2.66	0.44
17:N:37:PHE:CD2	17:N:37:PHE:N	2.84	0.44
6:B:160:LYS:CG	6:B:161:TRP:H	2.30	0.44
20:A:7026:LMU:H1B	20:A:7026:LMU:O6B	2.17	0.44
6:B:513:GLY:O	6:B:515:GLY:N	2.51	0.44
19:A:1759:CLA:CBB	19:A:1760:CLA:NC	2.81	0.43
5:A:515:TRP:CZ2	19:A:1782:CLA:HMC3	2.52	0.43
19:A:1783:CLA:H193	19:A:1783:CLA:H162	1.83	0.43
19:A:1813:CLA:CMB	19:A:1814:CLA:HMD1	2.48	0.43
5:A:346:LEU:O	5:A:347:TYR:HB2	2.17	0.43
5:A:365:LEU:O	5:A:369:THR:CG2	2.66	0.43
5:A:660:GLN:O	5:A:661:ALA:HB3	2.17	0.43
19:B:1747:CLA:C1A	19:B:1747:CLA:H12	2.48	0.43
19:B:1768:CLA:C8	19:B:1768:CLA:HBB2	2.45	0.43
6:B:178:HIS:C	6:B:180:SER:N	2.69	0.43
6:B:25:ILE:H	6:B:25:ILE:HG13	1.57	0.43
6:B:278:LEU:HD12	19:B:1746:CLA:HMA1	1.99	0.43
6:B:615:TYR:OH	6:B:621:ARG:NH2	2.50	0.43
7:C:51:CYS:N	25:C:1082:SF4:S4	2.86	0.43
5:A:584:PRO:CB	7:C:67:VAL:HB	2.48	0.43
6:B:297:ILE:HG21	11:G:21:PHE:HZ	1.82	0.43
11:G:24:PHE:C	11:G:26:PHE:N	2.71	0.43
11:G:43:HIS:HD1	11:G:43:HIS:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:15:LEU:HD12	13:I:18:ALA:HB3	2.00	0.43
16:L:65:VAL:C	16:L:67:PRO:HD2	2.37	0.43
3:3:97:PHE:C	3:3:98:ILE:CG2	2.83	0.43
17:N:82:PHE:H	17:N:82:PHE:HD2	1.66	0.43
5:A:24:ARG:HH12	5:A:29:THR:HA	1.77	0.43
1:1:25:ASP:O	1:1:26:PRO:C	2.55	0.43
19:2:1213:CLA:NC	19:2:1213:CLA:H43	2.32	0.43
2:2:62:ILE:HG13	2:2:66:GLU:OE2	2.18	0.43
3:3:111:TYR:HB2	3:3:112:THR:HG22	2.00	0.43
3:3:114:PHE:CZ	19:3:1221:CLA:HMB3	2.53	0.43
20:A:7041:LMU:O6'	20:A:7041:LMU:C1B	2.64	0.43
17:N:35:VAL:HG12	17:N:37:PHE:CZ	2.53	0.43
19:1:1145:CLA:H2	19:1:1145:CLA:H61	1.84	0.43
15:K:51:ASP:CB	15:K:52:PRO:CD	2.92	0.43
8:D:96:ILE:O	8:D:97:LYS:CB	2.66	0.43
4:4:179:ASP:H	4:4:184:HIS:CD2	2.36	0.43
4:4:123:GLN:CG	4:4:124:TYR:H	2.32	0.43
5:A:131:ILE:CG2	5:A:132:LEU:N	2.81	0.43
19:A:1759:CLA:HBB1	19:A:1760:CLA:C1C	2.47	0.43
19:A:1784:CLA:H52	19:A:1784:CLA:CMD	2.48	0.43
5:A:578:ARG:HG2	5:A:595:TRP:CD1	2.53	0.43
5:A:679:PHE:O	5:A:679:PHE:CD2	2.70	0.43
6:B:29:HIS:CB	19:B:1737:CLA:HBB2	2.48	0.43
19:B:1751:CLA:CBA	19:B:1752:CLA:O1A	2.66	0.43
19:B:1754:CLA:H61	19:B:1754:CLA:CMA	2.48	0.43
19:B:1762:CLA:CBB	23:B:1778:BCR:C23	2.96	0.43
19:B:1762:CLA:CBB	23:B:1778:BCR:H23C	2.48	0.43
19:B:1762:CLA:HBB2	23:B:1778:BCR:C25	2.48	0.43
6:B:274:ALA:O	6:B:278:LEU:HB2	2.18	0.43
6:B:50:HIS:HA	6:B:53:GLN:H	1.84	0.43
6:B:710:LEU:HA	6:B:713:PHE:HB3	2.00	0.43
11:G:43:HIS:CE1	11:G:45:GLU:CG	2.96	0.43
17:N:63:ASP:HA	17:N:64:ASP:O	2.17	0.43
19:1:1190:CLA:HBA1	19:1:1190:CLA:CHA	2.39	0.43
2:2:114:LEU:O	2:2:116:PRO:HD3	2.19	0.43
2:2:211:LYS:O	19:2:1218:CLA:C3B	2.66	0.43
4:4:147:LEU:O	4:4:148:GLU:O	2.36	0.43
20:A:7005:LMU:C5B	20:A:7005:LMU:O2B	2.66	0.43
20:A:7030:LMU:H41	20:A:7030:LMU:O6'	2.18	0.43
6:B:172:GLU:O	6:B:173:SER:C	2.56	0.43
2:2:208:PHE:O	2:2:209:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:33:ALA:C	10:F:35:ASP:H	2.20	0.43
5:A:571:ASP:O	5:A:574:ASN:ND2	2.51	0.43
2:2:159:LEU:O	2:2:160:ARG:C	2.56	0.43
13:I:4:LEU:O	13:I:4:LEU:HG	2.18	0.43
4:4:98:SER:O	4:4:102:GLU:CG	2.66	0.43
19:A:1761:CLA:H3A	19:A:1761:CLA:HBA1	1.68	0.43
19:A:1781:CLA:C6	19:A:1782:CLA:CED	2.93	0.43
5:A:716:VAL:O	19:A:1795:CLA:HMD3	2.18	0.43
5:A:73:GLU:HA	5:A:76:ARG:HD2	1.99	0.43
5:A:88:ILE:C	5:A:90:PHE:N	2.70	0.43
19:B:1744:CLA:H111	19:B:1744:CLA:H71	1.50	0.43
6:B:564:ARG:CZ	7:C:64:SER:OG	2.66	0.43
17:N:50:GLN:N	17:N:51:ASP:O	2.51	0.43
17:N:47:THR:HG1	17:N:54:LYS:HD3	1.79	0.43
17:N:70:GLU:O	17:N:72:LYS:NZ	2.51	0.43
2:2:96:ILE:O	2:2:100:VAL:CG1	2.66	0.43
3:3:114:PHE:CD1	19:3:1219:CLA:CHA	3.01	0.43
11:G:16:LEU:CD2	11:G:68:ILE:CG2	2.89	0.43
20:A:7036:LMU:H82	20:A:7036:LMU:C3	2.46	0.43
16:L:115:ALA:N	16:L:116:PRO:CD	2.77	0.43
5:A:631:GLN:O	5:A:632:GLY:C	2.56	0.43
16:L:58:LEU:CD2	16:L:153:TRP:CZ2	3.01	0.43
14:J:38:THR:O	14:J:39:PHE:CB	2.66	0.43
19:3:3008:CLA:HAA2	19:3:3008:CLA:HBD	2.00	0.43
4:4:118:ASP:HA	4:4:122:LYS:HA	1.99	0.43
4:4:139:ASN:HA	4:4:140:PRO:HD3	1.85	0.43
4:4:89:THR:O	4:4:92:VAL:CB	2.59	0.43
19:A:1782:CLA:H151	19:A:1782:CLA:H111	1.52	0.43
5:A:216:LEU:CD1	23:A:1803:BCR:H352	2.48	0.43
5:A:555:ILE:HG12	5:A:555:ILE:H	1.55	0.43
5:A:648:THR:C	5:A:650:ASN:H	2.21	0.43
5:A:84:GLY:O	5:A:87:SER:O	2.36	0.43
6:B:91:ILE:CD1	6:B:104:PHE:HE2	2.24	0.43
19:B:1735:CLA:HBC1	23:B:1778:BCR:C33	2.49	0.43
19:B:1763:CLA:H3A	19:B:1763:CLA:HBA1	1.63	0.43
6:B:183:PHE:HB3	6:B:284:PHE:CD2	2.52	0.43
6:B:285:LEU:HD11	19:B:1750:CLA:HBC2	1.98	0.43
6:B:416:GLU:O	6:B:420:SER:OG	2.36	0.43
6:B:590:VAL:O	6:B:593:TYR:HB3	2.18	0.43
6:B:625:TRP:C	6:B:625:TRP:CE3	2.92	0.43
13:I:11:LEU:HD13	13:I:11:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:70:ILE:CG1	4:4:71:ASN:N	2.80	0.43
17:N:61:LEU:O	17:N:62:SER:O	2.36	0.43
17:N:72:LYS:HZ1	17:N:74:LYS:CE	2.13	0.43
4:4:34:PRO:HB3	4:4:35:GLU:HB2	1.99	0.43
4:4:193:ILE:CG2	4:4:194:VAL:N	2.74	0.43
10:F:23:LYS:CB	10:F:24:LYS:NZ	2.80	0.43
20:R:1056:LMU:O5B	20:R:1056:LMU:C6'	2.66	0.43
16:L:121:THR:OG1	16:L:122:GLY:N	2.47	0.43
11:G:59:LYS:HA	11:G:59:LYS:HD3	1.83	0.43
5:A:582:ASP:OD1	7:C:53:ARG:NH2	2.52	0.43
19:J:1043:CLA:O1A	19:J:1043:CLA:C16	2.66	0.43
5:A:113:PRO:O	5:A:115:HIS:CD2	2.72	0.43
5:A:223:VAL:CG1	5:A:224:HIS:N	2.80	0.43
5:A:347:TYR:HE1	5:A:417:PHE:CZ	2.36	0.43
5:A:541:VAL:O	5:A:544:ILE:HG22	2.17	0.43
5:A:679:PHE:CE2	5:A:683:HIS:CD2	3.03	0.43
5:A:78:VAL:O	5:A:82:HIS:CB	2.65	0.43
5:A:85:GLN:O	5:A:88:ILE:HG22	2.18	0.43
6:B:707:LEU:HD11	19:B:1759:CLA:C9	2.49	0.43
6:B:431:PHE:CD2	19:B:1762:CLA:HMA3	2.54	0.43
23:B:1777:BCR:C8	23:B:1777:BCR:H311	2.48	0.43
6:B:317:ARG:HD3	6:B:410:ARG:HG2	2.00	0.43
6:B:438:VAL:O	6:B:442:VAL:HG23	2.17	0.43
7:C:64:SER:O	7:C:65:VAL:HB	2.19	0.43
11:G:48:ASP:N	11:G:49:THR:HG22	2.31	0.43
3:3:94:ARG:NH2	3:3:97:PHE:CE2	2.82	0.43
17:N:47:THR:O	17:N:52:LEU:O	2.36	0.43
5:A:250:LEU:O	5:A:252:ARG:HG2	2.19	0.43
1:1:144:LYS:NZ	19:1:1187:CLA:OBD	2.25	0.43
20:A:7013:LMU:H4'	20:A:7049:LMU:O6'	2.19	0.43
1:1:179:THR:HG21	4:4:87:SER:C	2.39	0.43
20:A:7025:LMU:C4	20:A:7025:LMU:O2'	2.67	0.43
5:A:530:LEU:HB2	5:A:531:PRO:CD	2.43	0.43
12:H:42:THR:O	12:H:45:ALA:N	2.52	0.43
20:A:7004:LMU:O6'	20:A:7004:LMU:H1'	2.18	0.43
14:J:32:PHE:HE2	14:J:33:PHE:CZ	2.36	0.43
5:A:685:VAL:CG1	5:A:741:GLY:HA2	2.44	0.43
5:A:87:SER:HA	5:A:90:PHE:HB2	1.99	0.43
6:B:81:PRO:HG2	6:B:360:PHE:CE1	2.52	0.43
9:E:46:PHE:CD2	9:E:47:LYS:N	2.86	0.43
16:L:136:TRP:O	16:L:140:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:82:PHE:N	17:N:82:PHE:CD2	2.86	0.43
10:F:20:GLN:NE2	10:F:21:ALA:N	2.67	0.43
11:G:60:SER:C	11:G:62:ASP:N	2.71	0.43
19:R:1054:CLA:CED	19:R:1054:CLA:C1A	2.96	0.43
21:3:1223:SUC:C1'	21:3:1223:SUC:H6'2	2.48	0.43
20:A:7038:LMU:H1B	20:A:7038:LMU:O6'	2.18	0.43
8:D:48:ILE:HA	8:D:100:PHE:HB3	1.99	0.43
19:4:1198:CLA:H161	19:4:1198:CLA:H122	1.41	0.43
19:4:1199:CLA:H92	19:4:1199:CLA:H61	1.88	0.43
5:A:147:SER:OG	19:A:1783:CLA:HED2	2.19	0.43
19:A:1789:CLA:H111	19:A:1789:CLA:H142	1.58	0.43
5:A:185:HIS:O	5:A:186:TYR:C	2.57	0.43
5:A:287:LEU:N	5:A:295:TRP:HE1	2.16	0.43
5:A:462:ILE:O	5:A:466:THR:OG1	2.34	0.43
5:A:57:LEU:O	5:A:61:ALA:HB2	2.18	0.43
5:A:709:TRP:CE3	5:A:710:ALA:N	2.87	0.43
6:B:334:LEU:HD22	19:B:1737:CLA:CHD	2.49	0.43
19:B:1739:CLA:H2	19:B:1739:CLA:H71	2.00	0.43
19:B:1743:CLA:C19	19:B:1748:CLA:OBD	2.66	0.43
19:B:1765:CLA:CBB	23:B:1777:BCR:C28	2.95	0.43
6:B:555:TYR:CE2	6:B:573:TRP:HA	2.54	0.43
11:G:28:ARG:NH2	11:G:28:ARG:CG	2.74	0.43
19:H:1079:CLA:OBD	19:H:1079:CLA:O1D	2.32	0.43
13:I:12:VAL:HG21	19:I:1031:CLA:CBA	2.49	0.43
13:I:26:LEU:HD22	13:I:30:LYS:HA	2.01	0.43
2:2:64:ILE:HG22	2:2:65:PRO:HD3	2.01	0.43
19:1:1308:CLA:CMA	19:1:1308:CLA:H2	2.48	0.43
20:A:7013:LMU:H42	20:A:7013:LMU:H11	1.67	0.43
20:A:7037:LMU:O3'	20:A:7037:LMU:C6'	2.67	0.43
20:A:7014:LMU:H1B	20:A:7014:LMU:H3'	1.25	0.43
20:A:7005:LMU:H72	20:A:7005:LMU:H42	1.48	0.43
6:B:31:PHE:HB2	6:B:42:LEU:CD1	2.49	0.43
5:A:58:HIS:HB3	19:A:1760:CLA:HBC1	2.00	0.43
22:A:1802:PQN:H251	19:B:1735:CLA:HMC1	2.01	0.43
5:A:495:THR:O	5:A:495:THR:OG1	2.37	0.43
6:B:177:HIS:CD2	19:B:1743:CLA:HMC2	2.54	0.43
19:B:1767:CLA:HBC3	19:B:1767:CLA:CMC	2.40	0.43
6:B:556:SER:O	24:B:1781:LMG:HC2	2.19	0.43
6:B:628:SER:O	6:B:629:SER:C	2.56	0.43
9:E:32:ARG:NH2	9:E:53:VAL:HA	2.33	0.43
16:L:88:ALA:O	16:L:90:GLY:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:24:ARG:O	5:A:25:ASP:C	2.55	0.43
16:L:164:PRO:N	16:L:165:TYR:CD1	2.86	0.43
8:D:80:LYS:HD3	8:D:112:LEU:HD21	2.01	0.43
2:2:100:VAL:HG22	2:2:101:PHE:H	1.84	0.43
2:2:54:TRP:CD1	19:2:1221:CLA:O1D	2.72	0.43
19:1:1146:CLA:HMD2	20:A:7001:LMU:H52	2.01	0.43
20:A:7013:LMU:H4'	20:A:7049:LMU:C6'	2.49	0.43
11:G:58:LEU:HB2	11:G:59:LYS:H	1.40	0.43
20:A:7027:LMU:H42	20:A:7027:LMU:H11	1.85	0.43
10:F:115:THR:O	10:F:116:GLN:CB	2.67	0.43
6:B:486:LEU:O	6:B:487:ASN:HB3	2.19	0.43
1:1:143:LEU:HD23	1:1:143:LEU:HA	1.89	0.43
4:4:53:LEU:O	4:4:54:GLY:C	2.57	0.43
19:A:1783:CLA:H18	19:A:1814:CLA:H18	2.00	0.43
23:A:1807:BCR:H24C	23:A:1807:BCR:H371	1.57	0.43
5:A:450:CYS:HB3	19:A:1817:CLA:HBA1	2.00	0.43
5:A:397:THR:HB	5:A:613:ILE:HG13	1.98	0.43
5:A:654:ARG:HG3	5:A:655:ASP:N	2.34	0.43
6:B:60:TRP:HH2	19:B:1758:CLA:CHB	2.32	0.43
19:A:1813:CLA:CAA	19:B:1784:CLA:HBB2	2.45	0.43
6:B:288:GLY:O	6:B:289:LEU:CB	2.66	0.43
5:A:447:ASN:ND2	6:B:678:LEU:HD21	2.34	0.43
6:B:708:VAL:C	6:B:710:LEU:O	2.57	0.43
19:B:1762:CLA:C4B	10:F:90:PHE:CE1	3.02	0.43
10:F:24:LYS:O	10:F:27:ALA:HB3	2.18	0.43
12:H:24:TYR:HB3	12:H:25:GLY:H	1.59	0.43
2:2:85:GLN:CA	2:2:85:GLN:OE1	2.61	0.43
21:B:8059:SUC:O2	21:B:8059:SUC:C1'	2.66	0.43
8:D:84:LEU:HD12	8:D:100:PHE:CZ	2.49	0.43
20:A:7026:LMU:C6B	20:A:7026:LMU:C2B	2.95	0.43
19:H:1081:CLA:H3A	19:H:1081:CLA:HBA2	1.55	0.43
6:B:42:LEU:O	6:B:43:TYR:C	2.57	0.43
5:A:348:GLU:O	5:A:350:LEU:N	2.51	0.43
1:1:34:ALA:O	1:1:35:ASN:C	2.57	0.43
1:1:63:LEU:HD22	1:1:63:LEU:H	1.84	0.43
19:4:1196:CLA:HAA1	19:4:1196:CLA:HBD	2.00	0.43
4:4:151:GLU:CA	4:4:154:ILE:HG23	2.40	0.43
5:A:110:LEU:O	5:A:113:PRO:HD3	2.19	0.43
5:A:128:GLY:HA3	6:B:446:PHE:HD2	1.83	0.43
5:A:132:LEU:HD21	5:A:674:ALA:HB2	2.00	0.43
5:A:462:ILE:HG22	19:A:1789:CLA:HMC3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1789:CLA:O2D	19:A:1789:CLA:H2A	2.18	0.43
19:A:1783:CLA:C18	23:A:1806:BCR:H17C	2.46	0.43
5:A:229:ILE:HG13	5:A:243:PRO:HB3	2.00	0.43
3:3:94:ARG:NH2	3:3:98:ILE:CD1	2.82	0.43
17:N:39:SER:OG	17:N:40:CYS:N	2.52	0.43
2:2:54:TRP:HZ2	2:2:109:ARG:CB	2.32	0.43
5:A:588:GLY:HA3	6:B:668:ARG:CD	2.28	0.43
7:C:44:ARG:NH2	8:D:127:ARG:NE	2.65	0.43
20:A:7037:LMU:H3O2	20:A:7037:LMU:C6'	2.32	0.43
20:A:7025:LMU:O5B	20:A:7025:LMU:C6'	2.57	0.43
5:A:119:SER:CB	5:A:136:VAL:HG21	2.48	0.43
2:2:181:HIS:CE1	19:2:1214:CLA:C4D	3.01	0.43
20:B:1782:LMU:H3'	20:B:1782:LMU:H1B	1.47	0.43
4:4:101:VAL:O	4:4:104:ARG:CD	2.67	0.42
5:A:182:GLY:CA	19:A:1767:CLA:HAC1	2.49	0.42
5:A:281:LEU:C	5:A:283:PHE:N	2.72	0.42
5:A:346:LEU:HD11	19:A:1779:CLA:HHD	2.01	0.42
5:A:417:PHE:C	5:A:417:PHE:CD1	2.92	0.42
5:A:606:TYR:HB2	5:A:739:LEU:CD2	2.49	0.42
6:B:86:PRO:C	6:B:115:ASN:HB3	2.40	0.42
19:B:1738:CLA:HHB	19:B:1759:CLA:CBB	2.30	0.42
6:B:290:MET:HG3	19:B:1751:CLA:C2C	2.49	0.42
23:B:1776:BCR:H15C	23:B:1776:BCR:H351	1.85	0.42
22:B:1773:PQN:H161	23:B:1780:BCR:H331	1.95	0.42
6:B:127:ILE:HD13	6:B:193:HIS:CE1	2.53	0.42
6:B:649:MET:HG2	23:B:1780:BCR:H381	2.01	0.42
19:H:1079:CLA:O2A	19:H:1079:CLA:CMA	2.61	0.42
23:L:1169:BCR:H341	23:L:1169:BCR:H11C	1.81	0.42
17:N:61:LEU:CD1	17:N:62:SER:N	2.80	0.42
3:3:132:TRP:CE3	3:3:155:GLU:HG2	2.26	0.42
2:2:70:LYS:O	2:2:71:LEU:C	2.57	0.42
2:2:73:ILE:HG22	2:2:73:ILE:O	2.19	0.42
14:J:13:VAL:CG1	14:J:15:SER:HB2	2.48	0.42
14:J:25:LEU:HA	14:J:28:GLU:HB2	2.01	0.42
5:A:197:GLN:HE22	5:A:351:THR:CB	2.26	0.42
19:I:1149:CLA:HBA2	19:I:1149:CLA:O1D	2.19	0.42
16:L:126:GLN:O	16:L:127:PRO:O	2.37	0.42
19:4:4014:CLA:CAA	19:4:4014:CLA:O2D	2.67	0.42
19:3:3011:CLA:H162	19:3:3011:CLA:H143	1.85	0.42
5:A:412:ALA:O	5:A:415:ALA:HB3	2.18	0.42
6:B:378:ILE:H	6:B:381:PHE:HD1	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:192:LEU:C	3:3:194:ILE:H	2.23	0.42
1:1:34:ALA:HB3	1:1:137:PRO:HB3	2.01	0.42
5:A:409:GLY:C	5:A:411:ALA:N	2.72	0.42
4:4:104:ARG:HD2	19:4:1208:CLA:C3C	2.42	0.42
19:A:1759:CLA:C1	19:A:1796:CLA:H61	2.49	0.42
5:A:361:ASN:ND2	19:A:1761:CLA:CED	2.81	0.42
5:A:259:TYR:HB3	5:A:260:PRO:CD	2.38	0.42
5:A:99:HIS:C	5:A:101:ALA:H	2.21	0.42
6:B:123:TRP:CZ3	19:B:1743:CLA:C19	2.98	0.42
6:B:431:PHE:HD2	19:B:1762:CLA:HMA3	1.83	0.42
6:B:198:ALA:H	6:B:200:PRO:HG2	1.83	0.42
6:B:230:TRP:O	6:B:231:ASN:C	2.56	0.42
6:B:387:PHE:O	6:B:391:PRO:CD	2.65	0.42
6:B:439:HIS:NE2	6:B:443:MET:SD	2.92	0.42
16:L:66:GLY:HA2	16:L:69:VAL:HG22	2.01	0.42
19:2:1217:CLA:HBD	19:2:1217:CLA:HAA1	2.01	0.42
2:2:56:MET:SD	2:2:169:LEU:HD23	2.59	0.42
4:4:194:VAL:HG12	4:4:195:GLN:HB3	1.98	0.42
20:A:7049:LMU:H112	20:A:7049:LMU:H82	1.80	0.42
7:C:44:ARG:NH2	8:D:127:ARG:CB	2.71	0.42
2:2:196:HIS:HB3	2:2:197:LEU:H	1.54	0.42
19:4:4014:CLA:CBC	19:4:4014:CLA:CMC	2.79	0.42
6:B:377:TYR:OH	6:B:717:TYR:HE1	2.02	0.42
6:B:503:GLU:O	6:B:507:SER:HB2	2.18	0.42
20:A:1811:LMU:O1'	20:A:1811:LMU:O6B	2.29	0.42
19:4:1198:CLA:O2D	19:4:1198:CLA:CAA	2.67	0.42
4:4:169:GLN:CA	4:4:169:GLN:NE2	2.70	0.42
4:4:99:HIS:ND1	4:4:103:ILE:HD13	2.34	0.42
5:A:127:VAL:HG21	19:A:1765:CLA:CBB	2.49	0.42
19:A:1768:CLA:HBD	19:A:1768:CLA:HAA1	1.99	0.42
23:A:1805:BCR:H17C	19:A:1814:CLA:C17	2.50	0.42
5:A:210:LEU:CD1	19:A:1769:CLA:CMB	2.94	0.42
5:A:210:LEU:HD11	19:A:1769:CLA:H42	2.01	0.42
5:A:277:TYR:CD2	5:A:278:ALA:N	2.87	0.42
5:A:338:PHE:HB2	19:A:1786:CLA:HBD	2.01	0.42
5:A:400:MET:O	5:A:609:ILE:HD12	2.19	0.42
5:A:472:ARG:O	5:A:474:GLN:CG	2.67	0.42
5:A:53:TRP:HA	5:A:56:ASN:CG	2.39	0.42
5:A:685:VAL:O	5:A:688:PHE:HB3	2.19	0.42
5:A:76:ARG:NH1	5:A:192:LYS:CG	2.77	0.42
6:B:124:TRP:HZ2	6:B:135:LEU:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:550:LYS:HG2	6:B:550:LYS:O	2.18	0.42
6:B:704:GLN:O	6:B:707:LEU:HB3	2.19	0.42
11:G:41:MET:O	11:G:42:SER:C	2.55	0.42
5:A:22:VAL:HG13	5:A:22:VAL:H	1.45	0.42
4:4:32:GLU:CA	4:4:32:GLU:OE2	2.68	0.42
3:3:182:LYS:O	3:3:186:ASN:N	2.33	0.42
3:3:49:ILE:O	3:3:49:ILE:HG23	2.18	0.42
2:2:168:ARG:HH21	2:2:171:MET:HG3	1.84	0.42
15:K:14:THR:HG23	15:K:15:THR:N	2.35	0.42
2:2:103:GLY:HA2	19:2:1221:CLA:HBB2	1.94	0.42
2:2:127:ASN:OD1	14:J:2:ARG:CG	2.67	0.42
10:F:30:LYS:O	10:F:31:LEU:CB	2.68	0.42
20:A:7033:LMU:C3'	20:A:7033:LMU:C6B	2.89	0.42
16:L:50:LEU:HG	16:L:51:LEU:CD2	2.49	0.42
6:B:301:ILE:O	6:B:301:ILE:CG2	2.67	0.42
16:L:107:PHE:HA	16:L:133:ALA:HB2	2.01	0.42
19:A:1760:CLA:C4A	19:A:1767:CLA:H71	2.49	0.42
5:A:210:LEU:CD1	19:A:1769:CLA:HHB	2.46	0.42
19:A:1793:CLA:H112	19:A:1793:CLA:H71	1.46	0.42
5:A:688:PHE:HD1	19:A:1815:CLA:CMB	2.33	0.42
5:A:347:TYR:CE1	5:A:417:PHE:CZ	3.07	0.42
5:A:682:ALA:HA	5:A:685:VAL:HG12	2.01	0.42
19:B:1764:CLA:CMC	19:B:1767:CLA:H2	2.49	0.42
6:B:441:ASP:OD1	6:B:617:MET:HB3	2.19	0.42
6:B:674:LEU:O	6:B:678:LEU:HB2	2.19	0.42
16:L:99:LEU:HB3	16:L:140:THR:HG21	2.02	0.42
16:L:84:GLY:HA3	16:L:155:CYS:CB	2.50	0.42
19:B:1770:CLA:H171	16:L:94:ILE:HG12	2.00	0.42
7:C:58:CYS:HA	7:C:59:PRO:HD2	1.60	0.42
8:D:27:PRO:HG2	8:D:75:LEU:HD23	2.00	0.42
4:4:194:VAL:CB	4:4:195:GLN:C	2.77	0.42
3:3:106:TYR:CB	3:3:107:TRP:HD1	2.31	0.42
21:2:1225:SUC:H5'	21:2:1225:SUC:O2	2.19	0.42
20:A:7023:LMU:H41	20:A:7023:LMU:H91	1.99	0.42
20:A:7030:LMU:C4	20:A:7030:LMU:O6'	2.67	0.42
19:1:1189:CLA:CB	19:1:1189:CLA:CBA	2.90	0.42
20:A:7026:LMU:H21	20:A:7026:LMU:O2'	2.18	0.42
19:4:1196:CLA:H41	19:4:1196:CLA:H62	1.84	0.42
4:4:122:LYS:HE2	4:4:150:LYS:CG	2.49	0.42
5:A:361:ASN:OD1	19:A:1761:CLA:OBD	2.38	0.42
19:A:1771:CLA:HMC1	19:A:1771:CLA:HBC3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:430:ASP:HA	5:A:434:ARG:HH21	1.84	0.42
5:A:603:PHE:CZ	5:A:693:LEU:CD2	3.02	0.42
5:A:652:TRP:O	5:A:656:PHE:HB3	2.19	0.42
23:B:1775:BCR:H341	23:B:1775:BCR:H11C	1.77	0.42
6:B:471:THR:O	6:B:472:TYR:C	2.58	0.42
8:D:137:ILE:HG13	8:D:137:ILE:H	1.55	0.42
11:G:30:ASN:ND2	11:G:31:MET:O	2.52	0.42
17:N:72:LYS:HG3	17:N:74:LYS:H	1.82	0.42
4:4:37:LEU:CA	4:4:39:TRP:CG	2.98	0.42
4:4:36:ASN:CB	4:4:39:TRP:CZ3	2.69	0.42
2:2:164:ILE:O	2:2:168:ARG:N	2.52	0.42
19:1:1143:CLA:C4	19:1:1143:CLA:O2A	2.67	0.42
3:3:66:MET:HE1	3:3:69:ALA:HB3	2.01	0.42
20:A:7013:LMU:C4'	20:A:7049:LMU:O6'	2.68	0.42
7:C:12:ILE:O	7:C:38:GLN:HG2	2.18	0.42
7:C:34:CYS:SG	7:C:39:ILE:HD12	2.59	0.42
2:2:203:THR:HG22	2:2:204:ILE:N	2.35	0.42
19:1:1149:CLA:CBD	19:1:1149:CLA:HAA1	2.49	0.42
14:J:9:SER:HB2	14:J:10:VAL:H	1.67	0.42
12:H:47:PHE:HD2	16:L:141:GLY:CA	2.32	0.42
16:L:49:PRO:HG3	16:L:131:GLN:NE2	2.35	0.42
7:C:25:VAL:HA	7:C:43:PRO:CD	2.50	0.42
20:A:1812:LMU:C5	20:A:1812:LMU:C1	2.96	0.42
6:B:633:ASN:HD22	6:B:636:THR:HB	1.85	0.42
12:H:32:TYR:HB3	12:H:33:ASN:H	1.62	0.42
20:A:1811:LMU:H12	20:A:1811:LMU:H41	1.79	0.42
6:B:479:SER:C	6:B:481:THR:H	2.19	0.42
4:4:51:ALA:O	4:4:55:VAL:HG13	2.19	0.42
5:A:163:GLN:C	5:A:165:TYR:N	2.72	0.42
19:A:1764:CLA:H142	23:A:1806:BCR:H14C	1.99	0.42
19:A:1773:CLA:HBA2	19:A:1773:CLA:H3A	1.21	0.42
19:A:1792:CLA:HBA2	19:A:1792:CLA:CBD	2.44	0.42
5:A:733:VAL:CG1	19:A:1796:CLA:C3D	2.97	0.42
5:A:703:LEU:HD13	5:A:707:ILE:HD11	2.01	0.42
5:A:76:ARG:NE	5:A:192:LYS:HA	2.34	0.42
6:B:225:LEU:HD22	6:B:230:TRP:CD1	2.54	0.42
6:B:460:ALA:O	6:B:461:GLN:C	2.57	0.42
6:B:592:PHE:CE2	19:B:1784:CLA:H62	2.54	0.42
6:B:365:PHE:HB3	6:B:602:TRP:CH2	2.54	0.42
6:B:710:LEU:H	6:B:713:PHE:H	1.67	0.42
8:D:79:ARG:H	8:D:82:GLN:HE21	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:1217:CLA:HBA2	19:2:1217:CLA:H3A	1.68	0.42
15:K:11:MET:O	15:K:15:THR:OG1	2.33	0.42
19:3:1218:CLA:CHD	19:3:1218:CLA:CBC	2.95	0.42
3:3:158:TYR:C	3:3:160:GLY:N	2.70	0.42
16:L:125:LYS:C	16:L:127:PRO:HD2	2.39	0.42
8:D:58:PHE:HE2	8:D:60:MET:HA	1.85	0.42
21:3:1223:SUC:C1'	21:3:1223:SUC:C6'	2.97	0.42
6:B:694:ARG:HH11	16:L:105:ALA:C	2.23	0.42
1:1:108:VAL:HG23	19:1:1195:CLA:NA	2.35	0.42
5:A:363:ALA:O	5:A:367:SER:HB3	2.19	0.42
2:2:198:ALA:O	2:2:199:ASP:CB	2.67	0.42
4:4:142:ASN:O	4:4:143:PHE:HB2	2.20	0.42
4:4:143:PHE:HB2	4:4:150:LYS:HE2	2.02	0.42
19:A:1762:CLA:C7	19:A:1762:CLA:H2	2.49	0.42
19:A:1770:CLA:CHC	23:A:1803:BCR:C18	2.97	0.42
19:A:1776:CLA:HMB2	19:A:1782:CLA:H92	2.01	0.42
19:A:1776:CLA:H102	23:A:1804:BCR:C21	2.50	0.42
23:A:1807:BCR:H271	13:I:12:VAL:CG1	2.49	0.42
5:A:183:TRP:C	5:A:185:HIS:H	2.23	0.42
5:A:241:GLU:O	5:A:242:ILE:HG23	2.20	0.42
5:A:705:GLU:O	5:A:706:SER:C	2.58	0.42
5:A:98:PHE:CD1	5:A:98:PHE:C	2.93	0.42
6:B:136:TYR:O	6:B:140:ILE:HD11	2.20	0.42
6:B:153:GLY:O	6:B:157:LEU:HB2	2.19	0.42
19:B:1738:CLA:H161	19:B:1738:CLA:H193	1.79	0.42
6:B:705:ALA:CB	22:B:1773:PQN:C8	2.97	0.42
19:B:1743:CLA:H42	23:B:1775:BCR:H10C	2.00	0.42
6:B:685:THR:HA	6:B:686:PRO:HD3	1.92	0.42
6:B:599:ILE:O	6:B:734:GLY:C	2.58	0.42
10:F:144:LEU:O	10:F:149:LEU:O	2.38	0.42
17:N:83:TRP:O	17:N:84:LYS:HG2	2.19	0.42
17:N:39:SER:O	17:N:40:CYS:HB2	2.19	0.42
20:A:7016:LMU:H1'	20:A:7016:LMU:H6D	1.72	0.42
1:1:54:VAL:O	1:1:56:GLY:N	2.53	0.42
10:F:47:GLU:N	10:F:50:LYS:HB2	2.34	0.42
8:D:114:PRO:HB2	8:D:115:LYS:H	1.68	0.42
8:D:118:VAL:HG13	8:D:119:TYR:H	1.84	0.42
10:F:151:ASP:HA	10:F:154:PHE:CB	2.47	0.42
5:A:499:ALA:O	5:A:501:GLY:N	2.42	0.42
16:L:43:TYR:O	16:L:44:ARG:CB	2.65	0.42
17:N:25:THR:HG22	17:N:26:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:684:ARG:HA	6:B:684:ARG:HD3	1.80	0.42
3:3:127:ARG:HG2	3:3:131:ASP:OD1	2.18	0.42
5:A:35:ALA:O	5:A:36:LYS:HB2	2.20	0.42
4:4:177:PRO:HB2	4:4:178:PHE:CD1	2.54	0.42
19:A:1763:CLA:HAA2	19:A:1765:CLA:O2D	2.20	0.42
19:A:1783:CLA:C7	23:A:1805:BCR:H371	2.47	0.42
19:A:1813:CLA:H71	19:A:1813:CLA:H111	1.75	0.42
19:A:1814:CLA:H11	6:B:616:LEU:CB	2.50	0.42
5:A:199:VAL:O	5:A:201:SER:N	2.53	0.42
5:A:270:PHE:CZ	19:A:1797:CLA:O2A	2.73	0.42
5:A:441:ALA:HA	5:A:444:SER:HB3	2.02	0.42
5:A:684:PHE:HD2	5:A:685:VAL:CA	2.32	0.42
19:B:1737:CLA:H62	19:B:1737:CLA:H102	1.59	0.42
19:B:1744:CLA:HBA2	19:B:1744:CLA:H3A	1.57	0.42
19:B:1767:CLA:H112	19:B:1767:CLA:H71	1.78	0.42
6:B:589:TRP:CD1	19:B:1784:CLA:H152	2.54	0.42
6:B:25:ILE:O	6:B:26:ALA:HB2	2.20	0.42
6:B:273:VAL:O	6:B:277:HIS:CD2	2.66	0.42
6:B:339:ALA:O	6:B:340:SER:CB	2.68	0.42
6:B:596:TRP:CZ3	6:B:613:SER:HB3	2.55	0.42
11:G:27:GLN:HG2	19:G:1099:CLA:C4D	2.49	0.42
4:4:69:ILE:C	4:4:71:ASN:N	2.70	0.42
11:G:88:THR:HG23	11:G:91:ASN:O	2.19	0.42
4:4:36:ASN:C	4:4:39:TRP:CE3	2.93	0.42
3:3:52:LYS:O	3:3:56:TYR:CB	2.68	0.42
10:F:131:PHE:O	10:F:132:ARG:C	2.58	0.42
12:H:37:SER:C	12:H:39:PHE:N	2.73	0.42
12:H:42:THR:HG22	12:H:45:ALA:CB	2.46	0.42
15:K:52:PRO:O	15:K:56:THR:HG22	2.19	0.42
21:B:8059:SUC:C1'	21:B:8059:SUC:H6'2	2.50	0.42
6:B:470:THR:H	6:B:501:ILE:HG23	1.84	0.42
5:A:535:GLY:O	5:A:539:PHE:HB2	2.20	0.42
20:A:7004:LMU:O6'	20:A:7004:LMU:C1'	2.67	0.42
12:H:63:SER:O	12:H:67:TYR:HB3	2.19	0.42
6:B:639:VAL:HG22	6:B:640:CYS:N	2.35	0.42
5:A:90:PHE:HB3	5:A:175:ALA:HB2	2.02	0.42
19:A:1796:CLA:HBA2	19:A:1796:CLA:H3A	1.60	0.42
5:A:242:ILE:HG12	5:A:243:PRO:HG3	2.01	0.42
5:A:390:ALA:CB	5:A:754:ILE:HD13	2.50	0.42
19:B:1738:CLA:H3A	19:B:1738:CLA:HBA1	1.78	0.42
19:B:1739:CLA:H13	19:B:1757:CLA:C12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:255:LEU:HD12	19:B:1746:CLA:O2D	2.20	0.42
19:B:1753:CLA:O1D	19:B:1753:CLA:OBD	2.37	0.42
19:B:1768:CLA:H41	23:B:1779:BCR:H323	2.02	0.42
6:B:493:TRP:CH2	19:B:1765:CLA:HMA2	2.55	0.42
6:B:67:HIS:CD2	6:B:71:GLN:HE22	2.37	0.42
6:B:720:THR:O	6:B:724:PHE:N	2.48	0.42
10:F:73:VAL:HG21	10:F:83:PHE:HB2	2.01	0.42
11:G:35:VAL:HG13	11:G:38:GLN:HB2	2.02	0.42
11:G:42:SER:CB	11:G:46:ALA:HB2	2.46	0.42
12:H:73:PRO:CD	21:H:1082:SUC:O6'	2.68	0.42
2:2:102:ILE:CG1	19:2:1222:CLA:HMD2	2.43	0.42
3:3:114:PHE:HE1	19:3:1219:CLA:C3D	2.33	0.42
19:2:1223:CLA:H152	19:2:1223:CLA:H111	1.14	0.42
10:F:123:VAL:HG13	14:J:7:TYR:N	2.34	0.42
10:F:41:ALA:O	10:F:44:ALA:O	2.38	0.42
7:C:31:TRP:HD1	7:C:32:GLY:N	2.18	0.42
20:A:7042:LMU:H11	20:A:7042:LMU:H71	2.01	0.42
20:A:7043:LMU:H62	20:A:7043:LMU:C11	2.49	0.42
20:A:7034:LMU:H1'	20:A:7034:LMU:O6'	2.19	0.42
15:K:74:ILE:CG2	15:K:75:VAL:HG22	2.41	0.42
6:B:503:GLU:HB3	6:B:507:SER:CA	2.50	0.42
20:A:7009:LMU:H102	20:A:7009:LMU:H71	1.38	0.42
5:A:539:PHE:CD2	5:A:539:PHE:C	2.93	0.42
6:B:607:SER:HA	6:B:610:ASN:HD22	1.85	0.42
5:A:409:GLY:C	5:A:411:ALA:H	2.23	0.42
6:B:605:ASN:HD22	6:B:605:ASN:C	2.23	0.42
4:4:123:GLN:HG2	4:4:124:TYR:H	1.84	0.42
4:4:127:PRO:HB2	4:4:143:PHE:HE1	1.83	0.42
5:A:131:ILE:HG21	6:B:446:PHE:HD1	1.84	0.42
19:A:1790:CLA:H3A	19:A:1790:CLA:HBA2	1.56	0.42
19:A:1764:CLA:H111	23:A:1806:BCR:C10	2.50	0.42
5:A:76:ARG:C	5:A:186:TYR:HD2	2.23	0.42
5:A:185:HIS:O	5:A:188:LYS:HG3	2.20	0.42
5:A:553:VAL:O	5:A:557:LEU:CB	2.67	0.42
19:B:1769:CLA:C1A	19:B:1769:CLA:O1D	2.62	0.42
6:B:255:LEU:N	6:B:255:LEU:HD23	2.34	0.42
6:B:291:TYR:HE1	19:B:1749:CLA:CED	2.32	0.42
6:B:304:ILE:HG22	19:B:1752:CLA:O1D	2.20	0.42
6:B:352:MET:SD	19:B:1758:CLA:OBD	2.78	0.42
6:B:693:TRP:CZ2	6:B:697:PRO:HG3	2.54	0.42
17:N:62:SER:O	17:N:66:ASP:CG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:36:ASN:O	4:4:39:TRP:CD2	2.73	0.42
2:2:72:GLY:C	2:2:74:LEU:N	2.69	0.42
1:1:54:VAL:C	1:1:56:GLY:H	2.23	0.42
19:1:1146:CLA:O1A	19:1:1146:CLA:C3A	2.68	0.42
6:B:476:ILE:HA	6:B:477:PRO:HD2	1.83	0.42
8:D:120:PRO:O	8:D:121:GLU:HB3	2.19	0.42
19:R:1055:CLA:H141	19:R:1055:CLA:H161	1.88	0.42
16:L:58:LEU:HA	16:L:146:GLY:O	2.20	0.42
1:1:135:LYS:HB3	1:1:136:ASP:H	1.54	0.42
6:B:681:ALA:O	6:B:683:GLU:N	2.53	0.42
5:A:502:THR:H	5:A:504:ALA:HB3	1.84	0.42
6:B:509:PHE:N	6:B:509:PHE:HD2	2.18	0.42
4:4:179:ASP:N	4:4:184:HIS:HD2	2.17	0.42
4:4:118:ASP:CA	4:4:122:LYS:HA	2.49	0.41
19:A:1761:CLA:C4B	19:A:1785:CLA:HMB2	2.50	0.41
5:A:123:VAL:O	19:A:1765:CLA:O1D	2.38	0.41
19:A:1790:CLA:C3D	19:A:1791:CLA:CAC	2.97	0.41
5:A:358:LEU:HD11	5:A:413:HIS:CD2	2.54	0.41
5:A:364:MET:CE	19:A:1782:CLA:H2	2.49	0.41
5:A:372:VAL:HG22	19:A:1774:CLA:H43	2.02	0.41
19:B:1737:CLA:H2	19:B:1737:CLA:H62	1.86	0.41
19:B:1753:CLA:HAC2	19:B:1753:CLA:HHD	1.83	0.41
19:B:1771:CLA:C2	22:B:1773:PQN:H251	2.50	0.41
6:B:606:VAL:C	6:B:608:GLN:N	2.72	0.41
6:B:70:TRP:H	6:B:70:TRP:HD1	1.66	0.41
11:G:43:HIS:ND1	11:G:43:HIS:N	2.68	0.41
23:I:1032:BCR:C39	23:L:1169:BCR:C40	2.97	0.41
13:I:24:LEU:HD23	23:L:1169:BCR:H23C	2.01	0.41
16:L:65:VAL:H	16:L:67:PRO:HD2	1.85	0.41
4:4:70:ILE:O	4:4:73:PRO:CD	2.66	0.41
2:2:162:LYS:CE	19:2:1215:CLA:OBD	2.68	0.41
2:2:102:ILE:HG22	19:2:1221:CLA:CBB	2.50	0.41
19:2:1221:CLA:HAC1	19:2:1221:CLA:HHD	1.87	0.41
11:G:16:LEU:HD12	11:G:17:PHE:CZ	2.55	0.41
2:2:178:TRP:N	2:2:178:TRP:CD1	2.88	0.41
8:D:101:TYR:CE1	8:D:114:PRO:HD3	2.55	0.41
8:D:49:THR:C	8:D:50:TRP:HD1	2.23	0.41
5:A:582:ASP:OD1	5:A:586:ARG:NH1	2.24	0.41
20:A:7033:LMU:H61	20:A:7033:LMU:H31	1.72	0.41
6:B:160:LYS:HG3	6:B:161:TRP:N	2.30	0.41
12:H:34:SER:OG	12:H:36:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:183:TYR:O	2:2:184:THR:C	2.58	0.41
4:4:121:PHE:CD1	4:4:143:PHE:HE2	2.32	0.41
19:A:1785:CLA:HBD	19:A:1785:CLA:HAA1	2.03	0.41
19:A:1813:CLA:H162	19:A:1813:CLA:H122	1.58	0.41
5:A:306:ILE:O	5:A:309:LEU:N	2.52	0.41
5:A:313:ALA:C	5:A:315:HIS:H	2.24	0.41
5:A:341:GLN:O	5:A:344:LYS:HB2	2.19	0.41
6:B:233:TYR:HD1	6:B:254:ILE:HG13	1.85	0.41
6:B:292:ARG:NH1	6:B:293:THR:H	2.18	0.41
6:B:606:VAL:C	6:B:608:GLN:H	2.24	0.41
6:B:580:VAL:HG13	6:B:710:LEU:HD21	2.01	0.41
6:B:646:TRP:CH2	6:B:726:ILE:HD13	2.55	0.41
19:A:1788:CLA:C15	23:L:1169:BCR:C36	2.98	0.41
19:A:1786:CLA:H2A	16:L:25:THR:HG21	2.02	0.41
16:L:30:SER:C	16:L:32:LEU:H	2.22	0.41
16:L:96:SER:OG	16:L:143:PHE:CD2	2.73	0.41
17:N:72:LYS:CE	17:N:74:LYS:HE3	2.38	0.41
5:A:251:ASN:C	5:A:253:ASP:N	2.65	0.41
3:3:111:TYR:HB2	3:3:112:THR:CG2	2.51	0.41
14:J:21:SER:O	14:J:22:LEU:C	2.58	0.41
6:B:660:GLY:O	6:B:663:PHE:O	2.39	0.41
6:B:247:THR:O	6:B:248:GLN:C	2.58	0.41
10:F:130:LEU:CD1	10:F:131:PHE:HD1	2.33	0.41
16:L:126:GLN:N	16:L:127:PRO:CD	2.82	0.41
3:3:206:VAL:HB	3:3:207:GLY:H	1.69	0.41
3:3:207:GLY:O	3:3:208:PRO:C	2.58	0.41
6:B:222:LEU:HD21	6:B:226:LEU:HD12	2.01	0.41
12:H:70:ALA:O	12:H:71:ASN:CB	2.68	0.41
2:2:77:PRO:O	17:N:3:ILE:CD1	2.68	0.41
11:G:14:LEU:HG	11:G:14:LEU:O	2.19	0.41
4:4:163:PHE:O	4:4:166:PHE:CB	2.66	0.41
5:A:145:ILE:HG23	19:A:1764:CLA:OBD	2.20	0.41
19:A:1774:CLA:CBB	19:A:1774:CLA:C8	2.93	0.41
5:A:372:VAL:HG22	19:A:1774:CLA:H41	2.00	0.41
5:A:40:PHE:N	5:A:44:ILE:HG21	2.35	0.41
5:A:553:VAL:H	5:A:556:LEU:CD1	2.31	0.41
5:A:650:ASN:O	5:A:653:LEU:HD13	2.19	0.41
19:B:1751:CLA:HBC3	23:B:1774:BCR:HC7	2.03	0.41
19:B:1753:CLA:CGD	19:B:1753:CLA:C2A	2.98	0.41
19:B:1761:CLA:CHD	19:B:1761:CLA:HBC2	2.44	0.41
19:B:1769:CLA:HBC2	19:B:1769:CLA:CMC	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:199:ILE:N	6:B:200:PRO:HD2	2.35	0.41
6:B:260:GLY:H	6:B:269:TRP:HE1	1.68	0.41
6:B:309:ILE:HA	6:B:310:PRO:HD3	1.77	0.41
6:B:407:VAL:HG23	19:B:1760:CLA:CMD	2.49	0.41
5:A:677:LEU:HD11	6:B:442:VAL:HG13	2.02	0.41
6:B:569:ASP:OD2	6:B:569:ASP:N	2.54	0.41
9:E:90:VAL:O	9:E:91:ALA:C	2.58	0.41
10:F:62:LEU:CD2	10:F:72:ILE:HD13	2.50	0.41
16:L:12:GLN:HA	16:L:13:PRO:HD3	1.85	0.41
8:D:30:ALA:HA	16:L:13:PRO:HG3	2.01	0.41
4:4:75:TRP:CE3	4:4:76:TYR:HB3	2.55	0.41
17:N:60:PHE:HA	17:N:61:LEU:O	2.20	0.41
17:N:82:PHE:N	17:N:82:PHE:HD2	2.17	0.41
2:2:112:ASP:C	2:2:114:LEU:N	2.72	0.41
14:J:21:SER:O	14:J:23:ALA:N	2.52	0.41
7:C:31:TRP:CD1	7:C:31:TRP:C	2.93	0.41
20:A:7041:LMU:H4'	20:A:7041:LMU:H2B	1.70	0.41
1:1:179:THR:OG1	4:4:87:SER:CB	2.69	0.41
12:H:23:VAL:O	12:H:24:TYR:C	2.59	0.41
19:2:1212:CLA:O1A	19:2:1212:CLA:C2	2.67	0.41
5:A:586:ARG:CG	7:C:49:VAL:HG21	2.38	0.41
5:A:374:GLN:C	5:A:376:MET:N	2.73	0.41
6:B:456:GLU:HA	6:B:514:PRO:HD3	2.03	0.41
18:R:26:UNK:C	18:R:28:UNK:N	2.81	0.41
4:4:53:LEU:O	4:4:56:ALA:N	2.53	0.41
12:H:30:SER:O	12:H:31:PRO:O	2.37	0.41
17:N:9:LYS:HB3	17:N:9:LYS:HE2	1.78	0.41
4:4:128:ALA:C	4:4:130:GLU:N	2.72	0.41
5:A:183:TRP:O	5:A:185:HIS:N	2.54	0.41
5:A:672:LEU:CD2	5:A:672:LEU:H	2.32	0.41
5:A:98:PHE:HD1	5:A:99:HIS:CD2	2.37	0.41
6:B:431:PHE:HE2	19:B:1762:CLA:HED3	1.85	0.41
6:B:290:MET:HA	19:B:1751:CLA:C3C	2.49	0.41
6:B:293:THR:O	6:B:295:PHE:CD2	2.73	0.41
6:B:564:ARG:NE	7:C:64:SER:OG	2.52	0.41
9:E:62:ARG:O	9:E:83:ALA:CB	2.69	0.41
11:G:34:GLN:O	11:G:36:PRO:N	2.53	0.41
16:L:10:VAL:HG13	16:L:12:GLN:HE22	1.85	0.41
17:N:63:ASP:N	17:N:64:ASP:CA	2.76	0.41
3:3:56:TYR:CD1	3:3:185:LYS:NZ	2.84	0.41
5:A:254:LEU:C	5:A:256:ALA:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:1213:CLA:O1D	19:2:1213:CLA:C2A	2.63	0.41
4:4:193:ILE:HG22	4:4:195:GLN:O	2.20	0.41
20:A:7001:LMU:H102	20:A:7001:LMU:H42	2.01	0.41
10:F:123:VAL:CG1	14:J:7:TYR:HB2	2.50	0.41
10:F:29:LEU:HB3	10:F:30:LYS:H	1.74	0.41
20:A:7041:LMU:H4B	20:A:7041:LMU:H1B	1.67	0.41
19:1:1148:CLA:OBD	19:1:1148:CLA:O1D	2.35	0.41
19:3:3011:CLA:H151	19:3:3011:CLA:H18	1.36	0.41
4:4:61:PRO:HA	4:4:65:THR:O	2.20	0.41
16:L:50:LEU:HD23	16:L:51:LEU:H	1.85	0.41
15:K:24:PHE:CB	15:K:52:PRO:HG2	2.46	0.41
21:B:8053:SUC:O5	21:B:8053:SUC:C5'	2.68	0.41
5:A:374:GLN:C	5:A:376:MET:H	2.24	0.41
6:B:262:HIS:HA	6:B:263:PRO:HD2	1.93	0.41
20:A:7019:LMU:H72	20:A:7019:LMU:H101	1.69	0.41
4:4:105:ARG:O	4:4:108:ASP:HB3	2.20	0.41
19:A:1774:CLA:CBB	19:A:1774:CLA:C7	2.97	0.41
19:A:1783:CLA:H71	23:A:1805:BCR:C37	2.48	0.41
5:A:382:TYR:HE2	19:A:1784:CLA:HED3	1.84	0.41
19:A:1786:CLA:HMB2	19:A:1787:CLA:C3D	2.51	0.41
19:A:1788:CLA:C2D	19:A:1789:CLA:H121	2.51	0.41
5:A:749:PHE:CD2	19:A:1813:CLA:HMD1	2.55	0.41
5:A:366:GLY:O	5:A:403:GLY:HA2	2.19	0.41
5:A:53:TRP:CA	5:A:56:ASN:HB2	2.44	0.41
19:B:1738:CLA:HED1	19:B:1759:CLA:H52	2.01	0.41
19:B:1764:CLA:C4C	19:B:1765:CLA:CBB	2.98	0.41
19:B:1764:CLA:NC	19:B:1765:CLA:HBB2	2.34	0.41
6:B:350:GLN:CD	19:B:1767:CLA:HBB2	2.41	0.41
6:B:289:LEU:HD21	19:B:1750:CLA:NA	2.35	0.41
6:B:317:ARG:HH12	6:B:407:VAL:N	2.18	0.41
9:E:55:VAL:CG2	9:E:65:VAL:HB	2.44	0.41
10:F:104:TYR:HD2	10:F:104:TYR:O	2.01	0.41
3:3:94:ARG:NH2	3:3:98:ILE:HD13	2.36	0.41
5:A:97:TYR:HA	5:A:153:TRP:CZ2	2.55	0.41
20:R:1056:LMU:H102	20:R:1056:LMU:H71	1.55	0.41
11:G:60:SER:O	11:G:62:ASP:N	2.53	0.41
5:A:639:ALA:O	5:A:641:ASN:N	2.54	0.41
5:A:560:VAL:O	5:A:563:ALA:HB2	2.21	0.41
18:R:8:UNK:CB	19:R:1054:CLA:HED1	2.51	0.41
8:D:28:ILE:O	8:D:66:ALA:CB	2.69	0.41
1:1:58:LEU:O	1:1:60:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:694:ARG:NH1	16:L:105:ALA:O	2.50	0.41
4:4:119:PRO:O	4:4:121:PHE:N	2.54	0.41
5:A:155:ALA:O	5:A:156:SER:C	2.59	0.41
19:A:1774:CLA:H62	19:A:1774:CLA:H93	1.30	0.41
19:A:1789:CLA:H18	19:L:1167:CLA:CMB	2.43	0.41
5:A:453:LEU:CB	5:A:547:PHE:HB2	2.35	0.41
5:A:702:GLU:HA	6:B:545:LYS:HE2	2.02	0.41
5:A:82:HIS:O	5:A:84:GLY:N	2.54	0.41
19:B:1736:CLA:HBC2	19:B:1736:CLA:HMC1	2.03	0.41
19:B:1749:CLA:C3	19:B:1754:CLA:H92	2.51	0.41
6:B:462:TRP:HZ3	19:B:1764:CLA:HBC1	1.86	0.41
6:B:471:THR:HB	6:B:472:TYR:CE1	2.56	0.41
6:B:510:LEU:HG	6:B:597:LYS:NZ	2.36	0.41
19:L:1167:CLA:HAC2	23:L:1169:BCR:HC42	2.02	0.41
16:L:14:LEU:CA	16:L:24:GLU:HG3	2.40	0.41
5:A:25:ASP:HA	5:A:27:ILE:H	1.85	0.41
4:4:30:LEU:O	4:4:32:GLU:OE1	2.38	0.41
3:3:112:THR:C	3:3:114:PHE:N	2.69	0.41
15:K:38:LEU:CG	15:K:39:LYS:CD	2.78	0.41
3:3:158:TYR:CB	3:3:159:PRO:CD	2.82	0.41
6:B:668:ARG:HH12	6:B:672:GLN:HG2	1.85	0.41
10:F:44:ALA:O	10:F:46:MET:N	2.53	0.41
16:L:160:VAL:O	16:L:160:VAL:CG2	2.66	0.41
12:H:40:PHE:O	12:H:41:GLU:C	2.59	0.41
4:4:83:TYR:HB3	4:4:84:PHE:H	1.53	0.41
3:3:153:SER:C	3:3:161:GLY:HA2	2.40	0.41
2:2:179:PHE:O	2:2:183:TYR:CD2	2.73	0.41
19:A:1764:CLA:H3A	19:A:1764:CLA:HBA2	1.39	0.41
19:A:1772:CLA:HAC2	19:A:1772:CLA:HHD	1.93	0.41
19:A:1763:CLA:HMB2	23:A:1806:BCR:H342	2.01	0.41
5:A:298:ASP:O	5:A:301:HIS:N	2.54	0.41
5:A:581:CYS:HB2	5:A:590:CYS:C	2.40	0.41
19:B:1735:CLA:H52	19:B:1735:CLA:C1C	2.51	0.41
19:B:1735:CLA:H201	10:F:104:TYR:CD1	2.56	0.41
19:A:1795:CLA:NC	19:B:1735:CLA:HBC2	2.35	0.41
6:B:645:VAL:HG11	19:B:1739:CLA:HMC1	2.02	0.41
6:B:189:ALA:HA	19:B:1745:CLA:HBB1	2.03	0.41
22:B:1773:PQN:H2M1	22:B:1773:PQN:H111	1.80	0.41
19:B:1758:CLA:H62	23:B:1776:BCR:HC7	2.02	0.41
6:B:434:LEU:O	6:B:438:VAL:HG13	2.21	0.41
6:B:353:TYR:CB	6:B:594:TRP:CH2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:77:MET:C	7:C:79:LEU:H	2.19	0.41
10:F:104:TYR:OH	10:F:122:ASP:N	2.42	0.41
19:A:1800:CLA:H91	23:L:1169:BCR:H10C	2.03	0.41
16:L:163:LEU:HD13	16:L:164:PRO:N	2.28	0.41
4:4:38:ARG:O	4:4:39:TRP:O	2.39	0.41
5:A:249:ILE:CG1	5:A:250:LEU:N	2.55	0.41
2:2:171:MET:SD	2:2:172:LEU:HA	2.60	0.41
2:2:70:LYS:HE3	2:2:70:LYS:HB3	1.62	0.41
10:F:21:ALA:O	10:F:23:LYS:N	2.54	0.41
10:F:44:ALA:HA	10:F:47:GLU:HB3	2.03	0.41
7:C:29:ILE:HG23	8:D:126:GLY:CA	2.44	0.41
20:A:7042:LMU:C7	20:A:7042:LMU:C2	2.92	0.41
20:A:7005:LMU:H3'	20:A:7005:LMU:H1B	1.30	0.41
19:3:3011:CLA:H142	19:3:3011:CLA:H92	2.03	0.41
8:D:102:ARG:CZ	8:D:110:GLN:HB2	2.51	0.41
5:A:532:ILE:N	5:A:533:PRO:HD3	2.34	0.41
19:1:1505:CLA:HAA2	19:1:1505:CLA:HBD	2.02	0.41
4:4:152:LYS:HA	4:4:152:LYS:HD2	1.73	0.41
8:D:53:PRO:HB2	8:D:54:LYS:H	1.66	0.41
4:4:163:PHE:O	4:4:164:LEU:C	2.58	0.41
19:A:1768:CLA:O1D	19:A:1769:CLA:HMC1	2.21	0.41
19:A:1784:CLA:H52	19:A:1784:CLA:HMD2	2.02	0.41
23:A:1806:BCR:H341	23:A:1806:BCR:H11C	1.80	0.41
5:A:236:GLY:O	5:A:237:VAL:HG22	2.20	0.41
5:A:538:ASP:O	5:A:542:HIS:CD2	2.73	0.41
5:A:747:TRP:HB2	19:A:1783:CLA:CBB	2.51	0.41
6:B:414:HIS:O	6:B:414:HIS:CD2	2.74	0.41
5:A:131:ILE:HG21	6:B:446:PHE:CD1	2.55	0.41
6:B:557:PHE:N	6:B:558:PRO:HD3	2.34	0.41
6:B:549:ASP:OD1	7:C:63:LEU:HD22	2.21	0.41
9:E:60:LYS:HG3	9:E:61:THR:OG1	2.21	0.41
23:B:1778:BCR:H391	10:F:90:PHE:N	2.36	0.41
17:N:79:SER:OG	17:N:80:ASN:N	2.53	0.41
19:1:1146:CLA:CMD	20:A:7001:LMU:H52	2.51	0.41
20:A:7039:LMU:H4B	20:A:7039:LMU:H1B	1.53	0.41
6:B:5:ILE:HG13	6:B:20:ARG:HH21	1.85	0.41
5:A:586:ARG:HB2	5:A:589:THR:OG1	2.21	0.41
20:A:7011:LMU:H52	20:A:7011:LMU:C1	2.48	0.41
3:3:120:LEU:O	3:3:123:PHE:HB3	2.21	0.41
4:4:107:GLN:HA	19:4:1196:CLA:C3A	2.50	0.41
4:4:128:ALA:CA	4:4:143:PHE:HZ	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:154:ILE:CG1	4:4:155:ALA:N	2.62	0.41
4:4:94:GLU:O	4:4:97:LEU:HB3	2.20	0.41
19:A:1787:CLA:H72	19:A:1801:CLA:HBA1	2.03	0.41
5:A:40:PHE:O	5:A:40:PHE:CD1	2.74	0.41
5:A:458:PHE:C	5:A:458:PHE:CD1	2.94	0.41
6:B:96:PHE:HZ	6:B:104:PHE:CE2	2.39	0.41
6:B:104:PHE:CZ	6:B:645:VAL:HG22	2.55	0.41
6:B:145:LEU:HD22	6:B:148:ILE:HD12	2.02	0.41
19:B:1738:CLA:CBC	19:B:1757:CLA:CMD	2.99	0.41
19:B:1741:CLA:HBC2	19:B:1741:CLA:HMC1	2.02	0.41
19:B:1762:CLA:H71	23:B:1779:BCR:H402	2.03	0.41
19:B:1765:CLA:HMB1	23:B:1777:BCR:C30	2.42	0.41
22:B:1773:PQN:H161	22:B:1773:PQN:H141	1.60	0.41
6:B:535:VAL:CG1	6:B:536:LYS:N	2.84	0.41
6:B:583:MET:HE2	6:B:583:MET:O	2.20	0.41
6:B:598:HIS:HB3	6:B:602:TRP:CH2	2.56	0.41
7:C:65:VAL:HG12	7:C:66:ARG:H	1.85	0.41
6:B:398:TYR:C	8:D:143:PRO:HG2	2.37	0.41
16:L:21:GLY:C	16:L:23:LEU:H	2.24	0.41
4:4:149:ALA:HB1	4:4:150:LYS:HE3	2.03	0.41
19:A:1771:CLA:HAA1	19:A:1771:CLA:HED2	2.03	0.41
19:A:1776:CLA:HBA1	19:A:1780:CLA:HBB2	2.00	0.41
5:A:405:PHE:O	19:A:1785:CLA:HMC1	2.21	0.41
19:A:1789:CLA:H161	19:A:1789:CLA:H202	1.80	0.41
19:A:1787:CLA:CBB	19:A:1793:CLA:H192	2.51	0.41
19:A:1798:CLA:H3A	19:A:1798:CLA:HBA1	1.13	0.41
19:A:1816:CLA:CAD	19:B:1784:CLA:HMB3	2.50	0.41
5:A:553:VAL:O	5:A:557:LEU:N	2.37	0.41
5:A:656:PHE:HB3	5:A:657:LEU:H	1.71	0.41
5:A:55:TRP:CD2	5:A:729:GLN:NE2	2.89	0.41
5:A:685:VAL:CG1	5:A:741:GLY:CA	2.99	0.41
19:B:1749:CLA:CHA	19:B:1749:CLA:HBA1	2.51	0.41
6:B:278:LEU:O	6:B:279:ALA:C	2.59	0.41
5:A:668:TYR:CD1	6:B:445:ALA:HB2	2.55	0.41
6:B:726:ILE:C	6:B:728:SER:H	2.23	0.41
16:L:90:GLY:O	16:L:94:ILE:N	2.49	0.41
16:L:64:LEU:CD2	16:L:91:LEU:HD22	2.51	0.41
3:3:94:ARG:HD2	3:3:94:ARG:HA	1.76	0.41
17:N:46:PHE:O	17:N:47:THR:CB	2.68	0.41
17:N:42:PHE:N	17:N:43:PRO:CD	2.83	0.41
4:4:37:LEU:O	4:4:38:ARG:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:40:PHE:CA	4:4:43:ALA:CB	2.97	0.41
18:R:35:UNK:CA	18:R:38:UNK:CB	2.97	0.41
19:2:2006:CLA:CB	19:2:2006:CLA:HHD	2.47	0.41
3:3:47:GLY:O	3:3:48:PHE:CD2	2.74	0.41
3:3:189:LEU:C	3:3:191:MET:N	2.74	0.41
3:3:49:ILE:CA	3:3:51:PRO:HD2	2.51	0.41
3:3:205:GLY:CA	5:A:252:ARG:NH1	2.67	0.41
2:2:102:ILE:CG2	2:2:106:GLU:HG3	2.50	0.41
19:3:1217:CLA:HMC1	19:3:1217:CLA:CB	2.22	0.41
2:2:128:ASN:CA	2:2:130:LEU:H	2.29	0.41
2:2:206:ALA:O	2:2:207:ALA:HB3	2.21	0.41
2:2:191:ASN:HB2	21:2:1225:SUC:C6	2.51	0.41
20:R:1056:LMU:H62	20:R:1056:LMU:H32	1.85	0.41
19:1:1148:CLA:H93	19:1:1148:CLA:H62	1.85	0.41
16:L:160:VAL:O	16:L:161:LEU:O	2.38	0.41
20:A:7010:LMU:C3'	20:A:7010:LMU:O2B	2.56	0.41
4:4:58:MET:SD	4:4:59:LEU:N	2.94	0.41
7:C:75:ARG:HH22	8:D:110:GLN:CD	2.24	0.41
21:B:8060:SUC:H5	21:B:8060:SUC:C1'	2.51	0.41
5:A:628:ILE:HG13	5:A:632:GLY:CA	2.48	0.41
6:B:529:THR:O	6:B:533:ILE:CG2	2.68	0.41
6:B:534:LEU:HD21	6:B:579:ALA:CB	2.51	0.41
2:2:37:ASP:HA	2:2:38:PRO:HD3	1.81	0.41
12:H:77:LEU:HB3	12:H:78:PRO:HD2	2.03	0.41
5:A:420:ARG:HB3	5:A:420:ARG:CZ	2.51	0.41
6:B:600:THR:O	6:B:605:ASN:O	2.38	0.41
4:4:159:LEU:HB3	4:4:160:MET:HE3	2.02	0.41
19:A:1788:CLA:HMD2	19:A:1789:CLA:H151	2.03	0.41
19:A:1796:CLA:C10	19:A:1815:CLA:H152	2.51	0.41
5:A:555:ILE:CG2	19:A:1817:CLA:HMD1	2.39	0.41
5:A:205:HIS:CE1	19:A:1769:CLA:CMC	3.02	0.41
5:A:220:ARG:O	5:A:221:HIS:CB	2.65	0.41
5:A:378:SER:O	5:A:379:MET:HG3	2.21	0.41
5:A:458:PHE:C	5:A:460:LEU:N	2.73	0.41
5:A:650:ASN:HA	5:A:653:LEU:HD13	2.03	0.41
5:A:664:VAL:HG23	5:A:665:ILE:HG23	2.02	0.41
5:A:665:ILE:C	5:A:665:ILE:HD12	2.41	0.41
6:B:140:ILE:O	6:B:144:PHE:HD1	2.04	0.41
19:B:1738:CLA:H62	24:B:1781:LMG:H351	2.02	0.41
6:B:183:PHE:CE1	19:B:1743:CLA:H71	2.54	0.41
19:B:1769:CLA:HBA2	19:B:1769:CLA:H11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1780:BCR:HC8	23:B:1780:BCR:H331	2.01	0.41
6:B:631:LEU:HG	6:B:632:ILE:HG23	2.03	0.41
6:B:551:LYS:HE2	8:D:143:PRO:HA	2.03	0.41
5:A:48:PRO:HB3	9:E:72:VAL:HG22	2.02	0.41
19:F:1157:CLA:CAD	19:F:1157:CLA:CED	2.99	0.41
11:G:45:GLU:O	11:G:46:ALA:O	2.38	0.41
16:L:26:PRO:C	16:L:28:THR:H	2.22	0.41
3:3:94:ARG:CZ	3:3:98:ILE:HD13	2.50	0.41
8:D:75:LEU:HD22	8:D:76:LYS:N	2.35	0.41
19:2:1217:CLA:H62	19:2:1217:CLA:H41	1.47	0.41
5:A:587:GLY:HA3	6:B:668:ARG:CZ	2.51	0.41
20:A:7021:LMU:O6'	20:A:7021:LMU:H41	2.20	0.41
20:A:7023:LMU:H91	20:A:7023:LMU:C3	2.50	0.41
20:R:1056:LMU:O6B	20:R:1056:LMU:C1B	2.67	0.41
12:H:25:GLY:HA3	12:H:27:ASP:CA	2.51	0.41
2:2:150:SER:HB3	2:2:151:ALA:H	1.51	0.41
19:4:1199:CLA:CMC	19:4:1199:CLA:HBC3	2.18	0.40
4:4:91:PHE:CE2	19:4:1207:CLA:C3C	3.01	0.40
4:4:120:ILE:HD12	4:4:120:ILE:H	1.85	0.40
4:4:143:PHE:N	4:4:150:LYS:CE	2.83	0.40
19:A:1761:CLA:H61	19:A:1761:CLA:H41	1.70	0.40
19:A:1776:CLA:HBA1	19:A:1780:CLA:CBB	2.51	0.40
5:A:206:HIS:C	5:A:211:LEU:HD23	2.42	0.40
5:A:211:LEU:HA	19:A:1774:CLA:HMC1	2.03	0.40
5:A:229:ILE:HG12	5:A:243:PRO:CB	2.50	0.40
5:A:227:LEU:HB3	5:A:258:LEU:HD21	2.03	0.40
5:A:343:HIS:O	5:A:346:LEU:HB2	2.20	0.40
19:B:1747:CLA:CAD	19:B:1756:CLA:CBB	2.92	0.40
19:B:1747:CLA:H3A	19:B:1747:CLA:HBA2	1.30	0.40
6:B:459:PHE:CD2	19:B:1768:CLA:C3D	3.04	0.40
6:B:292:ARG:CZ	6:B:297:ILE:H	2.34	0.40
6:B:460:ALA:O	6:B:463:ILE:N	2.55	0.40
6:B:492:ILE:CD1	6:B:492:ILE:N	2.80	0.40
5:A:703:LEU:HB2	6:B:536:LYS:HZ2	1.85	0.40
19:A:1817:CLA:C3B	6:B:659:THR:OG1	2.69	0.40
6:B:721:TYR:N	19:B:1784:CLA:O1D	2.53	0.40
23:B:1778:BCR:H372	10:F:93:ILE:HG22	2.03	0.40
11:G:23:PHE:CE2	11:G:24:PHE:HB2	2.56	0.40
14:J:19:PHE:C	14:J:19:PHE:CD2	2.93	0.40
16:L:92:VAL:O	16:L:96:SER:CB	2.69	0.40
17:N:65:LEU:O	17:N:67:LEU:CA	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:44:GLU:C	15:K:46:GLY:CA	2.88	0.40
4:4:193:ILE:O	4:4:194:VAL:C	2.59	0.40
7:C:28:MET:CG	7:C:38:GLN:HE21	2.32	0.40
2:2:197:LEU:HA	2:2:197:LEU:HD23	1.85	0.40
5:A:197:GLN:NE2	5:A:351:THR:O	2.53	0.40
20:A:7032:LMU:O1'	20:A:7032:LMU:C1B	2.69	0.40
20:A:7025:LMU:C2	20:A:7025:LMU:O2'	2.69	0.40
19:1:1192:CLA:H62	19:1:1192:CLA:H41	1.78	0.40
20:A:7009:LMU:H52	20:A:7009:LMU:H82	1.61	0.40
20:A:1811:LMU:H1'	20:A:1811:LMU:H21	1.61	0.40
5:A:173:VAL:HG23	5:A:174:PHE:N	2.36	0.40
5:A:90:PHE:HE2	5:A:178:MET:SD	2.44	0.40
5:A:692:PHE:HE2	19:A:1796:CLA:HBC3	1.78	0.40
5:A:652:TRP:CE2	19:A:1813:CLA:H142	2.56	0.40
5:A:308:ILE:HG22	5:A:309:LEU:H	1.81	0.40
5:A:64:PHE:HZ	5:A:77:LYS:HE3	1.84	0.40
5:A:687:ALA:O	19:A:1815:CLA:CBB	2.70	0.40
5:A:690:LEU:CD2	6:B:661:PHE:CE1	2.95	0.40
6:B:273:VAL:HG21	19:B:1748:CLA:HED2	2.02	0.40
19:B:1760:CLA:HED2	19:B:1760:CLA:CAA	2.51	0.40
6:B:185:VAL:HA	6:B:188:LEU:HB3	2.04	0.40
6:B:22:TRP:HA	6:B:25:ILE:HD11	2.03	0.40
6:B:568:CYS:C	6:B:570:ILE:HG23	2.42	0.40
6:B:598:HIS:O	6:B:599:ILE:C	2.59	0.40
7:C:79:LEU:HD22	7:C:81:TYR:O	2.21	0.40
8:D:31:GLY:HA2	16:L:13:PRO:HB2	2.00	0.40
16:L:9:GLN:O	16:L:11:ILE:N	2.54	0.40
4:4:72:VAL:O	4:4:72:VAL:HG22	2.21	0.40
4:4:76:TYR:O	4:4:77:ALA:HB3	2.22	0.40
19:2:2006:CLA:CAD	19:2:2006:CLA:CED	2.99	0.40
3:3:50:GLU:HG3	3:3:51:PRO:N	2.35	0.40
4:4:193:ILE:HG21	14:J:42:PHE:CD1	2.56	0.40
14:J:2:ARG:HB3	14:J:7:TYR:CE1	2.57	0.40
16:L:82:ALA:O	16:L:83:ALA:HB3	2.21	0.40
10:F:23:LYS:HA	10:F:23:LYS:HD2	1.82	0.40
20:A:7042:LMU:O6'	20:A:7042:LMU:H32	2.19	0.40
1:1:36:LEU:O	1:1:40:LYS:N	2.54	0.40
4:4:58:MET:SD	4:4:59:LEU:CA	3.09	0.40
21:3:1223:SUC:O6	21:3:1223:SUC:H5'	2.21	0.40
6:B:633:ASN:HA	6:B:633:ASN:HD22	1.67	0.40
6:B:14:GLN:N	6:B:14:GLN:HE21	2.14	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:183:TYR:CD2	2:2:184:THR:N	2.89	0.40
14:J:41:PHE:N	14:J:41:PHE:CD1	2.89	0.40
19:A:1767:CLA:H152	19:A:1767:CLA:H202	2.03	0.40
19:A:1774:CLA:C2A	19:A:1774:CLA:O1D	2.68	0.40
23:A:1805:BCR:C39	23:A:1805:BCR:C23	2.76	0.40
5:A:216:LEU:HD12	23:A:1803:BCR:H352	2.03	0.40
5:A:277:TYR:HD2	5:A:278:ALA:N	2.20	0.40
5:A:274:TRP:CZ2	5:A:278:ALA:HA	2.56	0.40
5:A:335:LYS:HG3	5:A:341:GLN:HA	2.02	0.40
5:A:550:HIS:O	5:A:552:THR:O	2.39	0.40
19:B:1736:CLA:HBB2	19:B:1738:CLA:CHA	2.51	0.40
7:C:62:PHE:HB3	7:C:63:LEU:H	1.59	0.40
9:E:40:ARG:N	9:E:46:PHE:CE1	2.85	0.40
9:E:90:VAL:CG1	9:E:90:VAL:O	2.69	0.40
9:E:90:VAL:HG12	9:E:90:VAL:O	2.21	0.40
13:I:29:GLU:HA	13:I:29:GLU:OE2	2.20	0.40
16:L:63:LEU:O	16:L:65:VAL:N	2.54	0.40
16:L:99:LEU:HD11	23:L:1169:BCR:C7	2.44	0.40
3:3:92:TRP:C	3:3:95:THR:OG1	2.59	0.40
4:4:36:ASN:C	4:4:39:TRP:CD2	2.95	0.40
19:2:2006:CLA:CHA	19:2:2006:CLA:CBA	2.99	0.40
8:D:45:PHE:C	8:D:46:TYR:CD2	2.92	0.40
2:2:57:LEU:O	2:2:60:ALA:HB3	2.21	0.40
2:2:126:PRO:HG3	2:2:129:LYS:HD2	2.03	0.40
7:C:12:ILE:O	7:C:12:ILE:HG22	2.21	0.40
6:B:211:ASN:ND2	6:B:214:ASP:OD1	2.55	0.40
5:A:506:GLY:O	5:A:507:ALA:CB	2.69	0.40
2:2:153:PRO:HB2	2:2:157:LYS:NZ	2.37	0.40
8:D:77:LEU:HD23	8:D:77:LEU:HA	1.81	0.40
5:A:575:LEU:HD12	5:A:575:LEU:H	1.85	0.40
19:A:1783:CLA:H102	23:A:1805:BCR:C37	2.44	0.40
19:A:1815:CLA:O2A	6:B:430:GLY:HA3	2.22	0.40
5:A:32:GLU:HG3	5:A:33:GLN:N	2.37	0.40
5:A:591:GLN:HA	5:A:591:GLN:NE2	2.28	0.40
6:B:86:PRO:O	6:B:115:ASN:HB3	2.22	0.40
6:B:152:ALA:HB2	19:B:1741:CLA:HMC3	2.02	0.40
6:B:424:TRP:HD1	19:B:1735:CLA:O1A	2.05	0.40
19:B:1747:CLA:H12	19:B:1747:CLA:NA	2.36	0.40
6:B:390:GLY:CA	23:B:1777:BCR:HC22	2.52	0.40
6:B:57:ILE:HG22	6:B:58:PHE:CD1	2.55	0.40
16:L:99:LEU:HD23	16:L:140:THR:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:CD1	17:N:63:ASP:CA	2.96	0.40
6:B:403:ASN:C	6:B:406:ASN:HB3	2.19	0.40
5:A:249:ILE:N	5:A:251:ASN:OD1	2.51	0.40
10:F:53:PHE:HB2	10:F:55:ASN:HD22	1.87	0.40
16:L:108:LYS:HE2	16:L:108:LYS:C	2.42	0.40
2:2:204:ILE:O	2:2:205:PHE:HB3	2.21	0.40
8:D:113:HIS:O	8:D:113:HIS:CD2	2.74	0.40
21:B:8059:SUC:C6'	21:B:8059:SUC:C1'	2.99	0.40
6:B:98:GLN:HE21	6:B:101:VAL:HG13	1.87	0.40
21:B:8053:SUC:O5	21:B:8053:SUC:H5'	2.21	0.40
6:B:525:LEU:HD22	6:B:529:THR:OG1	2.21	0.40
4:4:176:GLY:HA2	4:4:177:PRO:HD3	1.92	0.40
1:1:185:TRP:CZ2	19:1:1199:CLA:O2A	2.71	0.40
4:4:141:LEU:HB3	4:4:142:ASN:H	1.79	0.40
5:A:746:THR:OG1	19:A:1813:CLA:CGD	2.69	0.40
5:A:44:ILE:HG13	5:A:44:ILE:H	1.58	0.40
5:A:53:TRP:HA	5:A:56:ASN:ND2	2.37	0.40
5:A:714:LEU:HB2	5:A:716:VAL:HG13	2.03	0.40
5:A:723:ARG:O	19:A:1795:CLA:HBB1	2.21	0.40
19:B:1737:CLA:CBA	19:B:1737:CLA:HBD	2.48	0.40
19:B:1758:CLA:C6	23:B:1776:BCR:H322	2.52	0.40
19:B:1768:CLA:H62	19:B:1768:CLA:H101	1.88	0.40
22:B:1773:PQN:H302	23:L:1169:BCR:H24C	2.04	0.40
6:B:310:PRO:O	19:B:1772:CLA:CHD	2.69	0.40
6:B:559:CYS:SG	6:B:560:ASP:N	2.94	0.40
6:B:580:VAL:HG11	6:B:710:LEU:HD11	2.03	0.40
9:E:44:TYR:HB3	9:E:45:TRP:CZ3	2.57	0.40
7:C:17:CYS:O	7:C:58:CYS:HB2	2.21	0.40
2:2:62:ILE:O	2:2:66:GLU:HB2	2.22	0.40
4:4:192:THR:O	4:4:193:ILE:O	2.39	0.40
19:1:1142:CLA:OBD	19:1:1143:CLA:C1B	2.70	0.40
19:1:1143:CLA:HMD3	15:K:58:ALA:HB1	2.04	0.40
5:A:588:GLY:N	6:B:668:ARG:NH1	2.67	0.40
20:A:7039:LMU:H61	20:A:7039:LMU:H92	1.99	0.40
5:A:230:ASN:ND2	5:A:230:ASN:C	2.75	0.40
20:A:7043:LMU:H3'	20:A:7043:LMU:H1B	1.72	0.40
5:A:593:SER:OG	5:A:594:ALA:N	2.53	0.40
1:1:160:GLY:O	1:1:162:CYS:N	2.54	0.40
6:B:8:PHE:O	6:B:35:ASP:CG	2.60	0.40
6:B:377:TYR:O	6:B:378:ILE:CB	2.69	0.40
6:B:429:LEU:HA	6:B:429:LEU:HD23	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:159:PRO:O	6:B:163:PRO:HD3	2.21	0.40
3:3:194:ILE:HG13	19:3:1213:CLA:CMC	2.52	0.40

All (31) 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)
20:A:7008:LMU:C5B	21:B:8062:SUC:O1[1_654]	0.08	2.12
3:3:180:LYS:CD	6:B:490:ARG:CZ[1_556]	0.31	1.89
3:3:180:LYS:NZ	6:B:490:ARG:CD[1_556]	0.56	1.64
20:A:7008:LMU:O4'	21:B:8062:SUC:O2[1_654]	1.01	1.19
3:3:180:LYS:CG	6:B:490:ARG:NE[1_556]	1.05	1.15
3:3:180:LYS:CD	6:B:490:ARG:NH1[1_556]	1.09	1.11
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	1.49	0.71
20:A:7008:LMU:O2B	21:B:8062:SUC:O3'[1_654]	1.60	0.60
3:3:180:LYS:NZ	6:B:490:ARG:NE[1_556]	1.60	0.60
20:A:7008:LMU:O6B	21:B:8062:SUC:O2'[1_654]	1.73	0.47
20:A:7008:LMU:O6B	21:B:8062:SUC:O1'[1_654]	1.80	0.40
20:A:7008:LMU:C4'	21:B:8062:SUC:O4'[1_654]	1.86	0.34
20:A:7008:LMU:O5B	21:B:8062:SUC:O2'[1_654]	1.89	0.31
20:A:7008:LMU:C1'	21:B:8062:SUC:O4'[1_654]	1.90	0.30
20:A:7008:LMU:O3B	21:B:8062:SUC:O5[1_654]	1.92	0.28
4:4:126:LEU:O	16:L:78:GLU:N[1_655]	1.93	0.27
20:A:7008:LMU:C2B	21:B:8062:SUC:C1[1_654]	1.96	0.24
20:A:7009:LMU:O6B	20:R:1056:LMU:C10[1_654]	1.98	0.22
20:A:7008:LMU:C3B	21:B:8062:SUC:C5[1_654]	2.01	0.19
20:A:7008:LMU:C3B	21:B:8062:SUC:O3[1_654]	2.03	0.17
1:1:130:PRO:O	2:2:72:GLY:O[2_545]	2.04	0.16
19:1:1193:CLA:O2D	19:1:1142:CLA:C1[1_654]	2.04	0.16
20:A:7008:LMU:O6B	21:B:8062:SUC:O6'[1_654]	2.08	0.12
11:G:31:MET:SD	17:N:85:TRP:CE2[2_445]	2.08	0.12
20:A:7008:LMU:O6B	21:B:8062:SUC:C2'[1_654]	2.11	0.09
20:A:7008:LMU:O3B	21:B:8062:SUC:C5[1_654]	2.12	0.08
4:4:133:TYR:OH	16:L:156:PHE:O[1_655]	2.12	0.08
1:1:176:ASN:ND2	3:3:149:GLY:O[1_554]	2.13	0.07
20:A:7008:LMU:C6B	21:B:8062:SUC:C2'[1_654]	2.13	0.07
20:A:7008:LMU:O5B	21:B:8062:SUC:O5[1_654]	2.16	0.04
1:1:130:PRO:CA	2:2:72:GLY:O[2_545]	2.18	0.02

## 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%)	84 (52%)	39 (24%)	38 (24%)	0	1
2	2	174/269 (65%)	67 (38%)	51 (29%)	56 (32%)	0	0
3	3	145/276 (52%)	76 (52%)	36 (25%)	33 (23%)	0	1
4	4	164/251 (65%)	57 (35%)	44 (27%)	63 (38%)	0	0
5	A	726/758 (96%)	366 (50%)	187 (26%)	173 (24%)	0	1
6	B	731/734 (100%)	379 (52%)	204 (28%)	148 (20%)	0	1
7	C	79/81 (98%)	23 (29%)	31 (39%)	25 (32%)	0	0
8	D	136/212 (64%)	47 (35%)	48 (35%)	41 (30%)	0	0
9	E	63/143 (44%)	30 (48%)	15 (24%)	18 (29%)	0	0
10	F	152/231 (66%)	71 (47%)	40 (26%)	41 (27%)	0	0
11	G	93/167 (56%)	38 (41%)	27 (29%)	28 (30%)	0	0
12	H	67/144 (46%)	30 (45%)	16 (24%)	21 (31%)	0	0
13	I	28/40 (70%)	11 (39%)	10 (36%)	7 (25%)	0	1
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	1
15	K	82/131 (63%)	50 (61%)	13 (16%)	19 (23%)	0	1
16	L	160/216 (74%)	72 (45%)	49 (31%)	39 (24%)	0	1
17	N	83/170 (49%)	21 (25%)	19 (23%)	43 (52%)	0	0
All	All	3084/4108 (75%)	1441 (47%)	840 (27%)	803 (26%)	0	0

All (803) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU
1	1	73	GLU

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Mol	Chain	Res	Type
1	1	90	PRO
1	1	130	PRO
1	1	137	PRO
1	1	183	ASP
2	2	37	ASP
2	2	42	ARG
2	2	43	TRP
2	2	44	ASN
2	2	66	GLU
2	2	70	LYS
2	2	73	ILE
2	2	74	LEU
2	2	75	ASN
2	2	125	PHE
2	2	128	ASN
2	2	129	LYS
2	2	149	GLY
2	2	154	GLN
2	2	159	LEU
2	2	160	ARG
2	2	163	GLU
2	2	188	PRO
2	2	189	ILE
2	2	190	ASP
2	2	197	LEU
2	2	200	PRO
2	2	204	ILE
2	2	206	ALA
2	2	207	ALA
2	2	209	THR
2	2	210	PRO
3	3	48	PHE
3	3	49	ILE
3	3	94	ARG
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

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Mol	Chain	Res	Type
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	31	ALA
4	4	32	GLU
4	4	34	PRO
4	4	38	ARG
4	4	66	SER
4	4	69	ILE
4	4	73	PRO
4	4	74	LYS
4	4	82	GLU
4	4	84	PHE
4	4	87	SER
4	4	88	SER
4	4	91	PHE
4	4	107	GLN
4	4	115	VAL
4	4	121	PHE
4	4	122	LYS
4	4	125	SER
4	4	128	ALA
4	4	141	LEU
4	4	143	PHE
4	4	148	GLU
4	4	150	LYS
4	4	171	ASN
4	4	172	VAL
4	4	173	THR
4	4	175	LYS
4	4	193	ILE
5	A	22	VAL
5	A	28	LYS
5	A	35	ALA
5	A	36	LYS
5	A	40	PHE

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Mol	Chain	Res	Type
5	A	67	HIS
5	A	71	LEU
5	A	82	HIS
5	A	83	PHE
5	A	88	ILE
5	A	99	HIS
5	A	104	SER
5	A	156	SER
5	A	158	ILE
5	A	159	THR
5	A	160	SER
5	A	175	ALA
5	A	189	ALA
5	A	193	LEU
5	A	205	HIS
5	A	215	SER
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	283	PHE
5	A	286	GLY
5	A	307	ALA
5	A	310	PHE
5	A	317	TYR
5	A	329	ASP
5	A	339	THR
5	A	349	ILE
5	A	361	ASN
5	A	386	ALA
5	A	389	TYR
5	A	473	PRO
5	A	474	GLN
5	A	476	MET
5	A	477	PHE

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Mol	Chain	Res	Type
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	643	ALA
5	A	649	ILE
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	104	PHE
6	B	115	ASN
6	B	120	VAL
6	B	129	LEU
6	B	140	ILE
6	B	142	LEU
6	B	159	PRO
6	B	160	LYS
6	B	167	TRP

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Mol	Chain	Res	Type
6	B	182	LEU
6	B	187	SER
6	B	188	LEU
6	B	198	ALA
6	B	208	ARG
6	B	248	GLN
6	B	267	SER
6	B	293	THR
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	469	LYS
6	B	479	SER
6	B	490	ARG
6	B	494	LEU
6	B	495	PRO
6	B	506	ASN
6	B	512	ILE
6	B	528	HIS
6	B	545	LYS
6	B	555	TYR
6	B	569	ASP
6	B	587	ILE
6	B	603	ARG
6	B	610	ASN
6	B	629	SER
6	B	636	THR
6	B	639	VAL
6	B	661	PHE
6	B	662	MET
6	B	668	ARG
6	B	681	ALA
6	B	682	HIS

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Mol	Chain	Res	Type
6	B	691	ILE
6	B	710	LEU
6	B	732	LYS
6	B	733	PHE
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	70	TRP
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	110	GLN
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	139	LYS
8	D	151	LYS
8	D	153	PRO
9	E	46	PHE
9	E	54	ALA
9	E	60	LYS
9	E	65	VAL
9	E	72	VAL
9	E	73	ASN
9	E	86	GLU
9	E	87	VAL
9	E	89	GLU

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Mol	Chain	Res	Type
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
11	G	28	ARG
11	G	31	MET
11	G	34	GLN
11	G	38	GLN
11	G	47	GLY
11	G	50	ARG
11	G	59	LYS
11	G	61	ASN
11	G	70	ASP
11	G	74	TRP
11	G	81	VAL
11	G	86	LEU
11	G	93	TYR
11	G	94	ASP
12	H	15	ALA
12	H	20	GLN
12	H	21	TRP
12	H	23	VAL
12	H	24	TYR
12	H	31	PRO
12	H	41	GLU
12	H	46	PRO

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Mol	Chain	Res	Type
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	26	LEU
15	K	41	GLU
15	K	43	ARG
15	K	47	LEU
15	K	48	GLN
15	K	51	ASP
15	K	52	PRO
15	K	75	VAL
16	L	8	TYR
16	L	10	VAL
16	L	37	LEU
16	L	43	TYR
16	L	44	ARG
16	L	46	ALA
16	L	76	ASN
16	L	88	ALA
16	L	97	MET
16	L	121	THR
16	L	123	ARG
16	L	127	PRO
16	L	129	GLN
16	L	149	SER
16	L	158	MET
16	L	161	LEU
16	L	163	LEU
16	L	165	TYR
17	N	7	LEU
17	N	24	THR
17	N	27	ALA
17	N	28	ASN
17	N	40	CYS

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Mol	Chain	Res	Type
17	N	46	PHE
17	N	48	GLY
17	N	49	CYS
17	N	50	GLN
17	N	51	ASP
17	N	58	VAL
17	N	61	LEU
17	N	63	ASP
17	N	69	CYS
17	N	74	LYS
17	N	75	TYR
17	N	76	LYS
17	N	77	CYS
17	N	78	GLY
17	N	80	ASN
1	1	21	ASP
1	1	28	GLY
1	1	29	LEU
1	1	161	PHE
1	1	178	ALA
1	1	185	TRP
2	2	69	THR
2	2	71	LEU
2	2	81	THR
2	2	82	ALA
2	2	103	GLY
2	2	104	TRP
2	2	130	LEU
2	2	132	GLY
2	2	136	GLY
2	2	208	PHE
3	3	52	LYS
3	3	77	ILE
3	3	106	TYR
3	3	137	SER
3	3	162	PRO
3	3	208	PRO
4	4	45	LEU
4	4	59	LEU
4	4	70	ILE
4	4	71	ASN
4	4	127	PRO

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Mol	Chain	Res	Type
4	4	129	GLY
4	4	145	PRO
4	4	162	ALA
4	4	178	PHE
4	4	186	SER
4	4	188	PRO
5	A	25	ASP
5	A	39	HIS
5	A	60	ASP
5	A	69	SER
5	A	74	ILE
5	A	96	MET
5	A	130	GLU
5	A	157	GLY
5	A	200	GLU
5	A	210	LEU
5	A	242	ILE
5	A	243	PRO
5	A	266	ALA
5	A	278	ALA
5	A	282	THR
5	A	290	LEU
5	A	299	ILE
5	A	313	ALA
5	A	328	LYS
5	A	333	ALA
5	A	337	PRO
5	A	346	LEU
5	A	400	MET
5	A	404	GLY
5	A	421	ASP
5	A	424	PRO
5	A	427	ARG
5	A	428	TYR
5	A	429	ASN
5	A	431	LEU
5	A	433	ASP
5	A	439	ARG
5	A	511	THR
5	A	516	GLY
5	A	518	GLY
5	A	538	ASP

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Mol	Chain	Res	Type
5	A	574	ASN
5	A	592	VAL
5	A	594	ALA
5	A	624	VAL
5	A	640	GLY
5	A	661	ALA
5	A	717	ALA
6	B	99	PRO
6	B	105	THR
6	B	128	GLY
6	B	136	TYR
6	B	164	SER
6	B	179	LEU
6	B	224	PRO
6	B	225	LEU
6	B	231	ASN
6	B	237	PRO
6	B	247	THR
6	B	265	THR
6	B	292	ARG
6	B	309	ILE
6	B	330	ILE
6	B	437	TYR
6	B	464	GLN
6	B	474	PHE
6	B	480	SER
6	B	503	GLU
6	B	505	SER
6	B	539	LEU
6	B	554	GLY
6	B	599	ILE
6	B	657	TRP
6	B	664	LEU
6	B	690	LEU
7	C	10	THR
7	C	43	PRO
7	C	61	ASP
7	C	64	SER
8	D	26	SER
8	D	31	GLY
8	D	53	PRO
8	D	109	VAL

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Mol	Chain	Res	Type
8	D	129	GLY
8	D	130	VAL
8	D	132	LEU
8	D	146	VAL
9	E	30	PRO
9	E	35	LYS
9	E	42	GLU
9	E	53	VAL
9	E	64	PRO
9	E	90	VAL
10	F	114	PRO
10	F	126	ALA
10	F	132	ARG
11	G	33	LYS
11	G	63	PRO
11	G	80	ILE
11	G	84	TYR
11	G	85	ILE
11	G	87	ALA
12	H	17	THR
12	H	27	ASP
12	H	45	ALA
12	H	75	ASP
13	I	25	PHE
14	J	9	SER
14	J	37	LEU
14	J	39	PHE
15	K	27	ALA
15	K	35	THR
15	K	45	SER
15	K	73	GLY
15	K	79	LYS
16	L	24	GLU
16	L	27	VAL
16	L	63	LEU
16	L	89	ALA
16	L	108	LYS
16	L	120	LEU
16	L	125	LYS
16	L	128	ASP
16	L	147	GLY
17	N	2	VAL

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Mol	Chain	Res	Type
17	N	11	LYS
17	N	35	VAL
17	N	47	THR
17	N	54	LYS
17	N	64	ASP
17	N	66	ASP
17	N	68	GLU
17	N	81	VAL
17	N	82	PHE
17	N	83	TRP
1	1	78	PRO
1	1	79	GLY
1	1	118	PRO
2	2	91	THR
2	2	114	LEU
2	2	194	ALA
2	2	205	PHE
3	3	153	SER
3	3	157	ALA
4	4	35	GLU
4	4	119	PRO
4	4	139	ASN
5	A	23	ASP
5	A	31	PHE
5	A	45	ALA
5	A	57	LEU
5	A	105	ASN
5	A	124	TRP
5	A	144	GLN
5	A	155	ALA
5	A	184	PHE
5	A	213	LEU
5	A	263	ALA
5	A	276	LYS
5	A	354	TRP
5	A	373	ALA
5	A	426	THR
5	A	446	LEU
5	A	479	ASP
5	A	485	GLN
5	A	505	PRO
5	A	514	THR

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Mol	Chain	Res	Type
5	A	671	SER
6	B	103	ALA
6	B	153	GLY
6	B	161	TRP
6	B	230	TRP
6	B	294	ASN
6	B	335	GLY
6	B	371	LEU
6	B	379	ALA
6	B	451	LYS
6	B	468	GLY
6	B	481	THR
6	B	493	TRP
6	B	501	ILE
6	B	514	PRO
6	B	558	PRO
6	B	595	HIS
6	B	605	ASN
6	B	623	TYR
6	B	707	LEU
7	C	22	PRO
7	C	68	TYR
7	C	73	THR
8	D	55	GLU
8	D	63	GLY
8	D	128	GLN
8	D	150	GLY
9	E	88	GLU
10	F	11	SER
10	F	22	LEU
10	F	29	LEU
10	F	46	MET
10	F	53	PHE
10	F	63	CYS
10	F	138	VAL
10	F	153	ASN
11	G	96	SER
12	H	16	ASN
12	H	18	THR
12	H	37	SER
14	J	38	THR
15	K	32	ARG

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Mol	Chain	Res	Type
15	K	44	GLU
15	K	46	GLY
16	L	6	PRO
16	L	11	ILE
16	L	64	LEU
16	L	75	ARG
17	N	25	THR
17	N	42	PHE
17	N	43	PRO
17	N	53	ALA
17	N	62	SER
17	N	71	GLY
17	N	72	LYS
1	1	27	LEU
1	1	55	PRO
1	1	65	TYR
1	1	122	LYS
1	1	124	PRO
1	1	133	TYR
1	1	145	VAL
1	1	177	LEU
1	1	184	PRO
2	2	94	LEU
2	2	113	ILE
2	2	180	GLN
2	2	186	THR
2	2	202	ALA
3	3	75	PRO
3	3	93	PHE
3	3	141	GLN
3	3	156	PRO
3	3	169	PHE
4	4	60	LEU
4	4	77	ALA
4	4	123	GLN
4	4	126	LEU
4	4	131	VAL
4	4	177	PRO
4	4	187	ASP
4	4	192	THR
5	A	37	PRO
5	A	41	SER

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Mol	Chain	Res	Type
5	A	63	ASP
5	A	116	ILE
5	A	127	VAL
5	A	186	TYR
5	A	225	VAL
5	A	234	ASN
5	A	235	ALA
5	A	292	GLY
5	A	306	ILE
5	A	308	ILE
5	A	347	TYR
5	A	423	ASP
6	B	8	PHE
6	B	20	ARG
6	B	42	LEU
6	B	71	GLN
6	B	170	ASN
6	B	178	HIS
6	B	206	TYR
6	B	207	VAL
6	B	229	GLN
6	B	234	ALA
6	B	239	SER
6	B	240	SER
6	B	273	VAL
6	B	460	ALA
6	B	472	TYR
6	B	476	ILE
6	B	482	ASN
7	C	12	ILE
7	C	55	GLU
7	C	58	CYS
7	C	75	ARG
8	D	35	GLY
8	D	46	TYR
8	D	104	PHE
8	D	125	PRO
8	D	143	PRO
8	D	148	PHE
9	E	61	THR
10	F	34	ASP
10	F	44	ALA

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Mol	Chain	Res	Type
10	F	128	SER
10	F	151	ASP
10	F	152	ASN
11	G	20	ARG
11	G	56	SER
11	G	89	ALA
11	G	91	ASN
13	I	2	ILE
13	I	5	PRO
13	I	9	VAL
14	J	23	ALA
16	L	36	TYR
16	L	85	SER
16	L	86	LEU
16	L	112	PRO
16	L	154	ALA
17	N	21	ARG
17	N	34	THR
1	1	84	TYR
1	1	140	LEU
1	1	179	THR
2	2	45	VAL
2	2	120	ASN
2	2	140	GLY
2	2	168	ARG
4	4	72	VAL
4	4	83	TYR
4	4	85	ALA
4	4	90	LEU
4	4	112	PRO
4	4	130	GLU
5	A	73	GLU
5	A	114	THR
5	A	149	PHE
5	A	259	TYR
5	A	472	ARG
5	A	537	ALA
5	A	570	PRO
5	A	571	ASP
5	A	580	PRO
6	B	228	GLY
6	B	232	LEU

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Mol	Chain	Res	Type
6	B	278	LEU
6	B	361	ILE
6	B	475	ASP
6	B	477	PRO
6	B	559	CYS
6	B	592	PHE
6	B	730	SER
8	D	22	PRO
8	D	60	MET
9	E	84	LEU
10	F	39	ALA
10	F	61	LEU
10	F	73	VAL
10	F	83	PHE
11	G	23	PHE
11	G	36	PRO
15	K	29	SER
15	K	72	VAL
16	L	48	ASN
16	L	135	GLY
17	N	17	ASN
17	N	70	GLU
1	1	32	VAL
1	1	160	GLY
2	2	96	ILE
2	2	115	ASN
2	2	116	PRO
2	2	146	LEU
4	4	36	ASN
4	4	118	ASP
5	A	478	SER
5	A	584	PRO
5	A	586	ARG
5	A	718	PRO
5	A	754	ILE
6	B	219	PRO
6	B	222	LEU
6	B	318	GLY
6	B	391	PRO
6	B	596	TRP
6	B	711	VAL
7	C	24	ASP

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Mol	Chain	Res	Type
7	C	30	PRO
7	C	35	LYS
7	C	37	LYS
13	I	28	VAL
15	K	40	LEU
16	L	61	GLY
1	1	57	ILE
1	1	125	GLY
4	4	167	ILE
4	4	168	ILE
5	A	267	THR
5	A	531	PRO
5	A	637	ILE
5	A	721	GLN
5	A	742	GLY
6	B	400	PRO
6	B	557	PHE
8	D	27	PRO
10	F	37	ALA
2	2	187	GLY
4	4	135	GLY
4	4	154	ILE
5	A	229	ILE
5	A	500	PRO
6	B	217	PRO
11	G	64	VAL
1	1	64	GLY
1	1	77	LEU
1	1	89	VAL
1	1	173	PRO
12	H	72	ALA
2	2	135	VAL
5	A	190	ALA
5	A	223	VAL
5	A	632	GLY
8	D	67	ILE
15	K	69	ILE
17	N	59	PRO
4	4	137	ILE
5	A	249	ILE
6	B	94	PRO
6	B	162	LYS

### 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%)	100 (79%)	27 (21%)	1	7
2	2	140/216 (65%)	81 (58%)	59 (42%)	0	1
3	3	112/215 (52%)	76 (68%)	36 (32%)	0	2
4	4	138/201 (69%)	85 (62%)	53 (38%)	0	1
5	A	592/618 (96%)	410 (69%)	182 (31%)	0	3
6	B	598/600 (100%)	397 (66%)	201 (34%)	0	2
7	C	70/70 (100%)	41 (59%)	29 (41%)	0	1
8	D	118/173 (68%)	82 (70%)	36 (30%)	0	3
9	E	56/114 (49%)	38 (68%)	18 (32%)	0	2
10	F	127/190 (67%)	80 (63%)	47 (37%)	0	1
11	G	79/144 (55%)	53 (67%)	26 (33%)	0	2
12	H	57/115 (50%)	30 (53%)	27 (47%)	0	0
13	I	26/36 (72%)	22 (85%)	4 (15%)	3	20
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	3
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	3
16	L	125/169 (74%)	88 (70%)	37 (30%)	0	3
17	N	74/139 (53%)	43 (58%)	31 (42%)	0	1
All	All	2536/3331 (76%)	1694 (67%)	842 (33%)	0	2

All (842) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	17	SER
1	1	27	LEU
1	1	37	GLU
1	1	47	CYS
1	1	52	LEU
1	1	57	ILE
1	1	61	GLU

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Mol	Chain	Res	Type
1	1	63	LEU
1	1	72	GLN
1	1	84	TYR
1	1	85	LEU
1	1	105	ILE
1	1	110	HIS
1	1	111	GLN
1	1	117	ASP
1	1	120	LYS
1	1	121	LYS
1	1	129	ASP
1	1	133	TYR
1	1	134	SER
1	1	136	ASP
1	1	139	LYS
1	1	140	LEU
1	1	142	GLU
1	1	179	THR
1	1	181	LEU
1	1	183	ASP
2	2	37	ASP
2	2	39	GLU
2	2	53	ARG
2	2	57	LEU
2	2	63	PHE
2	2	66	GLU
2	2	67	PHE
2	2	69	THR
2	2	70	LYS
2	2	73	ILE
2	2	75	ASN
2	2	76	THR
2	2	79	TRP
2	2	80	TYR
2	2	85	GLN
2	2	86	GLU
2	2	87	TYR
2	2	89	THR
2	2	92	THR
2	2	95	PHE
2	2	97	VAL
2	2	98	GLU

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Mol	Chain	Res	Type
2	2	99	LEU
2	2	100	VAL
2	2	101	PHE
2	2	109	ARG
2	2	110	TRP
2	2	112	ASP
2	2	115	ASN
2	2	118	CYS
2	2	119	VAL
2	2	120	ASN
2	2	122	ASP
2	2	131	THR
2	2	137	TYR
2	2	143	PHE
2	2	144	ASP
2	2	146	LEU
2	2	150	SER
2	2	157	LYS
2	2	159	LEU
2	2	161	THR
2	2	162	LYS
2	2	164	ILE
2	2	169	LEU
2	2	171	MET
2	2	179	PHE
2	2	180	GLN
2	2	183	TYR
2	2	189	ILE
2	2	190	ASP
2	2	191	ASN
2	2	193	PHE
2	2	196	HIS
2	2	199	ASP
2	2	201	HIS
2	2	204	ILE
2	2	205	PHE
2	2	211	LYS
3	3	50	GLU
3	3	60	ILE
3	3	67	LEU
3	3	73	ILE
3	3	76	GLU

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Mol	Chain	Res	Type
3	3	78	LEU
3	3	92	TRP
3	3	93	PHE
3	3	94	ARG
3	3	97	PHE
3	3	98	ILE
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	180	LYS
3	3	185	LYS
3	3	188	ARG
3	3	191	MET
3	3	192	LEU
3	3	195	LEU
3	3	198	PHE
3	3	200	GLN
3	3	204	THR
3	3	209	TYR
3	3	210	GLN
4	4	32	GLU
4	4	33	ASP
4	4	35	GLU
4	4	38	ARG
4	4	45	LEU
4	4	49	ARG
4	4	50	TRP
4	4	52	MET
4	4	55	VAL
4	4	59	LEU
4	4	60	LEU

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Mol	Chain	Res	Type
4	4	64	PHE
4	4	66	SER
4	4	67	ILE
4	4	71	ASN
4	4	73	PRO
4	4	75	TRP
4	4	76	TYR
4	4	82	GLU
4	4	83	TYR
4	4	84	PHE
4	4	90	LEU
4	4	91	PHE
4	4	94	GLU
4	4	95	PHE
4	4	99	HIS
4	4	101	VAL
4	4	103	ILE
4	4	104	ARG
4	4	105	ARG
4	4	118	ASP
4	4	120	ILE
4	4	121	PHE
4	4	126	LEU
4	4	131	VAL
4	4	139	ASN
4	4	146	THR
4	4	147	LEU
4	4	150	LYS
4	4	151	GLU
4	4	158	ARG
4	4	159	LEU
4	4	160	MET
4	4	163	PHE
4	4	169	GLN
4	4	172	VAL
4	4	175	LYS
4	4	178	PHE
4	4	184	HIS
4	4	187	ASP
4	4	189	TRP
4	4	190	HIS
4	4	195	GLN

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Mol	Chain	Res	Type
5	A	21	LEU
5	A	22	VAL
5	A	23	ASP
5	A	24	ARG
5	A	26	PRO
5	A	27	ILE
5	A	28	LYS
5	A	29	THR
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	82	HIS
5	A	83	PHE
5	A	86	LEU
5	A	88	ILE
5	A	94	SER
5	A	103	PHE
5	A	107	GLU
5	A	111	ASN
5	A	114	THR
5	A	124	TRP
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	177	LEU
5	A	180	PHE
5	A	188	LYS
5	A	193	LEU

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Mol	Chain	Res	Type
5	A	197	GLN
5	A	203	LEU
5	A	207	LEU
5	A	213	LEU
5	A	223	VAL
5	A	224	HIS
5	A	227	LEU
5	A	230	ASN
5	A	231	GLN
5	A	232	PHE
5	A	238	ASP
5	A	242	ILE
5	A	248	PHE
5	A	249	ILE
5	A	251	ASN
5	A	253	ASP
5	A	254	LEU
5	A	255	LEU
5	A	261	SER
5	A	262	PHE
5	A	281	LEU
5	A	284	ARG
5	A	290	LEU
5	A	296	LEU
5	A	297	THR
5	A	298	ASP
5	A	304	LEU
5	A	308	ILE
5	A	316	MET
5	A	317	TYR
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
5	A	368	LEU
5	A	369	THR
5	A	375	HIS

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Mol	Chain	Res	Type
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	421	ASP
5	A	422	TYR
5	A	426	THR
5	A	427	ARG
5	A	430	ASP
5	A	433	ASP
5	A	434	ARG
5	A	438	HIS
5	A	439	ARG
5	A	440	ASP
5	A	446	LEU
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	496	HIS
5	A	498	LEU
5	A	520	LEU
5	A	521	VAL
5	A	523	VAL
5	A	529	LEU
5	A	530	LEU
5	A	532	ILE
5	A	536	THR

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Mol	Chain	Res	Type
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	568	LEU
5	A	569	ILE
5	A	575	LEU
5	A	577	PHE
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	622	SER
5	A	623	ASP
5	A	629	ASN
5	A	630	ASP
5	A	631	GLN
5	A	633	VAL
5	A	637	ILE
5	A	638	THR
5	A	641	ASN
5	A	642	PHE
5	A	644	GLN
5	A	645	SER
5	A	646	SER
5	A	653	LEU
5	A	654	ARG
5	A	660	GLN
5	A	663	GLN
5	A	673	SER
5	A	677	LEU
5	A	684	PHE
5	A	685	VAL
5	A	689	SER

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Mol	Chain	Res	Type
5	A	691	MET
5	A	692	PHE
5	A	697	ARG
5	A	703	LEU
5	A	704	ILE
5	A	707	ILE
5	A	715	LYS
5	A	723	ARG
5	A	726	SER
5	A	728	VAL
5	A	733	VAL
5	A	740	LEU
5	A	745	THR
5	A	754	ILE
6	B	3	LEU
6	B	4	ARG
6	B	5	ILE
6	B	9	SER
6	B	14	GLN
6	B	15	ASP
6	B	19	ARG
6	B	20	ARG
6	B	25	ILE
6	B	35	ASP
6	B	46	ILE
6	B	50	HIS
6	B	51	PHE
6	B	53	GLN
6	B	67	HIS
6	B	70	TRP
6	B	75	GLU
6	B	83	HIS
6	B	91	ILE
6	B	104	PHE
6	B	110	LEU
6	B	113	VAL
6	B	114	ASN
6	B	121	TYR
6	B	122	GLN
6	B	123	TRP
6	B	124	TRP
6	B	127	ILE

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Mol	Chain	Res	Type
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	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	195	VAL
6	B	203	ARG
6	B	206	TYR
6	B	208	ARG
6	B	210	ASN
6	B	214	ASP
6	B	215	VAL
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	272	ASP

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Mol	Chain	Res	Type
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	306	GLU
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	352	MET
6	B	353	TYR
6	B	361	ILE
6	B	363	GLN
6	B	364	ASP
6	B	365	PHE
6	B	374	HIS
6	B	382	ILE
6	B	384	THR
6	B	393	PHE
6	B	396	ARG
6	B	403	ASN
6	B	405	ASP
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

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Mol	Chain	Res	Type
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	457	PRO
6	B	458	ILE
6	B	461	GLN
6	B	471	THR
6	B	472	TYR
6	B	478	LEU
6	B	481	THR
6	B	486	LEU
6	B	492	ILE
6	B	494	LEU
6	B	501	ILE
6	B	502	ASN
6	B	504	ASN
6	B	508	LEU
6	B	509	PHE
6	B	510	LEU
6	B	512	ILE
6	B	516	ASP
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	542	ARG
6	B	544	SER
6	B	545	LYS
6	B	551	LYS
6	B	555	TYR
6	B	564	ARG
6	B	569	ASP
6	B	577	TYR
6	B	578	LEU

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Mol	Chain	Res	Type
6	B	583	MET
6	B	584	LEU
6	B	587	ILE
6	B	592	PHE
6	B	594	TRP
6	B	596	TRP
6	B	601	LEU
6	B	603	ARG
6	B	605	ASN
6	B	606	VAL
6	B	607	SER
6	B	608	GLN
6	B	611	GLU
6	B	615	TYR
6	B	616	LEU
6	B	617	MET
6	B	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	662	MET
6	B	664	LEU
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	692	ARG
6	B	702	ILE
6	B	703	VAL
6	B	712	HIS
6	B	715	VAL

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Mol	Chain	Res	Type
6	B	718	ILE
6	B	719	PHE
6	B	725	LEU
6	B	732	LYS
6	B	733	PHE
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	35	LYS
7	C	37	LYS
7	C	38	GLN
7	C	45	THR
7	C	48	CYS
7	C	52	LYS
7	C	54	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	27	PRO
8	D	28	ILE
8	D	41	GLN
8	D	44	GLU
8	D	46	TYR
8	D	47	VAL
8	D	49	THR

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Mol	Chain	Res	Type
8	D	50	TRP
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	90	LEU
8	D	92	SER
8	D	95	LYS
8	D	98	TYR
8	D	104	PHE
8	D	111	TYR
8	D	116	ASP
8	D	121	GLU
8	D	122	LYS
8	D	127	ARG
8	D	128	GLN
8	D	135	ARG
8	D	137	ILE
8	D	144	ILE
8	D	151	LYS
9	E	32	ARG
9	E	35	LYS
9	E	36	VAL
9	E	39	LEU
9	E	40	ARG
9	E	42	GLU
9	E	45	TRP
9	E	47	LYS
9	E	48	ASN
9	E	55	VAL
9	E	56	ASP
9	E	58	ASP
9	E	61	THR
9	E	68	ARG

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Mol	Chain	Res	Type
9	E	73	ASN
9	E	76	ASN
9	E	79	THR
9	E	90	VAL
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	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	91	LEU
10	F	92	TYR
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	115	THR
10	F	116	GLN
10	F	119	ILE
10	F	123	VAL

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Mol	Chain	Res	Type
10	F	135	SER
10	F	136	TRP
10	F	138	VAL
10	F	141	TYR
10	F	142	ARG
10	F	143	GLU
10	F	146	ASN
10	F	153	ASN
10	F	154	PHE
11	G	7	VAL
11	G	12	THR
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	38	GLN
11	G	39	ASN
11	G	41	MET
11	G	43	HIS
11	G	45	GLU
11	G	48	ASP
11	G	49	THR
11	G	50	ARG
11	G	55	VAL
11	G	58	LEU
11	G	62	ASP
11	G	71	VAL
11	G	83	TYR
11	G	88	THR
11	G	91	ASN
11	G	97	PHE
12	H	14	ILE
12	H	17	THR
12	H	21	TRP
12	H	24	TYR
12	H	32	TYR
12	H	33	ASN
12	H	35	LEU

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Mol	Chain	Res	Type
12	H	36	GLN
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
12	H	66	THR
12	H	67	TYR
12	H	69	SER
12	H	75	ASP
12	H	77	LEU
13	I	7	LEU
13	I	9	VAL
13	I	11	LEU
13	I	26	LEU
14	J	2	ARG
14	J	3	ASP
14	J	4	PHE
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	26	LEU
15	K	32	ARG

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Mol	Chain	Res	Type
15	K	33	LYS
15	K	39	LYS
15	K	40	LEU
15	K	43	ARG
15	K	44	GLU
15	K	52	PRO
15	K	55	PHE
15	K	68	HIS
15	K	69	ILE
15	K	72	VAL
15	K	84	LEU
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	32	LEU
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	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

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Mol	Chain	Res	Type
16	L	145	PHE
16	L	149	SER
16	L	152	THR
16	L	158	MET
16	L	163	LEU
16	L	165	TYR
17	N	3	ILE
17	N	4	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	46	PHE
17	N	49	CYS
17	N	50	GLN
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	65	LEU
17	N	66	ASP
17	N	67	LEU
17	N	68	GLU
17	N	75	TYR
17	N	79	SER
17	N	80	ASN
17	N	81	VAL
17	N	83	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	46	HIS

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Mol	Chain	Res	Type
1	1	111	GLN
1	1	150	ASN
2	2	44	ASN
2	2	115	ASN
2	2	128	ASN
2	2	181	HIS
2	2	191	ASN
3	3	105	ASN
3	3	126	HIS
3	3	165	ASN
4	4	71	ASN
4	4	139	ASN
4	4	169	GLN
4	4	180	ASN
5	A	58	HIS
5	A	99	HIS
5	A	121	GLN
5	A	129	GLN
5	A	144	GLN
5	A	187	HIS
5	A	197	GLN
5	A	224	HIS
5	A	230	ASN
5	A	231	GLN
5	A	361	ASN
5	A	398	HIS
5	A	447	ASN
5	A	464	ASN
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	631	GLN
5	A	636	HIS
5	A	641	ASN
5	A	660	GLN
5	A	683	HIS
5	A	701	GLN
5	A	711	HIS
5	A	729	GLN

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Mol	Chain	Res	Type
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	266	GLN
6	B	276	HIS
6	B	277	HIS
6	B	328	ASN
6	B	333	GLN
6	B	375	HIS
6	B	403	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	56	GLN
8	D	73	ASN
8	D	82	GLN
8	D	128	GLN
8	D	133	ASN
9	E	48	ASN
9	E	73	ASN
10	F	116	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
10	F	146	ASN
10	F	152	ASN
10	F	153	ASN
11	G	61	ASN
11	G	67	ASN
12	H	16	ASN
12	H	33	ASN
12	H	36	GLN
12	H	71	ASN
14	J	30	ASN
15	K	80	ASN
16	L	12	GLN
16	L	15	ASN
16	L	39	ASN
16	L	48	ASN
16	L	131	GLN
17	N	45	ASN
17	N	55	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 257 ligands modelled in this entry, 1 is unknown - leaving 256 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	1014	-	41,59,73	2.31	12 (29%)	44,96,113	4.39	16 (36%)
19	CLA	1	1142	-	36,54,73	2.39	11 (30%)	41,90,113	5.20	14 (34%)
19	CLA	1	1143	-	40,58,73	2.28	11 (27%)	44,95,113	4.93	18 (40%)
19	CLA	1	1145	-	45,63,73	2.24	10 (22%)	49,101,113	4.99	17 (34%)
19	CLA	1	1146	-	40,58,73	2.28	10 (25%)	44,95,113	4.80	20 (45%)
19	CLA	1	1148	-	45,63,73	2.16	11 (24%)	49,101,113	4.64	17 (34%)
19	CLA	1	1149	-	36,54,73	2.62	12 (33%)	42,90,113	4.67	22 (52%)
19	CLA	1	1187	1	36,54,73	2.33	11 (30%)	41,90,113	5.22	21 (51%)
19	CLA	1	1188	-	30,49,73	2.51	10 (33%)	34,84,113	5.23	15 (44%)
19	CLA	1	1189	-	37,55,73	2.45	13 (35%)	42,91,113	5.61	19 (45%)
19	CLA	1	1190	-	36,54,73	2.45	12 (33%)	41,90,113	5.30	20 (48%)
19	CLA	1	1191	-	24,44,73	2.89	8 (33%)	28,78,113	4.50	13 (46%)
19	CLA	1	1192	-	51,69,73	2.06	11 (21%)	56,108,113	4.02	18 (32%)
19	CLA	1	1193	-	41,59,73	2.40	13 (31%)	44,96,113	5.00	21 (47%)
19	CLA	1	1194	-	16,32,73	1.72	3 (18%)	21,54,113	3.12	12 (57%)
19	CLA	1	1195	-	16,32,73	1.71	3 (18%)	21,54,113	3.36	12 (57%)
19	CLA	1	1196	1	24,44,73	2.71	9 (37%)	28,78,113	4.50	12 (42%)
19	CLA	1	1197	-	41,59,73	2.52	14 (34%)	44,96,113	5.12	21 (47%)
19	CLA	1	1198	-	16,32,73	1.74	3 (18%)	21,54,113	3.14	11 (52%)
19	CLA	1	1199	-	41,59,73	2.49	15 (36%)	44,96,113	5.47	19 (43%)
19	CLA	1	1200	-	16,32,73	1.70	3 (18%)	21,54,113	3.38	11 (52%)
19	CLA	1	1307	-	16,32,73	1.72	3 (18%)	21,54,113	3.20	12 (57%)
19	CLA	1	1308	-	38,56,73	2.32	11 (28%)	42,92,113	4.93	16 (38%)
19	CLA	1	1309	-	16,32,73	1.76	3 (18%)	21,54,113	3.41	12 (57%)
19	CLA	1	1505	-	45,63,73	2.15	11 (24%)	49,101,113	4.63	19 (38%)
19	CLA	2	1212	-	41,59,73	2.35	11 (26%)	44,96,113	4.85	18 (40%)
19	CLA	2	1213	-	48,66,73	2.20	13 (27%)	52,104,113	4.66	20 (38%)
19	CLA	2	1214	-	16,32,73	1.74	6 (37%)	21,54,113	3.21	11 (52%)
19	CLA	2	1215	-	40,58,73	2.28	10 (25%)	44,95,113	4.49	16 (36%)
19	CLA	2	1216	-	16,32,73	1.68	3 (18%)	21,54,113	2.76	11 (52%)
19	CLA	2	1217	-	55,73,73	1.96	10 (18%)	61,113,113	4.09	19 (31%)
19	CLA	2	1218	-	16,32,73	1.77	6 (37%)	21,54,113	3.41	11 (52%)
19	CLA	2	1219	-	24,44,73	2.72	9 (37%)	28,78,113	4.86	13 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	2	1220	-	16,32,73	1.64	3 (18%)	21,54,113	3.03	11 (52%)
19	CLA	2	1221	2	40,58,73	2.36	12 (30%)	44,95,113	5.00	18 (40%)
19	CLA	2	1222	-	40,58,73	2.28	11 (27%)	44,95,113	4.98	19 (43%)
19	CLA	2	1223	-	51,69,73	2.02	11 (21%)	56,108,113	4.64	23 (41%)
20	LMU	2	1224	-	36,36,36	0.50	0	47,47,47	1.71	6 (12%)
21	SUC	2	1225	-	23,23,24	0.59	0	35,35,36	1.42	5 (14%)
19	CLA	2	2006	-	40,58,73	2.37	12 (30%)	44,95,113	4.87	17 (38%)
19	CLA	2	2010	-	16,32,73	1.63	3 (18%)	21,54,113	2.78	11 (52%)
19	CLA	3	1212	-	16,32,73	1.75	3 (18%)	21,54,113	3.02	11 (52%)
19	CLA	3	1213	-	24,44,73	2.80	7 (29%)	28,78,113	4.43	13 (46%)
19	CLA	3	1214	-	16,32,73	1.73	4 (25%)	21,54,113	3.19	11 (52%)
19	CLA	3	1215	-	16,32,73	1.75	3 (18%)	21,54,113	2.96	9 (42%)
19	CLA	3	1216	-	16,32,73	1.72	3 (18%)	21,54,113	3.17	12 (57%)
19	CLA	3	1217	-	32,50,73	2.49	10 (31%)	36,85,113	5.89	17 (47%)
19	CLA	3	1218	-	46,64,73	2.15	12 (26%)	50,102,113	4.62	19 (38%)
19	CLA	3	1219	-	16,32,73	1.67	3 (18%)	21,54,113	3.28	12 (57%)
19	CLA	3	1220	-	16,32,73	1.74	4 (25%)	21,54,113	3.49	11 (52%)
19	CLA	3	1221	-	55,73,73	1.96	11 (20%)	61,113,113	3.84	22 (36%)
19	CLA	3	1222	-	55,73,73	1.96	11 (20%)	61,113,113	4.25	18 (29%)
21	SUC	3	1223	-	24,24,24	0.51	0	36,36,36	1.45	5 (13%)
19	CLA	3	3001	-	16,32,73	1.79	3 (18%)	21,54,113	3.19	12 (57%)
19	CLA	3	3008	-	40,58,73	2.29	9 (22%)	44,95,113	4.66	17 (38%)
19	CLA	3	3011	-	55,73,73	1.93	13 (23%)	61,113,113	4.24	18 (29%)
19	CLA	3	3014	-	16,32,73	1.74	4 (25%)	21,54,113	3.42	12 (57%)
19	CLA	3	3015	-	16,32,73	1.69	3 (18%)	21,54,113	3.25	11 (52%)
19	CLA	4	1196	-	45,63,73	2.20	11 (24%)	49,101,113	4.64	19 (38%)
19	CLA	4	1197	-	24,44,73	2.83	9 (37%)	28,78,113	4.62	15 (53%)
19	CLA	4	1198	-	55,73,73	2.03	11 (20%)	61,113,113	4.23	20 (32%)
19	CLA	4	1199	-	45,63,73	2.14	10 (22%)	49,101,113	4.21	17 (34%)
19	CLA	4	1200	-	40,58,73	2.34	12 (30%)	44,95,113	5.16	18 (40%)
19	CLA	4	1201	-	42,60,73	2.34	11 (26%)	45,97,113	4.79	27 (60%)
19	CLA	4	1202	-	16,32,73	1.73	4 (25%)	21,54,113	3.14	11 (52%)
19	CLA	4	1203	-	16,32,73	1.74	5 (31%)	21,54,113	3.38	12 (57%)
19	CLA	4	1204	-	16,32,73	1.75	3 (18%)	21,54,113	3.12	11 (52%)
19	CLA	4	1205	-	40,58,73	2.32	12 (30%)	44,95,113	4.24	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	4	1206	-	55,73,73	1.98	13 (23%)	61,113,113	4.37	19 (31%)
19	CLA	4	1207	-	16,32,73	1.72	4 (25%)	21,54,113	3.18	11 (52%)
19	CLA	4	1208	-	16,32,73	1.68	3 (18%)	21,54,113	3.21	12 (57%)
19	CLA	4	1209	4	24,44,73	2.67	8 (33%)	28,78,113	4.88	16 (57%)
19	CLA	4	1210	4	16,32,73	1.78	4 (25%)	21,54,113	2.88	12 (57%)
19	CLA	4	1211	-	36,54,73	2.38	12 (33%)	41,90,113	4.74	15 (36%)
20	LMU	4	1212	-	36,36,36	0.71	1 (2%)	47,47,47	1.13	3 (6%)
19	CLA	4	4007	-	42,60,73	2.28	12 (28%)	45,97,113	5.06	20 (44%)
19	CLA	4	4014	-	37,55,73	2.34	12 (32%)	42,91,113	5.24	19 (45%)
19	CLA	A	1759	-	36,54,73	2.53	12 (33%)	41,90,113	5.17	15 (36%)
19	CLA	A	1760	19	45,63,73	2.27	11 (24%)	49,101,113	4.18	19 (38%)
19	CLA	A	1761	-	44,62,73	2.16	12 (27%)	47,99,113	3.98	17 (36%)
19	CLA	A	1762	-	46,64,73	2.10	10 (21%)	50,102,113	4.61	19 (38%)
19	CLA	A	1763	-	36,54,73	2.34	10 (27%)	41,90,113	5.26	18 (43%)
19	CLA	A	1764	5	50,68,73	2.11	12 (24%)	55,107,113	3.98	19 (34%)
19	CLA	A	1765	-	42,60,73	2.17	10 (23%)	45,97,113	4.48	19 (42%)
19	CLA	A	1766	-	32,53,73	2.49	10 (31%)	37,89,113	5.41	18 (48%)
19	CLA	A	1767	19,5	55,73,73	2.01	12 (21%)	61,113,113	3.80	19 (31%)
19	CLA	A	1768	5	44,62,73	2.13	10 (22%)	47,99,113	4.35	15 (31%)
19	CLA	A	1769	-	40,58,73	2.24	10 (25%)	44,95,113	4.67	18 (40%)
19	CLA	A	1770	-	16,32,73	1.80	6 (37%)	21,54,113	3.23	11 (52%)
19	CLA	A	1771	-	40,58,73	2.31	10 (25%)	44,95,113	4.83	19 (43%)
19	CLA	A	1772	-	44,62,73	2.18	12 (27%)	47,99,113	4.65	19 (40%)
19	CLA	A	1773	-	42,60,73	2.25	11 (26%)	45,97,113	4.99	15 (33%)
19	CLA	A	1774	-	50,68,73	2.20	13 (26%)	55,107,113	3.65	24 (43%)
19	CLA	A	1775	-	24,44,73	2.78	8 (33%)	28,78,113	4.53	14 (50%)
19	CLA	A	1776	-	48,66,73	2.11	10 (20%)	52,104,113	4.36	21 (40%)
19	CLA	A	1777	-	41,59,73	2.27	11 (26%)	44,96,113	4.74	17 (38%)
19	CLA	A	1778	5	32,50,73	2.44	10 (31%)	36,85,113	5.27	15 (41%)
19	CLA	A	1779	-	40,58,73	2.27	11 (27%)	44,95,113	4.48	17 (38%)
19	CLA	A	1780	-	48,66,73	2.03	11 (22%)	52,104,113	3.97	18 (34%)
19	CLA	A	1781	-	49,67,73	2.05	11 (22%)	53,105,113	4.42	18 (33%)
19	CLA	A	1782	-	55,73,73	1.90	11 (20%)	61,113,113	3.61	16 (26%)
19	CLA	A	1783	-	55,73,73	1.94	11 (20%)	61,113,113	4.36	16 (26%)
19	CLA	A	1784	5	45,63,73	2.17	11 (24%)	49,101,113	4.57	18 (36%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	A	1785	-	55,73,73	1.97	12 (21%)	61,113,113	3.85	19 (31%)
19	CLA	A	1786	-	40,58,73	2.31	12 (30%)	44,95,113	5.08	18 (40%)
19	CLA	A	1787	5	50,68,73	2.09	10 (20%)	55,107,113	4.20	19 (34%)
19	CLA	A	1788	-	55,73,73	1.94	11 (20%)	61,113,113	4.25	15 (24%)
19	CLA	A	1789	5	55,73,73	1.96	12 (21%)	61,113,113	4.61	25 (40%)
19	CLA	A	1790	5	40,58,73	2.25	10 (25%)	44,95,113	4.80	18 (40%)
19	CLA	A	1791	19,5	32,53,73	2.40	10 (31%)	37,89,113	5.47	18 (48%)
19	CLA	A	1792	-	36,54,73	2.41	10 (27%)	41,90,113	5.08	17 (41%)
19	CLA	A	1793	-	55,73,73	2.04	11 (20%)	61,113,113	4.24	19 (31%)
19	CLA	A	1794	-	37,55,73	2.40	11 (29%)	42,91,113	4.61	15 (35%)
19	CLA	A	1795	-	41,59,73	2.30	11 (26%)	44,96,113	4.92	18 (40%)
19	CLA	A	1796	-	55,73,73	1.98	10 (18%)	61,113,113	4.03	21 (34%)
19	CLA	A	1797	19	49,67,73	2.31	14 (28%)	53,105,113	4.16	21 (39%)
19	CLA	A	1798	-	45,63,73	2.15	11 (24%)	49,101,113	4.81	17 (34%)
19	CLA	A	1799	-	16,32,73	1.80	3 (18%)	21,54,113	3.39	12 (57%)
19	CLA	A	1800	-	55,73,73	1.92	11 (20%)	61,113,113	4.31	19 (31%)
19	CLA	A	1801	-	45,63,73	2.25	10 (22%)	49,101,113	4.42	20 (40%)
22	PQN	A	1802	-	34,34,34	1.49	2 (5%)	44,45,45	1.14	3 (6%)
23	BCR	A	1803	-	41,41,41	1.95	3 (7%)	56,56,56	5.47	20 (35%)
23	BCR	A	1804	-	41,41,41	2.01	3 (7%)	56,56,56	5.56	21 (37%)
23	BCR	A	1805	-	41,41,41	2.00	4 (9%)	56,56,56	5.70	26 (46%)
23	BCR	A	1806	-	41,41,41	1.92	3 (7%)	56,56,56	5.52	17 (30%)
23	BCR	A	1807	-	40,40,41	1.65	3 (7%)	50,53,56	4.35	19 (38%)
23	BCR	A	1808	-	41,41,41	2.51	6 (14%)	56,56,56	6.05	21 (37%)
23	BCR	A	1809	-	41,41,41	1.96	3 (7%)	56,56,56	5.69	21 (37%)
20	LMU	A	1810	-	36,36,36	0.68	0	47,47,47	1.33	7 (14%)
20	LMU	A	1811	-	36,36,36	0.66	1 (2%)	47,47,47	1.49	7 (14%)
20	LMU	A	1812	-	36,36,36	0.47	0	47,47,47	0.88	4 (8%)
19	CLA	A	1813	-	55,73,73	1.95	12 (21%)	61,113,113	4.36	19 (31%)
19	CLA	A	1814	-	55,73,73	1.99	12 (21%)	61,113,113	4.26	19 (31%)
19	CLA	A	1815	-	55,73,73	2.03	11 (20%)	61,113,113	4.18	17 (27%)
19	CLA	A	1816	-	44,62,73	2.18	11 (25%)	47,99,113	4.82	21 (44%)
19	CLA	A	1817	-	55,73,73	1.97	10 (18%)	61,113,113	4.17	17 (27%)
20	LMU	A	7001	-	36,36,36	0.66	0	47,47,47	1.65	9 (19%)
20	LMU	A	7003	-	36,36,36	0.48	0	47,47,47	0.75	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMU	A	7004	-	36,36,36	0.45	0	47,47,47	1.45	6 (12%)
20	LMU	A	7005	-	36,36,36	0.43	0	47,47,47	1.17	5 (10%)
20	LMU	A	7006	-	36,36,36	0.55	0	47,47,47	0.70	0
20	LMU	A	7008	21	36,36,36	1.08	3 (8%)	47,47,47	2.20	11 (23%)
20	LMU	A	7009	20	35,35,36	0.78	2 (5%)	46,46,47	1.85	11 (23%)
20	LMU	A	7010	-	36,36,36	0.54	0	47,47,47	0.89	2 (4%)
20	LMU	A	7011	-	36,36,36	0.46	0	47,47,47	1.55	6 (12%)
20	LMU	A	7013	20	36,36,36	0.56	0	47,47,47	1.01	2 (4%)
20	LMU	A	7014	-	36,36,36	0.84	1 (2%)	47,47,47	2.13	12 (25%)
20	LMU	A	7015	-	36,36,36	0.68	1 (2%)	47,47,47	1.35	4 (8%)
20	LMU	A	7016	-	36,36,36	0.49	0	47,47,47	1.50	6 (12%)
20	LMU	A	7017	-	36,36,36	0.63	0	47,47,47	1.90	14 (29%)
20	LMU	A	7019	-	36,36,36	0.75	1 (2%)	47,47,47	1.33	8 (17%)
20	LMU	A	7020	-	36,36,36	0.56	0	47,47,47	1.56	9 (19%)
20	LMU	A	7021	-	36,36,36	0.69	0	47,47,47	1.52	6 (12%)
20	LMU	A	7022	-	36,36,36	0.56	0	47,47,47	1.33	5 (10%)
20	LMU	A	7023	-	36,36,36	0.50	0	47,47,47	1.36	7 (14%)
20	LMU	A	7024	-	36,36,36	0.73	1 (2%)	47,47,47	1.46	8 (17%)
20	LMU	A	7025	-	36,36,36	0.51	0	47,47,47	1.26	6 (12%)
20	LMU	A	7026	-	36,36,36	0.84	1 (2%)	47,47,47	2.15	14 (29%)
20	LMU	A	7027	-	36,36,36	0.80	1 (2%)	47,47,47	1.63	11 (23%)
20	LMU	A	7028	-	36,36,36	0.50	0	47,47,47	1.05	3 (6%)
20	LMU	A	7030	-	36,36,36	0.59	0	47,47,47	1.67	8 (17%)
20	LMU	A	7031	-	36,36,36	0.45	0	47,47,47	1.29	4 (8%)
20	LMU	A	7032	-	36,36,36	0.71	1 (2%)	47,47,47	1.70	8 (17%)
20	LMU	A	7033	-	36,36,36	0.68	0	47,47,47	1.67	9 (19%)
20	LMU	A	7034	-	36,36,36	0.45	0	47,47,47	1.51	8 (17%)
20	LMU	A	7035	-	36,36,36	0.64	0	47,47,47	1.44	9 (19%)
20	LMU	A	7036	-	35,35,36	0.58	1 (2%)	46,46,47	1.37	5 (10%)
20	LMU	A	7037	-	36,36,36	0.60	0	47,47,47	1.90	13 (27%)
20	LMU	A	7038	-	36,36,36	0.69	0	47,47,47	1.77	11 (23%)
20	LMU	A	7039	-	36,36,36	0.60	0	47,47,47	1.64	8 (17%)
20	LMU	A	7040	-	36,36,36	0.66	1 (2%)	47,47,47	1.71	12 (25%)
20	LMU	A	7041	-	36,36,36	0.37	0	47,47,47	1.05	3 (6%)
20	LMU	A	7042	-	36,36,36	0.51	0	47,47,47	1.32	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMU	A	7043	-	36,36,36	0.59	1 (2%)	47,47,47	1.61	11 (23%)
20	LMU	A	7047	-	36,36,36	0.80	1 (2%)	47,47,47	1.24	4 (8%)
20	LMU	A	7049	20	36,36,36	0.49	0	47,47,47	0.97	2 (4%)
19	CLA	B	1735	-	55,73,73	2.01	11 (20%)	61,113,113	3.94	18 (29%)
19	CLA	B	1736	-	32,53,73	2.46	11 (34%)	37,89,113	4.93	14 (37%)
19	CLA	B	1737	-	51,69,73	1.98	12 (23%)	56,108,113	4.12	19 (33%)
19	CLA	B	1738	-	55,73,73	1.98	12 (21%)	61,113,113	4.25	22 (36%)
19	CLA	B	1739	-	50,68,73	2.11	11 (22%)	55,107,113	4.42	19 (34%)
19	CLA	B	1740	6	16,32,73	1.82	4 (25%)	21,54,113	2.96	11 (52%)
19	CLA	B	1741	6	44,62,73	2.39	11 (25%)	49,100,113	3.97	18 (36%)
19	CLA	B	1742	6	45,63,73	2.08	10 (22%)	49,101,113	4.52	18 (36%)
19	CLA	B	1743	-	55,73,73	1.97	10 (18%)	61,113,113	4.03	16 (26%)
19	CLA	B	1744	-	50,68,73	2.11	11 (22%)	55,107,113	4.06	16 (29%)
19	CLA	B	1745	6	50,68,73	2.03	10 (20%)	55,107,113	4.01	18 (32%)
19	CLA	B	1746	-	36,54,73	2.37	10 (27%)	41,90,113	4.54	16 (39%)
19	CLA	B	1747	-	43,61,73	2.21	11 (25%)	46,98,113	4.54	17 (36%)
19	CLA	B	1748	-	30,49,73	2.53	12 (40%)	34,84,113	6.00	17 (50%)
19	CLA	B	1749	-	51,69,73	1.96	11 (21%)	56,108,113	4.54	19 (33%)
19	CLA	B	1750	-	40,58,73	2.26	11 (27%)	44,95,113	4.93	15 (34%)
19	CLA	B	1751	-	36,54,73	2.37	11 (30%)	41,90,113	5.24	13 (31%)
19	CLA	B	1752	6	45,63,73	2.19	10 (22%)	49,101,113	4.69	18 (36%)
19	CLA	B	1753	-	55,73,73	2.08	14 (25%)	61,113,113	4.33	19 (31%)
19	CLA	B	1754	-	44,62,73	2.26	12 (27%)	47,99,113	4.56	19 (40%)
19	CLA	B	1755	-	48,66,73	2.09	11 (22%)	52,104,113	4.53	18 (34%)
19	CLA	B	1756	6	55,73,73	1.92	11 (20%)	61,113,113	4.21	19 (31%)
19	CLA	B	1757	-	55,73,73	1.99	11 (20%)	61,113,113	4.25	19 (31%)
19	CLA	B	1758	-	55,73,73	1.97	12 (21%)	61,113,113	3.89	20 (32%)
19	CLA	B	1759	-	55,73,73	1.96	12 (21%)	61,113,113	3.82	18 (29%)
19	CLA	B	1760	-	40,58,73	2.29	10 (25%)	44,95,113	4.66	17 (38%)
19	CLA	B	1761	10,6	40,58,73	2.35	14 (35%)	44,95,113	5.17	17 (38%)
19	CLA	B	1762	6	49,67,73	2.14	12 (24%)	53,105,113	4.33	18 (33%)
19	CLA	B	1763	6	40,58,73	2.28	12 (30%)	44,95,113	4.72	18 (40%)
19	CLA	B	1764	19	32,53,73	2.47	10 (31%)	37,89,113	5.33	13 (35%)
19	CLA	B	1765	19	32,53,73	2.47	10 (31%)	37,89,113	4.95	15 (40%)
19	CLA	B	1766	-	41,59,73	2.22	11 (26%)	44,96,113	4.97	20 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	B	1767	-	50,68,73	2.04	11 (22%)	55,107,113	4.30	14 (25%)
19	CLA	B	1768	6	55,73,73	1.90	11 (20%)	61,113,113	3.75	16 (26%)
19	CLA	B	1769	-	37,55,73	2.53	14 (37%)	42,91,113	5.43	18 (42%)
19	CLA	B	1770	-	55,73,73	1.94	11 (20%)	61,113,113	3.74	18 (29%)
19	CLA	B	1771	-	55,73,73	1.90	12 (21%)	61,113,113	3.69	18 (29%)
19	CLA	B	1772	-	24,44,73	2.77	8 (33%)	28,78,113	4.80	15 (53%)
22	PQN	B	1773	-	34,34,34	1.44	2 (5%)	44,45,45	1.28	6 (13%)
23	BCR	B	1774	-	41,41,41	1.86	3 (7%)	56,56,56	5.72	17 (30%)
23	BCR	B	1775	-	41,41,41	1.85	3 (7%)	56,56,56	5.19	24 (42%)
23	BCR	B	1776	-	41,41,41	1.75	3 (7%)	56,56,56	4.77	19 (33%)
23	BCR	B	1777	-	41,41,41	1.97	4 (9%)	56,56,56	5.55	20 (35%)
23	BCR	B	1778	-	41,41,41	2.00	3 (7%)	56,56,56	5.46	18 (32%)
23	BCR	B	1779	-	41,41,41	2.15	5 (12%)	56,56,56	5.72	23 (41%)
23	BCR	B	1780	-	41,41,41	1.94	3 (7%)	56,56,56	5.43	16 (28%)
24	LMG	B	1781	-	49,49,55	0.95	2 (4%)	57,57,63	1.08	2 (3%)
20	LMU	B	1782	-	26,26,36	0.75	1 (3%)	37,37,47	1.36	6 (16%)
25	SF4	B	1783	5,6	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	B	1784	-	55,73,73	1.93	11 (20%)	61,113,113	4.00	19 (31%)
21	SUC	B	8051	-	24,24,24	0.44	0	36,36,36	1.22	2 (5%)
21	SUC	B	8052	-	24,24,24	0.34	0	36,36,36	0.95	0
21	SUC	B	8053	-	23,23,24	0.62	0	35,35,36	1.41	6 (17%)
21	SUC	B	8054	-	24,24,24	0.57	0	36,36,36	0.99	2 (5%)
21	SUC	B	8055	-	24,24,24	0.45	0	36,36,36	1.25	4 (11%)
21	SUC	B	8056	-	24,24,24	0.49	0	36,36,36	1.20	6 (16%)
21	SUC	B	8059	-	24,24,24	0.51	0	36,36,36	1.22	2 (5%)
21	SUC	B	8060	-	24,24,24	0.48	0	36,36,36	0.98	2 (5%)
21	SUC	B	8061	-	24,24,24	0.51	0	36,36,36	1.63	9 (25%)
21	SUC	B	8062	20	24,24,24	1.05	2 (8%)	36,36,36	2.09	11 (30%)
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	2.59	8 (33%)	28,78,113	3.93	14 (50%)
19	CLA	F	1156	19	30,49,73	2.49	10 (33%)	34,84,113	5.48	16 (47%)
19	CLA	F	1157	19	43,61,73	2.51	17 (39%)	46,98,113	4.53	20 (43%)
19	CLA	G	1099	-	41,59,73	2.30	12 (29%)	44,96,113	4.33	17 (38%)
19	CLA	H	1079	-	48,66,73	2.15	12 (25%)	52,104,113	4.20	21 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	H	1080	-	45,63,73	2.16	10 (22%)	49,101,113	4.72	18 (36%)
19	CLA	H	1081	16	40,58,73	2.29	10 (25%)	44,95,113	4.94	16 (36%)
21	SUC	H	1082	-	24,24,24	0.43	0	36,36,36	0.90	1 (2%)
19	CLA	I	1031	-	50,68,73	2.04	11 (22%)	55,107,113	4.58	16 (29%)
23	BCR	I	1032	-	41,41,41	2.12	5 (12%)	56,56,56	6.12	27 (48%)
19	CLA	J	1043	-	51,69,73	2.00	11 (21%)	56,108,113	4.34	15 (26%)
19	CLA	L	1167	-	37,55,73	2.40	11 (29%)	42,91,113	5.14	17 (40%)
19	CLA	L	1168	-	40,58,73	2.36	12 (30%)	44,95,113	5.35	18 (40%)
23	BCR	L	1169	-	41,41,41	1.99	4 (9%)	56,56,56	5.63	16 (28%)
20	LMU	L	1170	-	36,36,36	0.69	1 (2%)	47,47,47	1.33	5 (10%)
19	CLA	R	1054	-	47,65,73	2.14	11 (23%)	50,103,113	4.77	20 (40%)
19	CLA	R	1055	-	55,73,73	2.01	10 (18%)	61,113,113	4.16	20 (32%)
20	LMU	R	1056	20	36,36,36	0.48	0	47,47,47	0.88	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1014	-	4/4/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1142	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1143	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	1	1145	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1146	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	1	1148	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1149	-	5/5/16/25	0/16/112/135	0/0/9/9
19	CLA	1	1187	1	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1188	-	3/3/15/25	0/8/106/135	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	0/15/113/135	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	-	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	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1196	1	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1197	-	4/4/17/25	1/21/119/135	0/0/9/9
19	CLA	1	1198	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1199	-	5/5/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1200	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1307	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1308	-	3/3/16/25	0/17/115/135	0/0/9/9
19	CLA	1	1309	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1505	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	2	1212	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	2	1213	-	4/4/18/25	0/29/127/135	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	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1219	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	2	1220	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1221	2	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1222	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1223	-	4/4/19/25	0/33/131/135	0/0/9/9
20	LMU	2	1224	-	-	0/21/61/61	0/2/2/2
21	SUC	2	1225	-	1/1/9/9	0/10/49/51	0/2/2/2
19	CLA	2	2006	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	2	2010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1212	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1213	-	3/3/14/25	0/0/96/135	0/0/9/9
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	-	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	3	1218	-	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	3	1219	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1220	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	1221	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1222	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	3	1223	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	3	3001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3008	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	3	3011	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	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
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	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1205	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	4	1206	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1207	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1208	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1209	4	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1210	4	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
20	LMU	4	1212	-	-	0/21/61/61	0/2/2/2
19	CLA	4	4007	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4014	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1759	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	1760	19	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1761	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1762	-	4/4/18/25	0/27/125/135	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	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	A	1765	-	3/3/17/25	0/22/120/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1766	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1767	19,5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1768	5	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1769	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1770	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	A	1771	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1772	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1773	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	1774	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	A	1775	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	A	1776	-	4/4/18/25	0/29/127/135	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	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1780	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	A	1781	-	4/4/18/25	1/30/128/135	0/0/9/9
19	CLA	A	1782	-	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	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	A	1788	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1789	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1790	5	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1791	19,5	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1792	-	3/3/16/25	0/15/113/135	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	19	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	A	1798	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	A	1799	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1800	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1801	-	4/4/18/25	0/25/123/135	0/0/9/9
22	PQN	A	1802	-	1/1/8/9	0/23/43/43	0/2/2/2
23	BCR	A	1803	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1804	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1805	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1806	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1807	-	-	0/29/60/63	0/2/2/2
23	BCR	A	1808	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1809	-	-	1/29/63/63	0/2/2/2
20	LMU	A	1810	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1811	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1812	-	-	0/21/61/61	0/2/2/2
19	CLA	A	1813	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1814	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1815	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1816	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1817	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	A	7001	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7003	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7004	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7005	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7006	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7008	21	-	0/21/61/61	0/2/2/2
20	LMU	A	7009	20	-	0/20/60/61	0/2/2/2
20	LMU	A	7010	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7011	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7013	20	-	0/21/61/61	0/2/2/2
20	LMU	A	7014	-	-	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	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7027	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMU	A	7028	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7030	-	-	1/21/61/61	0/2/2/2
20	LMU	A	7031	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7032	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7033	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7034	-	-	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
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	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7047	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7049	20	-	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	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	B	1738	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1739	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1740	6	3/3/7/25	0/0/66/135	0/0/8/9
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	-	4/4/19/25	0/31/129/135	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	-	3/3/17/25	0/23/121/135	0/0/9/9
19	CLA	B	1748	-	3/3/15/25	0/8/106/135	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	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1754	-	3/3/17/25	0/24/122/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1755	-	4/4/18/25	1/29/127/135	0/0/9/9
19	CLA	B	1756	6	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	10,6	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1762	6	4/4/18/25	0/30/128/135	0/0/9/9
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	1/16/114/135	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
22	PQN	B	1773	-	1/1/8/9	0/23/43/43	0/2/2/2
23	BCR	B	1774	-	-	2/29/63/63	0/2/2/2
23	BCR	B	1775	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1776	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1777	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1778	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1779	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1780	-	-	2/29/63/63	0/2/2/2
24	LMG	B	1781	-	-	0/44/64/70	0/1/1/1
20	LMU	B	1782	-	-	0/11/51/61	0/2/2/2
25	SF4	B	1783	5,6	-	0/0/48/48	0/6/5/5
19	CLA	B	1784	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	B	8051	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8052	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8053	-	1/1/9/9	0/10/49/51	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	H	1080	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	H	1081	16	3/3/17/25	0/19/117/135	0/0/9/9
21	SUC	H	1082	-	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
23	BCR	I	1032	-	-	0/29/63/63	0/2/2/2
19	CLA	J	1043	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	L	1167	-	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
23	BCR	L	1169	-	-	0/29/63/63	0/2/2/2
20	LMU	L	1170	-	-	0/21/61/61	0/2/2/2
19	CLA	R	1054	-	4/4/18/25	0/28/126/135	0/0/9/9
19	CLA	R	1055	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	R	1056	20	-	0/21/61/61	0/2/2/2

All (1783) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1808	BCR	C21-C22	-9.92	1.22	1.35
23	A	1808	BCR	C20-C21	-9.28	1.14	1.43
19	1	1191	CLA	CAB-C3B	-8.99	1.33	1.51
19	B	1741	CLA	CAB-C3B	-8.90	1.33	1.51
19	4	1197	CLA	CAB-C3B	-8.65	1.34	1.51
23	B	1779	BCR	C21-C22	-8.48	1.24	1.35
23	A	1803	BCR	C20-C21	-8.45	1.17	1.43
23	A	1804	BCR	C20-C21	-8.41	1.17	1.43
19	B	1772	CLA	CAB-C3B	-8.40	1.34	1.51
23	B	1778	BCR	C20-C21	-8.38	1.17	1.43
23	L	1169	BCR	C20-C21	-8.38	1.17	1.43
23	B	1779	BCR	C20-C21	-8.37	1.17	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1805	BCR	C20-C21	-8.34	1.17	1.43
23	A	1809	BCR	C20-C21	-8.33	1.17	1.43
19	1	1196	CLA	CAB-C3B	-8.32	1.34	1.51
19	A	1775	CLA	CAB-C3B	-8.27	1.34	1.51
23	B	1780	BCR	C20-C21	-8.27	1.18	1.43
19	2	1219	CLA	CAB-C3B	-8.26	1.34	1.51
23	B	1777	BCR	C20-C21	-8.22	1.18	1.43
23	A	1806	BCR	C20-C21	-8.22	1.18	1.43
23	A	1804	BCR	C21-C22	-8.20	1.24	1.35
19	1	1149	CLA	CAB-C3B	-8.18	1.35	1.51
19	4	1209	CLA	CAB-C3B	-8.13	1.35	1.51
19	3	1213	CLA	CAB-C3B	-8.12	1.35	1.51
23	I	1032	BCR	C20-C21	-8.10	1.18	1.43
23	B	1774	BCR	C20-C21	-8.09	1.18	1.43
23	I	1032	BCR	C21-C22	-8.03	1.25	1.35
23	B	1778	BCR	C21-C22	-8.01	1.25	1.35
23	B	1777	BCR	C21-C22	-7.92	1.25	1.35
23	A	1805	BCR	C21-C22	-7.91	1.25	1.35
23	A	1803	BCR	C21-C22	-7.82	1.25	1.35
23	A	1809	BCR	C21-C22	-7.78	1.25	1.35
19	A	1774	CLA	C3B-CAB	-7.73	1.31	1.47
23	L	1169	BCR	C21-C22	-7.71	1.25	1.35
23	B	1775	BCR	C20-C21	-7.69	1.19	1.43
23	A	1806	BCR	C21-C22	-7.68	1.25	1.35
19	A	1759	CLA	C3B-CAB	-7.65	1.31	1.47
23	B	1780	BCR	C21-C22	-7.63	1.25	1.35
19	A	1797	CLA	C3B-CAB	-7.45	1.32	1.47
23	B	1776	BCR	C20-C21	-7.42	1.20	1.43
19	2	1221	CLA	C3B-CAB	-7.34	1.32	1.47
19	B	1738	CLA	C3B-CAB	-7.25	1.32	1.47
23	B	1774	BCR	C21-C22	-7.18	1.26	1.35
19	A	1793	CLA	C3B-CAB	-7.17	1.32	1.47
23	A	1807	BCR	C21-C22	-7.16	1.26	1.35
19	B	1753	CLA	C3B-CAB	-7.07	1.32	1.47
19	B	1765	CLA	C3B-CAB	-7.02	1.32	1.47
19	A	1815	CLA	C3B-CAB	-7.01	1.32	1.47
19	B	1754	CLA	C3B-CAB	-6.96	1.33	1.47
19	B	1762	CLA	C3B-CAB	-6.96	1.33	1.47
19	B	1743	CLA	C3B-CAB	-6.91	1.33	1.47
19	J	1043	CLA	C3B-CAB	-6.90	1.33	1.47
19	B	1755	CLA	C3B-CAB	-6.86	1.33	1.47
19	A	1795	CLA	C3B-CAB	-6.85	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1752	CLA	C3B-CAB	-6.85	1.33	1.47
19	1	1190	CLA	C3B-CAB	-6.85	1.33	1.47
19	1	1197	CLA	C3B-CAB	-6.85	1.33	1.47
19	A	1764	CLA	C3B-CAB	-6.85	1.33	1.47
19	A	1781	CLA	C3B-CAB	-6.84	1.33	1.47
19	4	4014	CLA	C3B-CAB	-6.83	1.33	1.47
19	B	1735	CLA	C3B-CAB	-6.82	1.33	1.47
19	B	1739	CLA	C3B-CAB	-6.81	1.33	1.47
19	H	1079	CLA	C3B-CAB	-6.80	1.33	1.47
19	A	1784	CLA	C3B-CAB	-6.73	1.33	1.47
19	A	1783	CLA	C3B-CAB	-6.73	1.33	1.47
19	1	1189	CLA	C3B-CAB	-6.72	1.33	1.47
19	B	1766	CLA	C3B-CAB	-6.71	1.33	1.47
19	A	1816	CLA	C3B-CAB	-6.70	1.33	1.47
19	B	1756	CLA	C3B-CAB	-6.69	1.33	1.47
19	4	4007	CLA	C3B-CAB	-6.69	1.33	1.47
19	B	1767	CLA	C3B-CAB	-6.69	1.33	1.47
19	F	1155	CLA	CAB-C3B	-6.67	1.38	1.51
19	B	1758	CLA	C3B-CAB	-6.66	1.33	1.47
19	3	1221	CLA	C3B-CAB	-6.66	1.33	1.47
19	A	1792	CLA	C3B-CAB	-6.65	1.33	1.47
19	3	1218	CLA	C3B-CAB	-6.65	1.33	1.47
19	B	1764	CLA	C3B-CAB	-6.65	1.33	1.47
19	B	1744	CLA	C3B-CAB	-6.64	1.33	1.47
19	4	1201	CLA	C3B-CAB	-6.61	1.33	1.47
19	B	1768	CLA	C3B-CAB	-6.61	1.33	1.47
19	2	2006	CLA	C3B-CAB	-6.59	1.33	1.47
19	A	1760	CLA	C3B-CAB	-6.59	1.33	1.47
19	B	1737	CLA	C3B-CAB	-6.58	1.33	1.47
19	2	1213	CLA	C3B-CAB	-6.57	1.33	1.47
23	B	1775	BCR	C21-C22	-6.55	1.27	1.35
19	A	1814	CLA	C3B-CAB	-6.55	1.33	1.47
19	2	1212	CLA	C3B-CAB	-6.55	1.33	1.47
19	A	1817	CLA	C3B-CAB	-6.54	1.33	1.47
19	2	1223	CLA	C3B-CAB	-6.51	1.34	1.47
19	B	1761	CLA	C3B-CAB	-6.51	1.34	1.47
19	4	1206	CLA	C3B-CAB	-6.50	1.34	1.47
19	4	1198	CLA	C3B-CAB	-6.50	1.34	1.47
19	A	1794	CLA	C3B-CAB	-6.50	1.34	1.47
19	B	1748	CLA	C3B-CAB	-6.50	1.34	1.47
19	4	1196	CLA	C3B-CAB	-6.48	1.34	1.47
19	4	1211	CLA	C3B-CAB	-6.47	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	1217	CLA	C3B-CAB	-6.45	1.34	1.47
19	L	1167	CLA	C3B-CAB	-6.44	1.34	1.47
19	A	1767	CLA	C3B-CAB	-6.43	1.34	1.47
19	B	1757	CLA	C3B-CAB	-6.40	1.34	1.47
19	B	1771	CLA	C3B-CAB	-6.40	1.34	1.47
19	1	1308	CLA	C3B-CAB	-6.39	1.34	1.47
19	4	1200	CLA	C3B-CAB	-6.39	1.34	1.47
19	G	1099	CLA	C3B-CAB	-6.39	1.34	1.47
19	I	1031	CLA	C3B-CAB	-6.39	1.34	1.47
19	2	1217	CLA	C3B-CAB	-6.39	1.34	1.47
19	B	1769	CLA	C3B-CAB	-6.38	1.34	1.47
19	B	1763	CLA	C3B-CAB	-6.38	1.34	1.47
19	A	1800	CLA	C3B-CAB	-6.37	1.34	1.47
19	A	1765	CLA	C3B-CAB	-6.37	1.34	1.47
23	B	1776	BCR	C21-C22	-6.37	1.27	1.35
19	1	1148	CLA	C3B-CAB	-6.36	1.34	1.47
19	1	1199	CLA	C3B-CAB	-6.36	1.34	1.47
19	A	1763	CLA	C3B-CAB	-6.35	1.34	1.47
19	A	1780	CLA	C3B-CAB	-6.35	1.34	1.47
19	A	1773	CLA	C3B-CAB	-6.35	1.34	1.47
19	A	1801	CLA	C3B-CAB	-6.34	1.34	1.47
19	L	1168	CLA	C3B-CAB	-6.34	1.34	1.47
19	3	1222	CLA	C3B-CAB	-6.33	1.34	1.47
19	1	1146	CLA	C3B-CAB	-6.31	1.34	1.47
19	A	1787	CLA	C3B-CAB	-6.31	1.34	1.47
19	1	1142	CLA	C3B-CAB	-6.30	1.34	1.47
19	B	1760	CLA	C3B-CAB	-6.30	1.34	1.47
19	B	1784	CLA	C3B-CAB	-6.29	1.34	1.47
19	A	1778	CLA	C3B-CAB	-6.29	1.34	1.47
19	B	1749	CLA	C3B-CAB	-6.28	1.34	1.47
19	A	1796	CLA	C3B-CAB	-6.27	1.34	1.47
19	A	1813	CLA	C3B-CAB	-6.27	1.34	1.47
19	F	1156	CLA	C3B-CAB	-6.26	1.34	1.47
19	A	1788	CLA	C3B-CAB	-6.25	1.34	1.47
19	B	1750	CLA	C3B-CAB	-6.24	1.34	1.47
19	A	1798	CLA	C3B-CAB	-6.23	1.34	1.47
19	4	1199	CLA	C3B-CAB	-6.23	1.34	1.47
19	1	1193	CLA	C3B-CAB	-6.22	1.34	1.47
19	A	1772	CLA	C3B-CAB	-6.21	1.34	1.47
19	1	1143	CLA	C3B-CAB	-6.21	1.34	1.47
19	1	1192	CLA	C3B-CAB	-6.19	1.34	1.47
19	A	1786	CLA	C3B-CAB	-6.18	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1736	CLA	C3B-CAB	-6.18	1.34	1.47
19	F	1157	CLA	C3B-CAB	-6.17	1.34	1.47
19	2	1215	CLA	C3B-CAB	-6.16	1.34	1.47
19	1	1187	CLA	C3B-CAB	-6.13	1.34	1.47
19	1	1145	CLA	C3B-CAB	-6.09	1.34	1.47
19	R	1055	CLA	C3B-CAB	-6.09	1.34	1.47
19	H	1080	CLA	C3B-CAB	-6.08	1.34	1.47
19	A	1779	CLA	C3B-CAB	-6.08	1.34	1.47
19	B	1747	CLA	C3B-CAB	-6.07	1.34	1.47
19	A	1776	CLA	C3B-CAB	-6.05	1.35	1.47
19	A	1790	CLA	C3B-CAB	-6.04	1.35	1.47
19	1	1505	CLA	C3B-CAB	-6.03	1.35	1.47
19	4	1205	CLA	C3B-CAB	-6.03	1.35	1.47
19	A	1766	CLA	C3B-CAB	-6.01	1.35	1.47
19	A	1769	CLA	C3B-CAB	-6.00	1.35	1.47
19	1	1188	CLA	C3B-CAB	-5.99	1.35	1.47
19	A	1771	CLA	C3B-CAB	-5.97	1.35	1.47
19	B	1745	CLA	C3B-CAB	-5.95	1.35	1.47
19	A	1791	CLA	C3B-CAB	-5.94	1.35	1.47
19	A	1761	CLA	C3B-CAB	-5.94	1.35	1.47
19	B	1746	CLA	C3B-CAB	-5.92	1.35	1.47
19	A	1782	CLA	C3B-CAB	-5.90	1.35	1.47
19	B	1759	CLA	C3B-CAB	-5.90	1.35	1.47
19	2	1222	CLA	C3B-CAB	-5.90	1.35	1.47
19	H	1081	CLA	C3B-CAB	-5.87	1.35	1.47
19	R	1054	CLA	C3B-CAB	-5.86	1.35	1.47
19	A	1777	CLA	C3B-CAB	-5.86	1.35	1.47
19	A	1785	CLA	C3B-CAB	-5.82	1.35	1.47
19	3	3008	CLA	C3B-CAB	-5.82	1.35	1.47
19	1	1014	CLA	C3B-CAB	-5.79	1.35	1.47
19	B	1770	CLA	C3B-CAB	-5.73	1.35	1.47
19	A	1762	CLA	C3B-CAB	-5.73	1.35	1.47
23	A	1807	BCR	C20-C21	-5.69	1.26	1.43
19	B	1751	CLA	C3B-CAB	-5.67	1.35	1.47
19	A	1768	CLA	C3B-CAB	-5.48	1.36	1.47
19	3	3011	CLA	C3B-CAB	-5.39	1.36	1.47
19	B	1742	CLA	C3B-CAB	-5.31	1.36	1.47
19	B	1769	CLA	C4C-C3C	-5.20	1.35	1.45
19	B	1753	CLA	C4C-C3C	-4.97	1.36	1.45
19	3	1221	CLA	C4C-C3C	-4.95	1.36	1.45
19	B	1761	CLA	C4C-C3C	-4.87	1.36	1.45
19	2	2006	CLA	C4C-C3C	-4.85	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1201	CLA	C4C-C3C	-4.80	1.36	1.45
19	A	1789	CLA	C4C-C3C	-4.78	1.36	1.45
19	F	1157	CLA	C3A-C2A	-4.72	1.40	1.54
19	A	1789	CLA	C3B-CAB	-4.70	1.37	1.47
19	1	1199	CLA	C3A-C2A	-4.69	1.40	1.54
19	A	1774	CLA	C4C-C3C	-4.68	1.36	1.45
19	1	1014	CLA	C4C-C3C	-4.66	1.36	1.45
23	A	1808	BCR	C20-C19	-4.55	1.22	1.34
19	2	1212	CLA	C4C-C3C	-4.52	1.36	1.45
19	A	1789	CLA	C3B-C2B	-4.45	1.34	1.40
19	3	1217	CLA	C1C-C2C	-4.43	1.35	1.44
19	1	1197	CLA	C4C-C3C	-4.42	1.37	1.45
23	A	1808	BCR	C17-C18	-4.39	1.30	1.35
19	4	1200	CLA	C4C-C3C	-4.34	1.37	1.45
19	4	1205	CLA	C4C-C3C	-4.34	1.37	1.45
19	3	3011	CLA	C1C-C2C	-4.33	1.35	1.44
19	2	1213	CLA	C4C-C3C	-4.30	1.37	1.45
19	B	1748	CLA	C4C-C3C	-4.23	1.37	1.45
19	1	1189	CLA	C4C-C3C	-4.18	1.37	1.45
19	B	1737	CLA	C4C-C3C	-4.08	1.37	1.45
19	H	1079	CLA	C4C-C3C	-4.08	1.37	1.45
19	B	1741	CLA	C4C-C3C	-4.02	1.37	1.45
19	A	1789	CLA	C1C-C2C	-3.98	1.36	1.44
19	A	1774	CLA	C3B-C2B	-3.98	1.35	1.40
19	A	1772	CLA	C4C-C3C	-3.97	1.37	1.45
19	F	1157	CLA	C4C-C3C	-3.93	1.37	1.45
19	4	1206	CLA	C4C-C3C	-3.91	1.38	1.45
19	A	1759	CLA	C4C-C3C	-3.90	1.38	1.45
19	B	1761	CLA	C1C-C2C	-3.86	1.36	1.44
19	4	1201	CLA	C1C-C2C	-3.82	1.36	1.44
19	3	3011	CLA	C4C-C3C	-3.79	1.38	1.45
19	G	1099	CLA	C4C-C3C	-3.78	1.38	1.45
19	4	1198	CLA	C1C-C2C	-3.78	1.37	1.44
19	4	1211	CLA	C4C-C3C	-3.77	1.38	1.45
19	1	1146	CLA	C1C-C2C	-3.72	1.37	1.44
19	A	1765	CLA	C1C-C2C	-3.72	1.37	1.44
19	A	1813	CLA	C4C-C3C	-3.69	1.38	1.45
23	A	1804	BCR	C20-C19	-3.69	1.24	1.34
19	1	1199	CLA	C1C-C2C	-3.69	1.37	1.44
19	A	1795	CLA	C4C-C3C	-3.68	1.38	1.45
19	B	1743	CLA	C4C-C3C	-3.68	1.38	1.45
19	H	1079	CLA	C1C-C2C	-3.68	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1190	CLA	C4C-C3C	-3.67	1.38	1.45
19	A	1797	CLA	C1C-C2C	-3.67	1.37	1.44
19	J	1043	CLA	C1C-C2C	-3.66	1.37	1.44
23	I	1032	BCR	C30-C25	-3.64	1.48	1.53
19	A	1759	CLA	C3B-C2B	-3.64	1.35	1.40
19	1	1190	CLA	C1C-C2C	-3.64	1.37	1.44
19	1	1197	CLA	C3D-CAD	-3.63	1.35	1.45
19	1	1193	CLA	C2A-C1A	-3.62	1.44	1.52
19	B	1748	CLA	C1C-C2C	-3.61	1.37	1.44
19	1	1199	CLA	C4C-C3C	-3.59	1.38	1.45
23	B	1778	BCR	C20-C19	-3.57	1.25	1.34
23	L	1169	BCR	C20-C19	-3.57	1.25	1.34
19	4	1198	CLA	C4C-C3C	-3.55	1.38	1.45
19	A	1796	CLA	C4C-C3C	-3.55	1.38	1.45
19	4	4007	CLA	C4C-C3C	-3.55	1.38	1.45
19	4	1205	CLA	C1C-C2C	-3.53	1.37	1.44
19	A	1797	CLA	C4C-C3C	-3.53	1.38	1.45
19	F	1157	CLA	C2A-C1A	-3.52	1.45	1.52
19	2	1221	CLA	C4C-C3C	-3.52	1.38	1.45
19	2	1217	CLA	C1C-C2C	-3.51	1.37	1.44
19	A	1801	CLA	C4C-C3C	-3.50	1.38	1.45
19	1	1187	CLA	C1C-C2C	-3.49	1.37	1.44
19	1	1143	CLA	C4C-C3C	-3.49	1.38	1.45
19	B	1748	CLA	C3B-C2B	-3.47	1.35	1.40
23	B	1779	BCR	C20-C19	-3.46	1.25	1.34
19	A	1759	CLA	C1C-C2C	-3.46	1.37	1.44
19	B	1764	CLA	C4C-C3C	-3.45	1.38	1.45
19	A	1774	CLA	C1C-C2C	-3.45	1.37	1.44
23	A	1809	BCR	C20-C19	-3.44	1.25	1.34
19	B	1769	CLA	C1C-C2C	-3.44	1.37	1.44
19	2	1212	CLA	C1C-C2C	-3.44	1.37	1.44
19	B	1759	CLA	C4C-C3C	-3.44	1.38	1.45
19	B	1769	CLA	C3D-CAD	-3.43	1.36	1.45
19	2	1223	CLA	C4C-C3C	-3.42	1.38	1.45
23	A	1803	BCR	C20-C19	-3.40	1.25	1.34
19	3	1218	CLA	C1C-C2C	-3.40	1.37	1.44
19	2	1217	CLA	C4C-C3C	-3.40	1.38	1.45
23	A	1805	BCR	C20-C19	-3.39	1.25	1.34
19	B	1763	CLA	C1C-C2C	-3.37	1.37	1.44
19	B	1751	CLA	C4C-C3C	-3.37	1.38	1.45
19	4	1205	CLA	C3B-C2B	-3.36	1.35	1.40
19	B	1738	CLA	C1C-C2C	-3.35	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1780	BCR	C20-C19	-3.35	1.25	1.34
23	B	1777	BCR	C20-C19	-3.34	1.25	1.34
19	2	2006	CLA	C1C-C2C	-3.33	1.37	1.44
19	B	1766	CLA	C4C-C3C	-3.33	1.39	1.45
19	2	1221	CLA	C1C-C2C	-3.33	1.37	1.44
19	B	1756	CLA	C4C-C3C	-3.32	1.39	1.45
19	2	1213	CLA	C1C-C2C	-3.31	1.37	1.44
19	4	4007	CLA	C1C-C2C	-3.31	1.37	1.44
19	2	1213	CLA	C3B-C2B	-3.30	1.36	1.40
19	B	1739	CLA	C1C-C2C	-3.30	1.38	1.44
19	A	1782	CLA	C4C-C3C	-3.29	1.39	1.45
19	B	1758	CLA	C4C-C3C	-3.28	1.39	1.45
19	B	1741	CLA	C1C-C2C	-3.28	1.38	1.44
19	A	1817	CLA	C1C-C2C	-3.28	1.38	1.44
19	J	1043	CLA	C4C-C3C	-3.28	1.39	1.45
19	1	1146	CLA	C4C-C3C	-3.26	1.39	1.45
19	1	1148	CLA	C4C-C3C	-3.25	1.39	1.45
19	3	1222	CLA	C4C-C3C	-3.25	1.39	1.45
19	A	1795	CLA	C1C-C2C	-3.24	1.38	1.44
19	A	1767	CLA	C1C-C2C	-3.24	1.38	1.44
19	4	1199	CLA	C1C-C2C	-3.24	1.38	1.44
23	A	1806	BCR	C20-C19	-3.24	1.26	1.34
19	H	1081	CLA	C4C-C3C	-3.23	1.39	1.45
19	1	1143	CLA	C1C-C2C	-3.22	1.38	1.44
19	B	1762	CLA	C4C-C3C	-3.22	1.39	1.45
19	B	1766	CLA	C1C-C2C	-3.21	1.38	1.44
19	1	1197	CLA	C1C-C2C	-3.20	1.38	1.44
19	B	1737	CLA	C1C-C2C	-3.20	1.38	1.44
19	A	1769	CLA	C4C-C3C	-3.20	1.39	1.45
19	A	1788	CLA	C4C-C3C	-3.20	1.39	1.45
19	1	1142	CLA	C4C-C3C	-3.20	1.39	1.45
19	B	1749	CLA	C4C-C3C	-3.19	1.39	1.45
19	F	1157	CLA	CAA-C2A	-3.19	1.47	1.54
19	A	1791	CLA	C1C-C2C	-3.19	1.38	1.44
19	B	1768	CLA	C4C-C3C	-3.19	1.39	1.45
19	B	1763	CLA	C4C-C3C	-3.18	1.39	1.45
19	A	1815	CLA	C4C-C3C	-3.18	1.39	1.45
19	B	1765	CLA	C4C-C3C	-3.18	1.39	1.45
19	1	1187	CLA	C4C-C3C	-3.18	1.39	1.45
19	3	1218	CLA	C4C-C3C	-3.17	1.39	1.45
19	B	1755	CLA	C4C-C3C	-3.16	1.39	1.45
23	B	1774	BCR	C20-C19	-3.16	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1206	CLA	C1C-C2C	-3.16	1.38	1.44
19	A	1814	CLA	C4C-C3C	-3.16	1.39	1.45
19	A	1791	CLA	C4C-C3C	-3.15	1.39	1.45
19	F	1156	CLA	C4C-C3C	-3.15	1.39	1.45
19	4	1200	CLA	C1C-C2C	-3.15	1.38	1.44
19	1	1197	CLA	C3B-C2B	-3.15	1.36	1.40
19	B	1741	CLA	C3D-CAD	-3.14	1.36	1.45
19	F	1157	CLA	C1C-C2C	-3.13	1.38	1.44
19	B	1784	CLA	C4C-C3C	-3.13	1.39	1.45
19	A	1761	CLA	C1C-C2C	-3.12	1.38	1.44
19	A	1817	CLA	C4C-C3C	-3.11	1.39	1.45
23	I	1032	BCR	C20-C19	-3.11	1.26	1.34
19	B	1757	CLA	C4C-C3C	-3.11	1.39	1.45
19	I	1031	CLA	C4C-C3C	-3.10	1.39	1.45
19	4	1196	CLA	C4C-C3C	-3.10	1.39	1.45
19	A	1785	CLA	C4C-C3C	-3.09	1.39	1.45
19	A	1815	CLA	C1C-C2C	-3.09	1.38	1.44
19	A	1769	CLA	C1C-C2C	-3.09	1.38	1.44
23	B	1775	BCR	C20-C19	-3.07	1.26	1.34
19	1	1193	CLA	C4C-C3C	-3.06	1.39	1.45
19	A	1788	CLA	C1C-C2C	-3.05	1.38	1.44
19	B	1759	CLA	C1C-C2C	-3.04	1.38	1.44
19	B	1736	CLA	C4C-C3C	-3.04	1.39	1.45
19	A	1793	CLA	C4C-C3C	-3.04	1.39	1.45
19	1	1308	CLA	C4C-C3C	-3.02	1.39	1.45
19	4	1206	CLA	C3D-CAD	-3.02	1.37	1.45
19	L	1168	CLA	C4C-C3C	-3.02	1.39	1.45
19	1	1149	CLA	C1C-C2C	-3.01	1.38	1.44
19	A	1797	CLA	C3A-C2A	-3.00	1.45	1.54
19	B	1738	CLA	C4C-C3C	-3.00	1.39	1.45
19	1	1189	CLA	C1C-C2C	-3.00	1.38	1.44
19	A	1781	CLA	C4C-C3C	-3.00	1.39	1.45
19	A	1768	CLA	C4C-C3C	-2.99	1.39	1.45
19	F	1157	CLA	C3B-C2B	-2.99	1.36	1.40
19	A	1783	CLA	C4C-C3C	-2.99	1.39	1.45
19	B	1770	CLA	C4C-C3C	-2.99	1.39	1.45
19	4	4014	CLA	C1C-C2C	-2.99	1.38	1.44
19	B	1764	CLA	C1C-C2C	-2.98	1.38	1.44
19	3	3011	CLA	C3D-CAD	-2.98	1.37	1.45
19	B	1750	CLA	C4C-C3C	-2.97	1.39	1.45
19	A	1767	CLA	C4C-C3C	-2.96	1.39	1.45
19	A	1772	CLA	C1C-C2C	-2.94	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1762	CLA	C4C-C3C	-2.94	1.39	1.45
19	B	1754	CLA	C4C-C3C	-2.93	1.39	1.45
19	1	1014	CLA	C3D-CAD	-2.92	1.37	1.45
19	B	1739	CLA	C4C-C3C	-2.92	1.39	1.45
19	A	1794	CLA	C4C-C3C	-2.92	1.39	1.45
19	A	1763	CLA	C4C-C3C	-2.91	1.39	1.45
19	A	1816	CLA	C4C-C3C	-2.91	1.39	1.45
19	A	1764	CLA	C4C-C3C	-2.91	1.39	1.45
19	1	1308	CLA	C1C-C2C	-2.91	1.38	1.44
19	4	1197	CLA	C4C-C3C	-2.91	1.38	1.44
19	A	1778	CLA	C1C-C2C	-2.91	1.38	1.44
19	2	2006	CLA	C3D-CAD	-2.90	1.37	1.45
19	4	1211	CLA	C1C-C2C	-2.90	1.38	1.44
19	A	1760	CLA	C3B-C2B	-2.90	1.36	1.40
19	A	1787	CLA	C4C-C3C	-2.90	1.39	1.45
19	B	1742	CLA	C1C-C2C	-2.89	1.38	1.44
19	B	1758	CLA	C3B-C2B	-2.89	1.36	1.40
19	A	1773	CLA	C4C-C3C	-2.88	1.39	1.45
19	A	1779	CLA	C4C-C3C	-2.87	1.39	1.45
23	A	1808	BCR	C10-C9	-2.87	1.32	1.35
19	B	1738	CLA	C3B-C2B	-2.86	1.36	1.40
19	2	1222	CLA	C4C-C3C	-2.86	1.39	1.45
19	1	1189	CLA	C2A-C1A	-2.86	1.46	1.52
19	B	1753	CLA	C1C-C2C	-2.86	1.38	1.44
19	A	1772	CLA	C3B-C2B	-2.85	1.36	1.40
19	4	1198	CLA	C3B-C2B	-2.84	1.36	1.40
23	B	1779	BCR	C30-C25	-2.84	1.49	1.53
19	2	1218	CLA	C1C-NC	-2.83	1.32	1.37
19	B	1735	CLA	C4C-C3C	-2.83	1.39	1.45
19	A	1759	CLA	C3D-CAD	-2.83	1.37	1.45
19	B	1746	CLA	C1C-C2C	-2.82	1.38	1.44
19	H	1079	CLA	C3B-C2B	-2.82	1.36	1.40
19	B	1752	CLA	C1C-C2C	-2.82	1.38	1.44
19	A	1776	CLA	C1C-C2C	-2.81	1.38	1.44
19	B	1768	CLA	C1C-C2C	-2.81	1.38	1.44
19	A	1793	CLA	C1C-C2C	-2.80	1.39	1.44
19	F	1155	CLA	C1C-C2C	-2.80	1.39	1.44
19	A	1766	CLA	C4C-C3C	-2.80	1.40	1.45
19	B	1769	CLA	C3B-C2B	-2.80	1.36	1.40
19	A	1767	CLA	C3B-C2B	-2.79	1.36	1.40
19	A	1800	CLA	C4C-C3C	-2.79	1.40	1.45
19	B	1746	CLA	C4C-C3C	-2.79	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1777	CLA	C4C-C3C	-2.78	1.40	1.45
19	A	1792	CLA	C1C-C2C	-2.78	1.39	1.44
19	A	1775	CLA	C4C-C3C	-2.78	1.39	1.44
19	1	1192	CLA	C4C-C3C	-2.78	1.40	1.45
19	B	1748	CLA	C3D-CAD	-2.77	1.37	1.45
19	A	1772	CLA	C3D-CAD	-2.76	1.38	1.45
19	R	1054	CLA	C4C-C3C	-2.76	1.40	1.45
19	A	1786	CLA	C1C-C2C	-2.76	1.39	1.44
19	B	1784	CLA	C1C-C2C	-2.76	1.39	1.44
19	A	1789	CLA	C3D-CAD	-2.76	1.38	1.45
19	3	3011	CLA	C3B-C2B	-2.76	1.36	1.40
19	4	4007	CLA	C3B-C2B	-2.75	1.36	1.40
19	3	1217	CLA	C4C-C3C	-2.75	1.40	1.45
19	1	1145	CLA	C4C-C3C	-2.75	1.40	1.45
19	3	1222	CLA	C1C-C2C	-2.75	1.39	1.44
19	4	1206	CLA	C1C-NC	-2.74	1.33	1.37
19	1	1191	CLA	C1C-C2C	-2.74	1.39	1.44
19	A	1792	CLA	C4C-C3C	-2.74	1.40	1.45
19	2	1213	CLA	C3D-CAD	-2.74	1.38	1.45
19	A	1775	CLA	C1C-C2C	-2.74	1.39	1.44
19	A	1760	CLA	C4C-C3C	-2.74	1.40	1.45
19	A	1776	CLA	C4C-C3C	-2.73	1.40	1.45
19	B	1737	CLA	C3B-C2B	-2.73	1.36	1.40
19	A	1793	CLA	C3B-C2B	-2.73	1.36	1.40
19	A	1773	CLA	C1C-C2C	-2.72	1.39	1.44
19	B	1747	CLA	C1C-C2C	-2.72	1.39	1.44
19	A	1762	CLA	C1C-C2C	-2.72	1.39	1.44
19	A	1781	CLA	C1C-C2C	-2.72	1.39	1.44
23	B	1776	BCR	C20-C19	-2.72	1.27	1.34
19	A	1785	CLA	C3B-C2B	-2.71	1.36	1.40
19	A	1782	CLA	C1C-C2C	-2.71	1.39	1.44
19	3	1218	CLA	C3D-CAD	-2.71	1.38	1.45
19	A	1790	CLA	C1C-C2C	-2.71	1.39	1.44
19	A	1783	CLA	C1C-C2C	-2.70	1.39	1.44
19	B	1761	CLA	C3D-CAD	-2.70	1.38	1.45
19	A	1784	CLA	C3B-C2B	-2.70	1.36	1.40
19	4	1196	CLA	C1C-C2C	-2.70	1.39	1.44
19	R	1055	CLA	C4C-C3C	-2.70	1.40	1.45
19	4	4014	CLA	C3B-C2B	-2.69	1.36	1.40
19	F	1156	CLA	C1C-C2C	-2.69	1.39	1.44
19	A	1779	CLA	C1C-C2C	-2.69	1.39	1.44
19	1	1188	CLA	C4C-C3C	-2.68	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1768	CLA	C1C-C2C	-2.68	1.39	1.44
19	B	1735	CLA	C3B-C2B	-2.68	1.36	1.40
19	1	1188	CLA	C1C-C2C	-2.68	1.39	1.44
19	2	1223	CLA	C1C-C2C	-2.68	1.39	1.44
19	A	1794	CLA	C1C-C2C	-2.67	1.39	1.44
23	A	1807	BCR	C20-C19	-2.67	1.27	1.34
19	A	1764	CLA	C3B-C2B	-2.67	1.36	1.40
19	1	1505	CLA	C4C-C3C	-2.67	1.40	1.45
19	2	1215	CLA	C4C-C3C	-2.67	1.40	1.45
19	B	1747	CLA	C4C-C3C	-2.66	1.40	1.45
19	1	1187	CLA	C3D-CAD	-2.66	1.38	1.45
19	G	1099	CLA	C3B-C2B	-2.66	1.36	1.40
19	A	1797	CLA	C2A-C1A	-2.66	1.46	1.52
19	B	1754	CLA	C1C-C2C	-2.65	1.39	1.44
19	1	1014	CLA	C3B-C2B	-2.65	1.36	1.40
19	B	1784	CLA	C3B-C2B	-2.65	1.36	1.40
19	H	1079	CLA	C3D-CAD	-2.65	1.38	1.45
19	A	1771	CLA	C4C-C3C	-2.65	1.40	1.45
19	2	1218	CLA	C3C-C4C	-2.64	1.36	1.43
19	3	1221	CLA	C1C-C2C	-2.63	1.39	1.44
19	B	1752	CLA	C4C-C3C	-2.63	1.40	1.45
19	G	1099	CLA	C3D-CAD	-2.62	1.38	1.45
19	B	1742	CLA	C4C-C3C	-2.61	1.40	1.45
19	B	1757	CLA	C1C-C2C	-2.61	1.39	1.44
19	B	1760	CLA	C1C-C2C	-2.61	1.39	1.44
19	B	1753	CLA	C3B-C2B	-2.61	1.36	1.40
19	B	1770	CLA	C1C-C2C	-2.61	1.39	1.44
19	A	1784	CLA	C1C-C2C	-2.61	1.39	1.44
19	L	1167	CLA	C1C-C2C	-2.61	1.39	1.44
19	B	1736	CLA	C3B-C2B	-2.61	1.36	1.40
19	4	1200	CLA	C3B-C2B	-2.61	1.36	1.40
19	A	1766	CLA	C1C-C2C	-2.60	1.39	1.44
19	1	1142	CLA	C1C-C2C	-2.60	1.39	1.44
19	4	1211	CLA	C3B-C2B	-2.60	1.36	1.40
19	3	1218	CLA	C3B-C2B	-2.60	1.36	1.40
19	3	1213	CLA	C4C-C3C	-2.60	1.39	1.44
19	4	4007	CLA	C3D-CAD	-2.60	1.38	1.45
19	1	1145	CLA	C1C-C2C	-2.59	1.39	1.44
19	B	1744	CLA	C1C-C2C	-2.59	1.39	1.44
19	B	1761	CLA	C3B-C2B	-2.59	1.36	1.40
19	B	1755	CLA	C1C-C2C	-2.59	1.39	1.44
19	A	1814	CLA	C1C-C2C	-2.59	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1767	CLA	C1C-C2C	-2.58	1.39	1.44
19	A	1798	CLA	C4C-C3C	-2.58	1.40	1.45
19	B	1745	CLA	C4C-C3C	-2.57	1.40	1.45
19	A	1778	CLA	C4C-C3C	-2.57	1.40	1.45
19	1	1196	CLA	C4C-C3C	-2.56	1.39	1.44
19	2	1212	CLA	C3B-C2B	-2.55	1.37	1.40
19	B	1767	CLA	C4C-C3C	-2.55	1.40	1.45
19	A	1785	CLA	C1C-C2C	-2.55	1.39	1.44
19	1	1148	CLA	C1C-C2C	-2.54	1.39	1.44
19	1	1193	CLA	C3D-CAD	-2.54	1.38	1.45
19	B	1737	CLA	C3D-CAD	-2.54	1.38	1.45
19	A	1771	CLA	C1C-C2C	-2.54	1.39	1.44
19	F	1155	CLA	C4C-C3C	-2.54	1.39	1.44
19	3	3008	CLA	C4C-C3C	-2.53	1.40	1.45
19	G	1099	CLA	C1C-C2C	-2.52	1.39	1.44
19	B	1744	CLA	C3B-C2B	-2.52	1.37	1.40
19	B	1765	CLA	C1C-C2C	-2.52	1.39	1.44
19	1	1191	CLA	C4C-C3C	-2.51	1.39	1.44
19	2	1221	CLA	C3D-CAD	-2.51	1.38	1.45
19	A	1797	CLA	C3B-C2B	-2.51	1.37	1.40
19	B	1748	CLA	C1C-NC	-2.51	1.33	1.37
19	2	1221	CLA	C3B-C2B	-2.51	1.37	1.40
19	A	1813	CLA	C3B-C2B	-2.51	1.37	1.40
19	L	1167	CLA	C4C-C3C	-2.50	1.40	1.45
19	4	1211	CLA	C3D-CAD	-2.50	1.38	1.45
19	A	1780	CLA	C1C-C2C	-2.49	1.39	1.44
19	A	1774	CLA	C3D-CAD	-2.49	1.38	1.45
19	B	1759	CLA	C3D-CAD	-2.49	1.38	1.45
19	4	1197	CLA	C1C-C2C	-2.49	1.39	1.44
19	2	1218	CLA	C2C-C1C	-2.48	1.37	1.43
19	B	1751	CLA	C1C-C2C	-2.48	1.39	1.44
19	A	1761	CLA	C4C-C3C	-2.48	1.40	1.45
19	B	1760	CLA	C4C-C3C	-2.48	1.40	1.45
19	B	1744	CLA	C4C-C3C	-2.48	1.40	1.45
19	1	1197	CLA	CBD-CGD	-2.47	1.43	1.52
19	3	3011	CLA	C1C-NC	-2.47	1.33	1.37
19	B	1756	CLA	C1C-C2C	-2.46	1.39	1.44
19	A	1790	CLA	C4C-C3C	-2.46	1.40	1.45
19	B	1755	CLA	C3D-CAD	-2.46	1.38	1.45
19	A	1780	CLA	C3D-CAD	-2.45	1.38	1.45
19	2	1212	CLA	C1C-NC	-2.45	1.33	1.37
19	B	1759	CLA	C3B-C2B	-2.45	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	1054	CLA	C1C-C2C	-2.45	1.39	1.44
19	2	1222	CLA	C3D-CAD	-2.45	1.38	1.45
19	B	1771	CLA	C3B-C2B	-2.44	1.37	1.40
19	2	2006	CLA	C3B-C2B	-2.44	1.37	1.40
19	4	1209	CLA	C1C-C2C	-2.43	1.39	1.44
19	1	1192	CLA	C1C-C2C	-2.43	1.39	1.44
19	B	1771	CLA	C1C-C2C	-2.43	1.39	1.44
19	A	1784	CLA	C4C-C3C	-2.42	1.40	1.45
19	A	1761	CLA	C3B-C2B	-2.42	1.37	1.40
19	2	1222	CLA	C1C-C2C	-2.41	1.39	1.44
19	A	1787	CLA	C1C-C2C	-2.41	1.39	1.44
19	B	1763	CLA	C3D-CAD	-2.41	1.39	1.45
19	1	1014	CLA	C1C-C2C	-2.41	1.39	1.44
19	B	1762	CLA	C1C-C2C	-2.41	1.39	1.44
19	I	1031	CLA	C1C-C2C	-2.40	1.39	1.44
19	A	1816	CLA	C1C-C2C	-2.39	1.39	1.44
19	1	1193	CLA	C1C-C2C	-2.39	1.39	1.44
19	3	1221	CLA	C3D-CAD	-2.39	1.39	1.45
19	1	1149	CLA	C2A-C1A	-2.38	1.47	1.52
19	A	1777	CLA	C1C-C2C	-2.38	1.39	1.44
19	A	1800	CLA	C1C-C2C	-2.38	1.39	1.44
19	B	1750	CLA	C1C-C2C	-2.38	1.39	1.44
19	1	1190	CLA	C3D-CAD	-2.38	1.39	1.45
19	A	1780	CLA	C4C-C3C	-2.38	1.40	1.45
19	4	4014	CLA	C3D-CAD	-2.37	1.39	1.45
19	4	1196	CLA	C3D-CAD	-2.36	1.39	1.45
19	B	1743	CLA	C1C-C2C	-2.36	1.39	1.44
19	B	1769	CLA	C3D-C2D	-2.36	1.34	1.40
19	1	1189	CLA	C3D-CAD	-2.36	1.39	1.45
19	A	1765	CLA	C4C-C3C	-2.36	1.40	1.45
19	A	1796	CLA	C1C-C2C	-2.36	1.39	1.44
19	A	1813	CLA	C1C-C2C	-2.35	1.39	1.44
19	A	1770	CLA	C2C-C1C	-2.35	1.37	1.43
19	1	1193	CLA	C3A-C2A	-2.35	1.47	1.54
19	B	1758	CLA	C1C-C2C	-2.35	1.39	1.44
19	1	1505	CLA	C1C-C2C	-2.35	1.39	1.44
19	R	1055	CLA	C1C-C2C	-2.35	1.39	1.44
19	4	4014	CLA	C4C-C3C	-2.34	1.40	1.45
19	H	1080	CLA	C1C-C2C	-2.34	1.39	1.44
19	1	1196	CLA	C1C-C2C	-2.34	1.39	1.44
19	2	1213	CLA	C1C-NC	-2.34	1.33	1.37
19	A	1764	CLA	C1C-C2C	-2.33	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1760	CLA	C1C-C2C	-2.33	1.39	1.44
19	4	1205	CLA	C3D-CAD	-2.33	1.39	1.45
19	A	1801	CLA	C1C-C2C	-2.32	1.39	1.44
19	A	1798	CLA	C1C-C2C	-2.32	1.39	1.44
19	B	1757	CLA	C3D-CAD	-2.32	1.39	1.45
19	R	1054	CLA	C3D-CAD	-2.31	1.39	1.45
19	H	1079	CLA	C1C-NC	-2.31	1.33	1.37
19	2	1219	CLA	C1C-C2C	-2.30	1.40	1.44
19	B	1767	CLA	C3D-CAD	-2.30	1.39	1.45
19	B	1758	CLA	C3D-CAD	-2.30	1.39	1.45
19	1	1199	CLA	C1C-NC	-2.30	1.33	1.37
19	B	1762	CLA	C3D-CAD	-2.30	1.39	1.45
19	B	1766	CLA	C3D-CAD	-2.30	1.39	1.45
19	B	1772	CLA	C1C-C2C	-2.30	1.40	1.44
19	1	1190	CLA	C2A-C1A	-2.30	1.47	1.52
19	A	1797	CLA	C3D-CAD	-2.29	1.39	1.45
19	B	1771	CLA	C4C-C3C	-2.28	1.40	1.45
19	I	1031	CLA	C3D-CAD	-2.28	1.39	1.45
19	1	1189	CLA	C3B-C2B	-2.28	1.37	1.40
19	B	1736	CLA	C1C-C2C	-2.28	1.40	1.44
19	2	1219	CLA	C4C-C3C	-2.27	1.40	1.44
19	4	1201	CLA	C3D-CAD	-2.27	1.39	1.45
19	2	1223	CLA	C3D-CAD	-2.26	1.39	1.45
19	A	1795	CLA	C3B-C2B	-2.26	1.37	1.40
19	B	1772	CLA	C4C-C3C	-2.25	1.40	1.44
19	1	1199	CLA	C3A-C4A	-2.25	1.44	1.51
19	2	1214	CLA	C3C-C4C	-2.25	1.37	1.43
19	A	1766	CLA	C3B-C2B	-2.25	1.37	1.40
19	A	1761	CLA	C3D-CAD	-2.25	1.39	1.45
19	B	1753	CLA	C3D-CAD	-2.24	1.39	1.45
19	B	1735	CLA	C1C-C2C	-2.24	1.40	1.44
19	B	1751	CLA	C3D-CAD	-2.24	1.39	1.45
19	B	1740	CLA	C2C-C1C	-2.24	1.37	1.43
19	B	1745	CLA	C1C-C2C	-2.24	1.40	1.44
19	2	1215	CLA	C1C-C2C	-2.24	1.40	1.44
19	A	1800	CLA	C3D-CAD	-2.24	1.39	1.45
23	B	1779	BCR	C1-C6	-2.23	1.50	1.53
19	A	1782	CLA	C3D-CAD	-2.23	1.39	1.45
19	A	1781	CLA	C3D-CAD	-2.23	1.39	1.45
23	A	1805	BCR	C30-C25	-2.23	1.50	1.53
19	3	3014	CLA	C2C-C1C	-2.23	1.37	1.43
19	B	1754	CLA	C3B-C2B	-2.23	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1814	CLA	C3B-C2B	-2.22	1.37	1.40
19	B	1739	CLA	C3B-C2B	-2.22	1.37	1.40
23	I	1032	BCR	C1-C6	-2.22	1.50	1.53
19	A	1774	CLA	C1C-NC	-2.22	1.34	1.37
19	B	1749	CLA	C3D-CAD	-2.22	1.39	1.45
19	4	1203	CLA	C3C-C4C	-2.22	1.37	1.43
19	1	1148	CLA	C3D-CAD	-2.21	1.39	1.45
19	B	1754	CLA	C3D-CAD	-2.21	1.39	1.45
19	B	1749	CLA	C1C-C2C	-2.21	1.40	1.44
19	4	1207	CLA	C3C-C4C	-2.20	1.37	1.43
19	4	1198	CLA	CBD-CHA	-2.20	1.41	1.52
19	A	1814	CLA	C3D-CAD	-2.20	1.39	1.45
19	3	1214	CLA	C2C-C1C	-2.20	1.37	1.43
19	A	1777	CLA	C3D-CAD	-2.19	1.39	1.45
19	1	1308	CLA	C3D-CAD	-2.19	1.39	1.45
19	1	1149	CLA	C3D-CAD	-2.19	1.39	1.45
19	4	1209	CLA	C4C-C3C	-2.18	1.40	1.44
23	B	1777	BCR	C30-C25	-2.18	1.50	1.53
19	F	1156	CLA	C3D-CAD	-2.18	1.39	1.45
19	1	1199	CLA	C3B-C2B	-2.18	1.37	1.40
19	H	1081	CLA	C1C-C2C	-2.18	1.40	1.44
19	1	1143	CLA	C3D-CAD	-2.17	1.39	1.45
19	A	1813	CLA	C3D-CAD	-2.17	1.39	1.45
19	A	1798	CLA	C3B-C2B	-2.17	1.37	1.40
19	A	1764	CLA	C3D-CAD	-2.17	1.39	1.45
19	B	1765	CLA	C3D-CAD	-2.17	1.39	1.45
19	L	1168	CLA	C1C-C2C	-2.17	1.40	1.44
19	A	1794	CLA	C3B-C2B	-2.17	1.37	1.40
19	A	1763	CLA	C1C-C2C	-2.17	1.40	1.44
19	1	1505	CLA	C3D-CAD	-2.17	1.39	1.45
19	1	1199	CLA	C2A-C1A	-2.16	1.47	1.52
19	F	1157	CLA	CBD-CHA	-2.16	1.41	1.52
19	B	1769	CLA	C1C-NC	-2.16	1.34	1.37
19	3	1220	CLA	C2C-C1C	-2.16	1.38	1.43
19	B	1750	CLA	C3D-CAD	-2.16	1.39	1.45
19	B	1771	CLA	C3D-CAD	-2.16	1.39	1.45
19	B	1762	CLA	C3B-C2B	-2.16	1.37	1.40
19	B	1764	CLA	C3D-CAD	-2.16	1.39	1.45
19	1	1146	CLA	C3D-CAD	-2.16	1.39	1.45
19	4	1197	CLA	C3D-CAD	-2.15	1.39	1.45
19	A	1773	CLA	C3D-CAD	-2.15	1.39	1.45
19	B	1738	CLA	C3D-CAD	-2.15	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1785	CLA	C3D-CAD	-2.15	1.39	1.45
19	B	1761	CLA	C1C-NC	-2.15	1.34	1.37
19	A	1786	CLA	C4C-C3C	-2.15	1.41	1.45
23	L	1169	BCR	C17-C18	-2.14	1.32	1.35
23	A	1808	BCR	C14-C13	-2.14	1.32	1.35
19	1	1188	CLA	C3D-CAD	-2.14	1.39	1.45
19	4	1200	CLA	C3D-CAD	-2.14	1.39	1.45
19	4	1203	CLA	C2C-C1C	-2.13	1.38	1.43
19	H	1080	CLA	C4C-C3C	-2.13	1.41	1.45
19	L	1167	CLA	C3D-CAD	-2.11	1.39	1.45
19	A	1791	CLA	C3D-CAD	-2.11	1.39	1.45
19	A	1816	CLA	C3D-CAD	-2.10	1.39	1.45
19	F	1157	CLA	C3D-CAD	-2.10	1.39	1.45
19	A	1770	CLA	C3C-C4C	-2.10	1.38	1.43
19	A	1788	CLA	C3D-CAD	-2.10	1.39	1.45
19	A	1778	CLA	C3B-C2B	-2.09	1.37	1.40
19	2	1219	CLA	C3D-CAD	-2.09	1.39	1.45
19	4	1206	CLA	CAA-C2A	-2.09	1.49	1.54
19	B	1770	CLA	C3D-CAD	-2.08	1.39	1.45
19	3	3015	CLA	C3C-C4C	-2.08	1.38	1.43
19	4	1201	CLA	C3A-C2A	-2.08	1.48	1.54
19	A	1786	CLA	C3B-C2B	-2.08	1.37	1.40
19	1	1197	CLA	C3D-C2D	-2.07	1.35	1.40
19	3	1222	CLA	C3D-CAD	-2.07	1.39	1.45
19	A	1815	CLA	C3B-C2B	-2.07	1.37	1.40
19	2	1214	CLA	C1C-NC	-2.07	1.34	1.37
19	B	1756	CLA	C3D-CAD	-2.07	1.39	1.45
19	4	1199	CLA	C4C-C3C	-2.06	1.41	1.45
19	B	1768	CLA	C3D-CAD	-2.06	1.39	1.45
19	B	1747	CLA	C3D-CAD	-2.06	1.40	1.45
19	4	1202	CLA	C2C-C1C	-2.05	1.38	1.43
19	A	1770	CLA	C4C-NC	-2.05	1.34	1.37
19	2	1214	CLA	C2C-C1C	-2.05	1.38	1.43
19	3	1217	CLA	C3B-C2B	-2.05	1.37	1.40
19	1	1192	CLA	C3D-CAD	-2.04	1.40	1.45
19	L	1168	CLA	C3D-CAD	-2.04	1.40	1.45
19	B	1736	CLA	C3D-CAD	-2.03	1.40	1.45
19	1	1149	CLA	C4C-C3C	-2.03	1.41	1.45
19	A	1767	CLA	C3D-CAD	-2.03	1.40	1.45
19	1	1196	CLA	C3D-CAD	-2.03	1.40	1.45
19	A	1786	CLA	C3D-CAD	-2.02	1.40	1.45
19	A	1779	CLA	C3D-CAD	-2.02	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	1043	CLA	C3D-CAD	-2.02	1.40	1.45
19	A	1783	CLA	C3D-CAD	-2.02	1.40	1.45
19	L	1168	CLA	CBD-CGD	-2.01	1.45	1.52
19	B	1763	CLA	C3B-C2B	-2.01	1.37	1.40
20	A	7036	LMU	O1B-C4'	-2.01	1.38	1.43
19	2	2010	CLA	C3C-C4C	-2.00	1.38	1.43
19	B	1753	CLA	C1C-NC	-2.00	1.34	1.37
20	A	7015	LMU	O1'-C1'	2.00	1.43	1.40
20	L	1170	LMU	O1'-C1'	2.01	1.43	1.40
19	1	1190	CLA	C1B-CHB	2.01	1.45	1.39
20	A	7008	LMU	O4'-C4B	2.01	1.47	1.43
19	B	1761	CLA	C2-C3	2.02	1.38	1.32
19	4	1210	CLA	C1B-CHB	2.03	1.47	1.43
19	4	1202	CLA	CHA-C1A	2.05	1.47	1.41
19	A	1772	CLA	C1B-CHB	2.05	1.45	1.39
19	G	1099	CLA	C1B-CHB	2.05	1.45	1.39
19	B	1741	CLA	C1B-CHB	2.05	1.45	1.39
20	A	1811	LMU	O1'-C1'	2.07	1.43	1.40
20	A	7043	LMU	O1'-C1'	2.08	1.43	1.40
20	A	7009	LMU	O1'-C1'	2.08	1.43	1.40
19	A	1770	CLA	CHA-C1A	2.09	1.47	1.41
19	1	1195	CLA	CHA-C1A	2.10	1.47	1.41
19	1	1200	CLA	CHA-C1A	2.13	1.47	1.41
19	4	1206	CLA	C1B-CHB	2.13	1.45	1.39
20	A	7014	LMU	O2B-C2B	2.14	1.48	1.43
19	2	1223	CLA	C1B-CHB	2.15	1.45	1.39
21	B	8062	SUC	O2-C2	2.15	1.48	1.43
19	J	1043	CLA	C1B-CHB	2.16	1.45	1.39
19	3	3011	CLA	C1B-CHB	2.16	1.45	1.39
19	3	3014	CLA	CHA-C1A	2.16	1.47	1.41
19	A	1774	CLA	C1B-CHB	2.17	1.45	1.39
19	4	1208	CLA	CHA-C1A	2.18	1.47	1.41
19	B	1748	CLA	C1B-CHB	2.18	1.45	1.39
20	A	7024	LMU	O1'-C1'	2.19	1.44	1.40
19	A	1789	CLA	C1B-CHB	2.20	1.45	1.39
19	B	1736	CLA	C1B-CHB	2.21	1.45	1.39
19	A	1764	CLA	C1B-CHB	2.22	1.46	1.39
19	2	1218	CLA	CHA-C1A	2.22	1.47	1.41
20	A	7009	LMU	O6B-C6B	2.22	1.51	1.42
19	A	1793	CLA	C1B-CHB	2.22	1.46	1.39
19	A	1814	CLA	C1B-CHB	2.22	1.46	1.39
19	2	1220	CLA	CHA-C1A	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	1155	CLA	C1B-CHB	2.23	1.46	1.39
19	B	1760	CLA	C1B-CHB	2.24	1.46	1.39
19	1	1014	CLA	C1B-CHB	2.24	1.46	1.39
19	B	1738	CLA	C1B-CHB	2.28	1.46	1.39
19	2	1213	CLA	C1B-CHB	2.28	1.46	1.39
19	B	1754	CLA	C1B-CHB	2.29	1.46	1.39
19	3	1214	CLA	CHA-C1A	2.29	1.48	1.41
19	B	1740	CLA	CHA-C1A	2.30	1.48	1.41
19	1	1187	CLA	C1B-CHB	2.30	1.46	1.39
20	A	7008	LMU	C6B-C5B	2.31	1.60	1.51
19	3	1219	CLA	CHA-C1A	2.32	1.48	1.41
19	2	1214	CLA	CHA-C1A	2.32	1.48	1.41
19	2	1221	CLA	C1B-CHB	2.32	1.46	1.39
19	3	1214	CLA	C4B-CHC	2.33	1.48	1.43
19	A	1797	CLA	C1B-CHB	2.34	1.46	1.39
19	L	1167	CLA	C1B-CHB	2.34	1.46	1.39
19	4	4014	CLA	C1B-CHB	2.35	1.46	1.39
19	4	1207	CLA	CHA-C1A	2.36	1.48	1.41
19	A	1783	CLA	C1B-CHB	2.36	1.46	1.39
19	B	1769	CLA	C1B-CHB	2.36	1.46	1.39
19	1	1309	CLA	CHA-C1A	2.36	1.48	1.41
19	4	1203	CLA	CHA-C1A	2.36	1.48	1.41
19	3	1218	CLA	C1B-CHB	2.37	1.46	1.39
19	A	1776	CLA	C1B-CHB	2.37	1.46	1.39
19	4	1204	CLA	CHA-C1A	2.37	1.48	1.41
19	B	1751	CLA	C1B-CHB	2.38	1.46	1.39
19	A	1817	CLA	C1B-CHB	2.39	1.46	1.39
19	B	1766	CLA	C1B-CHB	2.39	1.46	1.39
19	2	2006	CLA	C1B-CHB	2.39	1.46	1.39
19	1	1307	CLA	CHA-C1A	2.39	1.48	1.41
19	1	1145	CLA	C1B-CHB	2.40	1.46	1.39
19	A	1795	CLA	C1B-CHB	2.40	1.46	1.39
19	1	1188	CLA	C1B-CHB	2.42	1.46	1.39
19	A	1815	CLA	C1B-CHB	2.43	1.46	1.39
19	3	1222	CLA	C1B-CHB	2.43	1.46	1.39
19	4	1209	CLA	C1B-CHB	2.43	1.46	1.39
19	4	1203	CLA	C4B-CHC	2.43	1.48	1.43
19	B	1743	CLA	C1B-CHB	2.44	1.46	1.39
19	2	1222	CLA	C1B-CHB	2.44	1.46	1.39
19	A	1799	CLA	CHA-C1A	2.44	1.48	1.41
21	B	8062	SUC	C1-C2	2.44	1.59	1.52
19	A	1767	CLA	C1B-CHB	2.46	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1779	CLA	C1B-CHB	2.46	1.46	1.39
19	A	1760	CLA	C1B-CHB	2.47	1.46	1.39
19	A	1769	CLA	C1B-CHB	2.47	1.46	1.39
19	A	1788	CLA	C1B-CHB	2.49	1.46	1.39
19	4	4007	CLA	C1B-CHB	2.49	1.46	1.39
19	A	1790	CLA	C1B-CHB	2.49	1.46	1.39
19	3	1212	CLA	CHA-C1A	2.49	1.48	1.41
19	2	1216	CLA	CHA-C1A	2.50	1.48	1.41
19	B	1762	CLA	C1B-CHB	2.50	1.46	1.39
20	A	7026	LMU	O1'-C1'	2.51	1.44	1.40
19	B	1737	CLA	C1B-CHB	2.51	1.46	1.39
19	B	1764	CLA	C1B-CHB	2.51	1.46	1.39
19	B	1739	CLA	C1B-CHB	2.51	1.46	1.39
19	1	1307	CLA	C4B-CHC	2.52	1.48	1.43
19	A	1762	CLA	C1B-CHB	2.52	1.46	1.39
19	A	1816	CLA	C1B-CHB	2.53	1.46	1.39
19	B	1770	CLA	C1B-CHB	2.53	1.46	1.39
20	4	1212	LMU	O1'-C1'	2.53	1.44	1.40
20	A	7027	LMU	O1'-C1'	2.53	1.44	1.40
19	A	1780	CLA	C1B-CHB	2.54	1.46	1.39
19	B	1784	CLA	C1B-CHB	2.54	1.46	1.39
19	A	1781	CLA	C1B-CHB	2.54	1.46	1.39
19	A	1768	CLA	C1B-CHB	2.55	1.46	1.39
19	H	1080	CLA	C1B-CHB	2.55	1.46	1.39
19	1	1308	CLA	C1B-CHB	2.55	1.46	1.39
19	B	1744	CLA	C1B-CHB	2.55	1.46	1.39
19	A	1787	CLA	C1B-CHB	2.55	1.46	1.39
19	A	1794	CLA	C1B-CHB	2.55	1.46	1.39
19	3	1215	CLA	CHA-C1A	2.56	1.48	1.41
19	F	1156	CLA	C1B-CHB	2.56	1.46	1.39
19	1	1148	CLA	C1B-CHB	2.56	1.46	1.39
19	A	1784	CLA	C1B-CHB	2.56	1.46	1.39
19	3	1220	CLA	CHA-C1A	2.56	1.48	1.41
19	B	1757	CLA	C1B-CHB	2.56	1.46	1.39
19	1	1189	CLA	C1B-CHB	2.56	1.46	1.39
19	B	1747	CLA	C1B-CHB	2.57	1.46	1.39
19	4	1210	CLA	CHA-C1A	2.58	1.48	1.41
19	B	1765	CLA	C1B-CHB	2.58	1.47	1.39
19	L	1168	CLA	C1B-CHB	2.58	1.47	1.39
20	A	7040	LMU	O1'-C1'	2.59	1.44	1.40
19	F	1157	CLA	C1B-CHB	2.60	1.47	1.39
19	F	1157	CLA	CMA-C3A	2.60	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1198	CLA	CHA-C1A	2.60	1.49	1.41
19	4	1197	CLA	C1B-CHB	2.60	1.47	1.39
19	2	1216	CLA	C4B-CHC	2.60	1.49	1.43
19	1	1199	CLA	CAA-CBA	2.60	1.61	1.52
19	A	1813	CLA	C1B-CHB	2.60	1.47	1.39
19	4	1196	CLA	C1B-CHB	2.60	1.47	1.39
19	B	1756	CLA	C1B-CHB	2.61	1.47	1.39
19	A	1798	CLA	C1B-CHB	2.61	1.47	1.39
20	B	1782	LMU	O1'-C1'	2.61	1.44	1.40
19	4	1199	CLA	C1B-CHB	2.61	1.47	1.39
19	B	1752	CLA	C1B-CHB	2.61	1.47	1.39
19	B	1753	CLA	C1B-CHB	2.62	1.47	1.39
19	2	1218	CLA	C4B-CHC	2.62	1.49	1.43
19	I	1031	CLA	C1B-CHB	2.62	1.47	1.39
19	A	1766	CLA	C1B-CHB	2.64	1.47	1.39
19	1	1194	CLA	CHA-C1A	2.65	1.49	1.41
19	3	1216	CLA	CHA-C1A	2.65	1.49	1.41
19	3	1213	CLA	C1B-CHB	2.65	1.47	1.39
19	1	1142	CLA	C1B-CHB	2.66	1.47	1.39
19	B	1735	CLA	C1B-CHB	2.66	1.47	1.39
19	A	1796	CLA	C1B-CHB	2.67	1.47	1.39
19	3	3008	CLA	C1B-CHB	2.68	1.47	1.39
19	1	1143	CLA	C1B-CHB	2.69	1.47	1.39
19	4	1211	CLA	C1B-CHB	2.69	1.47	1.39
19	2	1215	CLA	C1B-CHB	2.69	1.47	1.39
20	A	7019	LMU	O1'-C1'	2.69	1.45	1.40
19	3	1221	CLA	C1B-CHB	2.70	1.47	1.39
19	A	1791	CLA	C1B-CHB	2.70	1.47	1.39
19	1	1193	CLA	C1B-CHB	2.72	1.47	1.39
19	B	1763	CLA	C1B-CHB	2.72	1.47	1.39
19	2	1220	CLA	C4B-CHC	2.73	1.49	1.43
19	B	1748	CLA	OBD-CAD	2.73	1.26	1.22
19	3	1220	CLA	C4B-CHC	2.73	1.49	1.43
19	A	1759	CLA	C1B-CHB	2.74	1.47	1.39
19	A	1773	CLA	C1B-CHB	2.75	1.47	1.39
19	3	3001	CLA	CHA-C1A	2.75	1.49	1.41
19	A	1777	CLA	C1B-CHB	2.75	1.47	1.39
19	B	1740	CLA	C4B-CHC	2.75	1.49	1.43
19	B	1761	CLA	C1B-CHB	2.76	1.47	1.39
19	B	1755	CLA	C1B-CHB	2.76	1.47	1.39
19	B	1745	CLA	C1B-CHB	2.77	1.47	1.39
19	A	1785	CLA	C1B-CHB	2.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1771	CLA	C1B-CHB	2.77	1.47	1.39
20	A	7047	LMU	O1'-C1'	2.77	1.45	1.40
20	A	7032	LMU	O1'-C1'	2.78	1.45	1.40
19	B	1742	CLA	C1B-CHB	2.78	1.47	1.39
19	A	1782	CLA	C1B-CHB	2.79	1.47	1.39
19	1	1191	CLA	C1B-CHB	2.79	1.47	1.39
19	4	1205	CLA	C1B-CHB	2.79	1.47	1.39
19	A	1792	CLA	C1B-CHB	2.81	1.47	1.39
19	A	1775	CLA	C1B-CHB	2.82	1.47	1.39
19	3	3011	CLA	C4B-CHC	2.82	1.47	1.39
19	B	1737	CLA	OBD-CAD	2.82	1.26	1.22
20	A	7008	LMU	C4B-C3B	2.83	1.59	1.52
19	3	1217	CLA	C1B-CHB	2.84	1.47	1.39
19	R	1054	CLA	C1B-CHB	2.84	1.47	1.39
19	A	1786	CLA	C1B-CHB	2.84	1.47	1.39
19	A	1763	CLA	C1B-CHB	2.84	1.47	1.39
19	1	1187	CLA	C4B-CHC	2.85	1.47	1.39
19	1	1196	CLA	C1B-CHB	2.85	1.47	1.39
19	B	1746	CLA	C1B-CHB	2.86	1.47	1.39
19	B	1772	CLA	C1B-CHB	2.86	1.47	1.39
19	B	1750	CLA	C1B-CHB	2.87	1.47	1.39
19	A	1799	CLA	C4B-CHC	2.89	1.49	1.43
19	B	1759	CLA	C1B-CHB	2.90	1.47	1.39
19	1	1505	CLA	C1B-CHB	2.90	1.47	1.39
19	A	1761	CLA	C1B-CHB	2.90	1.47	1.39
19	1	1309	CLA	C4B-CHC	2.90	1.49	1.43
19	3	3015	CLA	C4B-CHC	2.92	1.49	1.43
19	2	2010	CLA	C4B-CHC	2.93	1.49	1.43
19	2	1214	CLA	C4B-CHC	2.93	1.49	1.43
19	4	1202	CLA	C4B-CHC	2.94	1.49	1.43
19	2	1219	CLA	C1B-CHB	2.94	1.48	1.39
19	4	1200	CLA	C1B-CHB	2.96	1.48	1.39
19	A	1765	CLA	C1B-CHB	2.96	1.48	1.39
19	B	1767	CLA	C1B-CHB	2.97	1.48	1.39
19	1	1200	CLA	C4B-CHC	2.97	1.49	1.43
19	B	1771	CLA	C1B-CHB	2.97	1.48	1.39
19	3	3014	CLA	C4B-CHC	2.97	1.49	1.43
19	H	1081	CLA	C1B-CHB	3.00	1.48	1.39
19	A	1774	CLA	OBD-CAD	3.00	1.26	1.22
19	3	1217	CLA	C4B-CHC	3.03	1.48	1.39
19	4	1207	CLA	C4B-CHC	3.04	1.50	1.43
19	B	1768	CLA	C1B-CHB	3.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1749	CLA	C1B-CHB	3.06	1.48	1.39
19	1	1197	CLA	C1B-CHB	3.06	1.48	1.39
19	A	1801	CLA	C1B-CHB	3.07	1.48	1.39
19	3	1219	CLA	C4B-CHC	3.07	1.50	1.43
19	3	1215	CLA	C4B-CHC	3.08	1.50	1.43
19	1	1190	CLA	C4B-CHC	3.09	1.48	1.39
19	A	1778	CLA	C1B-CHB	3.09	1.48	1.39
19	1	1189	CLA	O2A-CGA	3.10	1.42	1.33
19	1	1149	CLA	C1B-CHB	3.11	1.48	1.39
19	2	1217	CLA	C4B-CHC	3.11	1.48	1.39
19	A	1789	CLA	C4B-CHC	3.12	1.48	1.39
19	A	1759	CLA	C4B-CHC	3.14	1.48	1.39
19	B	1758	CLA	C1B-CHB	3.14	1.48	1.39
19	3	1216	CLA	C4B-CHC	3.15	1.50	1.43
19	1	1192	CLA	C1B-CHB	3.17	1.48	1.39
19	B	1761	CLA	C4B-CHC	3.19	1.48	1.39
19	2	1217	CLA	C1B-CHB	3.19	1.48	1.39
19	4	1208	CLA	C4B-CHC	3.21	1.50	1.43
19	1	1199	CLA	C4B-CHC	3.22	1.48	1.39
19	A	1770	CLA	C4B-CHC	3.22	1.50	1.43
19	4	1198	CLA	C4B-CHC	3.23	1.48	1.39
19	1	1198	CLA	C4B-CHC	3.23	1.50	1.43
19	A	1800	CLA	C1B-CHB	3.23	1.48	1.39
19	2	1218	CLA	CHD-C4C	3.25	1.48	1.41
19	4	1205	CLA	C4B-CHC	3.25	1.48	1.39
19	H	1079	CLA	C4B-CHC	3.25	1.48	1.39
19	R	1055	CLA	C1B-CHB	3.26	1.48	1.39
19	4	1204	CLA	C4B-CHC	3.26	1.50	1.43
19	1	1194	CLA	C4B-CHC	3.27	1.50	1.43
19	A	1765	CLA	C4B-CHC	3.28	1.48	1.39
19	B	1761	CLA	OBD-CAD	3.28	1.27	1.22
19	B	1753	CLA	OBD-CAD	3.32	1.27	1.22
19	2	1221	CLA	C4B-CHC	3.32	1.49	1.39
19	B	1769	CLA	OBD-CAD	3.33	1.27	1.22
19	A	1759	CLA	OBD-CAD	3.34	1.27	1.22
19	4	4007	CLA	C4B-CHC	3.35	1.49	1.39
19	1	1014	CLA	CHD-C4C	3.35	1.49	1.41
19	1	1142	CLA	O2A-C1	3.36	1.53	1.45
19	B	1753	CLA	C9-C8	3.37	1.64	1.52
19	A	1774	CLA	C4B-CHC	3.37	1.49	1.39
19	B	1768	CLA	C4B-CHC	3.38	1.49	1.39
19	4	1206	CLA	C4B-CHC	3.38	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	4014	CLA	C4B-CHC	3.38	1.49	1.39
19	4	1201	CLA	C4B-CHC	3.38	1.49	1.39
19	A	1789	CLA	CHD-C4C	3.38	1.49	1.41
19	2	1221	CLA	OBD-CAD	3.40	1.27	1.22
19	4	1199	CLA	C4B-CHC	3.40	1.49	1.39
19	2	2006	CLA	C4B-CHC	3.40	1.49	1.39
19	4	1205	CLA	OBD-CAD	3.40	1.27	1.22
19	2	1213	CLA	C4B-CHC	3.41	1.49	1.39
19	A	1797	CLA	C4B-CHC	3.41	1.49	1.39
19	3	1212	CLA	C4B-CHC	3.42	1.50	1.43
19	A	1795	CLA	C4B-CHC	3.43	1.49	1.39
19	3	1221	CLA	C4B-CHC	3.43	1.49	1.39
19	B	1738	CLA	C4B-CHC	3.44	1.49	1.39
19	1	1195	CLA	C4B-CHC	3.44	1.50	1.43
19	A	1761	CLA	C4B-CHC	3.46	1.49	1.39
19	B	1759	CLA	C4B-CHC	3.46	1.49	1.39
19	I	1031	CLA	OBD-CAD	3.47	1.27	1.22
19	1	1188	CLA	C4B-CHC	3.48	1.49	1.39
19	4	1200	CLA	C4B-CHC	3.50	1.49	1.39
19	B	1737	CLA	C4B-CHC	3.51	1.49	1.39
19	4	1206	CLA	OBD-CAD	3.51	1.27	1.22
19	F	1157	CLA	C4B-CHC	3.51	1.49	1.39
19	1	1149	CLA	C4B-CHC	3.53	1.49	1.39
19	B	1771	CLA	C4B-CHC	3.53	1.49	1.39
19	1	1197	CLA	C4B-CHC	3.55	1.49	1.39
19	1	1196	CLA	OBD-CAD	3.55	1.27	1.22
19	B	1763	CLA	C4B-CHC	3.55	1.49	1.39
19	3	3001	CLA	C4B-CHC	3.56	1.51	1.43
19	J	1043	CLA	C4B-CHC	3.56	1.49	1.39
19	B	1761	CLA	CHD-C4C	3.56	1.49	1.41
19	1	1146	CLA	C4B-CHC	3.57	1.49	1.39
19	A	1778	CLA	C4B-CHC	3.57	1.49	1.39
19	2	1223	CLA	O2A-CGA	3.57	1.44	1.33
19	A	1780	CLA	OBD-CAD	3.59	1.27	1.22
19	A	1817	CLA	C4B-CHC	3.60	1.49	1.39
19	1	1190	CLA	O2A-CGA	3.61	1.45	1.32
19	4	4007	CLA	O2A-CGA	3.62	1.44	1.33
19	B	1769	CLA	C4B-CHC	3.62	1.49	1.39
19	A	1794	CLA	C4B-CHC	3.62	1.49	1.39
19	B	1742	CLA	C4B-CHC	3.62	1.49	1.39
19	B	1739	CLA	C4B-CHC	3.63	1.49	1.39
19	B	1767	CLA	C4B-CHC	3.64	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1748	CLA	C4B-CHC	3.65	1.49	1.39
19	A	1790	CLA	C4B-CHC	3.65	1.49	1.39
19	B	1743	CLA	OBD-CAD	3.65	1.27	1.22
19	H	1079	CLA	CHD-C4C	3.65	1.49	1.41
19	2	1214	CLA	CHD-C4C	3.66	1.49	1.41
19	3	1218	CLA	C4B-CHC	3.66	1.49	1.39
19	4	1201	CLA	OBD-CAD	3.66	1.27	1.22
19	1	1142	CLA	O2A-CGA	3.67	1.45	1.32
19	A	1761	CLA	OBD-CAD	3.67	1.28	1.22
19	B	1752	CLA	C4B-CHC	3.67	1.50	1.39
19	3	1221	CLA	CHD-C4C	3.67	1.49	1.41
19	3	3011	CLA	O2A-CGA	3.68	1.44	1.33
19	A	1769	CLA	C4B-CHC	3.68	1.50	1.39
19	A	1800	CLA	C4B-CHC	3.68	1.50	1.39
19	B	1754	CLA	C4B-CHC	3.68	1.50	1.39
19	4	4007	CLA	OBD-CAD	3.69	1.28	1.22
19	A	1791	CLA	C4B-CHC	3.69	1.50	1.39
19	1	1143	CLA	C4B-CHC	3.69	1.50	1.39
19	A	1782	CLA	C4B-CHC	3.69	1.50	1.39
19	2	2010	CLA	CHD-C4C	3.70	1.49	1.41
19	A	1788	CLA	C4B-CHC	3.70	1.50	1.39
19	B	1753	CLA	C4B-CHC	3.70	1.50	1.39
19	B	1768	CLA	OBD-CAD	3.71	1.28	1.22
19	A	1786	CLA	C4B-CHC	3.71	1.50	1.39
19	B	1738	CLA	OBD-CAD	3.71	1.28	1.22
19	B	1749	CLA	OBD-CAD	3.72	1.28	1.22
19	B	1755	CLA	C4B-CHC	3.73	1.50	1.39
19	A	1793	CLA	C4B-CHC	3.73	1.50	1.39
19	1	1145	CLA	C4B-CHC	3.73	1.50	1.39
19	A	1784	CLA	C4B-CHC	3.74	1.50	1.39
19	A	1785	CLA	C4B-CHC	3.74	1.50	1.39
19	4	1200	CLA	CHD-C4C	3.74	1.50	1.41
19	A	1772	CLA	C4B-CHC	3.75	1.50	1.39
19	A	1800	CLA	O2A-CGA	3.75	1.44	1.33
19	A	1772	CLA	OBD-CAD	3.75	1.28	1.22
19	A	1782	CLA	OBD-CAD	3.75	1.28	1.22
19	3	3015	CLA	CHD-C4C	3.76	1.50	1.41
19	2	1222	CLA	C4B-CHC	3.76	1.50	1.39
19	A	1763	CLA	C4B-CHC	3.76	1.50	1.39
19	A	1767	CLA	C4B-CHC	3.77	1.50	1.39
19	B	1746	CLA	O2A-CGA	3.77	1.45	1.32
19	B	1766	CLA	C4B-CHC	3.77	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1766	CLA	O2A-CGA	3.77	1.44	1.33
19	A	1762	CLA	C4B-CHC	3.78	1.50	1.39
19	1	1308	CLA	C4B-CHC	3.78	1.50	1.39
19	2	1220	CLA	CHD-C4C	3.78	1.50	1.41
19	F	1157	CLA	O2A-CGA	3.78	1.44	1.33
19	B	1758	CLA	C4B-CHC	3.78	1.50	1.39
19	A	1814	CLA	C4B-CHC	3.78	1.50	1.39
19	A	1816	CLA	C4B-CHC	3.78	1.50	1.39
19	A	1798	CLA	C4B-CHC	3.79	1.50	1.39
19	B	1784	CLA	C4B-CHC	3.79	1.50	1.39
19	4	1196	CLA	C4B-CHC	3.80	1.50	1.39
19	A	1779	CLA	C4B-CHC	3.80	1.50	1.39
19	B	1769	CLA	CHD-C4C	3.80	1.50	1.41
19	4	1211	CLA	O2A-CGA	3.80	1.45	1.32
19	B	1765	CLA	C4B-CHC	3.81	1.50	1.39
19	1	1197	CLA	CHD-C4C	3.81	1.50	1.41
19	3	1218	CLA	OBD-CAD	3.82	1.28	1.22
19	A	1781	CLA	C4B-CHC	3.82	1.50	1.39
19	4	1211	CLA	CHD-C4C	3.83	1.50	1.41
19	B	1744	CLA	C4B-CHC	3.83	1.50	1.39
19	B	1756	CLA	C4B-CHC	3.83	1.50	1.39
19	A	1764	CLA	C4B-CHC	3.84	1.50	1.39
19	H	1079	CLA	OBD-CAD	3.84	1.28	1.22
19	B	1757	CLA	OBD-CAD	3.84	1.28	1.22
19	4	1197	CLA	C4B-CHC	3.84	1.50	1.39
19	A	1789	CLA	O2A-CGA	3.85	1.44	1.33
19	A	1815	CLA	C4B-CHC	3.85	1.50	1.39
19	1	1195	CLA	CHD-C4C	3.85	1.50	1.41
19	F	1155	CLA	C4B-CHC	3.85	1.50	1.39
19	B	1749	CLA	C4B-CHC	3.85	1.50	1.39
19	R	1054	CLA	C4B-CHC	3.86	1.50	1.39
19	3	1222	CLA	C4B-CHC	3.86	1.50	1.39
19	G	1099	CLA	C4B-CHC	3.86	1.50	1.39
19	4	1211	CLA	C4B-CHC	3.87	1.50	1.39
19	1	1014	CLA	C4B-CHC	3.87	1.50	1.39
19	B	1764	CLA	C4B-CHC	3.87	1.50	1.39
19	A	1783	CLA	C4B-CHC	3.88	1.50	1.39
19	A	1773	CLA	C4B-CHC	3.88	1.50	1.39
19	B	1760	CLA	C4B-CHC	3.88	1.50	1.39
19	A	1813	CLA	OBD-CAD	3.88	1.28	1.22
19	A	1787	CLA	C4B-CHC	3.88	1.50	1.39
19	1	1146	CLA	O2A-CGA	3.89	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1747	CLA	C4B-CHC	3.89	1.50	1.39
19	1	1187	CLA	O2A-CGA	3.89	1.46	1.32
19	1	1148	CLA	C4B-CHC	3.90	1.50	1.39
19	B	1750	CLA	C4B-CHC	3.90	1.50	1.39
19	A	1759	CLA	O2A-CGA	3.90	1.46	1.32
19	B	1735	CLA	C4B-CHC	3.90	1.50	1.39
19	A	1771	CLA	C4B-CHC	3.90	1.50	1.39
19	B	1784	CLA	O2A-CGA	3.90	1.45	1.33
19	A	1774	CLA	CHD-C4C	3.91	1.50	1.41
19	2	1212	CLA	CHD-C4C	3.91	1.50	1.41
19	A	1792	CLA	C4B-CHC	3.91	1.50	1.39
19	3	3011	CLA	CHC-C1C	3.91	1.47	1.35
19	B	1756	CLA	OBD-CAD	3.92	1.28	1.22
19	1	1505	CLA	C4B-CHC	3.92	1.50	1.39
19	B	1753	CLA	CHD-C4C	3.92	1.50	1.41
19	A	1760	CLA	C4B-CHC	3.92	1.50	1.39
19	1	1142	CLA	OBD-CAD	3.92	1.28	1.22
19	A	1781	CLA	OBD-CAD	3.92	1.28	1.22
19	B	1751	CLA	C4B-CHC	3.93	1.50	1.39
19	B	1738	CLA	O2A-CGA	3.93	1.45	1.33
19	A	1801	CLA	C4B-CHC	3.93	1.50	1.39
19	1	1189	CLA	C4B-CHC	3.93	1.50	1.39
19	1	1142	CLA	C4B-CHC	3.93	1.50	1.39
19	4	1205	CLA	CHD-C4C	3.94	1.50	1.41
19	B	1741	CLA	OBD-CAD	3.94	1.28	1.22
19	A	1780	CLA	C4B-CHC	3.94	1.50	1.39
19	2	1215	CLA	C4B-CHC	3.94	1.50	1.39
19	2	1223	CLA	C4B-CHC	3.94	1.50	1.39
19	B	1737	CLA	O2A-CGA	3.95	1.45	1.33
19	B	1741	CLA	C4B-CHC	3.95	1.50	1.39
19	A	1772	CLA	O2A-CGA	3.95	1.45	1.33
19	2	2006	CLA	CHD-C4C	3.95	1.50	1.41
19	2	1221	CLA	O2A-CGA	3.95	1.45	1.33
19	A	1775	CLA	C4B-CHC	3.95	1.50	1.39
19	B	1736	CLA	C4B-CHC	3.95	1.50	1.39
19	4	1210	CLA	C4B-CHC	3.95	1.51	1.43
19	R	1055	CLA	C4B-CHC	3.96	1.50	1.39
19	B	1761	CLA	O2A-CGA	3.96	1.45	1.33
19	1	1191	CLA	C4B-CHC	3.96	1.50	1.39
19	A	1763	CLA	O2A-CGA	3.96	1.46	1.32
19	1	1192	CLA	C4B-CHC	3.97	1.50	1.39
19	A	1767	CLA	OBD-CAD	3.98	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1770	CLA	C4B-CHC	3.98	1.50	1.39
19	A	1815	CLA	O2A-CGA	3.98	1.45	1.33
19	H	1080	CLA	C4B-CHC	3.98	1.50	1.39
19	A	1792	CLA	O2A-CGA	3.98	1.46	1.32
19	J	1043	CLA	O2A-CGA	3.99	1.45	1.33
19	J	1043	CLA	CHD-C4C	3.99	1.50	1.41
19	4	1211	CLA	OBD-CAD	3.99	1.28	1.22
19	A	1764	CLA	OBD-CAD	3.99	1.28	1.22
19	B	1771	CLA	OBD-CAD	3.99	1.28	1.22
19	A	1797	CLA	CHD-C4C	3.99	1.50	1.41
19	4	1205	CLA	O2A-CGA	4.00	1.45	1.33
19	1	1307	CLA	CHD-C4C	4.00	1.50	1.41
19	B	1746	CLA	C4B-CHC	4.00	1.50	1.39
19	2	1219	CLA	C4B-CHC	4.00	1.50	1.39
19	2	1216	CLA	CHD-C4C	4.01	1.50	1.41
19	B	1772	CLA	C4B-CHC	4.01	1.50	1.39
19	A	1783	CLA	O2A-CGA	4.01	1.45	1.33
19	A	1813	CLA	O2A-CGA	4.01	1.45	1.33
19	A	1817	CLA	OBD-CAD	4.01	1.28	1.22
19	4	1206	CLA	CHD-C4C	4.02	1.50	1.41
19	3	1216	CLA	CHD-C4C	4.02	1.50	1.41
19	A	1768	CLA	C4B-CHC	4.02	1.50	1.39
19	B	1741	CLA	CHD-C4C	4.02	1.50	1.41
19	A	1774	CLA	O2A-CGA	4.03	1.45	1.33
19	A	1766	CLA	C4B-CHC	4.03	1.50	1.39
19	2	2006	CLA	O2A-CGA	4.03	1.45	1.33
19	2	1212	CLA	C4B-CHC	4.03	1.50	1.39
24	B	1781	LMG	O7-C10	4.03	1.46	1.34
19	A	1772	CLA	CHD-C4C	4.03	1.50	1.41
19	1	1193	CLA	C4B-CHC	4.03	1.51	1.39
19	1	1143	CLA	O2A-CGA	4.04	1.45	1.33
19	B	1745	CLA	C4B-CHC	4.04	1.51	1.39
19	B	1750	CLA	OBD-CAD	4.04	1.28	1.22
19	A	1796	CLA	C4B-CHC	4.04	1.51	1.39
19	B	1757	CLA	C4B-CHC	4.04	1.51	1.39
19	4	1198	CLA	O2A-CGA	4.05	1.45	1.33
19	B	1741	CLA	O2D-CGD	4.05	1.43	1.33
19	2	2006	CLA	OBD-CAD	4.05	1.28	1.22
19	4	1203	CLA	CHD-C4C	4.06	1.50	1.41
19	B	1737	CLA	O2D-CGD	4.06	1.43	1.33
19	3	1213	CLA	C4B-CHC	4.06	1.51	1.39
19	A	1781	CLA	O2A-CGA	4.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3014	CLA	CHD-C4C	4.06	1.50	1.41
19	A	1770	CLA	CHD-C4C	4.07	1.50	1.41
19	2	1223	CLA	CHD-C4C	4.07	1.50	1.41
19	B	1758	CLA	O2A-CGA	4.07	1.45	1.33
19	B	1759	CLA	O2A-CGA	4.08	1.45	1.33
19	2	1215	CLA	OBD-CAD	4.08	1.28	1.22
19	B	1748	CLA	CHD-C4C	4.08	1.50	1.41
19	1	1190	CLA	OBD-CAD	4.08	1.28	1.22
19	A	1777	CLA	C4B-CHC	4.08	1.51	1.39
19	3	1221	CLA	OBD-CAD	4.09	1.28	1.22
19	L	1168	CLA	C4B-CHC	4.09	1.51	1.39
19	A	1776	CLA	C4B-CHC	4.09	1.51	1.39
19	I	1031	CLA	C4B-CHC	4.10	1.51	1.39
19	4	1206	CLA	O2A-CGA	4.10	1.45	1.33
19	1	1187	CLA	CHC-C1C	4.10	1.48	1.35
19	4	4014	CLA	OBD-CAD	4.11	1.28	1.22
19	B	1737	CLA	CHD-C4C	4.11	1.50	1.41
19	B	1767	CLA	OBD-CAD	4.12	1.28	1.22
19	B	1752	CLA	O2A-CGA	4.12	1.45	1.33
19	B	1761	CLA	CHC-C1C	4.12	1.48	1.35
19	4	1202	CLA	CHD-C4C	4.12	1.50	1.41
19	2	1212	CLA	O2A-CGA	4.12	1.45	1.33
19	B	1753	CLA	O2A-CGA	4.13	1.45	1.33
19	A	1813	CLA	C4B-CHC	4.13	1.51	1.39
19	A	1780	CLA	O2A-CGA	4.13	1.45	1.33
19	1	1187	CLA	CHD-C4C	4.13	1.50	1.41
19	A	1794	CLA	O2A-CGA	4.13	1.45	1.33
19	4	1209	CLA	C4B-CHC	4.13	1.51	1.39
19	2	1213	CLA	CHD-C4C	4.13	1.50	1.41
19	1	1146	CLA	OBD-CAD	4.13	1.28	1.22
19	B	1763	CLA	O2A-CGA	4.14	1.45	1.33
19	A	1784	CLA	OBD-CAD	4.14	1.28	1.22
19	B	1766	CLA	CHD-C4C	4.14	1.50	1.41
19	A	1762	CLA	O2A-CGA	4.14	1.45	1.33
19	L	1167	CLA	C4B-CHC	4.15	1.51	1.39
19	A	1759	CLA	CHD-C4C	4.15	1.51	1.41
19	4	1201	CLA	O2A-CGA	4.15	1.45	1.33
19	B	1741	CLA	O2A-CGA	4.15	1.45	1.33
19	4	1207	CLA	CHD-C4C	4.15	1.51	1.41
19	3	1219	CLA	CHD-C4C	4.16	1.51	1.41
19	1	1189	CLA	CHD-C4C	4.16	1.51	1.41
19	H	1081	CLA	C4B-CHC	4.16	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1196	CLA	C4B-CHC	4.16	1.51	1.39
19	B	1759	CLA	CHD-C4C	4.17	1.51	1.41
19	B	1749	CLA	CHD-C4C	4.17	1.51	1.41
19	4	1208	CLA	CHD-C4C	4.17	1.51	1.41
19	1	1192	CLA	CHD-C4C	4.17	1.51	1.41
19	A	1790	CLA	OBD-CAD	4.18	1.28	1.22
19	A	1813	CLA	CHD-C4C	4.19	1.51	1.41
19	4	1200	CLA	O2A-CGA	4.19	1.45	1.33
19	B	1762	CLA	C4B-CHC	4.19	1.51	1.39
19	3	1220	CLA	CHD-C4C	4.19	1.51	1.41
19	4	1210	CLA	CHD-C4C	4.19	1.51	1.41
19	2	1217	CLA	CHC-C1C	4.19	1.48	1.35
19	B	1768	CLA	O2A-CGA	4.19	1.45	1.33
19	2	1213	CLA	OBD-CAD	4.20	1.28	1.22
19	4	1196	CLA	O2A-CGA	4.20	1.46	1.33
19	B	1735	CLA	O2A-CGA	4.20	1.46	1.33
19	4	4014	CLA	O2A-CGA	4.20	1.46	1.33
19	A	1795	CLA	O2A-CGA	4.20	1.46	1.33
19	B	1756	CLA	O2A-CGA	4.21	1.46	1.33
19	B	1771	CLA	CHD-C4C	4.21	1.51	1.41
19	G	1099	CLA	O2A-CGA	4.21	1.46	1.33
19	B	1766	CLA	OBD-CAD	4.21	1.28	1.22
19	B	1758	CLA	CHD-C4C	4.22	1.51	1.41
19	3	3008	CLA	C4B-CHC	4.22	1.51	1.39
19	A	1769	CLA	OBD-CAD	4.22	1.28	1.22
19	1	1014	CLA	OBD-CAD	4.23	1.28	1.22
24	B	1781	LMG	O8-C28	4.23	1.46	1.33
19	B	1743	CLA	C4B-CHC	4.23	1.51	1.39
19	A	1798	CLA	O2A-CGA	4.23	1.46	1.33
19	A	1765	CLA	OBD-CAD	4.23	1.28	1.22
19	F	1157	CLA	CHD-C4C	4.24	1.51	1.41
19	B	1760	CLA	OBD-CAD	4.24	1.28	1.22
19	A	1765	CLA	CHC-C1C	4.24	1.48	1.35
19	3	1222	CLA	O2A-CGA	4.24	1.46	1.33
19	1	1308	CLA	OBD-CAD	4.25	1.28	1.22
19	3	1214	CLA	CHD-C4C	4.25	1.51	1.41
19	B	1763	CLA	OBD-CAD	4.25	1.28	1.22
19	2	1223	CLA	OBD-CAD	4.25	1.28	1.22
19	4	1197	CLA	CHD-C4C	4.26	1.51	1.41
19	3	1221	CLA	O2A-CGA	4.26	1.46	1.33
19	3	3011	CLA	CHD-C4C	4.26	1.51	1.41
19	2	1222	CLA	CHD-C4C	4.26	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1758	CLA	OBD-CAD	4.26	1.28	1.22
19	1	1194	CLA	CHD-C4C	4.26	1.51	1.41
19	3	1215	CLA	CHD-C4C	4.27	1.51	1.41
19	2	1219	CLA	OBD-CAD	4.27	1.28	1.22
19	A	1786	CLA	OBD-CAD	4.27	1.28	1.22
19	4	1209	CLA	CHD-C4C	4.28	1.51	1.41
19	B	1755	CLA	O2A-CGA	4.28	1.46	1.33
19	B	1757	CLA	O2A-CGA	4.28	1.46	1.33
19	B	1763	CLA	CHD-C4C	4.28	1.51	1.41
19	1	1308	CLA	O2A-CGA	4.28	1.46	1.33
19	B	1762	CLA	OBD-CAD	4.28	1.28	1.22
19	1	1198	CLA	CHD-C4C	4.29	1.51	1.41
19	B	1753	CLA	O2D-CGD	4.29	1.44	1.33
19	1	1199	CLA	O2A-CGA	4.30	1.46	1.33
19	3	1212	CLA	CHD-C4C	4.30	1.51	1.41
19	3	3011	CLA	OBD-CAD	4.31	1.28	1.22
19	A	1795	CLA	OBD-CAD	4.31	1.28	1.22
19	F	1156	CLA	C4B-CHC	4.31	1.51	1.39
19	3	1218	CLA	O2A-CGA	4.32	1.46	1.33
19	B	1784	CLA	OBD-CAD	4.32	1.28	1.22
19	A	1789	CLA	OBD-CAD	4.32	1.28	1.22
19	A	1776	CLA	OBD-CAD	4.32	1.29	1.22
19	B	1755	CLA	OBD-CAD	4.33	1.29	1.22
19	H	1079	CLA	O2A-CGA	4.33	1.46	1.33
19	3	1221	CLA	CHC-C1C	4.33	1.48	1.35
19	B	1745	CLA	OBD-CAD	4.33	1.29	1.22
19	A	1769	CLA	O2A-CGA	4.34	1.46	1.33
19	A	1788	CLA	O2A-CGA	4.34	1.46	1.33
19	B	1769	CLA	O2A-CGA	4.34	1.46	1.33
19	4	1196	CLA	CHD-C4C	4.34	1.51	1.41
19	J	1043	CLA	OBD-CAD	4.34	1.29	1.22
19	A	1816	CLA	OBD-CAD	4.34	1.29	1.22
19	1	1199	CLA	CHD-C4C	4.34	1.51	1.41
19	A	1773	CLA	OBD-CAD	4.34	1.29	1.22
19	A	1783	CLA	OBD-CAD	4.35	1.29	1.22
19	A	1796	CLA	O2A-CGA	4.35	1.46	1.33
19	1	1189	CLA	OBD-CAD	4.35	1.29	1.22
19	B	1751	CLA	O2A-CGA	4.35	1.47	1.32
19	A	1801	CLA	CHD-C4C	4.35	1.51	1.41
19	A	1814	CLA	OBD-CAD	4.36	1.29	1.22
19	1	1014	CLA	O2A-CGA	4.36	1.46	1.33
19	1	1200	CLA	CHD-C4C	4.36	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1739	CLA	OBD-CAD	4.36	1.29	1.22
19	A	1817	CLA	O2A-CGA	4.37	1.46	1.33
19	3	3008	CLA	O2A-CGA	4.37	1.46	1.33
19	2	1212	CLA	OBD-CAD	4.37	1.29	1.22
19	A	1776	CLA	O2A-CGA	4.37	1.46	1.33
19	1	1148	CLA	O2A-CGA	4.38	1.46	1.33
19	F	1156	CLA	CHD-C4C	4.38	1.51	1.41
19	3	1217	CLA	OBD-CAD	4.38	1.29	1.22
19	B	1772	CLA	CHD-C4C	4.38	1.51	1.41
19	3	3001	CLA	CHD-C4C	4.39	1.51	1.41
19	B	1743	CLA	O2A-CGA	4.39	1.46	1.33
19	1	1149	CLA	OBD-CAD	4.39	1.29	1.22
19	A	1782	CLA	CHD-C4C	4.40	1.51	1.41
19	G	1099	CLA	CHD-C4C	4.40	1.51	1.41
19	B	1764	CLA	OBD-CAD	4.40	1.29	1.22
19	A	1789	CLA	O2D-CGD	4.40	1.44	1.33
19	A	1814	CLA	CHD-C4C	4.40	1.51	1.41
19	1	1190	CLA	CHD-C4C	4.40	1.51	1.41
19	G	1099	CLA	OBD-CAD	4.41	1.29	1.22
19	B	1762	CLA	CHD-C4C	4.41	1.51	1.41
19	A	1779	CLA	OBD-CAD	4.41	1.29	1.22
19	A	1796	CLA	OBD-CAD	4.42	1.29	1.22
19	A	1785	CLA	O2A-CGA	4.42	1.46	1.33
19	B	1742	CLA	CHD-C4C	4.42	1.51	1.41
19	1	1199	CLA	CHC-C1C	4.42	1.49	1.35
19	L	1168	CLA	O2A-CGA	4.43	1.46	1.33
19	B	1743	CLA	CHD-C4C	4.43	1.51	1.41
19	B	1765	CLA	OBD-CAD	4.43	1.29	1.22
19	A	1795	CLA	CHD-C4C	4.43	1.51	1.41
19	2	1217	CLA	OBD-CAD	4.43	1.29	1.22
19	4	1204	CLA	CHD-C4C	4.43	1.51	1.41
19	4	1209	CLA	OBD-CAD	4.43	1.29	1.22
19	B	1742	CLA	O2A-CGA	4.43	1.46	1.33
19	A	1777	CLA	OBD-CAD	4.43	1.29	1.22
19	1	1145	CLA	OBD-CAD	4.43	1.29	1.22
19	4	1201	CLA	CHD-C4C	4.44	1.51	1.41
19	4	4014	CLA	O2D-CGD	4.44	1.44	1.33
19	3	1217	CLA	CHC-C1C	4.44	1.49	1.35
19	A	1793	CLA	O2A-CGA	4.44	1.46	1.33
19	B	1754	CLA	O2A-CGA	4.44	1.46	1.33
19	B	1771	CLA	O2A-CGA	4.44	1.46	1.33
19	A	1790	CLA	O2A-CGA	4.44	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1796	CLA	CHD-C4C	4.44	1.51	1.41
19	A	1797	CLA	OBD-CAD	4.45	1.29	1.22
19	1	1143	CLA	CHD-C4C	4.45	1.51	1.41
19	B	1745	CLA	O2A-CGA	4.45	1.46	1.33
19	1	1142	CLA	CHD-C4C	4.45	1.51	1.41
19	1	1192	CLA	O2A-CGA	4.45	1.46	1.33
19	A	1771	CLA	O2A-CGA	4.45	1.46	1.33
19	A	1800	CLA	CHD-C4C	4.46	1.51	1.41
19	A	1788	CLA	O2D-CGD	4.46	1.44	1.33
19	A	1782	CLA	O2A-CGA	4.46	1.46	1.33
19	B	1755	CLA	CHD-C4C	4.46	1.51	1.41
19	B	1748	CLA	O2D-CGD	4.47	1.44	1.33
19	1	1308	CLA	CHD-C4C	4.47	1.51	1.41
19	1	1505	CLA	O2A-CGA	4.47	1.46	1.33
19	L	1167	CLA	O2A-CGA	4.47	1.46	1.33
19	4	1200	CLA	OBD-CAD	4.47	1.29	1.22
19	3	1213	CLA	CHD-C4C	4.47	1.51	1.41
19	1	1505	CLA	OBD-CAD	4.47	1.29	1.22
19	H	1081	CLA	O2A-CGA	4.47	1.46	1.33
19	B	1759	CLA	OBD-CAD	4.47	1.29	1.22
19	1	1190	CLA	CHC-C1C	4.48	1.49	1.35
19	4	1196	CLA	OBD-CAD	4.48	1.29	1.22
19	B	1765	CLA	CHD-C4C	4.48	1.51	1.41
19	A	1816	CLA	O2A-CGA	4.48	1.46	1.33
19	A	1781	CLA	CHD-C4C	4.49	1.51	1.41
19	H	1081	CLA	CHD-C4C	4.49	1.51	1.41
19	B	1750	CLA	O2A-CGA	4.49	1.46	1.33
19	3	1218	CLA	CHD-C4C	4.49	1.51	1.41
19	A	1792	CLA	CHD-C4C	4.49	1.51	1.41
19	I	1031	CLA	CHD-C4C	4.49	1.51	1.41
19	B	1769	CLA	O2D-CGD	4.49	1.44	1.33
19	2	1215	CLA	O2A-CGA	4.49	1.46	1.33
19	A	1800	CLA	OBD-CAD	4.49	1.29	1.22
19	A	1765	CLA	O2A-CGA	4.49	1.46	1.33
19	A	1777	CLA	O2A-CGA	4.49	1.46	1.33
19	F	1157	CLA	CHC-C1C	4.49	1.49	1.35
19	H	1080	CLA	O2A-CGA	4.50	1.46	1.33
19	A	1759	CLA	CHC-C1C	4.50	1.49	1.35
19	2	1219	CLA	CHD-C4C	4.50	1.51	1.41
19	B	1751	CLA	CHD-C4C	4.50	1.51	1.41
19	A	1763	CLA	OBD-CAD	4.51	1.29	1.22
19	B	1745	CLA	CHD-C4C	4.51	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1146	CLA	CHD-C4C	4.51	1.51	1.41
19	1	1188	CLA	CHD-C4C	4.51	1.51	1.41
19	1	1193	CLA	CHD-C4C	4.51	1.51	1.41
19	B	1754	CLA	CHD-C4C	4.51	1.51	1.41
19	1	1148	CLA	CHD-C4C	4.51	1.51	1.41
19	2	1213	CLA	O2A-CGA	4.51	1.46	1.33
19	A	1768	CLA	OBD-CAD	4.51	1.29	1.22
19	H	1079	CLA	CHC-C1C	4.51	1.49	1.35
19	4	4007	CLA	CHD-C4C	4.52	1.51	1.41
19	L	1168	CLA	CHD-C4C	4.52	1.51	1.41
19	B	1760	CLA	O2A-CGA	4.52	1.46	1.33
19	B	1740	CLA	CHD-C4C	4.52	1.51	1.41
19	B	1756	CLA	CHD-C4C	4.53	1.51	1.41
19	A	1791	CLA	OBD-CAD	4.53	1.29	1.22
19	B	1762	CLA	O2A-CGA	4.53	1.47	1.33
19	1	1196	CLA	CHD-C4C	4.53	1.51	1.41
19	R	1055	CLA	CHD-C4C	4.53	1.51	1.41
19	1	1143	CLA	OBD-CAD	4.53	1.29	1.22
19	B	1750	CLA	CHD-C4C	4.54	1.51	1.41
19	A	1773	CLA	O2A-CGA	4.54	1.47	1.33
19	2	1217	CLA	CHD-C4C	4.54	1.51	1.41
19	2	1213	CLA	CHC-C1C	4.54	1.49	1.35
19	B	1746	CLA	CHD-C4C	4.54	1.51	1.41
19	4	1206	CLA	CHC-C1C	4.54	1.49	1.35
19	J	1043	CLA	O2D-CGD	4.54	1.44	1.33
19	A	1773	CLA	CHD-C4C	4.54	1.51	1.41
19	A	1797	CLA	CHC-C1C	4.54	1.49	1.35
19	3	1222	CLA	CHD-C4C	4.55	1.51	1.41
19	A	1769	CLA	CHD-C4C	4.55	1.51	1.41
19	A	1787	CLA	O2A-CGA	4.55	1.47	1.33
19	B	1735	CLA	OBD-CAD	4.56	1.29	1.22
19	L	1167	CLA	OBD-CAD	4.56	1.29	1.22
19	B	1770	CLA	OBD-CAD	4.56	1.29	1.22
19	B	1784	CLA	CHD-C4C	4.56	1.52	1.41
19	A	1788	CLA	OBD-CAD	4.56	1.29	1.22
19	B	1763	CLA	CHC-C1C	4.56	1.49	1.35
19	B	1752	CLA	OBD-CAD	4.56	1.29	1.22
19	B	1749	CLA	O2A-CGA	4.57	1.47	1.33
19	A	1775	CLA	CHD-C4C	4.58	1.52	1.41
19	B	1770	CLA	O2A-CGA	4.58	1.47	1.33
19	4	1211	CLA	O2D-CGD	4.58	1.44	1.33
19	A	1801	CLA	O2A-CGA	4.58	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	1217	CLA	O2A-CGA	4.58	1.47	1.33
19	B	1742	CLA	OBD-CAD	4.58	1.29	1.22
19	F	1155	CLA	OBD-CAD	4.59	1.29	1.22
19	A	1783	CLA	O2D-CGD	4.59	1.44	1.33
19	B	1764	CLA	CHD-C4C	4.59	1.52	1.41
19	A	1785	CLA	OBD-CAD	4.59	1.29	1.22
19	4	1198	CLA	OBD-CAD	4.59	1.29	1.22
19	F	1156	CLA	OBD-CAD	4.59	1.29	1.22
19	B	1748	CLA	CHC-C1C	4.59	1.49	1.35
19	4	1199	CLA	O2A-CGA	4.60	1.47	1.33
19	A	1794	CLA	CHD-C4C	4.60	1.52	1.41
19	B	1737	CLA	CHC-C1C	4.60	1.49	1.35
19	A	1764	CLA	CHD-C4C	4.60	1.52	1.41
19	1	1193	CLA	OBD-CAD	4.60	1.29	1.22
19	1	1505	CLA	CHD-C4C	4.60	1.52	1.41
19	H	1081	CLA	OBD-CAD	4.60	1.29	1.22
19	B	1767	CLA	CHD-C4C	4.60	1.52	1.41
19	B	1770	CLA	CHD-C4C	4.61	1.52	1.41
19	4	1205	CLA	CHC-C1C	4.61	1.49	1.35
19	B	1739	CLA	O2A-CGA	4.61	1.47	1.33
19	A	1798	CLA	OBD-CAD	4.61	1.29	1.22
19	B	1767	CLA	O2A-CGA	4.61	1.47	1.33
19	A	1768	CLA	CHD-C4C	4.61	1.52	1.41
19	1	1197	CLA	CHC-C1C	4.62	1.49	1.35
19	B	1771	CLA	CHC-C1C	4.62	1.49	1.35
19	A	1793	CLA	CHD-C4C	4.62	1.52	1.41
19	A	1784	CLA	CHD-C4C	4.62	1.52	1.41
19	A	1768	CLA	O2A-CGA	4.62	1.47	1.33
19	B	1744	CLA	O2A-CGA	4.62	1.47	1.33
19	1	1193	CLA	O2A-CGA	4.63	1.47	1.33
19	1	1148	CLA	OBD-CAD	4.63	1.29	1.22
19	A	1764	CLA	O2A-CGA	4.63	1.47	1.33
19	A	1785	CLA	CHD-C4C	4.63	1.52	1.41
19	4	1199	CLA	CHD-C4C	4.64	1.52	1.41
19	A	1817	CLA	CHD-C4C	4.64	1.52	1.41
19	H	1079	CLA	O2D-CGD	4.64	1.45	1.33
19	A	1816	CLA	CHD-C4C	4.64	1.52	1.41
19	A	1766	CLA	OBD-CAD	4.64	1.29	1.22
19	A	1767	CLA	O2A-CGA	4.64	1.47	1.33
19	B	1753	CLA	CHC-C1C	4.64	1.49	1.35
19	R	1054	CLA	CHD-C4C	4.64	1.52	1.41
19	J	1043	CLA	CHC-C1C	4.65	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1197	CLA	O2A-CGA	4.65	1.47	1.33
19	3	1222	CLA	OBD-CAD	4.65	1.29	1.22
19	1	1146	CLA	CHC-C1C	4.65	1.49	1.35
19	A	1793	CLA	OBD-CAD	4.65	1.29	1.22
19	1	1149	CLA	O2A-CGA	4.66	1.47	1.33
19	A	1789	CLA	CHC-C1C	4.66	1.49	1.35
19	A	1776	CLA	CHD-C4C	4.66	1.52	1.41
19	4	4007	CLA	CHC-C1C	4.66	1.49	1.35
19	A	1782	CLA	O2D-CGD	4.67	1.45	1.33
19	A	1774	CLA	CHC-C1C	4.67	1.50	1.35
19	A	1787	CLA	OBD-CAD	4.68	1.29	1.22
19	A	1759	CLA	O2D-CGD	4.68	1.45	1.33
19	F	1157	CLA	OBD-CAD	4.68	1.29	1.22
19	1	1187	CLA	OBD-CAD	4.68	1.29	1.22
19	4	1198	CLA	CHC-C1C	4.69	1.50	1.35
19	3	3008	CLA	OBD-CAD	4.69	1.29	1.22
19	4	1199	CLA	CHC-C1C	4.69	1.50	1.35
19	B	1755	CLA	O2D-CGD	4.69	1.45	1.33
19	B	1747	CLA	OBD-CAD	4.69	1.29	1.22
19	B	1768	CLA	O2D-CGD	4.69	1.45	1.33
19	A	1798	CLA	CHD-C4C	4.69	1.52	1.41
19	A	1774	CLA	O2D-CGD	4.70	1.45	1.33
19	A	1760	CLA	O2D-CGD	4.70	1.45	1.33
19	2	1215	CLA	CHD-C4C	4.70	1.52	1.41
19	B	1766	CLA	O2D-CGD	4.70	1.45	1.33
19	B	1747	CLA	O2A-CGA	4.71	1.47	1.33
19	R	1054	CLA	OBD-CAD	4.71	1.29	1.22
19	A	1778	CLA	CHC-C1C	4.71	1.50	1.35
19	B	1784	CLA	O2D-CGD	4.71	1.45	1.33
19	2	1222	CLA	OBD-CAD	4.71	1.29	1.22
19	B	1738	CLA	CHD-C4C	4.71	1.52	1.41
19	A	1788	CLA	CHD-C4C	4.72	1.52	1.41
19	A	1792	CLA	OBD-CAD	4.72	1.29	1.22
19	A	1780	CLA	CHD-C4C	4.72	1.52	1.41
19	A	1784	CLA	O2A-CGA	4.72	1.47	1.33
19	3	1218	CLA	O2D-CGD	4.72	1.45	1.33
19	2	2006	CLA	CHC-C1C	4.73	1.50	1.35
19	A	1761	CLA	CHC-C1C	4.73	1.50	1.35
19	A	1763	CLA	CHD-C4C	4.73	1.52	1.41
19	1	1143	CLA	CHC-C1C	4.73	1.50	1.35
19	B	1754	CLA	CHC-C1C	4.73	1.50	1.35
19	A	1781	CLA	O2D-CGD	4.73	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1762	CLA	CHD-C4C	4.73	1.52	1.41
19	I	1031	CLA	O2A-CGA	4.74	1.47	1.33
19	2	1221	CLA	CHC-C1C	4.74	1.50	1.35
19	A	1779	CLA	O2A-CGA	4.74	1.47	1.33
19	A	1771	CLA	OBD-CAD	4.74	1.29	1.22
19	1	1191	CLA	CHD-C4C	4.74	1.52	1.41
19	4	4014	CLA	CHC-C1C	4.74	1.50	1.35
19	A	1765	CLA	CHD-C4C	4.75	1.52	1.41
19	B	1768	CLA	CHC-C1C	4.75	1.50	1.35
19	1	1187	CLA	O2D-CGD	4.75	1.45	1.33
19	A	1791	CLA	CHD-C4C	4.75	1.52	1.41
19	A	1815	CLA	CHC-C1C	4.75	1.50	1.35
19	4	4014	CLA	CHD-C4C	4.76	1.52	1.41
19	R	1054	CLA	O2A-CGA	4.76	1.47	1.33
19	B	1738	CLA	CHC-C1C	4.76	1.50	1.35
19	B	1742	CLA	CHC-C1C	4.76	1.50	1.35
19	B	1736	CLA	CHD-C4C	4.76	1.52	1.41
19	F	1156	CLA	CHC-C1C	4.77	1.50	1.35
19	A	1769	CLA	O2D-CGD	4.77	1.45	1.33
19	A	1761	CLA	CHD-C4C	4.78	1.52	1.41
19	2	1221	CLA	CHD-C4C	4.78	1.52	1.41
19	B	1768	CLA	CHD-C4C	4.79	1.52	1.41
19	1	1197	CLA	OBD-CAD	4.79	1.29	1.22
19	B	1736	CLA	OBD-CAD	4.79	1.29	1.22
19	B	1759	CLA	CHC-C1C	4.79	1.50	1.35
19	B	1758	CLA	CHC-C1C	4.79	1.50	1.35
19	B	1756	CLA	O2D-CGD	4.80	1.45	1.33
19	A	1765	CLA	O2D-CGD	4.80	1.45	1.33
19	B	1752	CLA	CHD-C4C	4.80	1.52	1.41
19	4	1198	CLA	CHD-C4C	4.80	1.52	1.41
19	R	1055	CLA	O2A-CGA	4.80	1.47	1.33
19	A	1780	CLA	O2D-CGD	4.80	1.45	1.33
19	B	1744	CLA	CHD-C4C	4.81	1.52	1.41
19	3	1218	CLA	CHC-C1C	4.81	1.50	1.35
19	A	1795	CLA	CHC-C1C	4.81	1.50	1.35
19	1	1188	CLA	CHC-C1C	4.81	1.50	1.35
19	A	1760	CLA	CHD-C4C	4.82	1.52	1.41
19	A	1777	CLA	CHD-C4C	4.82	1.52	1.41
19	B	1762	CLA	O2D-CGD	4.82	1.45	1.33
19	B	1749	CLA	CHC-C1C	4.82	1.50	1.35
19	B	1749	CLA	O2D-CGD	4.83	1.45	1.33
19	1	1193	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1739	CLA	CHD-C4C	4.83	1.52	1.41
19	A	1779	CLA	CHC-C1C	4.83	1.50	1.35
19	L	1167	CLA	CHD-C4C	4.83	1.52	1.41
19	4	1206	CLA	O2D-CGD	4.83	1.45	1.33
19	1	1145	CLA	CHD-C4C	4.83	1.52	1.41
19	A	1767	CLA	CHC-C1C	4.83	1.50	1.35
19	A	1791	CLA	CHC-C1C	4.83	1.50	1.35
19	A	1799	CLA	CHD-C4C	4.84	1.52	1.41
19	B	1767	CLA	CHC-C1C	4.84	1.50	1.35
19	A	1814	CLA	O2A-CGA	4.84	1.47	1.33
19	A	1779	CLA	CHD-C4C	4.84	1.52	1.41
19	B	1747	CLA	CHD-C4C	4.84	1.52	1.41
19	B	1771	CLA	O2D-CGD	4.84	1.45	1.33
19	B	1767	CLA	O2D-CGD	4.85	1.45	1.33
19	4	1200	CLA	CHC-C1C	4.85	1.50	1.35
19	B	1752	CLA	CHC-C1C	4.85	1.50	1.35
19	1	1308	CLA	CHC-C1C	4.85	1.50	1.35
19	B	1739	CLA	CHC-C1C	4.86	1.50	1.35
19	A	1763	CLA	CHC-C1C	4.86	1.50	1.35
19	B	1741	CLA	CHC-C1C	4.87	1.50	1.35
19	B	1735	CLA	CHD-C4C	4.87	1.52	1.41
19	B	1746	CLA	OBD-CAD	4.87	1.29	1.22
19	1	1149	CLA	CHD-C4C	4.87	1.52	1.41
19	B	1758	CLA	O2D-CGD	4.87	1.45	1.33
19	B	1743	CLA	O2D-CGD	4.87	1.45	1.33
19	A	1783	CLA	CHC-C1C	4.87	1.50	1.35
19	1	1309	CLA	CHD-C4C	4.88	1.52	1.41
19	B	1755	CLA	CHC-C1C	4.88	1.50	1.35
19	A	1814	CLA	CHC-C1C	4.88	1.50	1.35
19	A	1788	CLA	CHC-C1C	4.88	1.50	1.35
19	4	1200	CLA	O2D-CGD	4.88	1.45	1.33
19	A	1783	CLA	CHD-C4C	4.88	1.52	1.41
19	1	1149	CLA	CHC-C1C	4.88	1.50	1.35
19	A	1786	CLA	O2A-CGA	4.88	1.48	1.33
19	2	1222	CLA	O2A-CGA	4.88	1.48	1.33
19	A	1793	CLA	O2D-CGD	4.89	1.45	1.33
19	A	1790	CLA	CHD-C4C	4.89	1.52	1.41
19	3	1213	CLA	OBD-CAD	4.89	1.29	1.22
19	A	1800	CLA	CHC-C1C	4.89	1.50	1.35
19	A	1813	CLA	CHC-C1C	4.89	1.50	1.35
19	4	1201	CLA	CHC-C1C	4.89	1.50	1.35
19	4	1209	CLA	CHC-C1C	4.89	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1772	CLA	CHC-C1C	4.89	1.50	1.35
19	A	1768	CLA	CHC-C1C	4.89	1.50	1.35
19	A	1786	CLA	CHD-C4C	4.90	1.52	1.41
19	1	1191	CLA	CHC-C1C	4.90	1.50	1.35
19	F	1155	CLA	CHD-C4C	4.91	1.52	1.41
19	A	1775	CLA	OBD-CAD	4.91	1.29	1.22
19	A	1762	CLA	CHC-C1C	4.91	1.50	1.35
19	3	3008	CLA	CHD-C4C	4.91	1.52	1.41
19	A	1795	CLA	O2D-CGD	4.91	1.45	1.33
19	B	1751	CLA	OBD-CAD	4.91	1.29	1.22
19	2	1213	CLA	O2D-CGD	4.91	1.45	1.33
19	B	1761	CLA	O2D-CGD	4.91	1.45	1.33
19	2	1212	CLA	O2D-CGD	4.91	1.45	1.33
19	2	1222	CLA	CHC-C1C	4.92	1.50	1.35
19	1	1142	CLA	O2D-CGD	4.92	1.45	1.33
19	A	1782	CLA	CHC-C1C	4.92	1.50	1.35
19	B	1784	CLA	CHC-C1C	4.92	1.50	1.35
19	4	1211	CLA	CHC-C1C	4.92	1.50	1.35
19	B	1738	CLA	O2D-CGD	4.93	1.45	1.33
19	A	1792	CLA	CHC-C1C	4.93	1.50	1.35
19	B	1756	CLA	CHC-C1C	4.93	1.50	1.35
19	B	1772	CLA	CHC-C1C	4.93	1.50	1.35
19	A	1764	CLA	O2D-CGD	4.93	1.45	1.33
19	A	1773	CLA	CHC-C1C	4.94	1.50	1.35
19	B	1757	CLA	CHD-C4C	4.94	1.52	1.41
19	B	1760	CLA	CHD-C4C	4.94	1.52	1.41
19	3	1217	CLA	CHD-C4C	4.94	1.52	1.41
19	B	1744	CLA	OBD-CAD	4.94	1.29	1.22
19	2	1223	CLA	CHC-C1C	4.95	1.50	1.35
19	3	1222	CLA	CHC-C1C	4.95	1.50	1.35
19	R	1054	CLA	CHC-C1C	4.95	1.50	1.35
19	A	1787	CLA	CHD-C4C	4.95	1.52	1.41
19	A	1785	CLA	CHC-C1C	4.95	1.50	1.35
19	A	1815	CLA	O2D-CGD	4.95	1.45	1.33
19	1	1192	CLA	CHC-C1C	4.95	1.50	1.35
19	B	1772	CLA	OBD-CAD	4.96	1.29	1.22
19	A	1790	CLA	CHC-C1C	4.96	1.50	1.35
19	3	3011	CLA	O2D-CGD	4.97	1.45	1.33
19	L	1167	CLA	CHC-C1C	4.97	1.50	1.35
19	2	1212	CLA	CHC-C1C	4.97	1.50	1.35
19	B	1750	CLA	O2D-CGD	4.97	1.45	1.33
19	A	1778	CLA	CHD-C4C	4.97	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1764	CLA	CHC-C1C	4.97	1.50	1.35
19	1	1189	CLA	O2D-CGD	4.97	1.45	1.33
19	A	1778	CLA	OBD-CAD	4.97	1.29	1.22
19	2	1219	CLA	CHC-C1C	4.97	1.50	1.35
19	A	1784	CLA	O2D-CGD	4.98	1.45	1.33
19	A	1775	CLA	CHC-C1C	4.98	1.50	1.35
19	B	1751	CLA	CHC-C1C	4.98	1.50	1.35
19	B	1746	CLA	CHC-C1C	4.98	1.50	1.35
19	A	1772	CLA	O2D-CGD	4.98	1.45	1.33
19	B	1766	CLA	CHC-C1C	4.98	1.51	1.35
19	F	1156	CLA	O2D-CGD	4.98	1.45	1.33
19	H	1080	CLA	OBD-CAD	4.98	1.30	1.22
19	1	1145	CLA	CHC-C1C	4.98	1.51	1.35
19	2	1223	CLA	O2D-CGD	4.99	1.45	1.33
19	1	1505	CLA	CHC-C1C	4.99	1.51	1.35
19	A	1786	CLA	O2D-CGD	4.99	1.45	1.33
19	B	1769	CLA	CHC-C1C	4.99	1.51	1.35
19	4	1199	CLA	OBD-CAD	4.99	1.30	1.22
19	L	1168	CLA	OBD-CAD	4.99	1.30	1.22
19	A	1761	CLA	O2A-CGA	4.99	1.48	1.33
19	A	1816	CLA	CHC-C1C	4.99	1.51	1.35
19	A	1814	CLA	O2D-CGD	5.00	1.46	1.33
19	1	1199	CLA	O2D-CGD	5.00	1.46	1.33
19	A	1794	CLA	O2D-CGD	5.00	1.46	1.33
19	L	1168	CLA	CHC-C1C	5.00	1.51	1.35
19	A	1762	CLA	OBD-CAD	5.00	1.30	1.22
19	A	1784	CLA	CHC-C1C	5.01	1.51	1.35
19	3	1221	CLA	O2D-CGD	5.01	1.46	1.33
19	1	1145	CLA	O2A-CGA	5.01	1.48	1.33
19	A	1786	CLA	CHC-C1C	5.01	1.51	1.35
19	1	1148	CLA	CHC-C1C	5.01	1.51	1.35
19	R	1055	CLA	CHC-C1C	5.01	1.51	1.35
19	B	1744	CLA	CHC-C1C	5.01	1.51	1.35
19	4	1196	CLA	CHC-C1C	5.01	1.51	1.35
19	B	1757	CLA	O2D-CGD	5.01	1.46	1.33
19	A	1817	CLA	CHC-C1C	5.01	1.51	1.35
19	A	1815	CLA	OBD-CAD	5.02	1.30	1.22
19	A	1760	CLA	OBD-CAD	5.02	1.30	1.22
19	2	1221	CLA	O2D-CGD	5.02	1.46	1.33
19	A	1780	CLA	CHC-C1C	5.03	1.51	1.35
19	1	1142	CLA	CHC-C1C	5.03	1.51	1.35
19	A	1816	CLA	O2D-CGD	5.03	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1781	CLA	CHC-C1C	5.03	1.51	1.35
19	H	1080	CLA	CHD-C4C	5.03	1.53	1.41
19	A	1797	CLA	O2A-CGA	5.03	1.48	1.33
19	B	1765	CLA	CHC-C1C	5.04	1.51	1.35
19	A	1785	CLA	O2D-CGD	5.04	1.46	1.33
19	F	1155	CLA	CHC-C1C	5.04	1.51	1.35
19	A	1771	CLA	CHC-C1C	5.04	1.51	1.35
19	A	1794	CLA	CHC-C1C	5.05	1.51	1.35
19	1	1148	CLA	O2D-CGD	5.05	1.46	1.33
19	1	1188	CLA	OBD-CAD	5.05	1.30	1.22
19	I	1031	CLA	O2D-CGD	5.05	1.46	1.33
19	A	1798	CLA	CHC-C1C	5.05	1.51	1.35
19	A	1800	CLA	O2D-CGD	5.05	1.46	1.33
19	A	1787	CLA	CHC-C1C	5.06	1.51	1.35
19	1	1014	CLA	CHC-C1C	5.06	1.51	1.35
19	B	1750	CLA	CHC-C1C	5.06	1.51	1.35
19	B	1736	CLA	O2D-CGD	5.06	1.46	1.33
19	A	1769	CLA	CHC-C1C	5.07	1.51	1.35
19	R	1055	CLA	OBD-CAD	5.07	1.30	1.22
19	A	1766	CLA	CHD-C4C	5.07	1.53	1.41
19	4	1197	CLA	CHC-C1C	5.07	1.51	1.35
19	B	1747	CLA	CHC-C1C	5.07	1.51	1.35
19	A	1767	CLA	O2D-CGD	5.08	1.46	1.33
19	A	1793	CLA	CHC-C1C	5.08	1.51	1.35
19	A	1815	CLA	CHD-C4C	5.08	1.53	1.41
19	H	1080	CLA	CHC-C1C	5.09	1.51	1.35
19	1	1191	CLA	OBD-CAD	5.09	1.30	1.22
19	B	1742	CLA	O2D-CGD	5.09	1.46	1.33
19	A	1801	CLA	CHC-C1C	5.09	1.51	1.35
19	A	1767	CLA	CHD-C4C	5.10	1.53	1.41
19	A	1760	CLA	O2A-CGA	5.10	1.48	1.33
19	B	1763	CLA	O2D-CGD	5.10	1.46	1.33
22	B	1773	PQN	C10-C5	5.10	1.48	1.40
19	B	1770	CLA	CHC-C1C	5.10	1.51	1.35
19	4	1199	CLA	O2D-CGD	5.10	1.46	1.33
19	4	1197	CLA	OBD-CAD	5.10	1.30	1.22
19	A	1792	CLA	O2D-CGD	5.10	1.46	1.33
19	A	1796	CLA	CHC-C1C	5.11	1.51	1.35
19	4	1201	CLA	O2D-CGD	5.11	1.46	1.33
19	A	1771	CLA	CHD-C4C	5.11	1.53	1.41
19	1	1197	CLA	O2D-CGD	5.12	1.46	1.33
19	B	1754	CLA	O2D-CGD	5.12	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1759	CLA	O2D-CGD	5.12	1.46	1.33
19	B	1760	CLA	CHC-C1C	5.13	1.51	1.35
19	A	1817	CLA	O2D-CGD	5.13	1.46	1.33
19	G	1099	CLA	CHC-C1C	5.13	1.51	1.35
19	A	1773	CLA	O2D-CGD	5.13	1.46	1.33
19	G	1099	CLA	O2D-CGD	5.14	1.46	1.33
19	1	1143	CLA	O2D-CGD	5.14	1.46	1.33
19	A	1813	CLA	O2D-CGD	5.14	1.46	1.33
19	B	1765	CLA	O2D-CGD	5.14	1.46	1.33
19	B	1746	CLA	O2D-CGD	5.14	1.46	1.33
19	2	1217	CLA	O2D-CGD	5.14	1.46	1.33
19	F	1157	CLA	O2D-CGD	5.14	1.46	1.33
19	A	1764	CLA	CHC-C1C	5.15	1.51	1.35
19	B	1739	CLA	O2D-CGD	5.15	1.46	1.33
19	A	1763	CLA	O2D-CGD	5.15	1.46	1.33
19	1	1308	CLA	O2D-CGD	5.15	1.46	1.33
19	I	1031	CLA	CHC-C1C	5.15	1.51	1.35
19	1	1193	CLA	CHC-C1C	5.15	1.51	1.35
19	1	1196	CLA	CHC-C1C	5.16	1.51	1.35
19	B	1757	CLA	CHC-C1C	5.16	1.51	1.35
19	A	1760	CLA	CHC-C1C	5.17	1.51	1.35
19	B	1770	CLA	O2D-CGD	5.17	1.46	1.33
19	3	1222	CLA	O2D-CGD	5.17	1.46	1.33
19	1	1189	CLA	CHC-C1C	5.17	1.51	1.35
19	B	1762	CLA	CHC-C1C	5.17	1.51	1.35
19	B	1735	CLA	CHC-C1C	5.17	1.51	1.35
19	B	1745	CLA	CHC-C1C	5.19	1.51	1.35
19	2	2006	CLA	O2D-CGD	5.19	1.46	1.33
19	A	1778	CLA	O2D-CGD	5.20	1.46	1.33
19	A	1787	CLA	O2D-CGD	5.20	1.46	1.33
19	B	1747	CLA	O2D-CGD	5.20	1.46	1.33
19	L	1167	CLA	O2D-CGD	5.20	1.46	1.33
19	B	1764	CLA	O2D-CGD	5.21	1.46	1.33
19	A	1777	CLA	CHC-C1C	5.21	1.51	1.35
19	A	1796	CLA	O2D-CGD	5.22	1.46	1.33
19	A	1768	CLA	O2D-CGD	5.22	1.46	1.33
19	A	1776	CLA	CHC-C1C	5.22	1.51	1.35
19	4	1205	CLA	O2D-CGD	5.23	1.46	1.33
19	A	1762	CLA	O2D-CGD	5.23	1.46	1.33
19	3	1217	CLA	O2D-CGD	5.23	1.46	1.33
19	H	1081	CLA	CHC-C1C	5.24	1.51	1.35
19	A	1791	CLA	O2D-CGD	5.24	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1751	CLA	O2D-CGD	5.25	1.46	1.33
19	A	1777	CLA	O2D-CGD	5.25	1.46	1.33
19	A	1779	CLA	O2D-CGD	5.26	1.46	1.33
19	A	1790	CLA	O2D-CGD	5.26	1.46	1.33
19	4	4007	CLA	O2D-CGD	5.26	1.46	1.33
19	B	1743	CLA	CHC-C1C	5.28	1.51	1.35
19	A	1794	CLA	OBD-CAD	5.28	1.30	1.22
19	B	1735	CLA	O2D-CGD	5.30	1.46	1.33
19	B	1736	CLA	CHC-C1C	5.30	1.52	1.35
19	A	1766	CLA	CHC-C1C	5.30	1.52	1.35
19	A	1801	CLA	O2D-CGD	5.32	1.46	1.33
19	A	1776	CLA	O2D-CGD	5.33	1.46	1.33
19	B	1752	CLA	O2D-CGD	5.33	1.46	1.33
19	1	1192	CLA	OBD-CAD	5.34	1.30	1.22
19	2	1215	CLA	CHC-C1C	5.34	1.52	1.35
19	A	1761	CLA	O2D-CGD	5.34	1.46	1.33
19	A	1798	CLA	O2D-CGD	5.34	1.46	1.33
19	H	1080	CLA	O2D-CGD	5.35	1.46	1.33
19	3	3008	CLA	CHC-C1C	5.35	1.52	1.35
19	L	1168	CLA	O2D-CGD	5.36	1.46	1.33
19	1	1190	CLA	O2D-CGD	5.37	1.46	1.33
19	1	1014	CLA	O2D-CGD	5.37	1.46	1.33
19	B	1744	CLA	O2D-CGD	5.38	1.46	1.33
19	2	1222	CLA	O2D-CGD	5.38	1.46	1.33
19	B	1745	CLA	O2D-CGD	5.38	1.46	1.33
22	A	1802	PQN	C10-C5	5.39	1.49	1.40
19	B	1754	CLA	OBD-CAD	5.40	1.30	1.22
19	R	1055	CLA	O2D-CGD	5.40	1.47	1.33
19	4	1198	CLA	O2D-CGD	5.41	1.47	1.33
19	4	1196	CLA	O2D-CGD	5.42	1.47	1.33
19	H	1081	CLA	O2D-CGD	5.42	1.47	1.33
19	1	1146	CLA	O2D-CGD	5.43	1.47	1.33
19	1	1199	CLA	OBD-CAD	5.44	1.30	1.22
19	A	1766	CLA	O2D-CGD	5.45	1.47	1.33
19	1	1505	CLA	O2D-CGD	5.46	1.47	1.33
19	2	1215	CLA	O2D-CGD	5.48	1.47	1.33
19	1	1192	CLA	O2D-CGD	5.49	1.47	1.33
19	A	1771	CLA	O2D-CGD	5.50	1.47	1.33
19	R	1054	CLA	O2D-CGD	5.50	1.47	1.33
19	1	1149	CLA	O2D-CGD	5.51	1.47	1.33
19	A	1797	CLA	O2D-CGD	5.52	1.47	1.33
19	B	1760	CLA	O2D-CGD	5.63	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	3008	CLA	O2D-CGD	5.63	1.47	1.33
19	A	1801	CLA	OBD-CAD	5.65	1.31	1.22
19	1	1145	CLA	O2D-CGD	5.71	1.47	1.33
19	1	1188	CLA	O2D-CGD	5.90	1.48	1.33
19	3	1213	CLA	CHC-C1C	5.93	1.53	1.35
22	A	1802	PQN	C3-C2	6.08	1.49	1.35
22	B	1773	PQN	C3-C2	6.13	1.49	1.35

All (3617) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1189	CLA	OBD-CAD-CBD	-17.99	98.80	125.94
19	1	1199	CLA	OBD-CAD-CBD	-17.48	99.56	125.94
19	A	1789	CLA	OBD-CAD-CBD	-17.41	99.66	125.94
19	B	1748	CLA	OBD-CAD-CBD	-17.02	100.26	125.94
19	A	1763	CLA	OBD-CAD-CBD	-16.60	100.89	125.94
19	A	1783	CLA	OBD-CAD-CBD	-14.89	103.47	125.94
19	A	1800	CLA	OBD-CAD-CBD	-14.49	104.08	125.94
19	4	4014	CLA	OBD-CAD-CBD	-14.43	104.16	125.94
19	4	1201	CLA	OBD-CAD-CBD	-14.40	104.20	125.94
19	3	1217	CLA	OBD-CAD-CBD	-14.32	104.33	125.94
19	1	1145	CLA	OBD-CAD-CBD	-14.28	104.39	125.94
19	2	1222	CLA	OBD-CAD-CBD	-14.03	104.77	125.94
19	4	1200	CLA	OBD-CAD-CBD	-13.89	104.98	125.94
19	B	1756	CLA	OBD-CAD-CBD	-13.83	105.06	125.94
19	A	1813	CLA	OBD-CAD-CBD	-13.80	105.11	125.94
19	H	1080	CLA	OBD-CAD-CBD	-13.72	105.23	125.94
19	B	1743	CLA	OBD-CAD-CBD	-13.67	105.31	125.94
19	B	1757	CLA	OBD-CAD-CBD	-13.62	105.39	125.94
19	4	1206	CLA	OBD-CAD-C3D	-13.57	100.66	128.35
19	A	1792	CLA	OBD-CAD-CBD	-13.56	105.47	125.94
19	A	1789	CLA	OBD-CAD-C3D	-13.44	100.92	128.35
19	2	1213	CLA	OBD-CAD-C3D	-13.35	101.12	128.35
19	B	1769	CLA	OBD-CAD-C3D	-13.10	101.62	128.35
19	4	4007	CLA	OBD-CAD-CBD	-13.01	106.31	125.94
19	B	1749	CLA	OBD-CAD-CBD	-12.93	106.43	125.94
19	3	1221	CLA	OBD-CAD-CBD	-12.93	106.43	125.94
19	A	1796	CLA	OBD-CAD-CBD	-12.85	106.55	125.94
19	3	3011	CLA	OBD-CAD-C3D	-12.78	102.28	128.35
19	I	1031	CLA	OBD-CAD-CBD	-12.75	106.71	125.94
19	R	1054	CLA	OBD-CAD-CBD	-12.71	106.75	125.94
19	A	1793	CLA	OBD-CAD-CBD	-12.67	106.82	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1772	CLA	OBD-CAD-CBD	-12.64	106.87	125.94
19	1	1149	CLA	CAB-C3B-C4B	-12.62	107.49	128.36
19	2	1221	CLA	OBD-CAD-CBD	-12.57	106.97	125.94
19	A	1766	CLA	OBD-CAD-CBD	-12.55	107.01	125.94
19	1	1014	CLA	OBD-CAD-CBD	-12.47	107.12	125.94
19	B	1784	CLA	OBD-CAD-CBD	-12.45	107.15	125.94
19	4	1197	CLA	CAB-C3B-C4B	-12.36	107.91	128.36
19	B	1741	CLA	CAB-C3B-C4B	-12.35	107.94	128.36
19	B	1764	CLA	OBD-CAD-CBD	-12.33	107.34	125.94
19	1	1142	CLA	OBD-CAD-CBD	-12.32	107.36	125.94
19	A	1816	CLA	OBD-CAD-CBD	-12.31	107.36	125.94
19	4	1206	CLA	OBD-CAD-CBD	-12.30	107.38	125.94
19	2	1219	CLA	CAB-C3B-C4B	-12.30	108.01	128.36
19	L	1167	CLA	OBD-CAD-CBD	-12.30	107.39	125.94
19	B	1772	CLA	CAB-C3B-C4B	-12.21	108.15	128.36
19	2	1215	CLA	OBD-CAD-CBD	-12.20	107.53	125.94
19	A	1781	CLA	OBD-CAD-CBD	-12.19	107.54	125.94
19	B	1750	CLA	OBD-CAD-CBD	-12.16	107.59	125.94
19	4	1209	CLA	CAB-C3B-C4B	-12.14	108.28	128.36
19	B	1763	CLA	OBD-CAD-CBD	-12.14	107.62	125.94
19	1	1190	CLA	OBD-CAD-CBD	-12.11	107.66	125.94
19	A	1785	CLA	OBD-CAD-CBD	-12.09	107.69	125.94
19	2	1221	CLA	OBD-CAD-C3D	-12.08	103.70	128.35
19	3	1218	CLA	OBD-CAD-CBD	-12.04	107.77	125.94
19	B	1755	CLA	OBD-CAD-CBD	-12.04	107.77	125.94
19	B	1757	CLA	OBD-CAD-C3D	-12.03	103.80	128.35
19	A	1759	CLA	OBD-CAD-C3D	-12.00	103.86	128.35
19	B	1769	CLA	OBD-CAD-CBD	-12.00	107.83	125.94
19	1	1197	CLA	OBD-CAD-C3D	-11.94	103.99	128.35
19	A	1786	CLA	OBD-CAD-CBD	-11.93	107.94	125.94
19	1	1199	CLA	OBD-CAD-C3D	-11.92	104.02	128.35
19	B	1761	CLA	OBD-CAD-CBD	-11.87	108.03	125.94
19	A	1791	CLA	OBD-CAD-C3D	-11.85	104.17	128.35
19	3	1218	CLA	OBD-CAD-C3D	-11.84	104.19	128.35
19	2	1223	CLA	OBD-CAD-CBD	-11.82	108.11	125.94
19	A	1762	CLA	OBD-CAD-CBD	-11.79	108.15	125.94
19	A	1759	CLA	OBD-CAD-CBD	-11.77	108.18	125.94
19	H	1081	CLA	OBD-CAD-CBD	-11.71	108.27	125.94
19	1	1149	CLA	OBD-CAD-CBD	-11.66	108.35	125.94
19	A	1776	CLA	OBD-CAD-CBD	-11.65	108.36	125.94
19	1	1505	CLA	OBD-CAD-CBD	-11.63	108.39	125.94
19	B	1737	CLA	OBD-CAD-CBD	-11.60	108.43	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1217	CLA	OBD-CAD-CBD	-11.54	108.53	125.94
19	3	1221	CLA	OBD-CAD-C3D	-11.51	104.87	128.35
19	A	1814	CLA	OBD-CAD-CBD	-11.50	108.59	125.94
23	A	1807	BCR	C24-C23-C22	-11.50	108.69	126.22
19	1	1149	CLA	OBD-CAD-C3D	-11.47	104.95	128.35
19	B	1741	CLA	OBD-CAD-C3D	-11.46	104.97	128.35
19	A	1784	CLA	OBD-CAD-CBD	-11.45	108.66	125.94
19	1	1196	CLA	CAB-C3B-C4B	-11.43	109.45	128.36
19	B	1760	CLA	OBD-CAD-CBD	-11.40	108.73	125.94
19	B	1753	CLA	OBD-CAD-CBD	-11.40	108.74	125.94
19	A	1772	CLA	OBD-CAD-C3D	-11.37	105.15	128.35
19	4	1196	CLA	OBD-CAD-C3D	-11.36	105.17	128.35
19	A	1777	CLA	OBD-CAD-C3D	-11.34	105.20	128.35
19	B	1751	CLA	OBD-CAD-CBD	-11.34	108.83	125.94
19	A	1791	CLA	OBD-CAD-CBD	-11.34	108.83	125.94
19	B	1752	CLA	OBD-CAD-CBD	-11.27	108.94	125.94
19	B	1748	CLA	OBD-CAD-C3D	-11.26	105.37	128.35
19	B	1751	CLA	OBD-CAD-C3D	-11.24	105.41	128.35
19	A	1788	CLA	OBD-CAD-CBD	-11.22	109.01	125.94
19	A	1786	CLA	OBD-CAD-C3D	-11.20	105.50	128.35
19	A	1795	CLA	OBD-CAD-CBD	-11.20	109.04	125.94
19	R	1055	CLA	OBD-CAD-CBD	-11.18	109.07	125.94
19	3	3011	CLA	OBD-CAD-CBD	-11.18	109.07	125.94
19	B	1763	CLA	OBD-CAD-C3D	-11.12	105.65	128.35
19	A	1778	CLA	OBD-CAD-CBD	-11.12	109.17	125.94
19	A	1773	CLA	OBD-CAD-CBD	-11.11	109.18	125.94
19	B	1739	CLA	OBD-CAD-CBD	-11.10	109.19	125.94
19	A	1781	CLA	OBD-CAD-C3D	-11.08	105.74	128.35
19	2	1213	CLA	OBD-CAD-CBD	-11.07	109.23	125.94
19	A	1766	CLA	OBD-CAD-C3D	-11.03	105.83	128.35
19	1	1193	CLA	OBD-CAD-CBD	-11.03	109.30	125.94
19	L	1168	CLA	OBD-CAD-CBD	-10.99	109.36	125.94
19	2	1222	CLA	OBD-CAD-C3D	-10.99	105.93	128.35
19	A	1764	CLA	OBD-CAD-C3D	-10.99	105.93	128.35
19	A	1761	CLA	OBD-CAD-C3D	-10.96	105.98	128.35
19	A	1775	CLA	CAB-C3B-C4B	-10.96	110.23	128.36
19	4	1198	CLA	OBD-CAD-C3D	-10.95	106.00	128.35
19	1	1188	CLA	OBD-CAD-CBD	-10.95	109.41	125.94
19	G	1099	CLA	OBD-CAD-C3D	-10.95	106.01	128.35
19	F	1157	CLA	OBD-CAD-C3D	-10.94	106.03	128.35
19	A	1800	CLA	OBD-CAD-C3D	-10.94	106.03	128.35
19	1	1189	CLA	OBD-CAD-C3D	-10.90	106.11	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1776	CLA	OBD-CAD-C3D	-10.87	106.16	128.35
19	1	1145	CLA	OBD-CAD-C3D	-10.87	106.17	128.35
19	1	1148	CLA	OBD-CAD-C3D	-10.86	106.19	128.35
19	3	1217	CLA	OBD-CAD-C3D	-10.85	106.21	128.35
19	1	1143	CLA	OBD-CAD-CBD	-10.84	109.58	125.94
19	L	1168	CLA	OBD-CAD-C3D	-10.83	106.26	128.35
19	B	1784	CLA	OBD-CAD-C3D	-10.82	106.28	128.35
19	A	1783	CLA	OBD-CAD-C3D	-10.82	106.28	128.35
19	J	1043	CLA	OBD-CAD-CBD	-10.81	109.63	125.94
19	F	1156	CLA	OBD-CAD-CBD	-10.79	109.65	125.94
19	B	1742	CLA	OBD-CAD-CBD	-10.79	109.66	125.94
19	1	1146	CLA	OBD-CAD-CBD	-10.78	109.67	125.94
19	4	1201	CLA	OBD-CAD-C3D	-10.76	106.39	128.35
19	A	1790	CLA	OBD-CAD-CBD	-10.75	109.72	125.94
19	B	1755	CLA	OBD-CAD-C3D	-10.75	106.42	128.35
19	4	1198	CLA	OBD-CAD-CBD	-10.74	109.73	125.94
19	2	1217	CLA	OBD-CAD-C3D	-10.73	106.45	128.35
19	A	1798	CLA	OBD-CAD-CBD	-10.71	109.77	125.94
19	F	1157	CLA	OBD-CAD-CBD	-10.70	109.80	125.94
19	1	1143	CLA	OBD-CAD-C3D	-10.69	106.54	128.35
19	A	1769	CLA	OBD-CAD-CBD	-10.66	109.85	125.94
19	A	1773	CLA	OBD-CAD-C3D	-10.63	106.66	128.35
19	B	1767	CLA	OBD-CAD-C3D	-10.62	106.67	128.35
19	1	1014	CLA	OBD-CAD-C3D	-10.60	106.71	128.35
19	4	1205	CLA	OBD-CAD-CBD	-10.55	110.01	125.94
19	F	1156	CLA	OBD-CAD-C3D	-10.55	106.83	128.35
19	G	1099	CLA	OBD-CAD-CBD	-10.53	110.05	125.94
19	1	1190	CLA	OBD-CAD-C3D	-10.52	106.88	128.35
19	3	1222	CLA	OBD-CAD-C3D	-10.52	106.88	128.35
19	I	1031	CLA	OBD-CAD-C3D	-10.49	106.95	128.35
19	A	1775	CLA	OBD-CAD-C3D	-10.48	106.96	128.35
19	A	1788	CLA	OBD-CAD-C3D	-10.47	106.99	128.35
19	A	1817	CLA	OBD-CAD-CBD	-10.47	110.14	125.94
19	R	1054	CLA	OBD-CAD-C3D	-10.45	107.03	128.35
19	H	1080	CLA	OBD-CAD-C3D	-10.44	107.05	128.35
19	A	1816	CLA	OBD-CAD-C3D	-10.44	107.05	128.35
19	A	1782	CLA	OBD-CAD-C3D	-10.43	107.07	128.35
19	B	1738	CLA	OBD-CAD-C3D	-10.41	107.10	128.35
19	B	1766	CLA	OBD-CAD-CBD	-10.40	110.24	125.94
19	B	1741	CLA	OBD-CAD-CBD	-10.38	110.28	125.94
19	A	1814	CLA	OBD-CAD-C3D	-10.35	107.23	128.35
19	A	1779	CLA	OBD-CAD-CBD	-10.35	110.32	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1197	CLA	OBD-CAD-C3D	-10.35	107.24	128.35
19	A	1779	CLA	OBD-CAD-C3D	-10.34	107.25	128.35
19	1	1142	CLA	OBD-CAD-C3D	-10.31	107.32	128.35
19	A	1785	CLA	OBD-CAD-C3D	-10.30	107.33	128.35
23	A	1808	BCR	C7-C8-C9	-10.29	110.52	126.22
19	A	1760	CLA	OBD-CAD-CBD	-10.29	110.41	125.94
19	A	1795	CLA	OBD-CAD-C3D	-10.28	107.37	128.35
19	B	1742	CLA	OBD-CAD-C3D	-10.28	107.37	128.35
19	1	1146	CLA	OBD-CAD-C3D	-10.28	107.38	128.35
19	3	1213	CLA	OBD-CAD-C3D	-10.26	107.41	128.35
19	1	1148	CLA	OBD-CAD-CBD	-10.26	110.46	125.94
19	2	1223	CLA	OBD-CAD-C3D	-10.25	107.44	128.35
19	A	1768	CLA	OBD-CAD-CBD	-10.20	110.54	125.94
19	A	1762	CLA	OBD-CAD-C3D	-10.20	107.54	128.35
19	4	1200	CLA	OBD-CAD-C3D	-10.19	107.55	128.35
19	B	1761	CLA	OBD-CAD-C3D	-10.15	107.64	128.35
19	A	1815	CLA	OBD-CAD-C3D	-10.14	107.66	128.35
19	B	1764	CLA	OBD-CAD-C3D	-10.14	107.66	128.35
19	1	1308	CLA	OBD-CAD-C3D	-10.06	107.83	128.35
19	B	1746	CLA	OBD-CAD-CBD	-10.04	110.80	125.94
19	1	1191	CLA	OBD-CAD-C3D	-10.00	107.94	128.35
19	B	1750	CLA	OBD-CAD-C3D	-10.00	107.95	128.35
19	L	1167	CLA	OBD-CAD-C3D	-9.99	107.96	128.35
19	B	1756	CLA	OBD-CAD-C3D	-9.99	107.97	128.35
19	2	1212	CLA	OBD-CAD-C3D	-9.96	108.03	128.35
19	A	1815	CLA	OBD-CAD-CBD	-9.95	110.92	125.94
19	A	1782	CLA	OBD-CAD-CBD	-9.93	110.95	125.94
19	B	1772	CLA	C3D-CAD-CBD	-9.90	101.14	107.75
19	1	1187	CLA	OBD-CAD-C3D	-9.86	108.22	128.35
19	2	2006	CLA	OBD-CAD-C3D	-9.78	108.39	128.35
19	4	1197	CLA	C3D-CAD-CBD	-9.77	101.22	107.75
19	B	1766	CLA	OBD-CAD-C3D	-9.77	108.42	128.35
19	B	1735	CLA	OBD-CAD-CBD	-9.76	111.21	125.94
19	B	1765	CLA	OBD-CAD-C3D	-9.74	108.47	128.35
19	B	1736	CLA	OBD-CAD-CBD	-9.74	111.24	125.94
19	H	1081	CLA	OBD-CAD-C3D	-9.74	108.48	128.35
19	B	1770	CLA	OBD-CAD-CBD	-9.72	111.27	125.94
19	4	1209	CLA	C3D-CAD-CBD	-9.71	101.27	107.75
19	4	1196	CLA	OBD-CAD-CBD	-9.70	111.30	125.94
19	2	1219	CLA	OBD-CAD-C3D	-9.66	108.63	128.35
23	A	1808	BCR	C15-C16-C17	-9.64	102.08	123.39
19	1	1191	CLA	CAB-C3B-C4B	-9.63	112.43	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1753	CLA	OBD-CAD-C3D	-9.62	108.72	128.35
19	A	1777	CLA	OBD-CAD-CBD	-9.62	111.42	125.94
19	3	1222	CLA	OBD-CAD-CBD	-9.58	111.49	125.94
19	A	1771	CLA	OBD-CAD-CBD	-9.56	111.50	125.94
19	B	1738	CLA	OBD-CAD-CBD	-9.56	111.52	125.94
19	B	1745	CLA	OBD-CAD-C3D	-9.54	108.89	128.35
19	1	1308	CLA	OBD-CAD-CBD	-9.52	111.58	125.94
19	A	1764	CLA	OBD-CAD-CBD	-9.49	111.62	125.94
19	A	1774	CLA	OBD-CAD-CBD	-9.45	111.67	125.94
19	1	1191	CLA	C3D-CAD-CBD	-9.45	101.43	107.75
19	A	1796	CLA	OBD-CAD-C3D	-9.44	109.08	128.35
19	1	1505	CLA	OBD-CAD-C3D	-9.43	109.10	128.35
19	4	1209	CLA	OBD-CAD-C3D	-9.43	109.12	128.35
19	A	1765	CLA	OBD-CAD-CBD	-9.40	111.75	125.94
19	2	1219	CLA	C3D-CAD-CBD	-9.37	101.49	107.75
19	A	1787	CLA	OBD-CAD-CBD	-9.36	111.81	125.94
19	A	1763	CLA	OBD-CAD-C3D	-9.36	109.25	128.35
19	B	1741	CLA	CAB-C3B-C2B	-9.35	106.02	125.14
19	2	1212	CLA	OBD-CAD-CBD	-9.32	111.87	125.94
19	1	1193	CLA	OBD-CAD-C3D	-9.31	109.35	128.35
19	A	1817	CLA	OBD-CAD-C3D	-9.29	109.39	128.35
19	A	1784	CLA	OBD-CAD-C3D	-9.26	109.45	128.35
19	B	1749	CLA	OBD-CAD-C3D	-9.26	109.47	128.35
19	B	1770	CLA	OBD-CAD-C3D	-9.25	109.48	128.35
19	1	1149	CLA	C3D-CAD-CBD	-9.22	94.56	107.60
19	A	1771	CLA	OBD-CAD-C3D	-9.22	109.55	128.35
19	4	1199	CLA	OBD-CAD-C3D	-9.21	109.56	128.35
19	A	1793	CLA	OBD-CAD-C3D	-9.21	109.57	128.35
19	B	1736	CLA	OBD-CAD-C3D	-9.20	109.57	128.35
19	B	1768	CLA	OBD-CAD-CBD	-9.19	112.07	125.94
19	B	1752	CLA	OBD-CAD-C3D	-9.16	109.67	128.35
19	3	1213	CLA	CAB-C3B-C4B	-9.14	113.24	128.36
19	A	1798	CLA	OBD-CAD-C3D	-9.08	109.82	128.35
19	F	1155	CLA	C3D-CAD-CBD	-9.08	101.68	107.75
19	1	1196	CLA	OBD-CAD-C3D	-9.06	109.87	128.35
19	B	1760	CLA	OBD-CAD-C3D	-9.05	109.89	128.35
19	3	1213	CLA	C3D-CAD-CBD	-9.04	101.71	107.75
19	1	1196	CLA	CAB-C3B-C2B	-9.04	106.66	125.14
19	A	1801	CLA	OBD-CAD-C3D	-8.99	110.00	128.35
19	A	1774	CLA	OBD-CAD-C3D	-8.98	110.02	128.35
23	I	1032	BCR	C24-C23-C22	-8.97	112.54	126.22
19	1	1192	CLA	OBD-CAD-C3D	-8.97	110.05	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1813	CLA	OBD-CAD-C3D	-8.96	110.06	128.35
19	A	1768	CLA	OBD-CAD-C3D	-8.94	110.12	128.35
19	B	1768	CLA	OBD-CAD-C3D	-8.93	110.12	128.35
19	B	1762	CLA	OBD-CAD-C3D	-8.93	110.13	128.35
19	4	1205	CLA	OBD-CAD-C3D	-8.93	110.13	128.35
19	4	4007	CLA	OBD-CAD-C3D	-8.91	110.17	128.35
19	B	1772	CLA	OBD-CAD-C3D	-8.90	110.20	128.35
19	B	1771	CLA	OBD-CAD-C3D	-8.88	110.24	128.35
19	B	1745	CLA	OBD-CAD-CBD	-8.81	112.64	125.94
19	1	1149	CLA	CAB-C3B-C2B	-8.80	107.14	125.14
19	1	1197	CLA	OBD-CAD-CBD	-8.77	112.70	125.94
19	A	1797	CLA	OBD-CAD-C3D	-8.75	110.50	128.35
19	B	1762	CLA	CAA-C2A-C3A	-8.71	88.19	113.22
19	1	1196	CLA	C3D-CAD-CBD	-8.71	101.93	107.75
19	A	1775	CLA	C3D-CAD-CBD	-8.69	101.94	107.75
19	1	1188	CLA	OBD-CAD-C3D	-8.69	110.63	128.35
19	B	1746	CLA	OBD-CAD-C3D	-8.67	110.65	128.35
19	4	4014	CLA	OBD-CAD-C3D	-8.66	110.67	128.35
19	A	1767	CLA	OBD-CAD-CBD	-8.66	112.87	125.94
23	A	1808	BCR	C15-C14-C13	-8.66	114.69	127.20
19	B	1765	CLA	OBD-CAD-CBD	-8.65	112.89	125.94
19	A	1792	CLA	OBD-CAD-C3D	-8.64	110.72	128.35
19	A	1769	CLA	OBD-CAD-C3D	-8.63	110.75	128.35
19	B	1772	CLA	CAB-C3B-C2B	-8.59	107.57	125.14
19	B	1759	CLA	OBD-CAD-C3D	-8.57	110.86	128.35
19	A	1780	CLA	OBD-CAD-C3D	-8.52	110.96	128.35
19	A	1778	CLA	OBD-CAD-C3D	-8.52	110.97	128.35
19	B	1747	CLA	OBD-CAD-CBD	-8.48	113.14	125.94
19	A	1765	CLA	OBD-CAD-C3D	-8.48	111.05	128.35
19	A	1790	CLA	OBD-CAD-C3D	-8.47	111.08	128.35
19	B	1743	CLA	OBD-CAD-C3D	-8.47	111.08	128.35
19	B	1758	CLA	OBD-CAD-C3D	-8.46	111.10	128.35
19	1	1014	CLA	C1D-CHD-C4C	-8.45	109.82	122.60
19	A	1761	CLA	OBD-CAD-CBD	-8.45	113.19	125.94
19	4	1199	CLA	OBD-CAD-CBD	-8.44	113.20	125.94
19	B	1744	CLA	OBD-CAD-CBD	-8.44	113.20	125.94
23	A	1809	BCR	C16-C17-C18	-8.43	115.02	127.20
23	A	1807	BCR	C7-C8-C9	-8.42	113.38	126.22
19	1	1192	CLA	OBD-CAD-CBD	-8.41	113.24	125.94
19	1	1014	CLA	C3D-CAD-CBD	-8.34	95.80	107.60
19	B	1747	CLA	OBD-CAD-C3D	-8.32	111.37	128.35
19	F	1155	CLA	OBD-CAD-C3D	-8.22	111.58	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1767	CLA	OBD-CAD-CBD	-8.17	113.61	125.94
23	B	1775	BCR	C24-C23-C22	-8.13	113.82	126.22
19	B	1762	CLA	OBD-CAD-CBD	-8.12	113.68	125.94
19	4	1198	CLA	C3D-CAD-CBD	-8.07	96.18	107.60
19	2	1219	CLA	CAB-C3B-C2B	-8.07	108.63	125.14
19	4	1209	CLA	CAB-C3B-C2B	-8.06	108.65	125.14
19	B	1737	CLA	OBD-CAD-C3D	-8.06	111.91	128.35
19	B	1771	CLA	OBD-CAD-CBD	-8.03	113.81	125.94
19	2	2006	CLA	OBD-CAD-CBD	-8.02	113.84	125.94
19	A	1789	CLA	C1D-CHD-C4C	-8.01	110.48	122.60
19	A	1780	CLA	OBD-CAD-CBD	-7.93	113.98	125.94
19	A	1775	CLA	CAB-C3B-C2B	-7.90	108.99	125.14
19	2	1212	CLA	C1D-CHD-C4C	-7.85	110.72	122.60
19	A	1801	CLA	OBD-CAD-CBD	-7.83	114.12	125.94
19	A	1787	CLA	OBD-CAD-C3D	-7.83	112.38	128.35
19	4	1211	CLA	OBD-CAD-C3D	-7.82	112.40	128.35
19	B	1758	CLA	OBD-CAD-CBD	-7.73	114.27	125.94
19	B	1744	CLA	OBD-CAD-C3D	-7.66	112.72	128.35
19	A	1774	CLA	C1D-CHD-C4C	-7.60	111.10	122.60
19	3	1213	CLA	CAB-C3B-C2B	-7.60	109.60	125.14
23	I	1032	BCR	C30-C25-C26	-7.55	111.57	122.66
19	A	1813	CLA	C3D-CAD-CBD	-7.53	96.95	107.60
19	2	1215	CLA	OBD-CAD-C3D	-7.52	113.00	128.35
19	4	1211	CLA	OBD-CAD-CBD	-7.51	114.60	125.94
19	1	1187	CLA	OBD-CAD-CBD	-7.51	114.61	125.94
19	3	3008	CLA	OBD-CAD-CBD	-7.45	114.70	125.94
19	A	1760	CLA	OBD-CAD-C3D	-7.40	113.26	128.35
19	3	3008	CLA	OBD-CAD-C3D	-7.40	113.26	128.35
19	F	1155	CLA	CAB-C3B-C4B	-7.39	116.14	128.36
19	B	1754	CLA	OBD-CAD-CBD	-7.39	114.79	125.94
19	J	1043	CLA	OBD-CAD-C3D	-7.39	113.28	128.35
19	A	1767	CLA	OBD-CAD-C3D	-7.37	113.31	128.35
19	4	1198	CLA	C1D-CHD-C4C	-7.32	111.52	122.60
19	2	1221	CLA	C4B-CHC-C1C	-7.30	113.59	129.26
19	3	1217	CLA	C4B-CHC-C1C	-7.27	113.64	129.26
19	B	1741	CLA	C1D-CHD-C4C	-7.27	111.60	122.60
19	4	1205	CLA	C1D-CHD-C4C	-7.21	111.69	122.60
23	A	1808	BCR	C3-C4-C5	-7.21	102.43	113.87
19	2	1217	CLA	C4B-CHC-C1C	-7.21	113.78	129.26
19	3	3011	CLA	C4B-CHC-C1C	-7.18	113.83	129.26
19	4	1197	CLA	CAB-C3B-C2B	-7.15	110.52	125.14
19	L	1168	CLA	C3D-CAD-CBD	-7.14	97.51	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1055	CLA	OBD-CAD-C3D	-7.13	113.80	128.35
19	A	1797	CLA	OBD-CAD-CBD	-7.12	115.19	125.94
19	1	1187	CLA	C4B-CHC-C1C	-7.11	114.00	129.26
19	3	1220	CLA	C3A-C4A-CHB	-7.10	116.89	124.06
19	1	1199	CLA	C1D-CHD-C4C	-7.06	111.91	122.60
19	1	1190	CLA	C4B-CHC-C1C	-7.01	114.19	129.26
19	2	2006	CLA	C4B-CHC-C1C	-7.01	114.20	129.26
23	I	1032	BCR	C16-C17-C18	-7.00	117.08	127.20
19	3	3014	CLA	C3A-C4A-CHB	-7.00	117.00	124.06
19	B	1761	CLA	C4B-CHC-C1C	-7.00	114.23	129.26
19	A	1789	CLA	C4B-CHC-C1C	-6.99	114.25	129.26
19	1	1197	CLA	C3D-CAD-CBD	-6.98	97.73	107.60
19	B	1769	CLA	C1D-CHD-C4C	-6.97	112.05	122.60
19	G	1099	CLA	C1D-CHD-C4C	-6.96	112.08	122.60
19	2	1218	CLA	C3A-C4A-CHB	-6.95	117.04	124.06
19	1	1197	CLA	C1D-CHD-C4C	-6.93	112.12	122.60
19	B	1739	CLA	OBD-CAD-C3D	-6.89	114.28	128.35
19	4	1206	CLA	C1D-CHD-C4C	-6.88	112.19	122.60
19	B	1735	CLA	OBD-CAD-C3D	-6.85	114.37	128.35
19	2	2006	CLA	C1D-CHD-C4C	-6.85	112.23	122.60
19	4	1201	CLA	C1D-CHD-C4C	-6.85	112.24	122.60
23	I	1032	BCR	C16-C15-C14	-6.83	108.28	123.39
19	1	1145	CLA	C3D-CAD-CBD	-6.83	97.94	107.60
19	1	1195	CLA	C3A-C4A-CHB	-6.83	117.16	124.06
19	A	1797	CLA	C4B-CHC-C1C	-6.83	114.59	129.26
19	1	1191	CLA	CAB-C3B-C2B	-6.82	111.20	125.14
19	H	1079	CLA	C1D-CHD-C4C	-6.80	112.31	122.60
19	H	1079	CLA	OBD-CAD-CBD	-6.80	115.68	125.94
19	4	1197	CLA	C1D-CHD-C4C	-6.79	112.33	122.60
19	3	3011	CLA	C1D-CHD-C4C	-6.78	112.34	122.60
19	4	1200	CLA	C1D-CHD-C4C	-6.78	112.35	122.60
19	B	1748	CLA	C1D-CHD-C4C	-6.74	112.41	122.60
19	A	1761	CLA	C4B-CHC-C1C	-6.69	114.88	129.26
20	A	7026	LMU	C3'-C4'-C5'	-6.69	95.71	110.84
20	A	7017	LMU	C1B-O1B-C4'	-6.69	100.53	118.01
23	B	1779	BCR	C15-C14-C13	-6.69	117.53	127.20
19	4	1199	CLA	C4B-CHC-C1C	-6.69	114.89	129.26
19	3	1221	CLA	C1D-CHD-C4C	-6.67	112.51	122.60
19	A	1795	CLA	C4B-CHC-C1C	-6.67	114.94	129.26
19	4	1205	CLA	C4B-CHC-C1C	-6.66	114.95	129.26
19	H	1079	CLA	C4B-CHC-C1C	-6.64	114.99	129.26
19	B	1784	CLA	C4B-CHC-C1C	-6.63	115.01	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1813	CLA	C4B-CHC-C1C	-6.59	115.10	129.26
19	B	1771	CLA	C4B-CHC-C1C	-6.58	115.12	129.26
19	1	1014	CLA	CHD-C4C-C3C	-6.57	114.78	124.94
19	A	1772	CLA	C1D-CHD-C4C	-6.56	112.67	122.60
19	1	1146	CLA	C4B-CHC-C1C	-6.56	115.16	129.26
19	4	4007	CLA	C4B-CHC-C1C	-6.56	115.17	129.26
19	A	1760	CLA	C4B-CHC-C1C	-6.54	115.22	129.26
19	2	1223	CLA	C1D-CHD-C4C	-6.53	112.72	122.60
19	A	1765	CLA	C4B-CHC-C1C	-6.52	115.26	129.26
19	H	1079	CLA	OBD-CAD-C3D	-6.51	115.07	128.35
19	1	1193	CLA	CBA-CAA-C2A	-6.50	95.40	113.73
19	A	1759	CLA	C4B-CHC-C1C	-6.49	115.32	129.26
19	B	1766	CLA	C1D-CHD-C4C	-6.49	112.78	122.60
19	1	1198	CLA	C3A-C4A-CHB	-6.48	117.52	124.06
19	4	4014	CLA	C4B-CHC-C1C	-6.47	115.36	129.26
19	A	1799	CLA	C3A-C4A-CHB	-6.47	117.53	124.06
19	4	1201	CLA	C4B-CHC-C1C	-6.47	115.37	129.26
19	B	1759	CLA	C4B-CHC-C1C	-6.45	115.40	129.26
19	4	1203	CLA	C3A-C4A-CHB	-6.45	117.55	124.06
19	1	1188	CLA	C4B-CHC-C1C	-6.45	115.41	129.26
19	F	1157	CLA	C1D-CHD-C4C	-6.44	112.86	122.60
19	4	1211	CLA	C1D-CHD-C4C	-6.41	112.90	122.60
19	B	1737	CLA	C4B-CHC-C1C	-6.40	115.52	129.26
19	B	1737	CLA	C1D-CHD-C4C	-6.40	112.92	122.60
19	1	1189	CLA	C4B-CHC-C1C	-6.40	115.52	129.26
19	4	1198	CLA	C4B-CHC-C1C	-6.40	115.52	129.26
19	2	1220	CLA	C3A-C4A-CHB	-6.38	117.62	124.06
19	B	1770	CLA	C4B-CHC-C1C	-6.35	115.61	129.26
23	A	1808	BCR	C10-C11-C12	-6.35	103.78	123.13
19	B	1761	CLA	C1D-CHD-C4C	-6.34	113.00	122.60
19	B	1739	CLA	O1D-CGD-CBD	-6.33	115.55	124.62
19	3	1216	CLA	C3A-C4A-CHB	-6.33	117.67	124.06
19	3	1219	CLA	C3A-C4A-CHB	-6.32	117.68	124.06
19	B	1753	CLA	C4B-CHC-C1C	-6.32	115.68	129.26
19	L	1168	CLA	C1D-CHD-C4C	-6.32	113.04	122.60
19	3	1221	CLA	C4B-CHC-C1C	-6.31	115.70	129.26
19	1	1197	CLA	C4B-CHC-C1C	-6.29	115.74	129.26
19	A	1792	CLA	C4B-CHC-C1C	-6.29	115.75	129.26
19	A	1778	CLA	C4B-CHC-C1C	-6.29	115.75	129.26
19	1	1309	CLA	C3A-C4A-CHB	-6.28	117.72	124.06
19	3	3015	CLA	C3A-C4A-CHB	-6.25	117.75	124.06
19	1	1199	CLA	C4B-CHC-C1C	-6.25	115.84	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1768	CLA	C4B-CHC-C1C	-6.25	115.84	129.26
19	3	1221	CLA	CHD-C4C-C3C	-6.24	115.29	124.94
19	1	1307	CLA	C3A-C4A-CHB	-6.24	117.76	124.06
19	B	1754	CLA	OBD-CAD-C3D	-6.22	115.66	128.35
19	1	1143	CLA	C4B-CHC-C1C	-6.21	115.91	129.26
19	4	4014	CLA	C3D-CAD-CBD	-6.21	98.81	107.60
19	A	1774	CLA	C4B-CHC-C1C	-6.20	115.93	129.26
19	A	1788	CLA	C4B-CHC-C1C	-6.20	115.94	129.26
19	J	1043	CLA	C1D-CHD-C4C	-6.20	113.22	122.60
19	J	1043	CLA	C4B-CHC-C1C	-6.18	115.99	129.26
19	B	1744	CLA	C4B-CHC-C1C	-6.17	116.00	129.26
19	A	1766	CLA	C4B-CHC-C1C	-6.16	116.03	129.26
19	A	1762	CLA	C4B-CHC-C1C	-6.15	116.04	129.26
19	B	1751	CLA	C1D-CHD-C4C	-6.15	113.30	122.60
19	3	3001	CLA	C3A-C4A-CHB	-6.15	117.85	124.06
19	2	1222	CLA	C1D-CHD-C4C	-6.14	113.31	122.60
19	B	1765	CLA	C4B-CHC-C1C	-6.13	116.09	129.26
19	1	1142	CLA	C1D-CHD-C4C	-6.13	113.33	122.60
19	B	1769	CLA	C4B-CHC-C1C	-6.12	116.11	129.26
19	1	1200	CLA	C3A-C4A-CHB	-6.12	117.88	124.06
19	B	1766	CLA	C4B-CHC-C1C	-6.11	116.14	129.26
19	B	1739	CLA	C4B-CHC-C1C	-6.10	116.15	129.26
19	A	1767	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	A	1779	CLA	C4B-CHC-C1C	-6.10	116.16	129.26
19	B	1743	CLA	C1D-CHD-C4C	-6.10	113.38	122.60
23	A	1809	BCR	C11-C10-C9	-6.09	118.40	127.20
19	R	1055	CLA	C4B-CHC-C1C	-6.08	116.21	129.26
19	B	1763	CLA	C1D-CHD-C4C	-6.07	113.42	122.60
23	A	1807	BCR	C3-C4-C5	-6.07	104.24	113.87
19	1	1194	CLA	C3A-C4A-CHB	-6.07	117.94	124.06
19	A	1791	CLA	C4B-CHC-C1C	-6.06	116.25	129.26
19	A	1784	CLA	C4B-CHC-C1C	-6.04	116.28	129.26
19	A	1814	CLA	C1D-CHD-C4C	-6.04	113.46	122.60
19	2	1219	CLA	C4B-CHC-C1C	-6.04	116.29	129.26
19	A	1793	CLA	C4B-CHC-C1C	-6.03	116.30	129.26
20	A	7014	LMU	C4B-C3B-C2B	-6.02	99.55	110.79
19	A	1782	CLA	C1D-CHD-C4C	-6.02	113.48	122.60
19	2	1222	CLA	C4B-CHC-C1C	-6.02	116.32	129.26
19	3	1215	CLA	C3A-C4A-CHB	-6.02	117.98	124.06
19	1	1149	CLA	C4B-CHC-C1C	-6.01	116.34	129.26
23	A	1809	BCR	C38-C26-C25	-6.01	118.70	124.61
19	A	1815	CLA	C4B-CHC-C1C	-6.01	116.35	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	1054	CLA	C4B-CHC-C1C	-6.00	116.36	129.26
19	I	1031	CLA	C1D-CHD-C4C	-5.99	113.53	122.60
19	B	1742	CLA	C4B-CHC-C1C	-5.99	116.39	129.26
19	B	1763	CLA	C4B-CHC-C1C	-5.99	116.39	129.26
19	B	1750	CLA	C4B-CHC-C1C	-5.99	116.40	129.26
19	B	1759	CLA	C1D-CHD-C4C	-5.98	113.55	122.60
19	4	1207	CLA	C3A-C4A-CHB	-5.97	118.03	124.06
19	1	1187	CLA	C1D-CHD-C4C	-5.97	113.56	122.60
19	B	1754	CLA	C1D-CHD-C4C	-5.97	113.57	122.60
19	B	1748	CLA	C4B-CHC-C1C	-5.96	116.45	129.26
19	A	1800	CLA	C4B-CHC-C1C	-5.96	116.45	129.26
19	1	1142	CLA	C4B-CHC-C1C	-5.95	116.47	129.26
19	1	1505	CLA	C4B-CHC-C1C	-5.95	116.48	129.26
19	4	1210	CLA	C3A-C4A-CHB	-5.95	118.06	124.06
19	B	1735	CLA	C4B-CHC-C1C	-5.95	116.49	129.26
19	A	1763	CLA	C4B-CHC-C1C	-5.93	116.51	129.26
19	A	1775	CLA	C4B-CHC-C1C	-5.93	116.51	129.26
19	A	1786	CLA	C4B-CHC-C1C	-5.93	116.52	129.26
19	B	1747	CLA	C4B-CHC-C1C	-5.93	116.52	129.26
19	2	1214	CLA	C3A-C4A-CHB	-5.93	118.08	124.06
19	B	1752	CLA	C4B-CHC-C1C	-5.92	116.53	129.26
19	B	1769	CLA	CHD-C4C-C3C	-5.91	115.80	124.94
19	B	1758	CLA	C1D-CHD-C4C	-5.91	113.66	122.60
19	A	1787	CLA	C4B-CHC-C1C	-5.91	116.57	129.26
19	A	1759	CLA	C1D-CHD-C4C	-5.91	113.66	122.60
19	3	1213	CLA	C1D-CHD-C4C	-5.90	113.67	122.60
19	A	1764	CLA	C4B-CHC-C1C	-5.90	116.58	129.26
19	A	1778	CLA	O1D-CGD-CBD	-5.90	116.16	124.62
19	1	1145	CLA	C4B-CHC-C1C	-5.90	116.58	129.26
19	B	1748	CLA	CAA-C2A-C3A	-5.89	102.10	116.20
19	A	1780	CLA	C4B-CHC-C1C	-5.89	116.61	129.26
19	B	1760	CLA	C4B-CHC-C1C	-5.89	116.62	129.26
19	1	1197	CLA	CHD-C4C-C3C	-5.88	115.85	124.94
19	2	1213	CLA	C1D-CHD-C4C	-5.88	113.70	122.60
20	A	7008	LMU	C1'-O5'-C5'	-5.88	102.33	113.75
19	B	1756	CLA	C1D-CHD-C4C	-5.88	113.70	122.60
19	B	1751	CLA	C4B-CHC-C1C	-5.87	116.65	129.26
19	3	1218	CLA	C4B-CHC-C1C	-5.86	116.68	129.26
19	3	1222	CLA	C1D-CHD-C4C	-5.85	113.75	122.60
19	B	1756	CLA	C4B-CHC-C1C	-5.85	116.70	129.26
19	A	1769	CLA	C4B-CHC-C1C	-5.84	116.71	129.26
19	L	1167	CLA	C4B-CHC-C1C	-5.84	116.72	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1781	CLA	C4B-CHC-C1C	-5.83	116.72	129.26
19	A	1785	CLA	C4B-CHC-C1C	-5.83	116.73	129.26
19	A	1769	CLA	C1D-CHD-C4C	-5.83	113.78	122.60
19	1	1192	CLA	C4B-CHC-C1C	-5.83	116.74	129.26
19	A	1782	CLA	C4B-CHC-C1C	-5.82	116.76	129.26
19	A	1814	CLA	C4B-CHC-C1C	-5.82	116.76	129.26
19	F	1156	CLA	C1D-CHD-C4C	-5.82	113.80	122.60
19	A	1794	CLA	C4B-CHC-C1C	-5.81	116.77	129.26
19	B	1749	CLA	C4B-CHC-C1C	-5.81	116.77	129.26
19	A	1790	CLA	C4B-CHC-C1C	-5.81	116.78	129.26
19	A	1797	CLA	C1D-CHD-C4C	-5.81	113.81	122.60
19	B	1764	CLA	C4B-CHC-C1C	-5.80	116.79	129.26
19	3	1222	CLA	C4B-CHC-C1C	-5.80	116.80	129.26
19	1	1191	CLA	C1D-CHD-C4C	-5.79	113.84	122.60
19	1	1308	CLA	C4B-CHC-C1C	-5.79	116.83	129.26
19	A	1816	CLA	C4B-CHC-C1C	-5.79	116.83	129.26
19	B	1761	CLA	CHD-C4C-C3C	-5.77	116.02	124.94
19	B	1754	CLA	C4B-CHC-C1C	-5.77	116.86	129.26
19	1	1308	CLA	C1D-CHD-C4C	-5.77	113.87	122.60
19	1	1191	CLA	C4B-CHC-C1C	-5.77	116.87	129.26
19	1	1192	CLA	C1D-CHD-C4C	-5.76	113.88	122.60
19	2	1213	CLA	C4B-CHC-C1C	-5.76	116.89	129.26
19	B	1758	CLA	C4B-CHC-C1C	-5.76	116.89	129.26
19	A	1791	CLA	C1D-CHD-C4C	-5.75	113.89	122.60
19	1	1148	CLA	C4B-CHC-C1C	-5.75	116.90	129.26
19	4	1196	CLA	C4B-CHC-C1C	-5.75	116.91	129.26
19	2	1217	CLA	C1D-CHD-C4C	-5.75	113.90	122.60
19	H	1080	CLA	C4B-CHC-C1C	-5.75	116.91	129.26
19	F	1155	CLA	C4B-CHC-C1C	-5.74	116.92	129.26
19	1	1193	CLA	C4B-CHC-C1C	-5.74	116.92	129.26
19	4	1211	CLA	C4B-CHC-C1C	-5.74	116.93	129.26
19	B	1738	CLA	C4B-CHC-C1C	-5.74	116.93	129.26
19	A	1796	CLA	C4B-CHC-C1C	-5.74	116.93	129.26
19	B	1759	CLA	OBD-CAD-CBD	-5.74	117.28	125.94
19	B	1755	CLA	C4B-CHC-C1C	-5.73	116.94	129.26
19	2	1215	CLA	C4B-CHC-C1C	-5.73	116.95	129.26
19	A	1777	CLA	C4B-CHC-C1C	-5.71	116.99	129.26
19	A	1774	CLA	CHD-C4C-C3C	-5.71	116.11	124.94
19	1	1143	CLA	C1D-CHD-C4C	-5.71	113.96	122.60
19	4	1205	CLA	O1D-CGD-CBD	-5.69	116.46	124.62
23	B	1775	BCR	C1-C6-C5	-5.69	114.30	122.66
19	4	1209	CLA	C1D-CHD-C4C	-5.68	114.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1214	CLA	C3A-C4A-CHB	-5.68	118.33	124.06
19	B	1762	CLA	C4B-CHC-C1C	-5.67	117.08	129.26
19	A	1817	CLA	C4B-CHC-C1C	-5.67	117.08	129.26
19	B	1746	CLA	C4B-CHC-C1C	-5.66	117.09	129.26
19	2	1218	CLA	C1D-CHD-C4C	-5.66	111.76	126.32
19	A	1768	CLA	C4B-CHC-C1C	-5.66	117.10	129.26
19	A	1801	CLA	C1D-CHD-C4C	-5.65	114.05	122.60
19	B	1762	CLA	C1D-CHD-C4C	-5.65	114.05	122.60
20	A	7033	LMU	C1B-O1B-C4'	-5.63	103.29	118.01
19	A	1775	CLA	C1D-CHD-C4C	-5.63	114.09	122.60
19	B	1764	CLA	C1D-CHD-C4C	-5.62	114.09	122.60
19	4	1200	CLA	C4B-CHC-C1C	-5.61	117.20	129.26
19	F	1157	CLA	C4B-CHC-C1C	-5.61	117.20	129.26
19	B	1743	CLA	C4B-CHC-C1C	-5.61	117.21	129.26
19	B	1749	CLA	C1D-CHD-C4C	-5.61	114.11	122.60
19	B	1767	CLA	C4B-CHC-C1C	-5.61	117.22	129.26
19	A	1776	CLA	C1D-CHD-C4C	-5.61	114.12	122.60
19	B	1753	CLA	CHD-C4C-C3C	-5.61	116.28	124.94
19	1	1148	CLA	C1D-CHD-C4C	-5.60	114.13	122.60
19	1	1190	CLA	C1D-CHD-C4C	-5.60	114.13	122.60
19	4	1208	CLA	C3A-C4A-CHB	-5.60	118.41	124.06
19	B	1738	CLA	C1D-CHD-C4C	-5.60	114.13	122.60
19	2	1223	CLA	C4B-CHC-C1C	-5.59	117.24	129.26
19	F	1155	CLA	C1D-CHD-C4C	-5.59	114.14	122.60
19	1	1196	CLA	C1D-CHD-C4C	-5.59	114.14	122.60
19	A	1773	CLA	C1D-CHD-C4C	-5.59	114.14	122.60
19	4	1196	CLA	C1D-CHD-C4C	-5.59	114.14	122.60
19	B	1772	CLA	C4B-CHC-C1C	-5.58	117.27	129.26
19	A	1773	CLA	C4B-CHC-C1C	-5.57	117.29	129.26
19	A	1798	CLA	C4B-CHC-C1C	-5.57	117.30	129.26
19	A	1795	CLA	C1D-CHD-C4C	-5.57	114.17	122.60
19	A	1767	CLA	C1D-CHD-C4C	-5.56	114.19	122.60
19	L	1167	CLA	CAA-C2A-C3A	-5.55	97.25	113.22
19	B	1745	CLA	C1D-CHD-C4C	-5.55	114.20	122.60
19	A	1794	CLA	OBD-CAD-CBD	-5.55	117.57	125.94
19	A	1771	CLA	C4B-CHC-C1C	-5.53	117.38	129.26
19	4	1203	CLA	C3B-C2B-C1B	-5.53	101.45	106.29
19	A	1768	CLA	C1D-CHD-C4C	-5.53	114.24	122.60
19	A	1801	CLA	C4B-CHC-C1C	-5.53	117.39	129.26
19	A	1761	CLA	C1D-CHD-C4C	-5.51	114.27	122.60
19	A	1783	CLA	C1D-CHD-C4C	-5.51	114.27	122.60
19	1	1196	CLA	C4B-CHC-C1C	-5.50	117.44	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1785	CLA	C1D-CHD-C4C	-5.49	114.30	122.60
20	A	7037	LMU	C1B-O5B-C5B	-5.48	103.10	113.75
19	3	1212	CLA	C3A-C4A-CHB	-5.48	118.52	124.06
19	H	1081	CLA	C1D-CHD-C4C	-5.48	114.30	122.60
19	H	1081	CLA	C4B-CHC-C1C	-5.48	117.48	129.26
19	A	1772	CLA	C4B-CHC-C1C	-5.47	117.50	129.26
19	L	1167	CLA	C1D-CHD-C4C	-5.46	114.34	122.60
19	4	1204	CLA	C3A-C4A-CHB	-5.46	118.55	124.06
19	B	1755	CLA	C1D-CHD-C4C	-5.46	114.34	122.60
19	A	1817	CLA	C1D-CHD-C4C	-5.45	114.36	122.60
19	4	4014	CLA	O1D-CGD-CBD	-5.44	116.83	124.62
19	B	1736	CLA	C4B-CHC-C1C	-5.44	117.58	129.26
19	B	1767	CLA	C1D-CHD-C4C	-5.43	114.39	122.60
19	L	1168	CLA	O1D-CGD-CBD	-5.42	116.85	124.62
19	B	1765	CLA	C1D-CHD-C4C	-5.42	114.39	122.60
19	2	1212	CLA	CHD-C4C-C3C	-5.42	116.56	124.94
19	B	1757	CLA	C4B-CHC-C1C	-5.42	117.62	129.26
19	B	1745	CLA	C4B-CHC-C1C	-5.42	117.62	129.26
19	A	1776	CLA	C4B-CHC-C1C	-5.41	117.63	129.26
19	1	1193	CLA	C1D-CHD-C4C	-5.41	114.42	122.60
19	B	1736	CLA	C1D-CHD-C4C	-5.40	114.42	122.60
19	1	1505	CLA	C1D-CHD-C4C	-5.40	114.44	122.60
19	A	1788	CLA	C1D-CHD-C4C	-5.39	114.45	122.60
19	4	1209	CLA	C4B-CHC-C1C	-5.38	117.69	129.26
19	4	1205	CLA	CHD-C4C-C3C	-5.38	116.62	124.94
19	A	1794	CLA	C1D-CHD-C4C	-5.38	114.46	122.60
19	B	1750	CLA	C1D-CHD-C4C	-5.37	114.47	122.60
19	2	1219	CLA	C1D-CHD-C4C	-5.37	114.47	122.60
19	A	1796	CLA	C1D-CHD-C4C	-5.37	114.47	122.60
19	3	3008	CLA	C4B-CHC-C1C	-5.36	117.75	129.26
19	4	1197	CLA	C4B-CHC-C1C	-5.36	117.75	129.26
19	A	1780	CLA	C1D-CHD-C4C	-5.36	114.50	122.60
19	A	1798	CLA	C1D-CHD-C4C	-5.36	114.50	122.60
19	4	1202	CLA	C3A-C4A-CHB	-5.36	118.65	124.06
19	B	1741	CLA	C4B-CHC-C1C	-5.36	117.75	129.26
19	1	1190	CLA	C3D-CAD-CBD	-5.35	100.03	107.60
19	A	1784	CLA	C1D-CHD-C4C	-5.34	114.52	122.60
19	2	2006	CLA	CHD-C4C-C3C	-5.33	116.70	124.94
19	3	3008	CLA	C1D-CHD-C4C	-5.33	114.53	122.60
23	I	1032	BCR	C1-C6-C5	-5.31	114.86	122.66
19	I	1031	CLA	C4B-CHC-C1C	-5.31	117.86	129.26
19	B	1757	CLA	C1D-CHD-C4C	-5.31	114.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	1080	CLA	C1D-CHD-C4C	-5.31	114.57	122.60
19	A	1781	CLA	C1D-CHD-C4C	-5.30	114.58	122.60
19	1	1014	CLA	C4B-CHC-C1C	-5.29	117.89	129.26
23	B	1775	BCR	C30-C25-C26	-5.29	114.89	122.66
19	B	1769	CLA	C3D-CAD-CBD	-5.29	100.12	107.60
19	4	4007	CLA	C1D-CHD-C4C	-5.28	114.61	122.60
19	2	1212	CLA	C4B-CHC-C1C	-5.28	117.92	129.26
23	B	1779	BCR	C24-C23-C22	-5.27	118.18	126.22
19	2	1218	CLA	C3C-C4C-CHD	-5.26	116.67	125.32
19	A	1800	CLA	C1D-CHD-C4C	-5.26	114.65	122.60
19	A	1765	CLA	C1D-CHD-C4C	-5.25	114.66	122.60
19	B	1752	CLA	C1D-CHD-C4C	-5.25	114.66	122.60
19	A	1816	CLA	C1D-CHD-C4C	-5.25	114.66	122.60
19	A	1778	CLA	C1D-CHD-C4C	-5.24	114.67	122.60
19	A	1813	CLA	C1D-CHD-C4C	-5.24	114.67	122.60
23	B	1775	BCR	C28-C27-C26	-5.24	105.55	113.87
23	I	1032	BCR	C11-C10-C9	-5.24	119.63	127.20
19	B	1743	CLA	CHD-C4C-C3C	-5.24	116.84	124.94
19	A	1777	CLA	C1D-CHD-C4C	-5.24	114.68	122.60
19	R	1054	CLA	C1D-CHD-C4C	-5.23	114.68	122.60
19	A	1793	CLA	C1D-CHD-C4C	-5.21	114.71	122.60
19	3	1213	CLA	C4B-CHC-C1C	-5.21	118.07	129.26
19	B	1751	CLA	CHD-C4C-C3C	-5.21	116.89	124.94
19	1	1189	CLA	C1D-CHD-C4C	-5.21	114.72	122.60
20	A	7032	LMU	C1B-C2B-C3B	-5.21	99.71	109.97
19	A	1813	CLA	CHD-C4C-C3C	-5.21	116.89	124.94
19	B	1753	CLA	C1D-CHD-C4C	-5.20	114.73	122.60
19	A	1778	CLA	C3D-CAD-CBD	-5.20	100.25	107.60
19	2	2006	CLA	C3D-CAD-CBD	-5.20	100.25	107.60
19	F	1156	CLA	C4B-CHC-C1C	-5.19	118.11	129.26
23	A	1805	BCR	C11-C10-C9	-5.17	119.72	127.20
19	G	1099	CLA	CHD-C4C-C3C	-5.17	116.95	124.94
19	G	1099	CLA	C4B-CHC-C1C	-5.16	118.17	129.26
23	B	1774	BCR	C11-C10-C9	-5.16	119.74	127.20
19	3	1216	CLA	C1D-CHD-C4C	-5.15	113.07	126.32
19	A	1790	CLA	C1D-CHD-C4C	-5.15	114.81	122.60
19	3	1218	CLA	C1D-CHD-C4C	-5.15	114.81	122.60
19	B	1746	CLA	C1D-CHD-C4C	-5.15	114.81	122.60
19	4	1211	CLA	CHD-C4C-C3C	-5.15	116.99	124.94
19	1	1145	CLA	C1D-CHD-C4C	-5.14	114.82	122.60
19	4	1198	CLA	CAA-C2A-C3A	-5.14	98.44	113.22
19	1	1193	CLA	CGD-CBD-CAD	-5.13	93.22	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1768	CLA	C1D-CHD-C4C	-5.13	114.84	122.60
23	A	1807	BCR	C4-C5-C6	-5.13	116.25	122.78
19	A	1779	CLA	C1D-CHD-C4C	-5.12	114.85	122.60
19	A	1760	CLA	C1D-CHD-C4C	-5.12	114.86	122.60
19	A	1797	CLA	C3D-CAD-CBD	-5.12	100.36	107.60
19	4	1206	CLA	C4B-CHC-C1C	-5.11	118.27	129.26
19	B	1741	CLA	C3D-CAD-CBD	-5.11	100.38	107.60
19	B	1772	CLA	C1D-CHD-C4C	-5.10	114.88	122.60
19	2	1214	CLA	C1D-CHD-C4C	-5.10	113.21	126.32
19	1	1188	CLA	C1D-CHD-C4C	-5.10	114.89	122.60
23	A	1804	BCR	C16-C17-C18	-5.10	119.84	127.20
19	L	1168	CLA	C4B-CHC-C1C	-5.09	118.32	129.26
19	1	1193	CLA	C3D-CAD-CBD	-5.09	100.40	107.60
19	B	1739	CLA	C1D-CHD-C4C	-5.08	114.92	122.60
19	4	1207	CLA	C1D-CHD-C4C	-5.08	113.26	126.32
19	1	1146	CLA	C1D-CHD-C4C	-5.07	114.92	122.60
19	2	2010	CLA	C1D-CHD-C4C	-5.07	113.27	126.32
20	A	7011	LMU	C1'-O5'-C5'	-5.04	103.96	113.75
19	1	1309	CLA	C2D-C3D-C4D	-5.04	101.86	106.30
23	A	1808	BCR	C34-C9-C10	-5.04	115.46	122.90
23	B	1776	BCR	C24-C23-C22	-5.03	118.55	126.22
19	B	1740	CLA	C3A-C4A-CHB	-5.03	118.98	124.06
19	A	1794	CLA	OBD-CAD-C3D	-5.02	118.10	128.35
19	A	1762	CLA	C1D-CHD-C4C	-5.02	115.00	122.60
19	B	1747	CLA	C1D-CHD-C4C	-5.02	115.01	122.60
19	2	1212	CLA	C3D-CAD-CBD	-5.02	100.51	107.60
19	A	1787	CLA	C1D-CHD-C4C	-5.01	115.02	122.60
19	A	1783	CLA	C4B-CHC-C1C	-5.01	118.50	129.26
19	A	1764	CLA	C1D-CHD-C4C	-5.00	115.03	122.60
19	3	3014	CLA	C2A-C1A-CHA	-5.00	113.73	122.58
19	A	1772	CLA	CHD-C4C-C3C	-5.00	117.22	124.94
19	2	1216	CLA	C3A-C4A-CHB	-5.00	119.01	124.06
19	R	1055	CLA	C1D-CHD-C4C	-4.99	115.05	122.60
19	B	1771	CLA	C1D-CHD-C4C	-4.99	115.05	122.60
19	A	1817	CLA	C3D-CAD-CBD	-4.99	100.54	107.60
19	4	1205	CLA	C3D-CAD-CBD	-4.98	100.55	107.60
19	F	1157	CLA	C3D-CAD-CBD	-4.98	100.55	107.60
19	1	1195	CLA	C3B-C2B-C1B	-4.98	101.93	106.29
22	B	1773	PQN	C11-C12-C13	-4.98	118.26	126.70
19	A	1792	CLA	C1D-CHD-C4C	-4.98	115.07	122.60
19	A	1786	CLA	C1D-CHD-C4C	-4.97	115.08	122.60
19	B	1742	CLA	C1D-CHD-C4C	-4.96	115.09	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1309	CLA	C2A-C1A-CHA	-4.96	113.79	122.58
19	3	1215	CLA	C1D-CHD-C4C	-4.95	113.60	126.32
19	2	1220	CLA	C1D-CHD-C4C	-4.93	113.65	126.32
19	A	1815	CLA	C1D-CHD-C4C	-4.92	115.16	122.60
19	1	1149	CLA	C1D-CHD-C4C	-4.91	115.17	122.60
19	4	4007	CLA	C3D-CAD-CBD	-4.91	100.65	107.60
19	A	1770	CLA	C3A-C4A-CHB	-4.91	119.10	124.06
19	A	1771	CLA	C1D-CHD-C4C	-4.90	115.19	122.60
20	A	7040	LMU	C1B-O1B-C4'	-4.89	105.22	118.01
19	A	1799	CLA	C3B-C2B-C1B	-4.89	102.01	106.29
23	A	1809	BCR	C33-C5-C6	-4.89	119.80	124.61
19	A	1770	CLA	C2A-C1A-CHA	-4.89	113.92	122.58
19	F	1155	CLA	CAB-C3B-C2B	-4.89	115.15	125.14
23	B	1774	BCR	C15-C14-C13	-4.89	120.14	127.20
19	B	1750	CLA	C3D-CAD-CBD	-4.88	100.70	107.60
19	R	1054	CLA	C3D-CAD-CBD	-4.88	100.70	107.60
19	4	1203	CLA	C1D-CHD-C4C	-4.87	113.78	126.32
20	A	7039	LMU	C1B-O5B-C5B	-4.87	104.30	113.75
19	A	1795	CLA	C3D-CAD-CBD	-4.86	100.72	107.60
20	A	7037	LMU	C4B-C3B-C2B	-4.85	101.74	110.79
19	3	1213	CLA	CHD-C4C-C3C	-4.84	116.72	124.83
23	B	1779	BCR	C30-C25-C26	-4.84	115.55	122.66
19	3	3015	CLA	C2A-C1A-CHA	-4.84	114.01	122.58
19	L	1168	CLA	CHD-C4C-C3C	-4.83	117.47	124.94
19	A	1779	CLA	C3D-CAD-CBD	-4.82	100.78	107.60
19	B	1767	CLA	O2D-CGD-O1D	-4.81	113.85	123.79
23	A	1804	BCR	C15-C14-C13	-4.81	120.25	127.20
19	A	1766	CLA	C1D-CHD-C4C	-4.80	115.34	122.60
20	A	7031	LMU	C4B-C3B-C2B	-4.80	101.84	110.79
20	A	7038	LMU	C3'-C4'-C5'	-4.79	100.00	110.84
19	1	1192	CLA	C3D-CAD-CBD	-4.79	100.82	107.60
19	1	1200	CLA	C2A-C1A-CHA	-4.79	114.10	122.58
19	3	1219	CLA	C3B-C2B-C1B	-4.77	102.11	106.29
19	2	1218	CLA	C3B-C2B-C1B	-4.77	102.12	106.29
19	2	1223	CLA	CHD-C4C-C3C	-4.76	117.58	124.94
19	1	1189	CLA	C2A-C1A-CHA	-4.76	115.12	123.89
19	B	1749	CLA	CHD-C4C-C3C	-4.76	117.58	124.94
23	B	1778	BCR	C11-C10-C9	-4.76	120.33	127.20
19	2	2006	CLA	C1-C2-C3	-4.76	118.91	126.71
19	3	3015	CLA	C1D-CHD-C4C	-4.76	114.09	126.32
23	B	1780	BCR	C15-C14-C13	-4.75	120.33	127.20
19	4	1202	CLA	C2A-C1A-CHA	-4.74	114.18	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1804	BCR	C24-C23-C22	-4.74	118.99	126.22
19	2	1214	CLA	C3C-C4C-CHD	-4.74	117.53	125.32
19	A	1763	CLA	C1D-CHD-C4C	-4.73	115.44	122.60
19	2	1215	CLA	C1D-CHD-C4C	-4.73	115.44	122.60
19	B	1737	CLA	CHD-C4C-C3C	-4.72	117.64	124.94
19	4	1206	CLA	CHD-C4C-C3C	-4.71	117.65	124.94
19	A	1801	CLA	CHD-C4C-C3C	-4.71	117.67	124.94
19	B	1784	CLA	C1D-CHD-C4C	-4.70	115.49	122.60
19	B	1735	CLA	C1D-CHD-C4C	-4.70	115.49	122.60
19	A	1770	CLA	C2D-C3D-C4D	-4.70	102.17	106.30
19	4	1204	CLA	C1D-CHD-C4C	-4.70	114.25	126.32
19	1	1192	CLA	CHD-C4C-C3C	-4.69	117.69	124.94
23	L	1169	BCR	C7-C8-C9	-4.69	119.06	126.22
19	B	1758	CLA	CHD-C4C-C3C	-4.69	117.69	124.94
23	I	1032	BCR	C27-C26-C25	-4.69	116.81	122.78
20	A	7014	LMU	C1'-C2'-C3'	-4.68	100.75	109.97
19	H	1079	CLA	CHD-C4C-C3C	-4.68	117.72	124.94
23	B	1779	BCR	C10-C11-C12	-4.67	108.89	123.13
19	A	1789	CLA	CHD-C4C-C3C	-4.67	117.72	124.94
19	B	1751	CLA	C3D-CAD-CBD	-4.67	101.00	107.60
19	1	1190	CLA	CMD-C2D-C3D	-4.66	115.98	125.09
19	3	3001	CLA	C1D-CHD-C4C	-4.66	114.34	126.32
19	4	1200	CLA	CHD-C4C-C3C	-4.65	117.75	124.94
19	1	1200	CLA	C3B-C2B-C1B	-4.65	102.22	106.29
19	A	1784	CLA	O1D-CGD-CBD	-4.65	117.96	124.62
19	1	1309	CLA	C3B-C2B-C1B	-4.65	102.22	106.29
19	1	1198	CLA	C1D-CHD-C4C	-4.65	114.37	126.32
19	1	1190	CLA	CAA-C2A-C3A	-4.64	99.86	113.22
19	3	1212	CLA	C1D-CHD-C4C	-4.64	114.39	126.32
19	3	1220	CLA	C2D-C3D-C4D	-4.63	102.22	106.30
19	1	1195	CLA	C1D-CHD-C4C	-4.62	114.44	126.32
19	2	2010	CLA	C3A-C4A-CHB	-4.61	119.40	124.06
19	4	1208	CLA	C2A-C1A-CHA	-4.61	114.41	122.58
19	A	1774	CLA	C3D-CAD-CBD	-4.60	101.09	107.60
19	3	3014	CLA	C2D-C3D-C4D	-4.60	102.25	106.30
19	3	1217	CLA	C1D-CHD-C4C	-4.60	115.64	122.60
20	A	7039	LMU	C1B-C2B-C3B	-4.59	100.92	109.97
23	A	1803	BCR	C15-C14-C13	-4.59	120.56	127.20
19	3	1220	CLA	C3B-C2B-C1B	-4.59	102.28	106.29
19	B	1769	CLA	CMD-C2D-C3D	-4.58	116.12	125.09
19	A	1788	CLA	C3D-CAD-CBD	-4.58	101.12	107.60
19	4	1210	CLA	C1D-CHD-C4C	-4.58	114.55	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1763	CLA	C3D-CAD-CBD	-4.58	101.13	107.60
19	2	1213	CLA	CHD-C4C-C3C	-4.57	117.88	124.94
19	H	1081	CLA	CHD-C4C-C3C	-4.56	117.89	124.94
19	3	1214	CLA	C2A-C1A-CHA	-4.55	114.52	122.58
23	A	1805	BCR	C33-C5-C6	-4.55	120.14	124.61
19	B	1746	CLA	C3D-CAD-CBD	-4.55	101.17	107.60
19	1	1307	CLA	C3B-C2B-C1B	-4.54	102.31	106.29
19	1	1194	CLA	C1D-CHD-C4C	-4.54	114.63	126.32
19	B	1753	CLA	C6-C5-C3	-4.54	102.53	112.48
19	B	1744	CLA	C1D-CHD-C4C	-4.53	115.74	122.60
19	B	1760	CLA	C1D-CHD-C4C	-4.53	115.75	122.60
23	B	1774	BCR	C33-C5-C6	-4.52	120.16	124.61
19	4	1206	CLA	CAA-CBA-CGA	-4.52	100.07	113.32
19	B	1771	CLA	C3D-CAD-CBD	-4.52	101.20	107.60
19	B	1741	CLA	CHD-C4C-C3C	-4.52	117.95	124.94
19	B	1762	CLA	C3D-CAD-CBD	-4.52	101.21	107.60
19	3	1219	CLA	C2A-C1A-CHA	-4.52	114.58	122.58
19	B	1757	CLA	O1D-CGD-CBD	-4.52	118.15	124.62
19	A	1815	CLA	C3D-CAD-CBD	-4.51	101.22	107.60
19	4	1208	CLA	C1D-CHD-C4C	-4.51	114.72	126.32
19	B	1748	CLA	CHD-C4C-C3C	-4.51	117.97	124.94
21	3	1223	SUC	C3-C4-C5	-4.51	102.34	110.20
19	A	1814	CLA	CHD-C4C-C3C	-4.51	117.98	124.94
23	A	1809	BCR	C16-C15-C14	-4.50	113.45	123.39
19	1	1189	CLA	CMD-C2D-C3D	-4.50	116.29	125.09
19	1	1200	CLA	C1D-CHD-C4C	-4.49	114.76	126.32
19	4	1204	CLA	C2A-C1A-CHA	-4.49	114.63	122.58
19	4	4014	CLA	C1D-CHD-C4C	-4.48	115.81	122.60
23	A	1804	BCR	C33-C5-C6	-4.48	120.20	124.61
19	B	1756	CLA	CHD-C4C-C3C	-4.48	118.02	124.94
19	2	1221	CLA	C1D-CHD-C4C	-4.47	115.83	122.60
19	B	1784	CLA	C3D-CAD-CBD	-4.47	101.28	107.60
19	B	1761	CLA	C3D-CAD-CBD	-4.47	101.28	107.60
19	2	1221	CLA	C3D-CAD-CBD	-4.46	101.29	107.60
19	2	2010	CLA	C3C-C4C-CHD	-4.46	117.98	125.32
19	B	1740	CLA	C2A-C1A-CHA	-4.45	114.69	122.58
19	A	1773	CLA	C3D-CAD-CBD	-4.45	101.30	107.60
19	2	1217	CLA	CHD-C4C-C3C	-4.44	118.07	124.94
19	3	3015	CLA	C3C-C4C-CHD	-4.44	118.02	125.32
19	A	1796	CLA	CHD-C4C-C3C	-4.44	118.08	124.94
23	B	1778	BCR	C15-C14-C13	-4.44	120.79	127.20
20	A	7026	LMU	C1B-O1B-C4'	-4.44	106.42	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1201	CLA	CHD-C4C-C3C	-4.43	118.09	124.94
19	3	1219	CLA	C1D-CHD-C4C	-4.43	114.92	126.32
19	B	1749	CLA	O1D-CGD-CBD	-4.42	118.29	124.62
19	3	1216	CLA	C3C-C4C-CHD	-4.41	118.06	125.32
19	3	1216	CLA	C3B-C2B-C1B	-4.41	102.43	106.29
19	B	1770	CLA	C1D-CHD-C4C	-4.41	115.92	122.60
19	A	1799	CLA	C2D-C3D-C4D	-4.41	102.42	106.30
19	2	1222	CLA	CHD-C4C-C3C	-4.40	118.14	124.94
20	2	1224	LMU	C1-O1'-C1'	-4.39	106.27	113.94
19	B	1749	CLA	C3D-CAD-CBD	-4.39	101.39	107.60
19	B	1742	CLA	C3D-CAD-CBD	-4.39	101.39	107.60
19	4	1211	CLA	O1D-CGD-CBD	-4.38	118.35	124.62
19	1	1193	CLA	CHD-C4C-C3C	-4.38	118.18	124.94
20	A	7040	LMU	O5B-C5B-C4B	-4.37	101.48	109.68
19	A	1784	CLA	C3D-CAD-CBD	-4.36	101.43	107.60
19	A	1782	CLA	CHD-C4C-C3C	-4.36	118.20	124.94
19	1	1195	CLA	C2A-C1A-CHA	-4.36	114.86	122.58
19	3	3001	CLA	C3B-C2B-C1B	-4.36	102.48	106.29
19	2	1213	CLA	C3D-CAD-CBD	-4.35	101.44	107.60
19	1	1308	CLA	C3D-CAD-CBD	-4.34	101.46	107.60
19	4	1211	CLA	C3D-CAD-CBD	-4.34	101.46	107.60
19	A	1800	CLA	CHD-C4C-C3C	-4.34	118.23	124.94
19	1	1149	CLA	O2D-CGD-O1D	-4.34	114.84	123.79
20	A	7009	LMU	C1B-O1B-C4'	-4.33	106.68	118.01
19	B	1739	CLA	C3D-CAD-CBD	-4.33	101.47	107.60
19	A	1797	CLA	CHD-C4C-C3C	-4.33	118.25	124.94
19	A	1759	CLA	CHD-C4C-C3C	-4.33	118.25	124.94
19	1	1188	CLA	C3D-CAD-CBD	-4.32	101.48	107.60
19	B	1759	CLA	CHD-C4C-C3C	-4.32	118.26	124.94
19	1	1194	CLA	C3B-C2B-C1B	-4.32	102.51	106.29
19	A	1759	CLA	O2D-CGD-O1D	-4.32	114.88	123.79
19	A	1793	CLA	C3D-CAD-CBD	-4.31	101.50	107.60
23	L	1169	BCR	C11-C10-C9	-4.31	120.97	127.20
19	A	1799	CLA	C2A-C1A-CHA	-4.31	114.94	122.58
19	4	1199	CLA	C3D-CAD-CBD	-4.31	101.51	107.60
19	2	1223	CLA	C3D-CAD-CBD	-4.31	101.51	107.60
19	4	1202	CLA	C2D-C3D-C4D	-4.31	102.51	106.30
19	3	3014	CLA	C3B-C2B-C1B	-4.30	102.53	106.29
19	B	1762	CLA	CHD-C4C-C3C	-4.30	118.30	124.94
19	B	1763	CLA	CHD-C4C-C3C	-4.30	118.30	124.94
19	B	1744	CLA	C3D-CAD-CBD	-4.30	101.52	107.60
23	A	1804	BCR	C11-C10-C9	-4.30	120.99	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	1221	CLA	CHD-C4C-C3C	-4.30	118.30	124.94
23	B	1780	BCR	C16-C17-C18	-4.29	120.99	127.20
19	B	1765	CLA	C3D-CAD-CBD	-4.29	101.53	107.60
19	4	1201	CLA	C3D-CAD-CBD	-4.29	101.53	107.60
19	1	1505	CLA	C3D-CAD-CBD	-4.28	101.54	107.60
19	B	1751	CLA	O1D-CGD-CBD	-4.28	118.49	124.62
19	3	1214	CLA	C1D-CHD-C4C	-4.28	115.31	126.32
23	I	1032	BCR	C34-C9-C10	-4.28	116.58	122.90
19	B	1737	CLA	CAA-C2A-C3A	-4.27	100.93	113.22
19	1	1307	CLA	C2A-C1A-CHA	-4.27	115.01	122.58
19	4	1198	CLA	CHD-C4C-C3C	-4.27	118.34	124.94
19	A	1783	CLA	C3D-CAD-CBD	-4.27	101.56	107.60
19	3	1221	CLA	O1D-CGD-CBD	-4.27	118.50	124.62
19	B	1766	CLA	CHD-C4C-C3C	-4.26	118.36	124.94
19	B	1750	CLA	CHD-C4C-C3C	-4.26	118.36	124.94
19	B	1770	CLA	CHD-C4C-C3C	-4.26	118.36	124.94
19	A	1789	CLA	C5-C3-C2	-4.26	112.98	121.05
19	B	1765	CLA	CHD-C4C-C3C	-4.26	118.36	124.94
19	4	1196	CLA	C3D-CAD-CBD	-4.25	101.58	107.60
19	3	1212	CLA	C2A-C1A-CHA	-4.25	115.05	122.58
19	A	1785	CLA	CHD-C4C-C3C	-4.25	118.37	124.94
19	F	1156	CLA	C3D-CAD-CBD	-4.25	101.59	107.60
19	A	1797	CLA	CMD-C2D-C3D	-4.24	116.79	125.09
19	4	1208	CLA	C2D-C3D-C4D	-4.24	102.57	106.30
19	A	1776	CLA	C3D-CAD-CBD	-4.24	101.60	107.60
19	B	1767	CLA	C3D-CAD-CBD	-4.24	101.61	107.60
19	R	1055	CLA	C3D-CAD-CBD	-4.24	101.61	107.60
19	1	1148	CLA	CHD-C4C-C3C	-4.24	118.39	124.94
19	B	1755	CLA	C3D-CAD-CBD	-4.24	101.61	107.60
19	B	1737	CLA	C3D-CAD-CBD	-4.23	101.61	107.60
19	3	1222	CLA	CHD-C4C-C3C	-4.23	118.41	124.94
23	A	1806	BCR	C11-C10-C9	-4.23	121.09	127.20
19	4	1197	CLA	CHD-C4C-C3C	-4.23	117.75	124.83
23	B	1778	BCR	C7-C8-C9	-4.23	119.77	126.22
19	1	1189	CLA	CHD-C4C-C3C	-4.22	118.42	124.94
19	A	1769	CLA	C3D-CAD-CBD	-4.21	101.64	107.60
19	F	1156	CLA	CHD-C4C-C3C	-4.21	118.44	124.94
19	B	1753	CLA	C3D-CAD-CBD	-4.21	101.65	107.60
19	3	1215	CLA	C3C-C4C-CHD	-4.21	118.40	125.32
19	3	1217	CLA	CHC-C1C-C2C	-4.21	115.29	126.35
23	I	1032	BCR	C38-C26-C25	-4.20	120.48	124.61
19	B	1766	CLA	C3D-CAD-CBD	-4.20	101.66	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1775	BCR	C38-C26-C25	-4.20	120.48	124.61
23	A	1803	BCR	C33-C5-C6	-4.20	120.48	124.61
19	1	1149	CLA	CMD-C2D-C3D	-4.19	116.88	125.09
19	B	1758	CLA	C3D-CAD-CBD	-4.19	101.67	107.60
19	1	1200	CLA	C2D-C3D-C4D	-4.19	102.61	106.30
19	2	1216	CLA	C2C-C1C-CHC	-4.19	117.71	125.15
20	A	7004	LMU	C1'-O5'-C5'	-4.18	105.63	113.75
23	A	1806	BCR	C15-C14-C13	-4.18	121.16	127.20
19	2	1218	CLA	C2A-C1A-CHA	-4.18	115.18	122.58
19	4	4007	CLA	CHD-C4C-C3C	-4.17	118.49	124.94
19	A	1798	CLA	C3D-CAD-CBD	-4.17	101.70	107.60
19	I	1031	CLA	CHD-C4C-C3C	-4.17	118.49	124.94
23	A	1805	BCR	C15-C14-C13	-4.17	121.17	127.20
19	3	1220	CLA	C2A-C1A-CHA	-4.17	115.20	122.58
19	1	1187	CLA	C3D-CAD-CBD	-4.16	101.71	107.60
19	B	1770	CLA	C3D-CAD-CBD	-4.16	101.71	107.60
19	4	1196	CLA	CHD-C4C-C3C	-4.16	118.51	124.94
19	A	1795	CLA	CAA-CBA-CGA	-4.16	101.14	113.32
19	3	3015	CLA	C3B-C2B-C1B	-4.16	102.65	106.29
19	A	1767	CLA	C3D-CAD-CBD	-4.16	101.72	107.60
23	B	1777	BCR	C11-C10-C9	-4.16	121.19	127.20
19	2	1214	CLA	C2A-C1A-CHA	-4.15	115.23	122.58
19	B	1740	CLA	C2D-C3D-C4D	-4.15	102.65	106.30
19	1	1197	CLA	O2A-CGA-O1A	-4.15	112.79	123.49
19	A	1771	CLA	C3D-CAD-CBD	-4.14	101.74	107.60
19	1	1199	CLA	CHD-C4C-C3C	-4.14	118.54	124.94
19	B	1763	CLA	O1D-CGD-CBD	-4.14	118.69	124.62
23	B	1779	BCR	C8-C7-C6	-4.14	114.88	127.32
19	4	1207	CLA	C3B-C2B-C1B	-4.14	102.67	106.29
19	1	1307	CLA	C1D-CHD-C4C	-4.13	115.69	126.32
19	B	1736	CLA	CHD-C4C-C3C	-4.13	118.55	124.94
19	3	1218	CLA	CMD-C2D-C3D	-4.13	117.00	125.09
19	4	4007	CLA	CAA-C2A-C3A	-4.13	101.33	113.22
19	A	1772	CLA	C3D-CAD-CBD	-4.13	101.76	107.60
19	B	1745	CLA	CHD-C4C-C3C	-4.12	118.58	124.94
19	1	1189	CLA	CAA-CBA-CGA	-4.11	101.28	113.32
23	A	1807	BCR	C38-C26-C25	-4.11	120.62	124.59
19	3	1218	CLA	O2D-CGD-O1D	-4.11	115.31	123.79
19	3	3011	CLA	CHD-C4C-C3C	-4.11	118.59	124.94
19	4	1207	CLA	C2A-C1A-CHA	-4.11	115.31	122.58
19	L	1167	CLA	C3D-CAD-CBD	-4.10	101.80	107.60
19	1	1142	CLA	CHD-C4C-C3C	-4.10	118.61	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1214	CLA	C2C-C1C-CHC	-4.09	117.88	125.15
19	A	1815	CLA	CMD-C2D-C3D	-4.09	117.09	125.09
19	3	3001	CLA	C2A-C1A-CHA	-4.09	115.34	122.58
19	2	1213	CLA	O1D-CGD-CBD	-4.09	118.77	124.62
23	B	1774	BCR	C7-C8-C9	-4.09	119.99	126.22
19	1	1505	CLA	CHD-C4C-C3C	-4.08	118.63	124.94
19	B	1771	CLA	CHD-C4C-C3C	-4.08	118.63	124.94
20	A	7036	LMU	C2'-C3'-C4'	-4.08	100.64	109.60
19	B	1752	CLA	C3D-CAD-CBD	-4.08	101.83	107.60
19	A	1795	CLA	CHD-C4C-C3C	-4.08	118.64	124.94
19	3	1220	CLA	C1D-CHD-C4C	-4.07	115.84	126.32
19	3	1215	CLA	C3B-C2B-C1B	-4.07	102.72	106.29
23	B	1776	BCR	C34-C9-C10	-4.07	116.88	122.90
19	3	1212	CLA	C3C-C4C-CHD	-4.07	118.62	125.32
19	2	2010	CLA	C2A-C1A-CHA	-4.07	115.37	122.58
19	B	1736	CLA	CMD-C2D-C3D	-4.07	117.13	125.09
19	3	1217	CLA	C2A-C1A-CHA	-4.07	116.40	123.89
19	1	1148	CLA	C3D-CAD-CBD	-4.06	101.86	107.60
19	3	1217	CLA	CAC-C3C-C2C	-4.06	120.39	127.51
19	3	1214	CLA	C3B-C2B-C1B	-4.06	102.74	106.29
19	B	1736	CLA	C3D-CAD-CBD	-4.06	101.86	107.60
19	2	2006	CLA	CMD-C2D-C3D	-4.06	117.16	125.09
19	B	1755	CLA	CHD-C4C-C3C	-4.05	118.68	124.94
19	4	1203	CLA	C2A-C1A-CHA	-4.05	115.40	122.58
19	A	1765	CLA	C3D-CAD-CBD	-4.05	101.87	107.60
23	B	1775	BCR	C27-C26-C25	-4.05	117.62	122.78
19	4	1210	CLA	C2A-C1A-CHA	-4.05	115.41	122.58
19	B	1759	CLA	C3D-CAD-CBD	-4.05	101.87	107.60
19	4	1208	CLA	C3B-C2B-C1B	-4.05	102.75	106.29
19	B	1743	CLA	C3D-CAD-CBD	-4.05	101.88	107.60
19	2	1216	CLA	C1D-CHD-C4C	-4.05	115.91	126.32
23	A	1804	BCR	C7-C8-C9	-4.04	120.05	126.22
23	B	1780	BCR	C11-C10-C9	-4.04	121.36	127.20
19	R	1054	CLA	CHD-C4C-C3C	-4.04	118.70	124.94
19	B	1745	CLA	C3D-CAD-CBD	-4.04	101.89	107.60
19	4	1204	CLA	C3B-C2B-C1B	-4.04	102.75	106.29
19	A	1769	CLA	CHD-C4C-C3C	-4.04	118.70	124.94
19	A	1816	CLA	CHD-C4C-C3C	-4.03	118.71	124.94
23	B	1778	BCR	C33-C5-C6	-4.03	120.65	124.61
19	A	1776	CLA	CMD-C2D-C3D	-4.02	117.22	125.09
23	B	1776	BCR	C27-C26-C25	-4.02	117.66	122.78
20	A	7027	LMU	C1B-O1B-C4'	-4.02	107.51	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1766	CLA	O2D-CGD-O1D	-4.01	115.51	123.79
19	R	1055	CLA	CHD-C4C-C3C	-4.01	118.74	124.94
19	A	1792	CLA	CAA-C2A-C3A	-4.01	101.69	113.22
19	F	1157	CLA	CHD-C4C-C3C	-4.01	118.75	124.94
19	A	1760	CLA	CHD-C4C-C3C	-4.01	118.75	124.94
19	4	1210	CLA	C3C-C4C-CHD	-4.01	118.73	125.32
19	A	1776	CLA	CHD-C4C-C3C	-4.01	118.75	124.94
19	B	1738	CLA	O2D-CGD-O1D	-4.00	115.52	123.79
19	A	1767	CLA	CMD-C2D-C3D	-4.00	117.26	125.09
20	A	7030	LMU	C3'-C4'-C5'	-3.99	101.81	110.84
19	1	1308	CLA	CHD-C4C-C3C	-3.99	118.77	124.94
23	B	1779	BCR	C16-C17-C18	-3.99	121.43	127.20
19	A	1773	CLA	CHD-C4C-C3C	-3.99	118.77	124.94
23	A	1809	BCR	C11-C12-C13	-3.99	114.58	126.32
19	A	1800	CLA	C6-C5-C3	-3.99	103.73	112.48
19	B	1769	CLA	O1D-CGD-CBD	-3.99	118.91	124.62
19	A	1798	CLA	CHD-C4C-C3C	-3.99	118.78	124.94
19	1	1189	CLA	CGD-CBD-CAD	-3.99	97.12	110.62
23	B	1779	BCR	C8-C9-C10	-3.99	112.56	118.98
19	A	1762	CLA	CHD-C4C-C3C	-3.98	118.79	124.94
19	4	1205	CLA	CBA-CAA-C2A	-3.98	102.50	113.73
20	A	7005	LMU	C1B-O1B-C4'	-3.98	107.61	118.01
19	F	1157	CLA	CBA-CAA-C2A	-3.98	102.52	113.73
19	A	1814	CLA	C3D-CAD-CBD	-3.98	101.98	107.60
19	A	1777	CLA	CHD-C4C-C3C	-3.97	118.80	124.94
19	1	1307	CLA	C2D-C3D-C4D	-3.97	102.81	106.30
19	B	1735	CLA	CHD-C4C-C3C	-3.97	118.81	124.94
19	A	1777	CLA	C3D-CAD-CBD	-3.97	101.99	107.60
20	A	7001	LMU	C3B-C4B-C5B	-3.97	103.28	110.20
19	4	1202	CLA	C3B-C2B-C1B	-3.96	102.82	106.29
19	1	1198	CLA	C3B-C2B-C1B	-3.96	102.82	106.29
19	B	1746	CLA	O1D-CGD-CBD	-3.96	118.95	124.62
19	B	1754	CLA	C3D-CAD-CBD	-3.96	102.00	107.60
19	A	1761	CLA	C3D-CAD-CBD	-3.96	102.00	107.60
23	A	1808	BCR	C24-C23-C22	-3.95	120.19	126.22
19	1	1194	CLA	C3C-C4C-CHD	-3.95	118.82	125.32
19	A	1792	CLA	C3D-CAD-CBD	-3.95	102.01	107.60
19	B	1764	CLA	CHD-C4C-C3C	-3.94	118.85	124.94
20	A	7020	LMU	C3'-C4'-C5'	-3.94	101.93	110.84
19	B	1757	CLA	CHD-C4C-C3C	-3.94	118.85	124.94
19	B	1764	CLA	C3D-CAD-CBD	-3.94	102.03	107.60
19	1	1195	CLA	C2D-C3D-C4D	-3.94	102.84	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1746	CLA	CHD-C4C-C3C	-3.94	118.86	124.94
20	2	1224	LMU	C1'-C2'-C3'	-3.93	102.22	109.97
19	A	1800	CLA	C3D-CAD-CBD	-3.93	102.04	107.60
19	2	1220	CLA	C3C-C4C-CHD	-3.92	118.86	125.32
19	A	1762	CLA	C3D-CAD-CBD	-3.92	102.05	107.60
19	H	1081	CLA	C3D-CAD-CBD	-3.92	102.05	107.60
19	B	1772	CLA	CAA-C2A-C3A	-3.92	106.81	116.20
19	1	1143	CLA	C3D-CAD-CBD	-3.92	102.06	107.60
19	A	1792	CLA	CMD-C2D-C3D	-3.91	117.43	125.09
19	1	1142	CLA	C3D-CAD-CBD	-3.91	102.06	107.60
19	3	1221	CLA	C3D-CAD-CBD	-3.91	102.06	107.60
19	3	3011	CLA	C3D-CAD-CBD	-3.91	102.06	107.60
19	A	1768	CLA	CHD-C4C-C3C	-3.91	118.89	124.94
19	A	1774	CLA	C6-C5-C3	-3.91	103.90	112.48
19	B	1735	CLA	CMD-C2D-C3D	-3.91	117.44	125.09
19	3	1215	CLA	C2C-C1C-CHC	-3.91	118.20	125.15
19	1	1195	CLA	C3C-C4C-CHD	-3.91	118.89	125.32
19	A	1785	CLA	C3D-CAD-CBD	-3.91	102.08	107.60
19	4	1206	CLA	C3D-CAD-CBD	-3.90	102.08	107.60
19	B	1742	CLA	C4-C3-C2	-3.90	115.84	123.50
23	A	1808	BCR	C19-C18-C17	-3.90	112.69	118.98
19	4	1205	CLA	CMD-C2D-C3D	-3.90	117.46	125.09
19	4	1203	CLA	C3C-C4C-CHD	-3.90	118.90	125.32
23	I	1032	BCR	C29-C30-C25	-3.90	104.19	110.36
19	1	1200	CLA	C3C-C4C-CHD	-3.90	118.91	125.32
19	A	1801	CLA	C3D-CAD-CBD	-3.90	102.09	107.60
19	A	1765	CLA	CHC-C1C-C2C	-3.89	116.11	126.35
19	A	1759	CLA	C3D-CAD-CBD	-3.89	102.09	107.60
19	4	1207	CLA	C3C-C4C-CHD	-3.89	118.92	125.32
19	4	1204	CLA	C3C-C4C-CHD	-3.89	118.92	125.32
19	A	1817	CLA	CHD-C4C-C3C	-3.89	118.94	124.94
23	A	1806	BCR	C7-C8-C9	-3.88	120.29	126.22
19	B	1760	CLA	C3D-CAD-CBD	-3.88	102.11	107.60
19	A	1790	CLA	C3D-CAD-CBD	-3.88	102.11	107.60
19	B	1756	CLA	C3D-CAD-CBD	-3.88	102.11	107.60
19	1	1146	CLA	CMD-C2D-C3D	-3.88	117.50	125.09
19	A	1775	CLA	CHD-C4C-C3C	-3.88	118.34	124.83
19	4	1200	CLA	C3D-CAD-CBD	-3.88	102.12	107.60
19	A	1781	CLA	C3D-CAD-CBD	-3.87	102.12	107.60
19	1	1188	CLA	CHD-C4C-C3C	-3.87	118.96	124.94
19	3	1214	CLA	C3C-C4C-CHD	-3.87	118.95	125.32
19	3	3014	CLA	C1D-CHD-C4C	-3.86	116.39	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1767	CLA	CAA-C2A-C3A	-3.86	102.12	113.22
19	B	1754	CLA	O2D-CGD-O1D	-3.85	115.83	123.79
19	1	1187	CLA	CMD-C2D-C3D	-3.85	117.55	125.09
23	B	1775	BCR	C3-C4-C5	-3.85	107.75	113.87
19	3	1222	CLA	C3D-CAD-CBD	-3.85	102.15	107.60
19	1	1198	CLA	C2A-C1A-CHA	-3.85	115.77	122.58
23	A	1805	BCR	C24-C23-C22	-3.84	120.36	126.22
19	1	1505	CLA	CMD-C2D-C3D	-3.84	117.57	125.09
20	A	7026	LMU	C2'-C3'-C4'	-3.84	101.17	109.60
19	1	1197	CLA	CMD-C2D-C3D	-3.84	117.58	125.09
19	A	1787	CLA	CHD-C4C-C3C	-3.83	119.02	124.94
19	4	1208	CLA	C3C-C4C-CHD	-3.83	119.02	125.32
19	B	1744	CLA	CMD-C2D-C3D	-3.83	117.60	125.09
19	G	1099	CLA	O2D-CGD-O1D	-3.82	115.89	123.79
23	A	1808	BCR	C33-C5-C6	-3.82	120.85	124.61
19	A	1781	CLA	CHD-C4C-C3C	-3.82	119.04	124.94
20	A	7008	LMU	C1B-C2B-C3B	-3.82	102.44	109.97
23	B	1774	BCR	C16-C17-C18	-3.82	121.68	127.20
19	A	1783	CLA	CHD-C4C-C3C	-3.82	119.04	124.94
23	B	1780	BCR	C24-C23-C22	-3.82	120.40	126.22
19	1	1193	CLA	CMD-C2D-C3D	-3.81	117.63	125.09
19	2	1216	CLA	C2A-C1A-CHA	-3.81	115.83	122.58
19	A	1782	CLA	C3D-CAD-CBD	-3.81	102.21	107.60
19	A	1764	CLA	CHD-C4C-C3C	-3.81	119.05	124.94
19	A	1794	CLA	O2D-CGD-O1D	-3.81	115.93	123.79
19	3	1216	CLA	C2A-C1A-CHA	-3.81	115.84	122.58
19	3	3008	CLA	CHD-C4C-C3C	-3.81	119.06	124.94
19	4	1207	CLA	C2C-C1C-CHC	-3.80	118.39	125.15
19	A	1763	CLA	C3D-CAD-CBD	-3.80	102.22	107.60
19	2	1222	CLA	C3D-CAD-CBD	-3.80	102.22	107.60
19	B	1738	CLA	C6-C5-C3	-3.80	104.15	112.48
23	B	1778	BCR	C38-C26-C25	-3.80	120.88	124.61
19	A	1763	CLA	CHD-C4C-C3C	-3.80	119.08	124.94
19	A	1777	CLA	CMD-C2D-C3D	-3.80	117.67	125.09
19	3	3001	CLA	C3C-C4C-CHD	-3.79	119.08	125.32
19	B	1753	CLA	C2A-C1A-CHA	-3.79	116.90	123.89
19	B	1736	CLA	O2D-CGD-O1D	-3.79	115.97	123.79
19	2	1216	CLA	C3C-C4C-CHD	-3.79	119.09	125.32
19	1	1197	CLA	CGD-CBD-CAD	-3.79	97.79	110.62
19	1	1196	CLA	CHD-C4C-C3C	-3.78	118.50	124.83
19	1	1194	CLA	C2A-C1A-CHA	-3.78	115.88	122.58
19	3	1215	CLA	C2A-C1A-CHA	-3.78	115.89	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1807	BCR	C37-C22-C21	-3.78	117.32	122.90
19	B	1753	CLA	CAA-C2A-C1A	-3.78	99.15	112.47
23	L	1169	BCR	C27-C26-C25	-3.77	117.97	122.78
19	B	1768	CLA	C3D-CAD-CBD	-3.77	102.27	107.60
19	3	1219	CLA	C3C-C4C-CHD	-3.77	119.12	125.32
19	B	1784	CLA	CHD-C4C-C3C	-3.76	119.13	124.94
19	A	1793	CLA	CMD-C2D-C3D	-3.76	117.73	125.09
19	1	1145	CLA	CHD-C4C-C3C	-3.76	119.13	124.94
19	4	1199	CLA	O1D-CGD-CBD	-3.76	119.23	124.62
21	B	8053	SUC	C1-O5-C5	-3.76	107.23	113.64
19	3	1220	CLA	C2C-C1C-CHC	-3.76	118.48	125.15
19	A	1791	CLA	C3D-CAD-CBD	-3.75	102.29	107.60
19	3	3011	CLA	CHC-C1C-C2C	-3.75	116.49	126.35
20	A	7036	LMU	C1B-O1B-C4'	-3.75	108.21	118.01
19	A	1766	CLA	CMD-C2D-C3D	-3.75	117.76	125.09
19	A	1788	CLA	CHD-C4C-C3C	-3.74	119.16	124.94
19	B	1768	CLA	CHD-C4C-C3C	-3.74	119.16	124.94
19	F	1155	CLA	CMD-C2D-C3D	-3.74	117.77	125.09
19	1	1189	CLA	C3D-CAD-CBD	-3.74	102.31	107.60
19	2	1213	CLA	CAA-C2A-C3A	-3.74	102.48	113.22
19	3	1212	CLA	C3B-C2B-C1B	-3.73	103.02	106.29
19	B	1767	CLA	CHD-C4C-C3C	-3.73	119.17	124.94
23	B	1777	BCR	C7-C8-C9	-3.73	120.53	126.22
19	2	1220	CLA	C2A-C1A-CHA	-3.73	115.97	122.58
19	2	1215	CLA	C3D-CAD-CBD	-3.73	102.33	107.60
23	A	1803	BCR	C16-C17-C18	-3.72	121.82	127.20
23	A	1803	BCR	C7-C8-C9	-3.72	120.54	126.22
19	A	1799	CLA	C1D-CHD-C4C	-3.72	116.75	126.32
19	3	3014	CLA	C2C-C1C-CHC	-3.72	118.54	125.15
19	B	1758	CLA	O2D-CGD-O1D	-3.72	116.11	123.79
19	A	1780	CLA	CHD-C4C-C3C	-3.71	119.21	124.94
19	3	1218	CLA	C4-C3-C2	-3.71	116.23	123.50
19	F	1157	CLA	CBC-CAC-C3C	-3.70	101.08	112.39
23	B	1776	BCR	C30-C25-C26	-3.70	117.22	122.66
23	L	1169	BCR	C15-C16-C17	-3.70	115.21	123.39
19	G	1099	CLA	C3D-CAD-CBD	-3.70	102.37	107.60
19	B	1772	CLA	CHD-C4C-C3C	-3.70	118.64	124.83
19	1	1190	CLA	CHD-C4C-C3C	-3.70	119.23	124.94
19	B	1754	CLA	CHD-C4C-C3C	-3.70	119.23	124.94
19	1	1196	CLA	CMD-C2D-C3D	-3.70	117.86	125.09
19	B	1748	CLA	CGD-CBD-CAD	-3.70	98.10	110.62
19	B	1764	CLA	CMD-C2D-C3D	-3.69	117.86	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1777	BCR	C16-C17-C18	-3.69	121.86	127.20
19	A	1768	CLA	C3D-CAD-CBD	-3.69	102.38	107.60
19	2	1215	CLA	CMD-C2D-C3D	-3.69	117.87	125.09
19	A	1775	CLA	CMD-C2D-C3D	-3.69	117.87	125.09
19	1	1187	CLA	CHC-C1C-C2C	-3.69	116.65	126.35
19	B	1770	CLA	CMD-C2D-C3D	-3.69	117.88	125.09
19	2	1219	CLA	CHD-C4C-C3C	-3.68	118.66	124.83
19	2	1218	CLA	C2C-C1C-CHC	-3.68	118.61	125.15
19	B	1740	CLA	C3B-C2B-C1B	-3.68	103.07	106.29
19	2	1214	CLA	C2C-C1C-CHC	-3.68	118.61	125.15
19	B	1757	CLA	CMD-C2D-C3D	-3.68	117.89	125.09
19	1	1143	CLA	CHD-C4C-C3C	-3.68	119.26	124.94
23	B	1774	BCR	C24-C23-C22	-3.67	120.62	126.22
19	L	1168	CLA	O2D-CGD-O1D	-3.67	116.20	123.79
19	A	1771	CLA	CMD-C2D-C3D	-3.67	117.91	125.09
19	1	1143	CLA	CMD-C2D-C3D	-3.67	117.92	125.09
19	B	1735	CLA	C3D-CAD-CBD	-3.67	102.41	107.60
19	3	1218	CLA	C3D-CAD-CBD	-3.66	102.42	107.60
19	A	1815	CLA	CHD-C4C-C3C	-3.66	119.28	124.94
19	A	1761	CLA	CHD-C4C-C3C	-3.66	119.28	124.94
19	B	1761	CLA	O2D-CGD-O1D	-3.66	116.23	123.79
19	A	1770	CLA	C3B-C2B-C1B	-3.66	103.09	106.29
19	A	1816	CLA	C5-C3-C2	-3.66	114.12	121.05
19	2	1215	CLA	CHD-C4C-C3C	-3.66	119.29	124.94
19	1	1191	CLA	CHD-C4C-C3C	-3.65	118.71	124.83
23	A	1803	BCR	C11-C10-C9	-3.65	121.92	127.20
19	B	1759	CLA	CMD-C2D-C3D	-3.65	117.95	125.09
19	B	1770	CLA	O1D-CGD-CBD	-3.65	119.39	124.62
19	3	1219	CLA	C2D-C3D-C4D	-3.65	103.09	106.30
19	B	1747	CLA	CHD-C4C-C3C	-3.65	119.31	124.94
19	A	1760	CLA	CMD-C2D-C3D	-3.64	117.96	125.09
23	A	1809	BCR	C7-C8-C9	-3.64	120.67	126.22
19	1	1194	CLA	C2D-C3D-C4D	-3.64	103.10	106.30
19	1	1198	CLA	C2D-C3D-C4D	-3.64	103.10	106.30
19	4	1197	CLA	CAA-C2A-C3A	-3.63	107.50	116.20
19	4	1199	CLA	CMD-C2D-C3D	-3.63	117.98	125.09
19	4	4014	CLA	CMD-C2D-C3D	-3.63	117.98	125.09
19	2	1220	CLA	C3B-C2B-C1B	-3.63	103.11	106.29
19	4	1199	CLA	CHC-C1C-C2C	-3.63	116.80	126.35
19	A	1793	CLA	CHD-C4C-C3C	-3.63	119.33	124.94
19	A	1792	CLA	CHD-C4C-C3C	-3.63	119.34	124.94
19	L	1167	CLA	CHD-C4C-C3C	-3.63	119.34	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1800	CLA	O1D-CGD-CBD	-3.63	119.42	124.62
23	B	1777	BCR	C28-C27-C26	-3.63	108.11	113.87
19	3	3015	CLA	C2D-C3D-C4D	-3.62	103.11	106.30
19	B	1740	CLA	C1D-CHD-C4C	-3.62	117.00	126.32
19	1	1199	CLA	CBA-CAA-C2A	-3.62	103.52	113.73
21	B	8062	SUC	O5-C5-C4	-3.62	102.89	109.68
19	I	1031	CLA	C3D-CAD-CBD	-3.62	102.48	107.60
23	B	1776	BCR	C16-C17-C18	-3.62	121.97	127.20
20	A	1811	LMU	C3B-C4B-C5B	-3.62	103.89	110.20
19	B	1755	CLA	CMD-C2D-C3D	-3.61	118.02	125.09
19	2	1217	CLA	CHC-C1C-C2C	-3.61	116.85	126.35
19	B	1747	CLA	C3D-CAD-CBD	-3.61	102.49	107.60
19	3	1220	CLA	C3C-C4C-CHD	-3.61	119.38	125.32
19	J	1043	CLA	CHD-C4C-C3C	-3.60	119.37	124.94
19	3	3001	CLA	C2D-C3D-C4D	-3.60	103.13	106.30
20	A	7008	LMU	C1'-C2'-C3'	-3.60	102.87	109.97
19	1	1198	CLA	C3C-C4C-CHD	-3.60	119.40	125.32
19	I	1031	CLA	O1D-CGD-CBD	-3.59	119.47	124.62
19	4	1202	CLA	C1D-CHD-C4C	-3.59	117.08	126.32
19	A	1786	CLA	C3D-CAD-CBD	-3.59	102.52	107.60
19	2	1214	CLA	C2D-C3D-C4D	-3.59	103.14	106.30
19	B	1750	CLA	CMD-C2D-C3D	-3.59	118.07	125.09
19	A	1766	CLA	O1D-CGD-CBD	-3.59	119.48	124.62
19	A	1794	CLA	CHD-C4C-C3C	-3.58	119.40	124.94
19	3	3008	CLA	C3D-CAD-CBD	-3.58	102.53	107.60
19	B	1767	CLA	CMD-C2D-C3D	-3.58	118.09	125.09
19	B	1757	CLA	C3D-CAD-CBD	-3.57	102.55	107.60
19	B	1761	CLA	CGD-CBD-CAD	-3.57	98.52	110.62
19	A	1814	CLA	O1D-CGD-CBD	-3.57	119.51	124.62
19	4	1206	CLA	CMD-C2D-C3D	-3.57	118.11	125.09
19	2	2010	CLA	C2C-C1C-CHC	-3.57	118.81	125.15
19	A	1764	CLA	C3D-CAD-CBD	-3.57	102.56	107.60
23	B	1779	BCR	C3-C4-C5	-3.56	108.22	113.87
19	A	1787	CLA	C3D-CAD-CBD	-3.56	102.57	107.60
19	1	1187	CLA	CHD-C4C-C3C	-3.56	119.45	124.94
19	B	1738	CLA	C3D-CAD-CBD	-3.55	102.57	107.60
19	A	1770	CLA	C2C-C1C-CHC	-3.54	118.85	125.15
20	A	7008	LMU	C1-O1'-C1'	-3.54	107.76	113.94
19	1	1148	CLA	CMD-C2D-C3D	-3.54	118.17	125.09
19	H	1081	CLA	O1D-CGD-CBD	-3.54	119.55	124.62
23	A	1805	BCR	C30-C25-C26	-3.53	117.47	122.66
19	A	1790	CLA	CMD-C2D-C3D	-3.53	118.18	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1806	BCR	C38-C26-C25	-3.53	121.14	124.61
19	4	1204	CLA	C2D-C3D-C4D	-3.53	103.20	106.30
19	1	1307	CLA	C3C-C4C-CHD	-3.53	119.52	125.32
19	A	1763	CLA	O1D-CGD-CBD	-3.52	119.58	124.62
23	L	1169	BCR	C24-C23-C22	-3.52	120.85	126.22
19	F	1155	CLA	CHD-C4C-C3C	-3.52	118.94	124.83
19	2	1214	CLA	C3B-C2B-C1B	-3.51	103.21	106.29
20	A	7037	LMU	C1B-O1B-C4'	-3.51	108.82	118.01
23	B	1779	BCR	C33-C5-C6	-3.51	121.15	124.61
19	A	1779	CLA	CHD-C4C-C3C	-3.51	119.52	124.94
19	R	1055	CLA	C4-C3-C2	-3.51	116.61	123.50
19	1	1198	CLA	C2C-C1C-CHC	-3.51	118.92	125.15
19	A	1780	CLA	CMD-C2D-C3D	-3.51	118.23	125.09
19	2	1222	CLA	O1D-CGD-CBD	-3.51	119.60	124.62
19	A	1762	CLA	CMD-C2D-C3D	-3.50	118.24	125.09
23	B	1777	BCR	C38-C26-C25	-3.50	121.17	124.61
19	A	1766	CLA	CHD-C4C-C3C	-3.50	119.54	124.94
19	B	1742	CLA	CMD-C2D-C3D	-3.50	118.25	125.09
19	H	1080	CLA	C3D-CAD-CBD	-3.49	102.66	107.60
19	H	1079	CLA	O2D-CGD-O1D	-3.49	116.59	123.79
19	B	1748	CLA	C3D-CAD-CBD	-3.48	102.67	107.60
20	A	7040	LMU	C3B-C4B-C5B	-3.48	104.13	110.20
20	2	1224	LMU	O5'-C5'-C4'	-3.47	102.41	109.75
19	A	1770	CLA	C1D-CHD-C4C	-3.47	117.39	126.32
19	A	1773	CLA	CMD-C2D-C3D	-3.47	118.30	125.09
19	2	1220	CLA	C2C-C1C-CHC	-3.47	118.98	125.15
19	2	1217	CLA	O2D-CGD-O1D	-3.47	116.62	123.79
19	A	1799	CLA	C2C-C1C-CHC	-3.47	118.98	125.15
19	B	1768	CLA	O2D-CGD-O1D	-3.47	116.63	123.79
19	3	3011	CLA	CMD-C2D-C3D	-3.46	118.31	125.09
19	A	1795	CLA	CMD-C2D-C3D	-3.46	118.31	125.09
19	R	1054	CLA	CMD-C2D-C3D	-3.46	118.31	125.09
19	A	1797	CLA	CHC-C1C-C2C	-3.46	117.24	126.35
19	4	4007	CLA	CMD-C2D-C3D	-3.46	118.32	125.09
19	B	1759	CLA	O1D-CGD-CBD	-3.46	119.67	124.62
19	A	1760	CLA	C3D-CAD-CBD	-3.45	102.71	107.60
19	A	1784	CLA	CHD-C4C-C3C	-3.45	119.61	124.94
23	A	1806	BCR	C24-C23-C22	-3.45	120.96	126.22
19	4	1198	CLA	CMD-C2D-C3D	-3.45	118.34	125.09
19	4	4007	CLA	CAA-CBA-CGA	-3.45	103.23	113.32
19	A	1798	CLA	O2D-CGD-O1D	-3.44	116.68	123.79
19	A	1778	CLA	CMD-C2D-C3D	-3.44	118.35	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1751	CLA	CMD-C2D-C3D	-3.44	118.36	125.09
19	4	1209	CLA	CHD-C4C-C3C	-3.44	119.07	124.83
23	I	1032	BCR	C8-C7-C6	-3.44	116.99	127.32
19	1	1146	CLA	C3D-CAD-CBD	-3.44	102.74	107.60
23	L	1169	BCR	C30-C25-C26	-3.44	117.61	122.66
19	F	1157	CLA	O2D-CGD-O1D	-3.44	116.70	123.79
19	1	1307	CLA	C2C-C1C-CHC	-3.43	119.05	125.15
19	A	1791	CLA	CMD-C2D-C3D	-3.43	118.38	125.09
19	B	1763	CLA	CMD-C2D-C3D	-3.43	118.38	125.09
19	3	1214	CLA	C2D-C3D-C4D	-3.43	103.28	106.30
19	B	1769	CLA	O2D-CGD-O1D	-3.43	116.71	123.79
19	A	1771	CLA	CHD-C4C-C3C	-3.43	119.65	124.94
20	A	7014	LMU	C1B-O1B-C4'	-3.43	109.06	118.01
19	A	1816	CLA	C3D-CAD-CBD	-3.42	102.75	107.60
19	2	1223	CLA	CAA-C2A-C3A	-3.42	103.38	113.22
19	A	1779	CLA	CMD-C2D-C3D	-3.42	118.40	125.09
19	R	1055	CLA	CMD-C2D-C3D	-3.42	118.40	125.09
19	4	1202	CLA	C2C-C1C-CHC	-3.42	119.08	125.15
19	A	1774	CLA	CMD-C2D-C3D	-3.42	118.41	125.09
19	2	1221	CLA	O1D-CGD-CBD	-3.41	119.73	124.62
20	A	7017	LMU	O5B-C5B-C4B	-3.41	103.28	109.68
19	B	1752	CLA	CMD-C2D-C3D	-3.41	118.43	125.09
19	3	1216	CLA	C2C-C1C-CHC	-3.40	119.11	125.15
19	4	1204	CLA	C2C-C1C-CHC	-3.40	119.11	125.15
19	A	1765	CLA	CMD-C2D-C3D	-3.40	118.44	125.09
19	L	1167	CLA	O2D-CGD-O1D	-3.40	116.77	123.79
19	A	1796	CLA	C3D-CAD-CBD	-3.40	102.80	107.60
19	3	3014	CLA	C3C-C4C-CHD	-3.39	119.74	125.32
23	A	1807	BCR	C16-C15-C14	-3.39	115.90	123.39
19	A	1790	CLA	CHD-C4C-C3C	-3.39	119.71	124.94
19	A	1793	CLA	O2D-CGD-O1D	-3.39	116.80	123.79
23	A	1805	BCR	C16-C17-C18	-3.38	122.31	127.20
19	A	1788	CLA	CMD-C2D-C3D	-3.38	118.47	125.09
19	4	1203	CLA	C2D-C3D-C4D	-3.38	103.33	106.30
19	2	1217	CLA	C3D-CAD-CBD	-3.38	102.82	107.60
19	A	1778	CLA	CHD-C4C-C3C	-3.38	119.72	124.94
19	1	1308	CLA	CMD-C2D-C3D	-3.37	118.49	125.09
19	A	1763	CLA	CMD-C2D-C3D	-3.37	118.49	125.09
19	1	1149	CLA	CHC-C1C-C2C	-3.37	117.48	126.35
19	1	1142	CLA	CMD-C2D-C3D	-3.37	118.50	125.09
19	1	1191	CLA	CMD-C2D-C3D	-3.37	118.50	125.09
19	A	1786	CLA	O1D-CGD-CBD	-3.37	119.79	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1748	CLA	CMD-C2D-C3D	-3.37	118.50	125.09
20	A	7031	LMU	C3B-C4B-C5B	-3.37	104.33	110.20
19	3	1212	CLA	C2C-C1C-CHC	-3.36	119.17	125.15
19	B	1765	CLA	CMD-C2D-C3D	-3.36	118.51	125.09
19	1	1188	CLA	CMD-C2D-C3D	-3.36	118.52	125.09
19	A	1759	CLA	O1D-CGD-CBD	-3.36	119.81	124.62
23	A	1807	BCR	C27-C26-C25	-3.35	118.51	122.74
19	2	1220	CLA	C2D-C3D-C4D	-3.35	103.35	106.30
19	H	1079	CLA	CAA-C2A-C3A	-3.35	103.58	113.22
19	2	1219	CLA	CMD-C2D-C3D	-3.35	118.54	125.09
19	B	1766	CLA	CMD-C2D-C3D	-3.35	118.54	125.09
19	A	1780	CLA	C3D-CAD-CBD	-3.35	102.86	107.60
19	4	1201	CLA	C6-C5-C3	-3.35	108.84	114.43
19	A	1817	CLA	CMD-C2D-C3D	-3.35	118.54	125.09
19	4	1201	CLA	CMD-C2D-C3D	-3.35	118.55	125.09
19	1	1200	CLA	C2C-C1C-CHC	-3.34	119.21	125.15
19	1	1190	CLA	O1D-CGD-CBD	-3.34	119.83	124.62
19	B	1742	CLA	CHD-C4C-C3C	-3.34	119.78	124.94
19	3	3015	CLA	C2C-C1C-CHC	-3.34	119.21	125.15
19	2	1221	CLA	CHC-C1C-C2C	-3.34	117.57	126.35
19	A	1764	CLA	CAA-C2A-C1A	-3.34	100.70	112.47
20	A	7009	LMU	O2'-C2'-C3'	-3.34	102.83	110.34
21	3	1223	SUC	C4-C3-C2	-3.33	104.57	110.79
19	4	4014	CLA	CBA-CAA-C2A	-3.33	104.33	113.73
23	B	1776	BCR	C37-C22-C21	-3.33	117.98	122.90
19	4	1197	CLA	CMD-C2D-C3D	-3.32	118.59	125.09
19	3	1222	CLA	CMD-C2D-C3D	-3.32	118.60	125.09
19	A	1766	CLA	C3D-CAD-CBD	-3.32	102.91	107.60
19	B	1753	CLA	O2D-CGD-O1D	-3.32	116.94	123.79
23	B	1774	BCR	C38-C26-C25	-3.31	121.35	124.61
19	1	1309	CLA	C2C-C1C-CHC	-3.31	119.26	125.15
19	B	1768	CLA	CMD-C2D-C3D	-3.31	118.61	125.09
19	B	1738	CLA	CMD-C2D-C3D	-3.31	118.62	125.09
19	A	1761	CLA	CHC-C1C-C2C	-3.30	117.67	126.35
19	A	1781	CLA	CMD-C2D-C3D	-3.30	118.63	125.09
19	A	1793	CLA	O1D-CGD-CBD	-3.30	119.89	124.62
20	A	7038	LMU	C2'-C3'-C4'	-3.30	102.35	109.60
19	2	1212	CLA	CMD-C2D-C3D	-3.30	118.64	125.09
19	A	1759	CLA	CHC-C1C-C2C	-3.30	117.68	126.35
19	B	1765	CLA	O1D-CGD-CBD	-3.30	119.90	124.62
19	A	1774	CLA	O2D-CGD-O1D	-3.30	116.98	123.79
19	3	1219	CLA	C2C-C1C-CHC	-3.30	119.29	125.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7028	LMU	C1B-O1B-C4'	-3.29	109.40	118.01
19	2	1223	CLA	CAA-C2A-C1A	-3.29	100.86	112.47
19	B	1747	CLA	CMD-C2D-C3D	-3.29	118.65	125.09
19	2	1223	CLA	O1D-CGD-CBD	-3.29	119.91	124.62
19	A	1796	CLA	O2D-CGD-O1D	-3.29	117.00	123.79
23	B	1777	BCR	C24-C23-C22	-3.29	121.20	126.22
19	B	1740	CLA	C2C-C1C-CHC	-3.29	119.31	125.15
19	B	1741	CLA	O1D-CGD-CBD	-3.29	119.91	124.62
19	A	1789	CLA	CBC-CAC-C3C	-3.29	102.36	112.39
19	B	1766	CLA	CAA-CBA-CGA	-3.28	103.71	113.32
19	F	1156	CLA	CMD-C2D-C3D	-3.28	118.67	125.09
19	A	1797	CLA	O1D-CGD-CBD	-3.28	119.92	124.62
19	A	1772	CLA	O1D-CGD-CBD	-3.28	119.92	124.62
19	A	1773	CLA	O1D-CGD-CBD	-3.28	119.92	124.62
19	B	1752	CLA	CHD-C4C-C3C	-3.28	119.88	124.94
19	4	1196	CLA	CMD-C2D-C3D	-3.27	118.69	125.09
20	A	7040	LMU	O3'-C3'-C2'	-3.27	102.97	110.34
19	A	1791	CLA	CHD-C4C-C3C	-3.27	119.89	124.94
23	B	1780	BCR	C7-C8-C9	-3.27	121.23	126.22
19	F	1156	CLA	CMA-C3A-C2A	-3.27	108.37	116.20
19	4	1199	CLA	C1D-CHD-C4C	-3.27	117.66	122.60
23	L	1169	BCR	C33-C5-C6	-3.27	121.40	124.61
19	A	1761	CLA	O1D-CGD-CBD	-3.26	119.95	124.62
19	2	1212	CLA	O1D-CGD-CBD	-3.26	119.95	124.62
19	A	1800	CLA	CMD-C2D-C3D	-3.26	118.72	125.09
23	B	1778	BCR	C16-C17-C18	-3.25	122.50	127.20
19	2	1213	CLA	CMD-C2D-C3D	-3.25	118.73	125.09
19	A	1785	CLA	O1D-CGD-CBD	-3.25	119.96	124.62
19	B	1759	CLA	O2D-CGD-O1D	-3.25	117.08	123.79
19	A	1791	CLA	O1D-CGD-CBD	-3.25	119.97	124.62
19	A	1770	CLA	C3C-C4C-CHD	-3.24	119.99	125.32
19	1	1199	CLA	CHC-C1C-C2C	-3.24	117.83	126.35
19	1	1309	CLA	C1D-CHD-C4C	-3.24	117.99	126.32
19	J	1043	CLA	CHC-C1C-C2C	-3.24	117.84	126.35
19	3	3001	CLA	C2C-C1C-CHC	-3.23	119.40	125.15
20	A	7032	LMU	C3B-C4B-C5B	-3.23	104.57	110.20
19	B	1761	CLA	O1D-CGD-CBD	-3.23	119.99	124.62
23	A	1809	BCR	C15-C14-C13	-3.23	122.53	127.20
19	A	1767	CLA	CHD-C4C-C3C	-3.23	119.95	124.94
23	B	1775	BCR	C16-C17-C18	-3.22	122.54	127.20
20	A	7034	LMU	O2B-C2B-C3B	-3.22	103.08	110.34
20	A	7016	LMU	C1'-O5'-C5'	-3.22	107.50	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1762	CLA	CMD-C2D-C3D	-3.22	118.80	125.09
19	B	1784	CLA	CAA-C2A-C3A	-3.22	103.97	113.22
19	4	1198	CLA	CHC-C1C-C2C	-3.21	117.90	126.35
19	4	1207	CLA	C2D-C3D-C4D	-3.21	103.47	106.30
19	4	4014	CLA	CHC-C1C-C2C	-3.21	117.91	126.35
19	4	1210	CLA	C3B-C2B-C1B	-3.21	103.48	106.29
19	B	1764	CLA	O1D-CGD-CBD	-3.21	120.03	124.62
19	A	1769	CLA	C1-C2-C3	-3.21	121.46	126.71
19	3	1213	CLA	CMD-C2D-C3D	-3.20	118.82	125.09
19	A	1761	CLA	CMD-C2D-C3D	-3.20	118.83	125.09
19	L	1167	CLA	CMD-C2D-C3D	-3.20	118.83	125.09
19	A	1778	CLA	CHC-C1C-C2C	-3.19	117.95	126.35
19	1	1189	CLA	CAA-C2A-C1A	-3.19	101.22	112.47
20	A	7034	LMU	C1B-O5B-C5B	-3.19	107.55	113.75
19	1	1189	CLA	O2D-CGD-O1D	-3.19	117.21	123.79
19	1	1194	CLA	C2C-C1C-CHC	-3.19	119.48	125.15
19	B	1741	CLA	CBA-CAA-C2A	-3.19	104.74	113.73
19	1	1146	CLA	CHD-C4C-C3C	-3.19	120.02	124.94
20	A	7035	LMU	C3'-C4'-C5'	-3.19	103.64	110.84
19	A	1797	CLA	O2D-CGD-O1D	-3.19	117.21	123.79
19	B	1744	CLA	CHD-C4C-C3C	-3.18	120.02	124.94
19	A	1796	CLA	CAA-C2A-C3A	-3.18	104.07	113.22
19	4	1209	CLA	CAA-C2A-C3A	-3.18	108.58	116.20
19	B	1746	CLA	CMD-C2D-C3D	-3.18	118.88	125.09
19	4	1210	CLA	C2C-C1C-CHC	-3.17	119.51	125.15
19	1	1187	CLA	CBA-CAA-C2A	-3.17	104.78	113.73
20	A	7001	LMU	O5B-C5B-C4B	-3.16	103.75	109.68
19	B	1738	CLA	CHC-C1C-C2C	-3.16	118.03	126.35
19	4	1202	CLA	C3C-C4C-CHD	-3.16	120.12	125.32
19	A	1815	CLA	O2D-CGD-O1D	-3.16	117.26	123.79
23	B	1777	BCR	C33-C5-C6	-3.16	121.50	124.61
23	A	1803	BCR	C24-C23-C22	-3.16	121.40	126.22
19	3	3008	CLA	CMD-C2D-C3D	-3.15	118.92	125.09
19	4	4007	CLA	CHC-C1C-C2C	-3.15	118.06	126.35
19	1	1145	CLA	CMD-C2D-C3D	-3.15	118.93	125.09
19	A	1799	CLA	C3C-C4C-CHD	-3.15	120.14	125.32
19	4	1203	CLA	C2C-C1C-CHC	-3.15	119.56	125.15
19	B	1762	CLA	O2D-CGD-O1D	-3.15	117.29	123.79
19	3	1218	CLA	CHD-C4C-C3C	-3.14	120.09	124.94
19	1	1188	CLA	CHC-C1C-C2C	-3.14	118.09	126.35
19	A	1791	CLA	CHC-C1C-C2C	-3.13	118.11	126.35
23	A	1807	BCR	C28-C27-C26	-3.13	108.89	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1747	CLA	O2D-CGD-O1D	-3.13	117.33	123.79
19	H	1079	CLA	C6-C5-C3	-3.13	105.61	112.48
19	2	1217	CLA	O1D-CGD-CBD	-3.13	120.14	124.62
19	4	1200	CLA	O2D-CGD-O1D	-3.13	117.33	123.79
19	A	1787	CLA	CMD-C2D-C3D	-3.13	118.97	125.09
19	2	1223	CLA	CBA-CAA-C2A	-3.13	104.91	113.73
19	2	1221	CLA	C1-C2-C3	-3.13	121.58	126.71
19	A	1783	CLA	CMD-C2D-C3D	-3.13	118.97	125.09
19	B	1772	CLA	CMA-C3A-C2A	-3.12	108.72	116.20
19	B	1740	CLA	C3C-C4C-CHD	-3.12	120.18	125.32
19	1	1145	CLA	CMA-C3A-C2A	-3.12	100.57	114.35
19	B	1760	CLA	O2D-CGD-O1D	-3.11	117.36	123.79
19	B	1741	CLA	CMD-C2D-C3D	-3.11	119.00	125.09
19	4	1210	CLA	C2D-C3D-C4D	-3.11	103.56	106.30
19	2	1223	CLA	C4-C3-C2	-3.11	117.40	123.50
19	1	1192	CLA	O1D-CGD-CBD	-3.11	120.17	124.62
19	H	1079	CLA	CHC-C1C-C2C	-3.11	118.18	126.35
19	B	1735	CLA	O2D-CGD-O1D	-3.11	117.38	123.79
19	A	1784	CLA	O2D-CGD-O1D	-3.11	117.38	123.79
19	A	1766	CLA	C2A-C1A-CHA	-3.11	118.17	123.89
19	B	1738	CLA	CHD-C4C-C3C	-3.10	120.15	124.94
23	B	1775	BCR	C34-C9-C10	-3.10	118.32	122.90
19	B	1744	CLA	O1D-CGD-CBD	-3.10	120.18	124.62
19	3	3008	CLA	O1D-CGD-CBD	-3.10	120.18	124.62
19	B	1784	CLA	CBA-CAA-C2A	-3.10	104.99	113.73
19	A	1789	CLA	CHC-C1C-C2C	-3.10	118.20	126.35
23	A	1804	BCR	C30-C25-C26	-3.10	118.11	122.66
19	B	1756	CLA	CMD-C2D-C3D	-3.09	119.04	125.09
19	4	1206	CLA	C4-C3-C2	-3.09	117.43	123.50
19	B	1742	CLA	CHC-C1C-C2C	-3.09	118.22	126.35
19	B	1760	CLA	CMD-C2D-C3D	-3.09	119.04	125.09
19	A	1813	CLA	CMD-C2D-C3D	-3.08	119.06	125.09
19	B	1745	CLA	C4-C3-C2	-3.08	117.45	123.50
19	A	1798	CLA	CMD-C2D-C3D	-3.08	119.07	125.09
19	1	1199	CLA	O1D-CGD-CBD	-3.08	120.21	124.62
19	A	1790	CLA	C1-C2-C3	-3.08	121.67	126.71
19	3	1212	CLA	C2D-C3D-C4D	-3.07	103.60	106.30
23	B	1775	BCR	C33-C5-C6	-3.07	121.59	124.61
20	A	7042	LMU	C1B-O1B-C4'	-3.07	109.98	118.01
19	A	1795	CLA	CAA-C2A-C1A	-3.07	101.64	112.47
19	4	1208	CLA	C2C-C1C-CHC	-3.07	119.70	125.15
19	B	1756	CLA	O1D-CGD-CBD	-3.07	120.22	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1805	BCR	C40-C30-C25	-3.06	105.50	110.30
19	A	1768	CLA	CMD-C2D-C3D	-3.06	119.10	125.09
19	A	1797	CLA	CGD-CBD-CAD	-3.06	100.25	110.62
19	1	1187	CLA	O1D-CGD-CBD	-3.06	120.24	124.62
19	B	1750	CLA	O1D-CGD-CBD	-3.06	120.24	124.62
21	B	8061	SUC	C4-C3-C2	-3.06	105.09	110.79
23	B	1777	BCR	C15-C14-C13	-3.05	122.78	127.20
19	H	1080	CLA	CHD-C4C-C3C	-3.05	120.22	124.94
19	A	1789	CLA	C3D-CAD-CBD	-3.05	103.28	107.60
19	3	1216	CLA	C2D-C3D-C4D	-3.05	103.62	106.30
20	A	7017	LMU	C1B-O5B-C5B	-3.05	107.83	113.75
19	A	1765	CLA	O1D-CGD-CBD	-3.04	120.26	124.62
20	A	7037	LMU	C3B-C4B-C5B	-3.04	104.89	110.20
19	B	1759	CLA	CHC-C1C-C2C	-3.04	118.35	126.35
19	B	1737	CLA	C6-C5-C3	-3.04	105.81	112.48
19	4	1205	CLA	CHC-C1C-C2C	-3.04	118.36	126.35
19	1	1146	CLA	CHC-C1C-C2C	-3.04	118.36	126.35
19	B	1758	CLA	O1D-CGD-CBD	-3.04	120.27	124.62
20	A	7020	LMU	C1-O1'-C1'	-3.04	108.64	113.94
19	B	1739	CLA	CHD-C4C-C3C	-3.04	120.25	124.94
19	A	1801	CLA	C4-C3-C2	-3.03	117.54	123.50
19	B	1743	CLA	O1D-CGD-CBD	-3.03	120.27	124.62
19	B	1768	CLA	O1D-CGD-CBD	-3.03	120.28	124.62
23	I	1032	BCR	C2-C1-C6	-3.03	105.56	110.36
19	B	1748	CLA	O2D-CGD-O1D	-3.03	117.53	123.79
21	B	8053	SUC	C1-C2-C3	-3.03	104.00	109.97
19	A	1795	CLA	CHC-C1C-C2C	-3.03	118.38	126.35
19	A	1767	CLA	CHC-C1C-C2C	-3.03	118.38	126.35
20	A	7008	LMU	O5B-C5B-C4B	-3.03	104.00	109.68
23	A	1805	BCR	C7-C8-C9	-3.02	121.61	126.22
19	2	1221	CLA	CMD-C2D-C3D	-3.02	119.18	125.09
19	A	1816	CLA	O2D-CGD-O1D	-3.02	117.55	123.79
19	A	1781	CLA	O2D-CGD-O1D	-3.01	117.56	123.79
23	A	1805	BCR	C27-C26-C25	-3.01	118.94	122.78
19	1	1142	CLA	O2D-CGD-O1D	-3.01	117.57	123.79
19	H	1080	CLA	O1D-CGD-CBD	-3.01	120.30	124.62
23	B	1779	BCR	C37-C22-C21	-3.01	118.45	122.90
19	A	1759	CLA	CMD-C2D-C3D	-3.01	119.20	125.09
23	A	1808	BCR	C4-C5-C6	-3.01	118.95	122.78
19	A	1786	CLA	CHC-C1C-C2C	-3.00	118.45	126.35
19	A	1785	CLA	O2D-CGD-O1D	-3.00	117.59	123.79
19	A	1786	CLA	CMD-C2D-C3D	-3.00	119.22	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1190	CLA	CHC-C1C-C2C	-3.00	118.46	126.35
23	I	1032	BCR	C33-C5-C6	-3.00	121.66	124.61
19	A	1789	CLA	CAA-C2A-C3A	-2.99	104.61	113.22
19	A	1769	CLA	CMD-C2D-C3D	-2.99	119.24	125.09
19	A	1785	CLA	CMD-C2D-C3D	-2.99	119.24	125.09
20	A	7009	LMU	C1B-C2B-C3B	-2.99	104.08	109.97
20	A	7037	LMU	O2'-C2'-C1'	-2.99	103.47	110.02
19	B	1739	CLA	CHC-C1C-C2C	-2.99	118.50	126.35
19	A	1772	CLA	CMD-C2D-C3D	-2.98	119.25	125.09
19	A	1762	CLA	O2D-CGD-O1D	-2.98	117.64	123.79
19	B	1761	CLA	CHC-C1C-C2C	-2.98	118.52	126.35
19	1	1143	CLA	CHC-C1C-C2C	-2.98	118.52	126.35
19	1	1187	CLA	CAA-C2A-C3A	-2.98	104.66	113.22
19	A	1771	CLA	CAA-C2A-C3A	-2.98	104.66	113.22
20	A	7009	LMU	O1B-C4'-C5'	-2.97	101.50	109.32
19	B	1743	CLA	CMD-C2D-C3D	-2.97	119.28	125.09
19	3	1222	CLA	O2D-CGD-O1D	-2.97	117.66	123.79
23	L	1169	BCR	C37-C22-C21	-2.97	118.51	122.90
19	A	1777	CLA	O2D-CGD-O1D	-2.97	117.66	123.79
19	1	1145	CLA	CAA-C2A-C3A	-2.97	104.68	113.22
19	A	1789	CLA	O1D-CGD-CBD	-2.97	120.37	124.62
19	A	1786	CLA	O2D-CGD-O1D	-2.96	117.67	123.79
20	A	7011	LMU	C1'-C2'-C3'	-2.96	104.14	109.97
19	B	1737	CLA	CMD-C2D-C3D	-2.96	119.30	125.09
19	1	1309	CLA	C3C-C4C-CHD	-2.96	120.45	125.32
19	A	1788	CLA	CHC-C1C-C2C	-2.96	118.58	126.35
23	B	1779	BCR	C27-C26-C25	-2.95	119.02	122.78
19	A	1771	CLA	O2D-CGD-O1D	-2.95	117.70	123.79
19	B	1759	CLA	C2A-C1A-CHA	-2.95	118.46	123.89
19	A	1777	CLA	O1D-CGD-CBD	-2.94	120.40	124.62
23	B	1775	BCR	C11-C10-C9	-2.93	122.96	127.20
23	A	1803	BCR	C38-C26-C25	-2.93	121.73	124.61
19	A	1817	CLA	CHC-C1C-C2C	-2.93	118.64	126.35
19	B	1737	CLA	CGD-CBD-CAD	-2.93	100.69	110.62
19	3	1217	CLA	C3D-CAD-CBD	-2.93	103.45	107.60
19	B	1771	CLA	CHC-C1C-C2C	-2.93	118.64	126.35
19	1	1145	CLA	CHC-C1C-C2C	-2.93	118.65	126.35
21	B	8060	SUC	C2'-O1-C1	-2.93	109.82	117.53
19	3	1217	CLA	CMD-C2D-C3D	-2.93	119.36	125.09
19	G	1099	CLA	CMD-C2D-C3D	-2.92	119.37	125.09
19	2	1222	CLA	CHC-C1C-C2C	-2.92	118.66	126.35
19	1	1187	CLA	O2D-CGD-O1D	-2.92	117.76	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1801	CLA	O2D-CGD-O1D	-2.92	117.76	123.79
19	B	1763	CLA	CHC-C1C-C2C	-2.92	118.67	126.35
23	A	1809	BCR	C23-C24-C25	-2.92	118.55	127.32
19	B	1749	CLA	CMD-C2D-C3D	-2.92	119.38	125.09
19	A	1764	CLA	CMD-C2D-C3D	-2.91	119.39	125.09
19	A	1764	CLA	C6-C5-C3	-2.91	106.09	112.48
21	B	8056	SUC	C1-C2-C3	-2.91	104.23	109.97
19	A	1816	CLA	CMD-C2D-C3D	-2.91	119.40	125.09
19	4	1201	CLA	O2A-CGA-O1A	-2.91	115.98	123.49
23	A	1806	BCR	C16-C17-C18	-2.91	123.00	127.20
19	3	1217	CLA	O2D-CGD-O1D	-2.91	117.79	123.79
19	3	1221	CLA	O2D-CGD-O1D	-2.91	117.79	123.79
19	4	1206	CLA	O1D-CGD-CBD	-2.91	120.46	124.62
23	L	1169	BCR	C3-C4-C5	-2.90	109.26	113.87
21	B	8059	SUC	C4-C3-C2	-2.90	105.37	110.79
19	B	1743	CLA	CBA-CAA-C2A	-2.90	105.55	113.73
19	A	1769	CLA	CHC-C1C-C2C	-2.90	118.72	126.35
19	A	1790	CLA	CHC-C1C-C2C	-2.90	118.73	126.35
21	B	8062	SUC	C6'-C5'-C4'	-2.90	108.23	115.08
19	A	1779	CLA	C1-C2-C3	-2.90	121.96	126.71
19	4	1201	CLA	CHC-C1C-C2C	-2.90	118.73	126.35
23	A	1805	BCR	C3-C4-C5	-2.89	109.28	113.87
19	B	1739	CLA	CMD-C2D-C3D	-2.89	119.43	125.09
19	4	1199	CLA	O2D-CGD-O1D	-2.89	117.82	123.79
19	4	1201	CLA	C4-C3-C2	-2.89	117.82	123.50
19	B	1760	CLA	CHD-C4C-C3C	-2.89	120.47	124.94
19	1	1146	CLA	O2A-CGA-O1A	-2.89	116.04	123.49
19	I	1031	CLA	CMD-C2D-C3D	-2.89	119.44	125.09
19	G	1099	CLA	O1D-CGD-CBD	-2.89	120.48	124.62
19	L	1167	CLA	CHC-C1C-C2C	-2.89	118.76	126.35
19	A	1786	CLA	CHD-C4C-C3C	-2.88	120.48	124.94
19	B	1768	CLA	CHC-C1C-C2C	-2.88	118.77	126.35
19	B	1771	CLA	CMD-C2D-C3D	-2.88	119.45	125.09
19	1	1197	CLA	CAA-C2A-C1A	-2.88	102.32	112.47
19	A	1764	CLA	O2D-CGD-O1D	-2.88	117.85	123.79
19	2	1222	CLA	CGD-CBD-CAD	-2.88	100.87	110.62
21	B	8062	SUC	C1-O5-C5	-2.88	108.16	113.75
19	H	1080	CLA	O2D-CGD-O1D	-2.87	117.86	123.79
19	1	1146	CLA	O2D-CGD-O1D	-2.87	117.86	123.79
19	L	1167	CLA	CGD-CBD-CAD	-2.87	100.91	110.62
19	B	1752	CLA	CHC-C1C-C2C	-2.87	118.81	126.35
19	3	1222	CLA	O2A-CGA-O1A	-2.86	116.11	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1043	CLA	C3D-CAD-CBD	-2.86	103.56	107.60
19	4	1209	CLA	CMD-C2D-C3D	-2.86	119.50	125.09
19	B	1744	CLA	CHC-C1C-C2C	-2.86	118.84	126.35
20	A	7009	LMU	O1B-C4'-C3'	-2.86	99.80	107.17
19	A	1793	CLA	CHC-C1C-C2C	-2.85	118.86	126.35
19	A	1784	CLA	CHC-C1C-C2C	-2.85	118.86	126.35
19	2	2006	CLA	CHC-C1C-C2C	-2.85	118.86	126.35
19	1	1148	CLA	O2D-CGD-O1D	-2.84	117.92	123.79
20	A	7004	LMU	C1B-O5B-C5B	-2.84	108.23	113.75
19	A	1767	CLA	C11-C12-C13	-2.84	106.06	115.49
19	A	1801	CLA	CMD-C2D-C3D	-2.84	119.53	125.09
19	B	1766	CLA	CHC-C1C-C2C	-2.84	118.88	126.35
19	H	1079	CLA	C3D-CAD-CBD	-2.84	103.58	107.60
19	2	1223	CLA	O2D-CGD-O1D	-2.84	117.93	123.79
23	B	1780	BCR	C11-C12-C13	-2.84	117.97	126.32
19	H	1080	CLA	CMD-C2D-C3D	-2.84	119.54	125.09
19	A	1794	CLA	CHC-C1C-C2C	-2.84	118.89	126.35
19	B	1784	CLA	CHC-C1C-C2C	-2.83	118.90	126.35
21	B	8062	SUC	C1'-C2'-C3'	-2.83	104.92	114.49
19	A	1774	CLA	C6-C7-C8	-2.83	106.09	115.49
21	B	8061	SUC	C3-C4-C5	-2.83	105.27	110.20
19	4	4007	CLA	C4-C3-C2	-2.82	117.96	123.50
19	B	1739	CLA	CAA-C2A-C3A	-2.82	105.10	113.22
19	A	1782	CLA	O2D-CGD-O1D	-2.82	117.97	123.79
19	1	1187	CLA	CAC-C3C-C2C	-2.82	122.57	127.51
19	1	1143	CLA	O1D-CGD-CBD	-2.82	120.58	124.62
19	F	1157	CLA	CHC-C1C-C2C	-2.82	118.94	126.35
19	1	1197	CLA	CHC-C1C-C2C	-2.82	118.94	126.35
19	A	1760	CLA	O2A-CGA-O1A	-2.81	116.23	123.49
19	B	1772	CLA	CMD-C2D-C3D	-2.81	119.58	125.09
19	2	1218	CLA	C2D-C3D-C4D	-2.81	103.83	106.30
19	1	1146	CLA	C1-C2-C3	-2.81	122.10	126.71
19	2	1213	CLA	O2D-CGD-O1D	-2.81	117.99	123.79
19	R	1054	CLA	O2A-CGA-O1A	-2.81	116.25	123.49
19	B	1762	CLA	O1D-CGD-CBD	-2.81	120.60	124.62
19	B	1754	CLA	CHC-C1C-C2C	-2.80	118.98	126.35
19	A	1760	CLA	O2D-CGD-O1D	-2.80	118.00	123.79
19	A	1772	CLA	O2A-CGA-O1A	-2.80	116.26	123.49
19	F	1157	CLA	CMD-C2D-C3D	-2.80	119.61	125.09
19	2	1217	CLA	C2A-C1A-CHA	-2.80	118.73	123.89
20	A	7042	LMU	C4B-C3B-C2B	-2.80	105.57	110.79
19	4	1201	CLA	CBA-CAA-C2A	-2.80	105.85	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1803	BCR	C23-C24-C25	-2.79	118.92	127.32
19	2	1216	CLA	C2D-C3D-C4D	-2.79	103.84	106.30
19	1	1199	CLA	O2D-CGD-O1D	-2.79	118.03	123.79
19	A	1774	CLA	O2A-CGA-O1A	-2.78	116.31	123.49
23	A	1804	BCR	C27-C26-C25	-2.78	119.24	122.78
19	3	1218	CLA	O1D-CGD-CBD	-2.77	120.65	124.62
19	4	1211	CLA	CGD-CBD-CAD	-2.77	101.23	110.62
19	3	1218	CLA	CHC-C1C-C2C	-2.77	119.06	126.35
19	1	1192	CLA	CMD-C2D-C3D	-2.77	119.67	125.09
19	1	1308	CLA	CHC-C1C-C2C	-2.77	119.06	126.35
19	H	1081	CLA	O2D-CGD-O1D	-2.77	118.07	123.79
19	2	1223	CLA	CAA-CBA-CGA	-2.77	105.20	113.32
20	A	7042	LMU	C1'-C2'-C3'	-2.77	104.52	109.97
19	2	1213	CLA	CHC-C1C-C2C	-2.77	119.07	126.35
23	A	1807	BCR	C10-C11-C12	-2.76	114.70	123.13
19	2	1216	CLA	C3B-C2B-C1B	-2.76	103.87	106.29
23	A	1803	BCR	C4-C5-C6	-2.76	119.26	122.78
19	A	1787	CLA	O2D-CGD-O1D	-2.76	118.09	123.79
19	A	1813	CLA	CAA-C2A-C3A	-2.76	105.29	113.22
19	B	1754	CLA	CMD-C2D-C3D	-2.76	119.70	125.09
23	A	1808	BCR	C37-C22-C21	-2.75	118.83	122.90
19	F	1156	CLA	CAA-C2A-C3A	-2.75	109.61	116.20
19	A	1789	CLA	O2D-CGD-O1D	-2.75	118.11	123.79
19	1	1190	CLA	CAA-C2A-C1A	-2.75	102.76	112.47
23	A	1808	BCR	C7-C6-C5	-2.75	115.07	121.37
19	4	1209	CLA	CMA-C3A-C2A	-2.75	109.61	116.20
21	B	8062	SUC	O5-C1-C2	-2.75	104.63	110.28
19	R	1055	CLA	CHC-C1C-C2C	-2.74	119.14	126.35
19	A	1765	CLA	O2D-CGD-O1D	-2.74	118.13	123.79
19	A	1773	CLA	CHC-C1C-C2C	-2.74	119.15	126.35
19	H	1080	CLA	CHC-C1C-C2C	-2.73	119.16	126.35
19	4	1200	CLA	O2A-CGA-O1A	-2.73	116.44	123.49
23	B	1778	BCR	C1-C6-C5	-2.73	118.66	122.66
19	1	1014	CLA	CMD-C2D-C3D	-2.73	119.76	125.09
19	1	1199	CLA	CGD-CBD-CAD	-2.72	101.39	110.62
23	B	1779	BCR	C15-C16-C17	-2.72	117.37	123.39
19	B	1753	CLA	CMD-C2D-C3D	-2.72	119.77	125.09
19	A	1798	CLA	CHC-C1C-C2C	-2.72	119.20	126.35
19	B	1747	CLA	CHC-C1C-C2C	-2.72	119.20	126.35
19	3	1221	CLA	C6-C5-C3	-2.72	106.52	112.48
19	4	4014	CLA	O2D-CGD-O1D	-2.72	118.18	123.79
19	1	1149	CLA	CHD-C4C-C3C	-2.71	120.75	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7004	LMU	O5'-C1'-C2'	-2.71	104.71	110.28
19	A	1771	CLA	CHC-C1C-C2C	-2.71	119.22	126.35
19	B	1767	CLA	CHC-C1C-C2C	-2.71	119.23	126.35
23	B	1775	BCR	C37-C22-C21	-2.71	118.90	122.90
19	R	1054	CLA	CHC-C1C-C2C	-2.71	119.23	126.35
19	A	1774	CLA	CAA-C2A-C3A	-2.71	105.44	113.22
19	A	1798	CLA	O1D-CGD-CBD	-2.70	120.75	124.62
19	A	1792	CLA	O2D-CGD-O1D	-2.70	118.22	123.79
19	A	1762	CLA	CHC-C1C-C2C	-2.70	119.26	126.35
19	A	1792	CLA	CHC-C1C-C2C	-2.70	119.26	126.35
20	A	7041	LMU	C4B-C3B-C2B	-2.69	105.76	110.79
19	B	1760	CLA	CHC-C1C-C2C	-2.69	119.26	126.35
19	A	1793	CLA	CAA-C2A-C1A	-2.69	102.97	112.47
19	B	1770	CLA	CAA-C2A-C3A	-2.69	105.48	113.22
21	2	1225	SUC	O2-C2-C3	-2.69	104.28	110.34
19	B	1760	CLA	C1-C2-C3	-2.69	122.30	126.71
19	2	2010	CLA	C3B-C2B-C1B	-2.68	103.94	106.29
19	B	1766	CLA	O1D-CGD-CBD	-2.68	120.78	124.62
19	A	1763	CLA	C2A-C1A-CHA	-2.68	118.94	123.89
19	A	1774	CLA	O1D-CGD-CBD	-2.68	120.78	124.62
23	B	1778	BCR	C23-C24-C25	-2.68	119.27	127.32
22	A	1802	PQN	C21-C20-C18	-2.68	106.61	115.49
19	B	1762	CLA	CAA-CBA-CGA	-2.67	105.49	113.32
19	A	1780	CLA	CHC-C1C-C2C	-2.67	119.32	126.35
19	2	1219	CLA	CAA-C2A-C3A	-2.67	109.80	116.20
19	A	1767	CLA	CAA-C2A-C1A	-2.67	103.05	112.47
19	B	1759	CLA	CMA-C3A-C2A	-2.66	102.56	114.35
19	B	1745	CLA	O2D-CGD-O1D	-2.66	118.29	123.79
19	A	1768	CLA	CHC-C1C-C2C	-2.66	119.35	126.35
19	B	1741	CLA	CAA-C2A-C3A	-2.66	105.56	113.22
19	A	1815	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
19	B	1746	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
19	B	1737	CLA	C11-C10-C8	-2.66	106.68	115.49
19	A	1776	CLA	CHC-C1C-C2C	-2.66	119.37	126.35
19	A	1814	CLA	O2A-CGA-O1A	-2.65	116.64	123.49
19	3	1222	CLA	CHC-C1C-C2C	-2.65	119.37	126.35
19	H	1079	CLA	CMD-C2D-C3D	-2.65	119.90	125.09
19	A	1762	CLA	C2A-C1A-CHA	-2.65	119.00	123.89
19	A	1782	CLA	CHC-C1C-C2C	-2.65	119.38	126.35
19	A	1766	CLA	CMA-C3A-C2A	-2.65	102.64	114.35
19	2	1217	CLA	CMD-C2D-C3D	-2.64	119.92	125.09
19	B	1737	CLA	CHC-C1C-C2C	-2.64	119.40	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1738	CLA	CAA-C2A-C3A	-2.64	105.62	113.22
19	1	1195	CLA	C2C-C1C-CHC	-2.64	120.46	125.15
19	A	1795	CLA	O2D-CGD-O1D	-2.63	118.36	123.79
19	A	1801	CLA	O1D-CGD-CBD	-2.63	120.85	124.62
19	A	1775	CLA	CHC-C1C-C2C	-2.63	119.44	126.35
19	1	1505	CLA	CHC-C1C-C2C	-2.63	119.44	126.35
23	A	1805	BCR	C28-C27-C26	-2.63	109.70	113.87
23	A	1806	BCR	C30-C25-C26	-2.62	118.81	122.66
19	4	4014	CLA	CHD-C4C-C3C	-2.62	120.89	124.94
19	4	4007	CLA	CAA-C2A-C1A	-2.62	103.24	112.47
23	A	1805	BCR	C1-C6-C5	-2.62	118.82	122.66
19	R	1054	CLA	C4-C3-C2	-2.61	118.37	123.50
23	A	1803	BCR	C28-C27-C26	-2.61	109.72	113.87
21	B	8060	SUC	C6'-C5'-C4'	-2.61	108.91	115.08
19	F	1156	CLA	O2D-CGD-O1D	-2.61	118.41	123.79
19	3	1221	CLA	C4-C3-C2	-2.60	118.39	123.50
19	4	1209	CLA	CHC-C1C-C2C	-2.60	119.50	126.35
19	A	1788	CLA	O2D-CGD-O1D	-2.60	118.42	123.79
19	L	1168	CLA	CMD-C2D-C3D	-2.60	120.00	125.09
20	A	7023	LMU	C1'-O5'-C5'	-2.60	108.69	113.75
19	2	1223	CLA	C11-C10-C8	-2.60	106.86	115.49
23	A	1805	BCR	C38-C26-C25	-2.60	122.05	124.61
19	F	1155	CLA	CAA-C2A-C3A	-2.60	109.98	116.20
19	B	1771	CLA	O2A-CGA-O1A	-2.60	116.78	123.49
19	B	1754	CLA	CGD-CBD-CAD	-2.60	101.82	110.62
21	2	1225	SUC	O4'-C4'-C3'	-2.60	103.75	112.01
19	A	1779	CLA	CHC-C1C-C2C	-2.60	119.52	126.35
19	A	1796	CLA	CMD-C2D-C3D	-2.59	120.01	125.09
19	2	2006	CLA	CBC-CAC-C3C	-2.59	104.47	112.39
19	A	1764	CLA	CAA-C2A-C3A	-2.59	105.76	113.22
19	1	1308	CLA	O2D-CGD-O1D	-2.59	118.44	123.79
23	A	1807	BCR	C24-C25-C26	-2.59	115.43	121.37
23	A	1804	BCR	C11-C12-C13	-2.59	118.69	126.32
23	B	1778	BCR	C37-C22-C21	-2.59	119.07	122.90
19	2	1212	CLA	O2D-CGD-O1D	-2.59	118.45	123.79
19	3	3011	CLA	O2D-CGD-O1D	-2.58	118.45	123.79
19	H	1080	CLA	C4-C3-C2	-2.57	118.45	123.50
20	A	7042	LMU	C1'-O5'-C5'	-2.57	108.75	113.75
19	1	1193	CLA	O1D-CGD-CBD	-2.57	120.94	124.62
20	A	7032	LMU	C4B-C3B-C2B	-2.57	106.00	110.79
23	A	1804	BCR	C38-C26-C25	-2.57	122.08	124.61
19	B	1763	CLA	CAA-CBA-CGA	-2.57	105.80	113.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1758	CLA	CHC-C1C-C2C	-2.57	119.60	126.35
19	1	1190	CLA	C2A-C1A-CHA	-2.57	119.16	123.89
23	A	1806	BCR	C33-C5-C6	-2.56	122.09	124.61
19	2	1215	CLA	CHC-C1C-C2C	-2.56	119.61	126.35
19	A	1787	CLA	O1D-CGD-CBD	-2.56	120.95	124.62
23	A	1804	BCR	C28-C27-C26	-2.56	109.80	113.87
19	B	1769	CLA	CAA-CBA-CGA	-2.56	105.81	113.32
19	A	1789	CLA	CMD-C2D-C3D	-2.56	120.08	125.09
19	1	1191	CLA	CHC-C1C-C2C	-2.56	119.62	126.35
19	B	1766	CLA	C4-C3-C2	-2.56	118.48	123.50
21	2	1225	SUC	O5-C5-C4	-2.56	105.09	109.53
23	B	1776	BCR	C15-C14-C13	-2.56	123.51	127.20
19	A	1793	CLA	CAA-C2A-C3A	-2.55	105.88	113.22
20	A	7033	LMU	C3'-C4'-C5'	-2.55	105.08	110.84
19	A	1793	CLA	C2A-C1A-CHA	-2.55	119.19	123.89
19	A	1781	CLA	CHC-C1C-C2C	-2.54	119.66	126.35
19	B	1764	CLA	CHC-C1C-C2C	-2.54	119.66	126.35
19	1	1308	CLA	O1D-CGD-CBD	-2.54	120.98	124.62
19	A	1785	CLA	CHC-C1C-C2C	-2.54	119.67	126.35
19	4	1196	CLA	CHC-C1C-C2C	-2.54	119.67	126.35
20	A	7021	LMU	C6B-C5B-C4B	-2.54	106.75	113.02
23	B	1779	BCR	C1-C6-C5	-2.54	118.93	122.66
19	F	1155	CLA	CHC-C1C-C2C	-2.53	119.69	126.35
19	A	1760	CLA	CHC-C1C-C2C	-2.53	119.69	126.35
22	B	1773	PQN	C14-C13-C12	-2.53	118.53	123.50
19	A	1794	CLA	O1D-CGD-CBD	-2.53	120.99	124.62
19	2	1219	CLA	CHC-C1C-C2C	-2.53	119.70	126.35
19	A	1814	CLA	CHC-C1C-C2C	-2.53	119.70	126.35
19	B	1741	CLA	O2D-CGD-O1D	-2.53	118.57	123.79
19	1	1148	CLA	O1D-CGD-CBD	-2.53	121.00	124.62
20	A	7024	LMU	C3B-C4B-C5B	-2.53	105.79	110.20
23	A	1803	BCR	C8-C7-C6	-2.52	119.74	127.32
19	1	1142	CLA	CHC-C1C-C2C	-2.52	119.72	126.35
19	4	1198	CLA	CBC-CAC-C3C	-2.52	104.70	112.39
19	A	1766	CLA	CHC-C1C-C2C	-2.52	119.74	126.35
19	A	1783	CLA	O2D-CGD-O1D	-2.51	118.60	123.79
19	A	1794	CLA	CMD-C2D-C3D	-2.51	120.18	125.09
19	3	1213	CLA	CAA-C2A-C3A	-2.51	110.19	116.20
19	B	1749	CLA	C4-C3-C2	-2.51	118.57	123.50
19	A	1763	CLA	CAA-C2A-C1A	-2.51	103.62	112.47
19	1	1189	CLA	CHC-C1C-C2C	-2.51	119.75	126.35
19	A	1817	CLA	CAA-C2A-C3A	-2.51	106.00	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1199	CLA	CMD-C2D-C3D	-2.51	120.18	125.09
23	B	1774	BCR	C23-C24-C25	-2.51	119.79	127.32
19	B	1750	CLA	CHC-C1C-C2C	-2.51	119.76	126.35
19	1	1143	CLA	O2A-CGA-O1A	-2.51	117.03	123.49
19	4	1198	CLA	C11-C10-C8	-2.50	107.18	115.49
19	A	1784	CLA	CMD-C2D-C3D	-2.50	120.19	125.09
19	A	1815	CLA	C2A-C1A-CHA	-2.50	119.28	123.89
19	B	1768	CLA	CBC-CAC-C3C	-2.50	104.75	112.39
19	A	1782	CLA	CMD-C2D-C3D	-2.50	120.20	125.09
20	A	7020	LMU	C1'-O5'-C5'	-2.50	108.89	113.75
23	A	1805	BCR	C35-C13-C14	-2.50	119.21	122.90
20	A	7004	LMU	C1B-C2B-C3B	-2.50	105.05	109.97
19	B	1748	CLA	CHC-C1C-C2C	-2.50	119.78	126.35
19	A	1780	CLA	C4-C3-C2	-2.50	118.60	123.50
19	A	1814	CLA	CMD-C2D-C3D	-2.50	120.20	125.09
20	A	7008	LMU	O5'-C1'-C2'	-2.50	105.15	110.28
23	B	1776	BCR	C33-C5-C6	-2.50	122.15	124.61
19	A	1800	CLA	CHC-C1C-C2C	-2.50	119.79	126.35
19	4	1200	CLA	CHC-C1C-C2C	-2.50	119.79	126.35
19	1	1505	CLA	O1D-CGD-CBD	-2.50	121.05	124.62
23	A	1809	BCR	C36-C18-C17	-2.49	119.22	122.90
19	1	1193	CLA	CHC-C1C-C2C	-2.49	119.80	126.35
19	B	1742	CLA	O2D-CGD-O1D	-2.49	118.65	123.79
19	A	1789	CLA	CAC-C3C-C2C	-2.49	123.14	127.51
19	B	1772	CLA	CHC-C1C-C2C	-2.49	119.80	126.35
19	A	1769	CLA	O1D-CGD-CBD	-2.49	121.06	124.62
19	B	1765	CLA	CHC-C1C-C2C	-2.49	119.81	126.35
23	A	1804	BCR	C4-C5-C6	-2.49	119.61	122.78
19	F	1156	CLA	CHC-C1C-C2C	-2.49	119.81	126.35
19	A	1792	CLA	O1D-CGD-CBD	-2.49	121.06	124.62
19	A	1791	CLA	CAC-C3C-C2C	-2.49	123.15	127.51
19	3	3011	CLA	O1D-CGD-CBD	-2.48	121.06	124.62
19	1	1143	CLA	CBC-CAC-C3C	-2.48	104.81	112.39
19	3	3008	CLA	O2A-CGA-O1A	-2.48	117.09	123.49
19	1	1192	CLA	CHC-C1C-C2C	-2.48	119.83	126.35
23	A	1804	BCR	C3-C4-C5	-2.47	109.94	113.87
19	B	1751	CLA	CHC-C1C-C2C	-2.47	119.84	126.35
20	A	7011	LMU	C4B-C3B-C2B	-2.47	106.17	110.79
19	A	1762	CLA	CAA-C2A-C1A	-2.47	103.75	112.47
19	I	1031	CLA	CHC-C1C-C2C	-2.47	119.85	126.35
19	4	1197	CLA	CMA-C3A-C2A	-2.47	110.29	116.20
19	A	1789	CLA	C11-C10-C8	-2.47	107.30	115.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1222	CLA	C4-C3-C2	-2.47	118.66	123.50
19	A	1787	CLA	CHC-C1C-C2C	-2.46	119.87	126.35
19	B	1769	CLA	C2C-C1C-NC	-2.46	108.41	110.24
19	4	4014	CLA	O2A-CGA-O1A	-2.46	117.14	123.49
19	F	1157	CLA	O1D-CGD-CBD	-2.46	121.10	124.62
19	1	1148	CLA	CHC-C1C-C2C	-2.46	119.89	126.35
23	B	1775	BCR	C4-C5-C6	-2.46	119.65	122.78
19	2	1213	CLA	CAA-C2A-C1A	-2.46	103.81	112.47
19	B	1748	CLA	CMA-C3A-C2A	-2.46	110.32	116.20
19	4	1211	CLA	CBA-CAA-C2A	-2.45	106.81	113.73
19	1	1197	CLA	O2D-CGD-O1D	-2.45	118.72	123.79
20	A	7030	LMU	C3B-C4B-C5B	-2.45	105.92	110.20
19	B	1770	CLA	CHC-C1C-C2C	-2.44	119.92	126.35
19	4	1200	CLA	CMD-C2D-C3D	-2.44	120.32	125.09
23	B	1780	BCR	C30-C25-C26	-2.44	119.08	122.66
19	A	1765	CLA	CHD-C4C-C3C	-2.44	121.18	124.94
19	4	1201	CLA	O1D-CGD-CBD	-2.43	121.13	124.62
23	A	1804	BCR	C8-C7-C6	-2.43	120.01	127.32
19	A	1780	CLA	O2A-CGA-O1A	-2.43	117.22	123.49
19	A	1785	CLA	CAA-C2A-C1A	-2.43	103.89	112.47
23	B	1780	BCR	C33-C5-C6	-2.43	122.22	124.61
19	3	1222	CLA	O1D-CGD-CBD	-2.43	121.14	124.62
20	A	7043	LMU	C6'-C5'-C4'	-2.43	106.18	113.25
19	A	1764	CLA	CHC-C1C-C2C	-2.43	119.97	126.35
23	B	1778	BCR	C20-C19-C18	-2.42	119.19	126.32
19	A	1790	CLA	O2D-CGD-O1D	-2.42	118.79	123.79
19	A	1768	CLA	O2D-CGD-O1D	-2.42	118.79	123.79
19	A	1796	CLA	O2A-CGA-O1A	-2.42	117.25	123.49
19	A	1789	CLA	O2A-CGA-O1A	-2.42	117.25	123.49
19	B	1769	CLA	CHC-C1C-C2C	-2.42	119.99	126.35
20	A	7001	LMU	O3B-C3B-C4B	-2.41	104.90	110.34
23	B	1779	BCR	C35-C13-C14	-2.41	119.34	122.90
20	A	7035	LMU	O5'-C5'-C4'	-2.41	104.65	109.75
19	H	1081	CLA	CMD-C2D-C3D	-2.41	120.37	125.09
19	A	1814	CLA	C4-C3-C2	-2.41	118.77	123.50
19	B	1769	CLA	C2A-C1A-CHA	-2.41	119.45	123.89
19	2	1212	CLA	CHC-C1C-C2C	-2.41	120.02	126.35
20	A	7041	LMU	C1B-O5B-C5B	-2.41	109.07	113.75
20	A	7049	LMU	C1B-O1B-C4'	-2.41	111.72	118.01
19	2	1221	CLA	C2A-C1A-CHA	-2.41	119.45	123.89
23	L	1169	BCR	C28-C27-C26	-2.40	110.05	113.87
19	A	1797	CLA	O2A-CGA-O1A	-2.40	117.29	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1758	CLA	O2A-CGA-O1A	-2.40	117.29	123.49
21	B	8053	SUC	O5-C1-C2	-2.40	105.35	110.28
19	H	1079	CLA	O2A-CGA-O1A	-2.40	117.30	123.49
21	B	8055	SUC	C6-C5-C4	-2.40	107.10	113.02
19	B	1738	CLA	C16-C15-C13	-2.40	107.54	115.49
19	A	1771	CLA	C1-C2-C3	-2.40	122.78	126.71
19	1	1196	CLA	CHC-C1C-C2C	-2.40	120.05	126.35
19	B	1757	CLA	O2A-CGA-O1A	-2.39	117.32	123.49
19	B	1755	CLA	CHC-C1C-C2C	-2.39	120.06	126.35
21	B	8053	SUC	C6-C5-C4	-2.39	108.38	113.08
19	L	1167	CLA	O1D-CGD-CBD	-2.39	121.20	124.62
23	A	1807	BCR	C16-C17-C18	-2.39	123.75	127.20
19	1	1505	CLA	CGD-CBD-CAD	-2.39	102.53	110.62
19	3	1221	CLA	C6-C7-C8	-2.39	107.57	115.49
19	A	1766	CLA	O2D-CGD-O1D	-2.39	118.86	123.79
19	3	1221	CLA	C2A-C1A-CHA	-2.38	119.50	123.89
23	B	1780	BCR	C27-C26-C25	-2.38	119.75	122.78
19	B	1762	CLA	CHC-C1C-C2C	-2.38	120.09	126.35
19	A	1774	CLA	CHC-C1C-C2C	-2.38	120.09	126.35
23	B	1777	BCR	C27-C26-C25	-2.38	119.75	122.78
23	B	1776	BCR	C35-C13-C14	-2.38	119.39	122.90
19	2	1215	CLA	CAA-C2A-C3A	-2.38	106.38	113.22
19	A	1777	CLA	CHC-C1C-C2C	-2.38	120.10	126.35
19	R	1054	CLA	O2D-CGD-O1D	-2.38	118.88	123.79
19	B	1749	CLA	CHC-C1C-C2C	-2.38	120.10	126.35
23	B	1780	BCR	C38-C26-C25	-2.37	122.28	124.61
23	A	1806	BCR	C8-C7-C6	-2.37	120.19	127.32
19	B	1754	CLA	O1D-CGD-CBD	-2.37	121.22	124.62
19	3	3008	CLA	CHC-C1C-C2C	-2.37	120.11	126.35
20	A	7037	LMU	O1'-C1'-C2'	-2.37	105.05	108.04
19	A	1790	CLA	O1D-CGD-CBD	-2.36	121.23	124.62
19	B	1758	CLA	CMD-C2D-C3D	-2.36	120.47	125.09
23	B	1778	BCR	C30-C25-C26	-2.36	119.19	122.66
19	4	1211	CLA	CHC-C1C-C2C	-2.36	120.14	126.35
19	2	1222	CLA	CMD-C2D-C3D	-2.36	120.47	125.09
20	A	7023	LMU	C1-O1'-C1'	-2.36	109.82	113.94
19	B	1757	CLA	CAA-C2A-C1A	-2.36	104.15	112.47
19	A	1769	CLA	CAA-C2A-C1A	-2.36	104.15	112.47
19	3	1221	CLA	CMD-C2D-C3D	-2.36	120.47	125.09
19	B	1757	CLA	CAA-C2A-C3A	-2.36	106.44	113.22
22	B	1773	PQN	C16-C15-C13	-2.36	107.31	112.48
23	B	1779	BCR	C4-C5-C6	-2.36	119.78	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1782	CLA	O1D-CGD-CBD	-2.36	121.25	124.62
19	H	1079	CLA	O1D-CGD-CBD	-2.35	121.25	124.62
23	A	1805	BCR	C37-C22-C21	-2.35	119.43	122.90
19	A	1816	CLA	CHC-C1C-C2C	-2.35	120.17	126.35
19	B	1755	CLA	O2D-CGD-O1D	-2.35	118.94	123.79
23	A	1804	BCR	C23-C24-C25	-2.35	120.26	127.32
19	A	1760	CLA	C3B-C4B-NB	-2.35	106.17	109.21
19	B	1784	CLA	O2D-CGD-O1D	-2.35	118.94	123.79
19	A	1797	CLA	C4-C3-C2	-2.35	118.89	123.50
19	2	1221	CLA	CAA-C2A-C3A	-2.35	106.47	113.22
19	J	1043	CLA	CMD-C2D-C3D	-2.35	120.50	125.09
19	B	1735	CLA	CHC-C1C-C2C	-2.34	120.19	126.35
20	A	7032	LMU	O5'-C1'-C2'	-2.34	105.47	110.28
21	B	8061	SUC	C1'-C2'-C3'	-2.34	106.60	114.49
19	B	1758	CLA	C11-C12-C13	-2.34	107.74	115.49
19	R	1054	CLA	O1D-CGD-CBD	-2.34	121.27	124.62
19	A	1783	CLA	O2A-CGA-O1A	-2.33	117.47	123.49
19	2	1213	CLA	C4-C3-C2	-2.33	118.93	123.50
20	A	7036	LMU	C4B-C3B-C2B	-2.33	106.44	110.79
20	A	7034	LMU	C1B-O1B-C4'	-2.33	111.92	118.01
19	B	1756	CLA	C2A-C1A-CHA	-2.33	119.60	123.89
19	A	1763	CLA	O2D-CGD-O1D	-2.33	118.98	123.79
20	A	7038	LMU	C6B-C5B-C4B	-2.33	107.28	113.02
19	L	1168	CLA	C1-C2-C3	-2.33	122.90	126.71
23	B	1774	BCR	C8-C7-C6	-2.33	120.33	127.32
19	B	1745	CLA	CHC-C1C-C2C	-2.32	120.24	126.35
23	B	1774	BCR	C28-C27-C26	-2.32	110.18	113.87
22	B	1773	PQN	C2M-C2-C3	-2.32	119.14	124.10
19	B	1756	CLA	CHC-C1C-C2C	-2.32	120.25	126.35
19	B	1736	CLA	O1D-CGD-CBD	-2.32	121.30	124.62
19	B	1757	CLA	CHC-C1C-C2C	-2.32	120.25	126.35
19	B	1752	CLA	O1D-CGD-CBD	-2.32	121.30	124.62
19	B	1736	CLA	CHC-C1C-C2C	-2.32	120.26	126.35
19	B	1735	CLA	C2A-C1A-CHA	-2.32	119.62	123.89
19	4	1199	CLA	CAC-C3C-C2C	-2.31	123.45	127.51
20	A	7039	LMU	O5B-C5B-C6B	-2.31	100.51	106.36
23	A	1803	BCR	C1-C6-C5	-2.31	119.27	122.66
19	1	1142	CLA	C2A-C1A-CHA	-2.31	119.63	123.89
19	A	1776	CLA	CAA-C2A-C3A	-2.31	106.57	113.22
21	B	8062	SUC	O5-C1-O1	-2.31	102.20	109.96
23	B	1774	BCR	C27-C26-C25	-2.31	119.84	122.78
19	A	1796	CLA	C4-C3-C2	-2.31	118.97	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1812	LMU	C1-O1'-C1'	-2.31	109.91	113.94
19	2	1212	CLA	O2A-CGA-O1A	-2.31	117.54	123.49
19	A	1779	CLA	CAA-C2A-C3A	-2.31	106.59	113.22
21	B	8056	SUC	O1-C2'-C1'	-2.30	102.30	109.69
20	A	7020	LMU	C3B-C4B-C5B	-2.30	106.18	110.20
19	A	1772	CLA	CHC-C1C-C2C	-2.30	120.29	126.35
19	R	1055	CLA	O2A-CGA-O1A	-2.30	117.55	123.49
19	A	1773	CLA	O2D-CGD-O1D	-2.30	119.03	123.79
20	A	7017	LMU	O4'-C4B-C5B	-2.30	103.14	109.24
20	A	7026	LMU	O5'-C5'-C4'	-2.30	104.89	109.75
19	4	1206	CLA	CHC-C1C-C2C	-2.30	120.31	126.35
19	A	1781	CLA	O1D-CGD-CBD	-2.29	121.33	124.62
19	G	1099	CLA	CHC-C1C-C2C	-2.29	120.32	126.35
20	A	7040	LMU	O3B-C3B-C2B	-2.29	105.17	110.34
20	A	7005	LMU	C1'-C2'-C3'	-2.29	105.45	109.97
19	2	1223	CLA	CHC-C1C-C2C	-2.29	120.33	126.35
19	A	1774	CLA	CAA-C2A-C1A	-2.29	104.39	112.47
21	B	8054	SUC	O1'-C1'-C2'	-2.29	104.60	111.91
19	A	1776	CLA	O2D-CGD-O1D	-2.28	119.07	123.79
19	A	1801	CLA	CHC-C1C-C2C	-2.28	120.34	126.35
23	A	1808	BCR	C23-C24-C25	-2.28	120.46	127.32
23	A	1803	BCR	C27-C26-C25	-2.28	119.87	122.78
19	1	1192	CLA	O2D-CGD-O1D	-2.28	119.08	123.79
19	B	1741	CLA	CHC-C1C-C2C	-2.28	120.35	126.35
19	2	1221	CLA	CAA-C2A-C1A	-2.28	104.43	112.47
19	2	1213	CLA	O2A-CGA-O1A	-2.28	117.61	123.49
23	A	1806	BCR	C28-C27-C26	-2.28	110.25	113.87
19	A	1763	CLA	CHC-C1C-C2C	-2.27	120.38	126.35
23	B	1777	BCR	C11-C12-C13	-2.27	119.63	126.32
19	H	1081	CLA	CHC-C1C-C2C	-2.27	120.38	126.35
19	4	1197	CLA	CHC-C1C-C2C	-2.27	120.38	126.35
19	B	1755	CLA	C4-C3-C2	-2.27	119.05	123.50
19	2	2010	CLA	C2D-C3D-C4D	-2.27	104.31	106.30
19	A	1776	CLA	O1D-CGD-CBD	-2.27	121.37	124.62
20	A	7016	LMU	C1-O1'-C1'	-2.27	109.98	113.94
19	4	1200	CLA	C1-C2-C3	-2.27	123.00	126.71
23	B	1777	BCR	C23-C24-C25	-2.26	120.53	127.32
20	A	7022	LMU	O1B-C1B-O5B	-2.26	104.96	110.68
19	B	1737	CLA	O2D-CGD-O1D	-2.26	119.13	123.79
19	1	1197	CLA	O1D-CGD-CBD	-2.26	121.39	124.62
23	B	1779	BCR	C36-C18-C17	-2.26	119.57	122.90
19	J	1043	CLA	O2D-CGD-O1D	-2.25	119.14	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1765	CLA	O2D-CGD-O1D	-2.25	119.15	123.79
19	1	1190	CLA	O2A-CGA-O1A	-2.25	115.61	123.02
19	B	1756	CLA	O2D-CGD-O1D	-2.25	119.15	123.79
19	A	1783	CLA	CHC-C1C-C2C	-2.25	120.45	126.35
20	A	7026	LMU	O6'-C6'-C5'	-2.24	103.92	111.33
19	A	1765	CLA	O2A-CGA-O1A	-2.24	117.71	123.49
19	A	1780	CLA	O1D-CGD-CBD	-2.24	121.41	124.62
19	B	1745	CLA	CMD-C2D-C3D	-2.24	120.71	125.09
19	A	1791	CLA	O2D-CGD-O1D	-2.24	119.17	123.79
19	4	1196	CLA	C4-C3-C2	-2.24	119.11	123.50
19	A	1800	CLA	C6-C7-C8	-2.24	108.06	115.49
19	A	1780	CLA	O2D-CGD-O1D	-2.24	119.17	123.79
20	A	1812	LMU	C1B-O1B-C4'	-2.24	112.16	118.01
19	R	1055	CLA	O1D-CGD-CBD	-2.23	121.42	124.62
19	A	1796	CLA	C2A-C1A-CHA	-2.23	119.77	123.89
23	B	1778	BCR	C24-C23-C22	-2.23	122.81	126.22
19	3	3008	CLA	O2D-CGD-O1D	-2.23	119.18	123.79
23	A	1807	BCR	C12-C13-C14	-2.23	115.39	118.98
19	B	1758	CLA	CMA-C3A-C2A	-2.23	104.49	114.35
19	4	1198	CLA	O2A-CGA-O1A	-2.23	117.74	123.49
20	A	7039	LMU	O5B-C1B-C2B	-2.23	105.71	110.28
19	A	1792	CLA	C2A-C1A-CHA	-2.23	119.78	123.89
20	A	7004	LMU	C1B-O1B-C4'	-2.23	112.19	118.01
23	A	1809	BCR	C8-C7-C6	-2.23	120.63	127.32
23	B	1780	BCR	C28-C27-C26	-2.22	110.34	113.87
19	1	1014	CLA	C4-C3-C2	-2.22	119.14	123.50
23	A	1805	BCR	C8-C7-C6	-2.22	120.65	127.32
19	1	1193	CLA	O2D-CGD-O1D	-2.22	119.22	123.79
20	A	7014	LMU	C1-O1'-C1'	-2.21	110.07	113.94
23	A	1806	BCR	C27-C26-C25	-2.21	119.96	122.78
19	4	4007	CLA	O2D-CGD-O1D	-2.21	119.22	123.79
19	B	1739	CLA	O2A-CGA-O1A	-2.21	117.78	123.49
19	A	1767	CLA	O2D-CGD-O1D	-2.21	119.22	123.79
19	B	1738	CLA	O1D-CGD-CBD	-2.21	121.45	124.62
21	B	8061	SUC	O3'-C3'-C4'	-2.21	105.34	113.29
19	B	1753	CLA	O2A-CGA-O1A	-2.21	117.79	123.49
23	L	1169	BCR	C8-C7-C6	-2.21	120.68	127.32
19	A	1778	CLA	O2D-CGD-O1D	-2.21	119.23	123.79
19	2	1223	CLA	CMD-C2D-C3D	-2.21	120.77	125.09
23	B	1777	BCR	C37-C22-C21	-2.20	119.65	122.90
23	B	1777	BCR	C4-C5-C6	-2.20	119.97	122.78
23	B	1779	BCR	C28-C27-C26	-2.20	110.38	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1754	CLA	CBC-CAC-C3C	-2.20	105.68	112.39
19	B	1771	CLA	O2D-CGD-O1D	-2.20	119.25	123.79
19	B	1754	CLA	CAA-CBA-CGA	-2.20	106.88	113.32
19	1	1505	CLA	C4-C3-C2	-2.20	119.19	123.50
19	2	1215	CLA	O1D-CGD-CBD	-2.19	121.48	124.62
19	B	1749	CLA	O2D-CGD-O1D	-2.19	119.26	123.79
19	4	1201	CLA	CMB-C2B-C1B	-2.19	124.74	128.36
19	A	1813	CLA	C3B-C4B-NB	-2.19	106.38	109.21
19	A	1796	CLA	CHC-C1C-C2C	-2.19	120.60	126.35
19	A	1775	CLA	CAA-C2A-C3A	-2.19	110.96	116.20
19	A	1771	CLA	O2A-CGA-O1A	-2.18	117.85	123.49
23	A	1805	BCR	C23-C24-C25	-2.18	120.75	127.32
19	3	3011	CLA	C11-C10-C8	-2.18	108.24	115.49
19	B	1784	CLA	CMD-C2D-C3D	-2.18	120.81	125.09
23	B	1778	BCR	C3-C4-C5	-2.18	110.40	113.87
23	B	1775	BCR	C29-C30-C25	-2.18	106.91	110.36
19	B	1746	CLA	O2D-CGD-O1D	-2.18	119.29	123.79
19	A	1785	CLA	C2A-C1A-CHA	-2.18	119.87	123.89
23	B	1780	BCR	C20-C19-C18	-2.18	119.91	126.32
19	A	1816	CLA	O1D-CGD-CBD	-2.18	121.50	124.62
19	B	1757	CLA	C2A-C1A-CHA	-2.17	119.88	123.89
23	A	1806	BCR	C23-C24-C25	-2.17	120.79	127.32
19	A	1801	CLA	C2A-C1A-CHA	-2.17	119.89	123.89
23	B	1776	BCR	C3-C4-C5	-2.17	110.43	113.87
23	A	1809	BCR	C37-C22-C21	-2.17	119.70	122.90
19	F	1156	CLA	C2A-C1A-CHA	-2.16	119.90	123.89
19	4	1211	CLA	CMD-C2D-C3D	-2.16	120.86	125.09
19	A	1789	CLA	C3B-C4B-NB	-2.16	106.42	109.21
19	B	1743	CLA	CHC-C1C-C2C	-2.16	120.67	126.35
19	G	1099	CLA	CBA-CAA-C2A	-2.16	107.64	113.73
19	A	1813	CLA	CHC-C1C-C2C	-2.16	120.67	126.35
19	A	1798	CLA	C4-C3-C2	-2.15	119.28	123.50
23	A	1805	BCR	C34-C9-C10	-2.15	119.72	122.90
20	A	7040	LMU	O2'-C2'-C3'	-2.15	105.50	110.34
23	A	1803	BCR	C15-C16-C17	-2.15	118.64	123.39
19	1	1187	CLA	CGD-CBD-CAD	-2.15	103.35	110.62
19	A	1765	CLA	C5-C3-C2	-2.15	116.98	121.05
20	A	7014	LMU	O5B-C1B-C2B	-2.15	105.87	110.28
23	B	1775	BCR	C15-C14-C13	-2.14	124.10	127.20
20	A	7011	LMU	O5'-C1'-C2'	-2.14	105.88	110.28
23	B	1778	BCR	C11-C12-C13	-2.14	120.02	126.32
19	B	1750	CLA	CMA-C3A-C2A	-2.14	104.88	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1748	CLA	O1D-CGD-CBD	-2.14	121.56	124.62
23	B	1777	BCR	C29-C30-C25	-2.13	106.98	110.36
19	A	1817	CLA	O1D-CGD-CBD	-2.13	121.56	124.62
19	1	1192	CLA	C4-C3-C2	-2.13	119.31	123.50
23	B	1774	BCR	C3-C4-C5	-2.13	110.48	113.87
19	A	1787	CLA	O2A-CGA-O1A	-2.13	118.00	123.49
19	A	1785	CLA	O2A-CGA-O1A	-2.13	118.00	123.49
19	1	1191	CLA	CAA-C2A-C3A	-2.13	111.11	116.20
19	B	1752	CLA	C5-C3-C2	-2.12	117.02	121.05
19	1	1149	CLA	O2A-CGA-O1A	-2.12	118.01	123.49
19	B	1746	CLA	CAC-C3C-C2C	-2.12	123.79	127.51
20	A	7005	LMU	O3'-C3'-C4'	-2.12	104.85	109.87
23	A	1805	BCR	C4-C5-C6	-2.12	120.08	122.78
19	B	1770	CLA	O2A-CGA-O1A	-2.12	118.02	123.49
19	1	1505	CLA	O2A-CGA-O1A	-2.12	118.03	123.49
19	2	1222	CLA	O2A-CGA-O1A	-2.12	118.03	123.49
20	A	7019	LMU	O2'-C2'-C3'	-2.12	105.57	110.34
19	A	1762	CLA	O1D-CGD-CBD	-2.12	121.59	124.62
19	A	1789	CLA	C11-C12-C13	-2.12	108.47	115.49
19	A	1790	CLA	O2A-CGA-O1A	-2.11	118.03	123.49
19	3	1218	CLA	CAC-C3C-C2C	-2.11	123.80	127.51
23	B	1777	BCR	C30-C25-C26	-2.11	119.56	122.66
19	B	1738	CLA	O2A-CGA-O1A	-2.11	118.05	123.49
19	B	1741	CLA	CAA-CBA-CGA	-2.11	107.15	113.32
23	A	1805	BCR	C11-C12-C13	-2.10	120.12	126.32
19	B	1761	CLA	CAA-C2A-C3A	-2.10	107.17	113.22
19	A	1783	CLA	C11-C10-C8	-2.10	108.51	115.49
23	A	1803	BCR	C30-C25-C26	-2.10	119.57	122.66
19	L	1168	CLA	CHC-C1C-C2C	-2.10	120.82	126.35
19	1	1199	CLA	O2A-CGA-O1A	-2.10	118.07	123.49
19	B	1742	CLA	C2A-C1A-CHA	-2.10	120.02	123.89
19	A	1794	CLA	CAA-CBA-CGA	-2.10	107.18	113.32
19	A	1772	CLA	O2D-CGD-O1D	-2.10	119.46	123.79
20	A	7017	LMU	O3'-C3'-C2'	-2.10	105.62	110.34
19	B	1763	CLA	O2A-CGA-O1A	-2.10	118.08	123.49
19	A	1796	CLA	C6-C7-C8	-2.09	108.56	115.49
20	A	7003	LMU	C1B-O1B-C4'	-2.09	112.55	118.01
23	A	1809	BCR	C20-C19-C18	-2.09	120.17	126.32
19	4	1201	CLA	CBC-CAC-C3C	-2.09	106.02	112.39
19	1	1146	CLA	O1D-CGD-CBD	-2.09	121.63	124.62
19	A	1782	CLA	C2A-C1A-CHA	-2.08	120.05	123.89
20	A	7039	LMU	O5B-C5B-C4B	-2.08	105.78	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1800	CLA	O2D-CGD-O1D	-2.08	119.50	123.79
19	R	1055	CLA	CGD-CBD-CAD	-2.08	103.59	110.62
19	A	1769	CLA	O2D-CGD-O1D	-2.08	119.50	123.79
20	A	7025	LMU	O2'-C2'-C3'	-2.08	105.66	110.34
19	4	1205	CLA	CBC-CAC-C3C	-2.07	106.06	112.39
23	A	1809	BCR	C24-C23-C22	-2.07	123.06	126.22
19	A	1815	CLA	O2A-CGA-O1A	-2.07	118.14	123.49
19	H	1079	CLA	CBA-CAA-C2A	-2.07	107.89	113.73
19	4	1196	CLA	O1D-CGD-CBD	-2.07	121.66	124.62
21	B	8055	SUC	O4'-C4'-C5'	-2.07	104.84	111.05
19	A	1791	CLA	C2A-C1A-CHA	-2.07	120.08	123.89
19	1	1143	CLA	C2A-C1A-CHA	-2.07	120.08	123.89
23	B	1775	BCR	C36-C18-C17	-2.06	119.85	122.90
23	B	1774	BCR	C4-C5-C6	-2.06	120.15	122.78
19	A	1774	CLA	C2A-C1A-CHA	-2.06	120.09	123.89
23	A	1808	BCR	C20-C19-C18	-2.06	120.26	126.32
19	2	1212	CLA	C2A-C1A-CHA	-2.06	120.09	123.89
21	B	8054	SUC	C2'-O1-C1	-2.06	112.11	117.53
19	I	1031	CLA	O2A-CGA-O1A	-2.05	118.19	123.49
23	A	1804	BCR	C15-C16-C17	-2.05	118.86	123.39
19	B	1756	CLA	C4-C3-C2	-2.05	119.48	123.50
19	B	1738	CLA	CMA-C3A-C2A	-2.05	105.29	114.35
20	A	7015	LMU	O5B-C5B-C4B	-2.04	105.84	109.68
23	A	1809	BCR	C28-C27-C26	-2.04	110.63	113.87
19	A	1781	CLA	C2A-C1A-CHA	-2.04	120.13	123.89
19	4	1201	CLA	C2C-C1C-NC	-2.04	108.73	110.24
19	4	1198	CLA	C6-C5-C3	-2.04	108.01	112.48
19	4	1196	CLA	O2A-CGA-O1A	-2.04	118.23	123.49
23	B	1776	BCR	C28-C27-C26	-2.04	110.64	113.87
19	A	1774	CLA	C2C-C1C-NC	-2.04	108.73	110.24
19	B	1739	CLA	O2D-CGD-O1D	-2.04	119.59	123.79
19	B	1763	CLA	O2D-CGD-O1D	-2.04	119.59	123.79
19	B	1745	CLA	O1D-CGD-CBD	-2.03	121.71	124.62
19	1	1148	CLA	C2A-C1A-CHA	-2.03	120.15	123.89
23	B	1776	BCR	C16-C15-C14	-2.02	118.92	123.39
20	A	7035	LMU	C2'-C3'-C4'	-2.02	105.16	109.60
19	1	1189	CLA	CBC-CAC-C3C	-2.02	106.22	112.39
21	B	8056	SUC	O1-C1-C2	-2.02	101.61	108.36
19	A	1764	CLA	O1D-CGD-CBD	-2.02	121.72	124.62
20	A	7014	LMU	O3'-C3'-C2'	-2.02	105.79	110.34
19	2	1217	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
19	A	1793	CLA	O2A-CGA-O1A	-2.02	118.28	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1755	CLA	C2A-C1A-CHA	-2.02	120.17	123.89
19	2	1223	CLA	C11-C12-C13	-2.02	108.80	115.49
20	A	7039	LMU	C1'-C2'-C3'	-2.02	106.00	109.97
20	A	7030	LMU	C1'-C2'-C3'	-2.02	106.00	109.97
19	B	1739	CLA	C4-C3-C2	-2.02	119.54	123.50
19	3	1221	CLA	CHC-C1C-C2C	-2.02	121.05	126.35
19	A	1786	CLA	O2A-CGA-O1A	-2.01	118.30	123.49
19	A	1813	CLA	C6-C7-C8	-2.01	108.82	115.49
23	A	1805	BCR	C20-C19-C18	-2.01	120.40	126.32
19	A	1795	CLA	CBC-CAC-C3C	-2.01	106.25	112.39
20	A	7025	LMU	C3B-C4B-C5B	-2.01	106.70	110.20
19	B	1752	CLA	C2A-C1A-CHA	-2.01	120.19	123.89
19	4	1200	CLA	CAC-C3C-C2C	-2.01	123.99	127.51
19	A	1776	CLA	C5-C3-C2	-2.01	117.25	121.05
19	A	1775	CLA	C2A-C1A-CHA	-2.00	120.19	123.89
23	B	1780	BCR	C1-C6-C5	-2.00	119.72	122.66
23	I	1032	BCR	C12-C13-C14	-2.00	115.76	118.98
23	A	1806	BCR	C11-C12-C13	-2.00	120.43	126.32
19	2	1223	CLA	C2A-C1A-CHA	-2.00	120.20	123.89
19	B	1739	CLA	C4A-NA-C1A	2.00	108.94	106.36
19	2	2006	CLA	O2A-CGA-CBA	2.00	118.00	111.90
19	B	1753	CLA	CMB-C2B-C3B	2.00	129.00	125.09
21	H	1082	SUC	O5-C5-C6	2.00	111.42	106.36
20	A	7001	LMU	C4B-C3B-C2B	2.00	114.53	110.79
20	A	7033	LMU	O1'-C1'-C2'	2.00	110.57	108.04
19	2	2010	CLA	C2A-C1A-NA	2.01	115.05	110.36
19	L	1168	CLA	CAC-C3C-C4C	2.01	127.74	124.83
19	B	1749	CLA	CHB-C4A-NA	2.01	127.29	124.51
19	A	1766	CLA	CHB-C4A-NA	2.01	127.29	124.51
20	A	1812	LMU	O1'-C1'-C2'	2.01	110.58	108.04
19	A	1763	CLA	CHB-C4A-NA	2.01	127.30	124.51
20	A	7013	LMU	O1'-C1'-C2'	2.02	110.59	108.04
19	4	1208	CLA	C2B-C3B-C4B	2.02	108.05	106.29
23	B	1776	BCR	C2-C1-C6	2.02	113.56	110.36
23	I	1032	BCR	C23-C22-C21	2.02	122.24	118.98
19	3	3014	CLA	C2B-C3B-C4B	2.02	108.06	106.29
19	A	1769	CLA	C5-C3-C4	2.02	119.61	114.64
21	B	8056	SUC	O1-C2'-C3'	2.02	115.09	108.04
19	2	1222	CLA	CED-O2D-CGD	2.02	120.74	115.99
20	4	1212	LMU	O5'-C5'-C6'	2.02	111.47	106.36
21	B	8056	SUC	O5-C5-C6	2.03	111.47	106.36
19	4	1209	CLA	CMC-C2C-C1C	2.03	128.16	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1190	CLA	CMB-C2B-C3B	2.03	129.06	125.09
19	B	1771	CLA	CMB-C2B-C1B	2.03	131.73	128.36
19	B	1784	CLA	CGD-CBD-CAD	2.03	117.52	110.62
21	2	1225	SUC	O5-C1-C2	2.04	114.45	110.28
19	A	1776	CLA	CMB-C2B-C3B	2.04	129.07	125.09
20	A	7022	LMU	O5'-C5'-C4'	2.04	114.05	109.75
19	R	1055	CLA	CHB-C4A-NA	2.04	127.33	124.51
19	A	1779	CLA	CAC-C3C-C4C	2.04	127.79	124.83
23	A	1809	BCR	C37-C22-C23	2.05	121.50	118.10
20	B	1782	LMU	O5'-C5'-C4'	2.05	114.07	109.75
19	A	1801	CLA	CED-O2D-CGD	2.05	120.79	115.99
19	3	1218	CLA	O2A-CGA-CBA	2.05	118.14	111.90
19	A	1786	CLA	CBA-CAA-C2A	2.05	119.52	113.73
19	A	1813	CLA	CGD-CBD-CAD	2.05	117.57	110.62
19	3	3011	CLA	CED-O2D-CGD	2.05	120.81	115.99
19	2	1222	CLA	C4A-NA-C1A	2.05	109.01	106.36
19	B	1747	CLA	C4-C3-C5	2.05	118.55	115.41
20	A	7032	LMU	O5B-C5B-C6B	2.06	111.55	106.36
19	A	1772	CLA	CMB-C2B-C3B	2.06	129.11	125.09
19	A	1774	CLA	C4-C3-C5	2.06	118.55	115.41
23	B	1776	BCR	C1-C6-C7	2.06	121.59	115.82
19	3	1219	CLA	C2B-C3B-C4B	2.06	108.09	106.29
19	1	1197	CLA	C4A-NA-C1A	2.06	109.03	106.36
19	B	1759	CLA	C4A-NA-C1A	2.06	109.03	106.36
19	4	1210	CLA	C2B-C3B-C4B	2.06	108.09	106.29
19	A	1779	CLA	CMB-C2B-C3B	2.06	129.12	125.09
20	A	7031	LMU	O2B-C2B-C1B	2.06	114.55	110.02
19	B	1754	CLA	CMC-C2C-C1C	2.07	128.22	125.02
19	B	1772	CLA	CMC-C2C-C1C	2.07	128.22	125.02
19	A	1796	CLA	CMC-C2C-C1C	2.07	128.22	125.02
20	A	7020	LMU	C6'-C5'-C4'	2.07	119.26	113.25
20	A	7017	LMU	C1'-C2'-C3'	2.07	114.05	109.97
19	4	1198	CLA	C4-C3-C5	2.07	118.57	115.41
19	3	1215	CLA	C2B-C3B-C4B	2.07	108.10	106.29
19	A	1779	CLA	O2A-CGA-CBA	2.07	118.22	111.90
19	1	1193	CLA	C4A-NA-C1A	2.08	109.05	106.36
21	B	8061	SUC	O5-C5-C4	2.08	113.59	109.68
19	B	1767	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	I	1032	BCR	C29-C28-C27	2.08	116.79	111.53
20	A	7043	LMU	C2'-C3'-C4'	2.09	114.18	109.60
19	B	1784	CLA	C4-C3-C5	2.09	118.59	115.41
19	R	1054	CLA	CHB-C4A-NA	2.09	127.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	8056	SUC	O2'-C2'-C1'	2.09	113.66	107.98
23	B	1775	BCR	C36-C18-C19	2.09	121.57	118.10
20	A	7025	LMU	O5B-C1B-C2B	2.09	114.57	110.28
19	A	1792	CLA	CMB-C2B-C3B	2.09	129.18	125.09
19	A	1769	CLA	O2A-CGA-CBA	2.09	118.27	111.90
20	A	7034	LMU	C1'-C2'-C3'	2.09	114.09	109.97
21	B	8053	SUC	O1-C2'-C3'	2.09	115.33	108.04
19	A	1797	CLA	CED-O2D-CGD	2.09	120.90	115.99
19	2	1217	CLA	CED-O2D-CGD	2.09	120.90	115.99
19	1	1146	CLA	CED-O2D-CGD	2.10	120.90	115.99
19	1	1189	CLA	O2A-CGA-CBA	2.10	118.29	111.90
23	A	1809	BCR	C33-C5-C4	2.10	117.40	113.43
19	R	1055	CLA	C5-C3-C2	2.10	125.03	121.05
19	R	1055	CLA	CBA-CAA-C2A	2.10	119.65	113.73
19	1	1146	CLA	C5-C3-C4	2.10	119.80	114.64
19	A	1784	CLA	CAC-C3C-C4C	2.10	127.88	124.83
20	A	7042	LMU	O1B-C4'-C5'	2.10	114.83	109.32
19	R	1054	CLA	CAA-CBA-CGA	2.10	119.47	113.32
23	B	1777	BCR	C37-C22-C23	2.10	121.60	118.10
20	A	7023	LMU	O5B-C5B-C6B	2.11	111.68	106.36
19	H	1081	CLA	CHB-C4A-NA	2.11	127.43	124.51
19	B	1771	CLA	CAA-CBA-CGA	2.11	119.49	113.32
19	A	1771	CLA	CED-O2D-CGD	2.11	120.94	115.99
19	4	1200	CLA	CHB-C4A-NA	2.11	127.43	124.51
19	I	1031	CLA	C4-C3-C5	2.11	118.63	115.41
19	A	1763	CLA	CAC-C3C-C4C	2.11	127.90	124.83
19	4	4014	CLA	CAA-C2A-C3A	2.11	119.29	113.22
19	1	1192	CLA	CED-O2D-CGD	2.12	120.95	115.99
19	1	1187	CLA	C2C-C1C-NC	2.12	111.82	110.24
19	A	1801	CLA	CHB-C4A-NA	2.12	127.44	124.51
19	2	2006	CLA	C4A-NA-C1A	2.12	109.10	106.36
19	B	1769	CLA	CHB-C4A-NA	2.12	127.45	124.51
20	A	7042	LMU	O5'-C5'-C6'	2.12	111.72	106.36
19	B	1743	CLA	CHB-C4A-NA	2.12	127.45	124.51
19	A	1800	CLA	CHB-C4A-NA	2.12	127.45	124.51
20	A	7026	LMU	C1B-C2B-C3B	2.12	114.16	109.97
23	A	1804	BCR	C1-C6-C7	2.13	121.78	115.82
19	A	1816	CLA	CMC-C2C-C1C	2.13	128.31	125.02
19	A	1790	CLA	CED-O2D-CGD	2.13	120.99	115.99
19	A	1787	CLA	CED-O2D-CGD	2.13	120.99	115.99
19	A	1759	CLA	C4A-NA-C1A	2.13	109.12	106.36
20	A	7023	LMU	C3'-C4'-C5'	2.14	115.67	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1307	CLA	C2B-C3B-C4B	2.14	108.16	106.29
19	B	1765	CLA	CHB-C4A-NA	2.14	127.47	124.51
19	3	1221	CLA	CHB-C4A-NA	2.14	127.48	124.51
19	B	1755	CLA	C4-C3-C5	2.15	118.69	115.41
19	A	1801	CLA	CMC-C2C-C1C	2.15	128.34	125.02
19	A	1800	CLA	C4-C3-C5	2.15	118.69	115.41
23	A	1803	BCR	C1-C6-C7	2.15	121.84	115.82
20	A	7019	LMU	C1B-C2B-C3B	2.15	114.21	109.97
23	A	1805	BCR	C1-C6-C7	2.15	121.85	115.82
21	B	8061	SUC	O2'-C2'-C1'	2.15	113.84	107.98
20	L	1170	LMU	O1B-C4'-C3'	2.16	112.75	107.17
19	4	1203	CLA	C2B-C3B-C4B	2.17	108.18	106.29
19	3	3001	CLA	C2B-C3B-C4B	2.17	108.18	106.29
19	B	1756	CLA	CMB-C2B-C3B	2.17	129.33	125.09
19	A	1772	CLA	CED-O2D-CGD	2.17	121.08	115.99
19	3	1217	CLA	C3B-C4B-NB	2.17	112.02	109.21
20	A	7040	LMU	C2'-C3'-C4'	2.18	114.38	109.60
23	L	1169	BCR	C33-C5-C4	2.18	117.56	113.43
19	A	1768	CLA	CED-O2D-CGD	2.18	121.11	115.99
20	A	7019	LMU	O1'-C1'-C2'	2.18	110.80	108.04
20	A	7035	LMU	C1'-C2'-C3'	2.18	114.28	109.97
19	B	1749	CLA	CAA-C2A-C1A	2.18	120.17	112.47
19	A	1815	CLA	CGD-CBD-CAD	2.18	118.03	110.62
23	B	1779	BCR	C38-C26-C27	2.19	117.57	113.43
19	B	1738	CLA	CAC-C3C-C4C	2.19	128.00	124.83
20	A	7027	LMU	O5'-C1'-C2'	2.19	114.77	110.28
19	3	3011	CLA	O2A-CGA-CBA	2.19	118.57	111.90
19	2	1218	CLA	C3D-C2D-C1D	2.19	108.23	106.30
20	A	7005	LMU	C1'-O5'-C5'	2.19	118.00	113.75
20	A	1810	LMU	O5B-C5B-C4B	2.19	113.80	109.68
20	A	7001	LMU	O2'-C2'-C1'	2.20	114.83	110.02
20	A	7027	LMU	C3B-C4B-C5B	2.20	114.03	110.20
20	A	7021	LMU	O5B-C5B-C4B	2.20	113.81	109.68
19	1	1190	CLA	CAC-C3C-C4C	2.20	128.02	124.83
19	H	1081	CLA	O2A-CGA-CBA	2.20	118.60	111.90
19	A	1764	CLA	O2A-CGA-CBA	2.20	118.61	111.90
19	A	1817	CLA	CED-O2D-CGD	2.21	121.17	115.99
19	4	1206	CLA	CED-O2D-CGD	2.21	121.17	115.99
19	1	1193	CLA	CMB-C2B-C3B	2.21	129.42	125.09
19	B	1747	CLA	CED-O2D-CGD	2.21	121.18	115.99
23	I	1032	BCR	C19-C18-C17	2.22	122.55	118.98
19	B	1761	CLA	C4A-NA-C1A	2.22	109.22	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7042	LMU	O5B-C5B-C6B	2.22	111.96	106.36
19	B	1763	CLA	CMB-C2B-C3B	2.22	129.43	125.09
19	H	1080	CLA	CED-O2D-CGD	2.22	121.20	115.99
23	A	1806	BCR	C30-C25-C24	2.22	122.05	115.82
19	1	1014	CLA	O2A-CGA-CBA	2.22	118.68	111.90
19	4	1197	CLA	CMB-C2B-C3B	2.23	129.69	125.14
20	A	7026	LMU	O2B-C2B-C1B	2.23	114.90	110.02
19	2	1216	CLA	C3D-C4D-ND	2.23	112.10	110.13
19	L	1168	CLA	CHB-C4A-NA	2.23	127.59	124.51
19	A	1791	CLA	CED-O2D-CGD	2.23	121.22	115.99
19	1	1143	CLA	CED-O2D-CGD	2.23	121.22	115.99
19	1	1194	CLA	C2B-C3B-C4B	2.23	108.24	106.29
20	A	7047	LMU	C1B-C2B-C3B	2.23	114.37	109.97
20	B	1782	LMU	C3B-C4B-C5B	2.23	114.09	110.20
19	B	1752	CLA	O2A-CGA-CBA	2.23	118.70	111.90
19	F	1157	CLA	O2A-CGA-CBA	2.23	118.70	111.90
20	L	1170	LMU	O1'-C1'-C2'	2.23	110.86	108.04
19	A	1788	CLA	CMB-C2B-C3B	2.23	129.46	125.09
20	A	1811	LMU	C1B-C2B-C3B	2.24	114.38	109.97
19	B	1738	CLA	C4-C3-C5	2.24	118.83	115.41
19	A	1776	CLA	CGD-CBD-CAD	2.24	118.22	110.62
19	1	1308	CLA	CED-O2D-CGD	2.24	121.25	115.99
19	A	1800	CLA	CAC-C3C-C4C	2.24	128.09	124.83
20	A	7039	LMU	O4'-C4B-C3B	2.24	115.39	110.34
20	A	7023	LMU	C1B-C2B-C3B	2.25	114.40	109.97
19	A	1786	CLA	CAC-C3C-C4C	2.25	128.09	124.83
20	A	7022	LMU	O1'-C1'-C2'	2.25	110.88	108.04
20	A	7033	LMU	O5B-C5B-C6B	2.25	112.04	106.36
19	B	1760	CLA	CAC-C3C-C4C	2.25	128.10	124.83
19	B	1744	CLA	CAC-C3C-C4C	2.25	128.10	124.83
19	2	1213	CLA	CED-O2D-CGD	2.25	121.28	115.99
19	4	4007	CLA	O2A-CGA-CBA	2.26	118.77	111.90
19	B	1758	CLA	CMB-C2B-C1B	2.26	132.10	128.36
19	A	1786	CLA	CHB-C4A-NA	2.26	127.63	124.51
20	A	7035	LMU	O1'-C1'-C2'	2.26	110.89	108.04
20	A	7017	LMU	O5B-C1B-C2B	2.26	114.92	110.28
19	B	1755	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	A	1800	CLA	O2A-CGA-CBA	2.27	118.81	111.90
20	A	7010	LMU	O5'-C5'-C6'	2.27	112.10	106.36
20	A	7034	LMU	C3B-C4B-C5B	2.27	114.16	110.20
19	A	1771	CLA	CGD-CBD-CAD	2.28	118.34	110.62
20	A	7040	LMU	C1B-C2B-C3B	2.28	114.46	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1792	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	B	1761	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	I	1032	BCR	C7-C6-C5	2.28	126.60	121.37
19	A	1774	CLA	CHB-C4A-NA	2.29	127.67	124.51
19	B	1759	CLA	O2A-CGA-CBA	2.29	118.87	111.90
20	B	1782	LMU	O1B-C4'-C3'	2.29	113.07	107.17
19	A	1781	CLA	C4-C3-C5	2.29	118.90	115.41
19	B	1758	CLA	C4A-NA-C1A	2.29	109.32	106.36
23	B	1775	BCR	C30-C25-C24	2.29	122.23	115.82
19	B	1766	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	4	1209	CLA	CAC-C3C-C4C	2.29	128.57	125.02
19	4	1201	CLA	CGD-CBD-CAD	2.29	118.39	110.62
19	B	1750	CLA	CHB-C4A-NA	2.29	127.68	124.51
20	A	7040	LMU	C1'-C2'-C3'	2.29	114.49	109.97
19	1	1195	CLA	C2B-C3B-C4B	2.29	108.29	106.29
20	A	7019	LMU	O5B-C5B-C6B	2.30	112.16	106.36
19	A	1782	CLA	O2A-CGA-CBA	2.30	118.89	111.90
20	A	7037	LMU	O3B-C3B-C2B	2.30	115.51	110.34
19	1	1309	CLA	C2B-C3B-C4B	2.30	108.30	106.29
20	A	7010	LMU	O1'-C1'-C2'	2.30	110.95	108.04
19	B	1767	CLA	O2A-CGA-CBA	2.30	118.92	111.90
19	2	1216	CLA	C3D-C2D-C1D	2.30	108.33	106.30
19	4	1197	CLA	CHB-C4A-NA	2.31	127.70	124.51
20	A	7017	LMU	O1B-C1B-C2B	2.31	113.73	108.10
19	A	1776	CLA	O2A-CGA-CBA	2.31	118.95	111.90
19	B	1749	CLA	CMC-C2C-C1C	2.32	128.60	125.02
19	2	1220	CLA	C3D-C4D-ND	2.32	112.18	110.13
19	A	1813	CLA	CMC-C2C-C1C	2.32	128.60	125.02
19	B	1737	CLA	C4-C3-C5	2.32	118.95	115.41
19	B	1755	CLA	O2A-CGA-CBA	2.32	118.96	111.90
19	A	1765	CLA	C2C-C1C-NC	2.32	111.97	110.24
23	B	1775	BCR	C23-C22-C21	2.32	122.72	118.98
20	A	1812	LMU	O5'-C5'-C6'	2.33	112.25	106.36
20	A	7027	LMU	C3'-C4'-C5'	2.33	116.11	110.84
19	2	2006	CLA	CED-O2D-CGD	2.34	121.48	115.99
19	B	1747	CLA	CMB-C2B-C3B	2.34	129.67	125.09
19	1	1505	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	A	1785	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	B	1756	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	L	1170	LMU	O5'-C5'-C6'	2.35	112.30	106.36
19	1	1196	CLA	CHB-C4A-NA	2.35	127.77	124.51
20	A	7038	LMU	O3'-C3'-C2'	2.36	115.64	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7043	LMU	O5'-C5'-C6'	2.36	112.32	106.36
22	A	1802	PQN	C2M-C2-C1	2.36	120.10	116.27
23	A	1807	BCR	C35-C13-C12	2.36	122.02	118.10
19	1	1188	CLA	CAA-C2A-C1A	2.36	118.70	112.17
20	A	7033	LMU	C1'-C2'-C3'	2.37	114.63	109.97
21	B	8061	SUC	O2'-C5'-C6'	2.37	115.73	108.57
20	A	7035	LMU	O5'-C5'-C6'	2.37	112.34	106.36
19	4	1206	CLA	O2A-CGA-CBA	2.37	119.12	111.90
19	4	1201	CLA	C4-C3-C5	2.38	119.04	115.41
19	A	1816	CLA	CAC-C3C-C4C	2.38	128.28	124.83
19	B	1760	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	B	1744	CLA	CED-O2D-CGD	2.38	121.58	115.99
19	B	1742	CLA	O2A-CGA-CBA	2.38	119.16	111.90
20	A	7047	LMU	C1'-O5'-C5'	2.38	118.37	113.75
19	1	1197	CLA	CHB-C4A-NA	2.39	127.81	124.51
20	A	7037	LMU	C1'-C2'-C3'	2.39	114.67	109.97
19	3	1217	CLA	CED-O2D-CGD	2.40	121.61	115.99
23	B	1780	BCR	C38-C26-C27	2.40	117.98	113.43
20	A	7033	LMU	O5'-C5'-C6'	2.40	112.42	106.36
19	2	1215	CLA	CED-O2D-CGD	2.40	121.62	115.99
19	B	1753	CLA	C9-C8-C10	2.40	120.30	111.08
19	A	1761	CLA	CAC-C3C-C4C	2.40	128.31	124.83
19	A	1799	CLA	C2B-C3B-C4B	2.40	108.39	106.29
19	A	1763	CLA	CMC-C2C-C1C	2.40	128.74	125.02
20	A	7028	LMU	O5B-C5B-C6B	2.40	112.43	106.36
19	A	1787	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	A	7027	LMU	O5'-C5'-C6'	2.41	112.44	106.36
19	4	1196	CLA	O2D-CGD-CBD	2.41	114.60	111.30
19	A	1760	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	4	1201	CLA	CED-O2D-CGD	2.41	121.65	115.99
19	A	1785	CLA	O2A-CGA-CBA	2.41	119.25	111.90
20	A	7040	LMU	O5B-C1B-C2B	2.42	115.23	110.28
19	1	1148	CLA	CHB-C4A-NA	2.42	127.85	124.51
20	A	7035	LMU	O1B-C4'-C5'	2.42	115.67	109.32
19	B	1763	CLA	CED-O2D-CGD	2.42	121.66	115.99
19	B	1761	CLA	O2A-CGA-CBA	2.42	119.27	111.90
23	I	1032	BCR	C35-C13-C12	2.42	122.12	118.10
19	A	1774	CLA	CGD-CBD-CAD	2.42	118.83	110.62
19	4	1196	CLA	CAC-C3C-C4C	2.42	128.34	124.83
19	1	1145	CLA	CGD-CBD-CAD	2.42	118.83	110.62
19	B	1769	CLA	CED-O2D-CGD	2.42	121.67	115.99
19	B	1762	CLA	O2A-CGA-CBA	2.42	119.28	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1142	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	A	1816	CLA	CAA-C2A-C1A	2.43	121.04	112.47
19	F	1157	CLA	CMA-C3A-C2A	2.43	125.10	114.35
19	1	1149	CLA	CAA-C2A-C1A	2.43	121.04	112.47
20	A	7043	LMU	O5'-C1'-C2'	2.43	115.26	110.28
19	B	1748	CLA	CHB-C4A-NA	2.43	127.88	124.51
20	A	7043	LMU	O1B-C4'-C3'	2.43	113.45	107.17
19	A	1797	CLA	CAA-C2A-C3A	2.43	120.22	113.22
21	3	1223	SUC	C1-O5-C5	2.44	118.48	113.75
20	A	7024	LMU	O5B-C5B-C6B	2.44	112.52	106.36
21	B	8062	SUC	O2-C2-C1	2.44	115.37	110.02
19	A	1816	CLA	O2A-CGA-CBA	2.44	119.34	111.90
19	1	1143	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	3	1213	CLA	CMC-C2C-C1C	2.44	128.80	125.02
19	3	1213	CLA	CHB-C4A-NA	2.45	127.89	124.51
19	1	1197	CLA	CED-O2D-CGD	2.45	121.73	115.99
19	B	1735	CLA	O2A-CGA-CBA	2.45	119.35	111.90
19	A	1796	CLA	CMB-C2B-C3B	2.45	129.88	125.09
19	A	1766	CLA	CED-O2D-CGD	2.45	121.74	115.99
20	A	7009	LMU	O5'-C5'-C6'	2.45	112.56	106.36
19	1	1148	CLA	C4-C3-C5	2.45	119.16	115.41
19	A	1784	CLA	CGD-CBD-CAD	2.46	118.95	110.62
20	A	7008	LMU	O4'-C4B-C5B	2.46	115.76	109.24
19	A	1813	CLA	O2A-CGA-CBA	2.46	119.39	111.90
19	F	1156	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	A	1814	CLA	CED-O2D-CGD	2.46	121.77	115.99
19	L	1168	CLA	CAA-C2A-C1A	2.46	121.16	112.47
19	A	1782	CLA	CHB-C4A-NA	2.47	127.92	124.51
20	A	7019	LMU	O5'-C5'-C4'	2.47	114.95	109.75
19	B	1759	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	B	1771	CLA	C4-C3-C5	2.47	119.18	115.41
19	A	1791	CLA	CAC-C3C-C4C	2.47	128.42	124.83
19	1	1191	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	B	1768	CLA	O2A-CGA-CBA	2.47	119.44	111.90
19	2	1217	CLA	CGD-CBD-CAD	2.48	119.02	110.62
19	B	1745	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	B	1770	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	B	1744	CLA	O2A-CGA-CBA	2.48	119.46	111.90
19	A	1778	CLA	CHB-C4A-NA	2.48	127.95	124.51
19	B	1784	CLA	CMB-C2B-C3B	2.48	129.95	125.09
19	A	1777	CLA	CHB-C4A-NA	2.48	127.95	124.51
19	1	1148	CLA	O2A-CGA-CBA	2.49	119.48	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	3008	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	R	1055	CLA	CAA-CBA-CGA	2.50	120.63	113.32
19	A	1760	CLA	CMB-C2B-C3B	2.50	129.97	125.09
19	1	1014	CLA	CAA-C2A-C1A	2.50	121.28	112.47
21	B	8055	SUC	C1-O5-C5	2.51	118.61	113.75
20	A	7030	LMU	O5B-C5B-C6B	2.51	112.70	106.36
23	B	1776	BCR	C23-C22-C21	2.51	123.03	118.98
19	1	1505	CLA	CED-O2D-CGD	2.51	121.88	115.99
19	A	1767	CLA	CAA-CBA-CGA	2.52	120.68	113.32
19	B	1766	CLA	O2A-CGA-CBA	2.52	119.58	111.90
19	B	1747	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	A	1775	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	A	1790	CLA	O2A-CGA-CBA	2.53	119.62	111.90
19	B	1743	CLA	O2A-CGA-CBA	2.54	119.62	111.90
19	A	1781	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	B	1755	CLA	CAC-C3C-C4C	2.54	128.52	124.83
19	B	1756	CLA	O2A-CGA-CBA	2.54	119.65	111.90
19	A	1762	CLA	CED-O2D-CGD	2.55	121.96	115.99
19	A	1789	CLA	CMB-C2B-C1B	2.55	132.58	128.36
19	4	1206	CLA	CMB-C2B-C3B	2.55	130.07	125.09
22	B	1773	PQN	C14-C13-C15	2.55	119.30	115.41
19	B	1766	CLA	CAC-C3C-C4C	2.55	128.53	124.83
19	A	1793	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	B	1778	BCR	C38-C26-C27	2.56	118.28	113.43
19	2	1221	CLA	CHB-C4A-NA	2.56	128.05	124.51
19	2	1215	CLA	O2A-CGA-CBA	2.56	119.70	111.90
19	A	1761	CLA	CHB-C4A-NA	2.56	128.06	124.51
19	B	1752	CLA	CHB-C4A-NA	2.56	128.06	124.51
19	3	1216	CLA	C3D-C4D-ND	2.56	112.41	110.13
19	4	4007	CLA	C4-C3-C5	2.57	119.33	115.41
20	A	1811	LMU	C1'-C2'-C3'	2.57	115.03	109.97
20	B	1782	LMU	O5B-C5B-C4B	2.57	114.50	109.68
19	I	1031	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	1	1308	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	B	1742	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	A	1764	CLA	CMB-C2B-C3B	2.57	130.12	125.09
20	A	7037	LMU	O1B-C1B-C2B	2.57	114.37	108.10
19	1	1149	CLA	CGD-CBD-CAD	2.57	119.35	110.62
20	A	7038	LMU	O5'-C5'-C6'	2.58	112.87	106.36
19	A	1797	CLA	CHB-C4A-NA	2.58	128.07	124.51
19	A	1767	CLA	O2A-CGA-CBA	2.58	119.76	111.90
19	B	1760	CLA	CGD-CBD-CAD	2.58	119.37	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1099	CLA	O2A-CGA-CBA	2.58	119.77	111.90
20	A	7017	LMU	O5'-C5'-C6'	2.58	112.88	106.36
19	1	1145	CLA	CED-O2D-CGD	2.58	122.05	115.99
19	A	1776	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	A	1777	CLA	CED-O2D-CGD	2.59	122.05	115.99
19	B	1745	CLA	CED-O2D-CGD	2.59	122.06	115.99
20	A	7008	LMU	O1B-C1B-O5B	2.59	117.23	110.68
19	B	1735	CLA	CHB-C4A-NA	2.59	128.09	124.51
20	A	7049	LMU	O1'-C1'-C2'	2.59	111.31	108.04
23	B	1775	BCR	C1-C6-C7	2.59	123.08	115.82
20	A	7035	LMU	O5'-C1'-C2'	2.60	115.61	110.28
19	A	1767	CLA	CMB-C2B-C1B	2.60	132.67	128.36
22	B	1773	PQN	C2M-C2-C1	2.60	120.50	116.27
19	2	2010	CLA	C3D-C4D-ND	2.61	112.44	110.13
19	A	1776	CLA	CED-O2D-CGD	2.61	122.11	115.99
19	A	1795	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	A	1766	CLA	CMB-C2B-C3B	2.61	130.19	125.09
19	A	1816	CLA	C6-C5-C3	2.61	118.21	112.48
19	1	1199	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	A	1788	CLA	CHB-C4A-NA	2.61	128.13	124.51
20	A	7017	LMU	O5'-C1'-C2'	2.62	115.64	110.28
19	1	1149	CLA	CAC-C3C-C4C	2.62	128.63	124.83
20	A	7034	LMU	C1B-C2B-C3B	2.62	115.13	109.97
19	B	1772	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	A	1787	CLA	CMB-C2B-C3B	2.62	130.22	125.09
23	A	1803	BCR	C38-C26-C27	2.62	118.40	113.43
19	A	1773	CLA	CHB-C4A-NA	2.63	128.15	124.51
20	A	7021	LMU	C1B-O1B-C4'	2.64	124.90	118.01
19	A	1760	CLA	CBA-CAA-C2A	2.64	121.19	113.73
19	A	1814	CLA	C4-C3-C5	2.64	119.44	115.41
20	A	7001	LMU	O1B-C4'-C5'	2.64	116.27	109.32
19	1	1188	CLA	CHB-C4A-NA	2.65	128.17	124.51
19	A	1771	CLA	CHB-C4A-NA	2.65	128.18	124.51
19	B	1742	CLA	CAC-C3C-C4C	2.66	128.69	124.83
19	B	1771	CLA	CHB-C4A-NA	2.66	128.19	124.51
19	2	1219	CLA	CHB-C4A-NA	2.66	128.19	124.51
19	A	1813	CLA	CMB-C2B-C3B	2.66	130.30	125.09
19	F	1157	CLA	C4-C3-C5	2.66	119.48	115.41
19	3	1221	CLA	CHC-C1C-NC	2.67	128.69	123.67
19	A	1784	CLA	O2A-CGA-CBA	2.67	120.03	111.90
19	4	1210	CLA	C3D-C4D-ND	2.67	112.50	110.13
20	A	7027	LMU	C1'-O5'-C5'	2.67	118.93	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1217	CLA	CHB-C4A-NA	2.67	128.21	124.51
20	A	7033	LMU	C4B-C3B-C2B	2.67	115.78	110.79
20	A	7038	LMU	O1B-C1B-C2B	2.68	114.61	108.10
19	1	1188	CLA	CMB-C2B-C3B	2.68	130.32	125.09
21	B	8062	SUC	O5-C5-C6	2.68	113.12	106.36
23	A	1809	BCR	C35-C13-C12	2.68	122.56	118.10
23	B	1777	BCR	C33-C5-C4	2.69	118.52	113.43
19	3	1216	CLA	C2B-C3B-C4B	2.69	108.64	106.29
20	A	7036	LMU	O5B-C5B-C6B	2.69	113.15	106.36
20	A	7026	LMU	O3'-C3'-C2'	2.69	116.40	110.34
19	A	1762	CLA	CHB-C4A-NA	2.69	128.24	124.51
19	2	1214	CLA	C3D-C2D-C1D	2.70	108.68	106.30
19	A	1795	CLA	CMB-C2B-C3B	2.70	130.38	125.09
20	A	7016	LMU	C4B-C3B-C2B	2.70	115.84	110.79
19	A	1794	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	B	1765	CLA	CMB-C2B-C3B	2.71	130.38	125.09
19	A	1762	CLA	O2A-CGA-CBA	2.71	120.16	111.90
20	2	1224	LMU	O1B-C1B-C2B	2.71	114.71	108.10
19	B	1746	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	B	1737	CLA	CHB-C4A-NA	2.72	128.27	124.51
20	A	7043	LMU	C1'-O5'-C5'	2.72	119.02	113.75
19	L	1168	CLA	O2A-CGA-CBA	2.72	120.18	111.90
19	4	1207	CLA	C3D-C2D-C1D	2.72	108.69	106.30
19	3	3015	CLA	C3D-C2D-C1D	2.72	108.70	106.30
19	B	1753	CLA	CHC-C1C-NC	2.72	128.79	123.67
20	A	1810	LMU	C3'-C4'-C5'	2.72	117.00	110.84
20	A	7019	LMU	C3'-C4'-C5'	2.73	117.00	110.84
19	3	1218	CLA	CHB-C4A-NA	2.73	128.29	124.51
19	B	1753	CLA	O2A-CGA-CBA	2.73	120.22	111.90
19	B	1744	CLA	CHB-C4A-NA	2.73	128.29	124.51
21	B	8059	SUC	O3-C3-C4	2.73	116.49	110.34
20	L	1170	LMU	O5B-C5B-C4B	2.74	114.82	109.68
19	B	1766	CLA	CMB-C2B-C3B	2.74	130.44	125.09
19	B	1752	CLA	CED-O2D-CGD	2.75	122.44	115.99
19	A	1784	CLA	C4-C3-C5	2.75	119.61	115.41
19	4	1196	CLA	CHB-C4A-NA	2.75	128.32	124.51
19	B	1741	CLA	CHB-C4A-NA	2.76	128.32	124.51
20	A	7030	LMU	O1B-C4'-C5'	2.76	116.57	109.32
19	1	1199	CLA	O2A-CGA-CBA	2.76	120.31	111.90
23	A	1804	BCR	C38-C26-C27	2.76	118.66	113.43
23	B	1779	BCR	C2-C1-C6	2.76	114.73	110.36
20	A	7027	LMU	O1B-C1B-C2B	2.76	114.82	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7014	LMU	O2B-C2B-C1B	2.76	116.07	110.02
19	A	1761	CLA	O2A-CGA-CBA	2.76	120.31	111.90
20	A	7008	LMU	O1B-C1B-C2B	2.77	114.83	108.10
19	A	1780	CLA	CHB-C4A-NA	2.77	128.34	124.51
19	G	1099	CLA	C4-C3-C5	2.77	118.82	115.68
19	A	1768	CLA	CHB-C4A-NA	2.77	128.34	124.51
19	1	1146	CLA	CMB-C2B-C3B	2.77	130.50	125.09
19	4	1206	CLA	C4-C3-C5	2.78	119.65	115.41
19	3	3008	CLA	CED-O2D-CGD	2.78	122.50	115.99
19	B	1764	CLA	CHB-C4A-NA	2.78	128.35	124.51
20	A	7025	LMU	C2'-C3'-C4'	2.78	115.70	109.60
19	2	1215	CLA	CHB-C4A-NA	2.78	128.36	124.51
19	B	1743	CLA	C4-C3-C5	2.78	119.65	115.41
20	A	7026	LMU	O1'-C1'-C2'	2.79	111.56	108.04
20	A	1810	LMU	O5'-C5'-C4'	2.79	115.63	109.75
19	3	1221	CLA	O2A-CGA-CBA	2.79	120.41	111.90
19	2	1218	CLA	C3D-C4D-ND	2.79	112.61	110.13
20	A	7011	LMU	O5B-C5B-C6B	2.79	113.42	106.36
21	3	1223	SUC	O5-C1-C2	2.79	116.01	110.28
20	A	7014	LMU	O5B-C5B-C6B	2.80	113.42	106.36
19	A	1813	CLA	CHC-C1C-NC	2.80	128.94	123.67
20	A	7037	LMU	O5'-C5'-C6'	2.80	113.44	106.36
20	B	1782	LMU	C2'-C3'-C4'	2.80	115.75	109.60
19	A	1784	CLA	CHB-C4A-NA	2.80	128.39	124.51
19	B	1763	CLA	O2A-CGA-CBA	2.81	120.45	111.90
23	B	1775	BCR	C33-C5-C4	2.81	118.75	113.43
19	4	4007	CLA	C4A-NA-C1A	2.81	109.99	106.36
23	I	1032	BCR	C30-C25-C24	2.81	123.69	115.82
19	A	1762	CLA	CMB-C2B-C3B	2.81	130.59	125.09
19	L	1168	CLA	CHC-C1C-NC	2.81	128.97	123.67
21	B	8055	SUC	O5-C5-C6	2.82	113.47	106.36
19	B	1757	CLA	CHB-C4A-NA	2.82	128.41	124.51
19	3	1222	CLA	CHB-C4A-NA	2.82	128.41	124.51
20	A	7008	LMU	O5B-C5B-C6B	2.82	113.49	106.36
19	A	1777	CLA	O2A-CGA-CBA	2.82	120.50	111.90
20	A	7014	LMU	O5'-C1'-O1'	2.82	116.85	110.05
19	1	1190	CLA	CHB-C4A-NA	2.83	128.42	124.51
19	B	1749	CLA	C4-C3-C5	2.83	119.73	115.41
19	A	1817	CLA	O2A-CGA-CBA	2.83	120.53	111.90
20	R	1056	LMU	O1'-C1'-C2'	2.83	111.62	108.04
23	B	1774	BCR	C38-C26-C27	2.84	118.81	113.43
19	4	1196	CLA	O2A-CGA-CBA	2.84	120.55	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1221	CLA	CMC-C2C-C1C	2.84	129.41	125.02
19	A	1765	CLA	CAC-C3C-C4C	2.84	128.95	124.83
19	B	1749	CLA	CHC-C1C-NC	2.84	129.01	123.67
19	4	1211	CLA	CHB-C4A-NA	2.84	128.44	124.51
19	F	1156	CLA	CHC-C1C-NC	2.84	129.02	123.67
19	B	1770	CLA	C4-C3-C5	2.84	119.75	115.41
19	4	4014	CLA	O2A-CGA-CBA	2.84	120.56	111.90
21	B	8061	SUC	O5-C5-C6	2.84	113.54	106.36
19	A	1760	CLA	C4-C3-C5	2.85	119.76	115.41
19	H	1080	CLA	O2A-CGA-CBA	2.85	120.59	111.90
19	A	1801	CLA	C4-C3-C5	2.85	119.77	115.41
20	A	7019	LMU	C1'-C2'-C3'	2.86	115.61	109.97
19	A	1780	CLA	O2A-CGA-CBA	2.86	120.61	111.90
19	1	1189	CLA	CHB-C4A-NA	2.86	128.47	124.51
19	H	1080	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	A	1808	BCR	C37-C22-C23	2.86	122.86	118.10
20	A	7017	LMU	C3B-C4B-C5B	2.86	115.19	110.20
19	B	1757	CLA	C4-C3-C5	2.87	119.78	115.41
19	1	1195	CLA	CHC-C1C-NC	2.87	128.91	123.78
19	B	1745	CLA	O2A-CGA-CBA	2.88	120.66	111.90
19	3	1212	CLA	C3D-C2D-C1D	2.88	108.83	106.30
19	L	1167	CLA	O2A-CGA-CBA	2.88	120.67	111.90
19	A	1768	CLA	O2A-CGA-CBA	2.88	120.67	111.90
19	A	1815	CLA	O2A-CGA-CBA	2.88	120.67	111.90
20	A	7017	LMU	O5B-C5B-C6B	2.88	113.64	106.36
20	A	1810	LMU	C3B-C4B-C5B	2.88	115.22	110.20
20	A	7009	LMU	C3'-C4'-C5'	2.88	117.36	110.84
23	A	1806	BCR	C38-C26-C27	2.88	118.90	113.43
19	B	1749	CLA	O2A-CGA-CBA	2.88	120.69	111.90
19	B	1770	CLA	CMB-C2B-C3B	2.89	130.73	125.09
20	A	7032	LMU	C3'-C4'-C5'	2.89	117.37	110.84
19	B	1762	CLA	CHB-C4A-NA	2.89	128.50	124.51
20	A	7037	LMU	O4'-C4B-C5B	2.89	116.90	109.24
20	A	7038	LMU	O5B-C5B-C4B	2.90	115.12	109.68
20	A	7027	LMU	C6B-C5B-C4B	2.90	120.17	113.02
19	1	1308	CLA	O2A-CGA-CBA	2.90	120.74	111.90
23	B	1778	BCR	C33-C5-C4	2.90	118.93	113.43
20	A	7024	LMU	O5'-C5'-C6'	2.90	113.69	106.36
19	A	1761	CLA	CED-O2D-CGD	2.90	122.80	115.99
19	2	1222	CLA	CAA-C2A-C1A	2.91	122.73	112.47
19	A	1794	CLA	O2A-CGA-CBA	2.91	120.76	111.90
19	4	1206	CLA	CHC-C1C-NC	2.91	129.16	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7020	LMU	O5B-C1B-C2B	2.92	116.27	110.28
20	A	7020	LMU	O1'-C1'-C2'	2.92	111.73	108.04
19	A	1798	CLA	CED-O2D-CGD	2.92	122.84	115.99
19	1	1193	CLA	O2A-CGA-CBA	2.92	120.81	111.90
19	A	1776	CLA	C4-C3-C5	2.93	119.88	115.41
19	A	1796	CLA	CHC-C1C-NC	2.93	129.18	123.67
23	A	1805	BCR	C38-C26-C27	2.93	118.98	113.43
19	A	1783	CLA	CHB-C4A-NA	2.93	128.56	124.51
19	3	1221	CLA	CMB-C2B-C3B	2.93	130.83	125.09
19	3	1213	CLA	CHC-C1C-NC	2.94	129.20	123.67
19	A	1779	CLA	CHB-C4A-NA	2.94	128.58	124.51
20	A	1810	LMU	O1'-C1'-C2'	2.94	111.75	108.04
19	2	2006	CLA	CHB-C4A-NA	2.94	128.58	124.51
21	3	1223	SUC	O3-C3-C2	2.95	116.97	110.34
19	3	3011	CLA	CHB-C4A-NA	2.95	128.59	124.51
20	A	7047	LMU	O1'-C1'-C2'	2.95	111.76	108.04
19	4	1209	CLA	CHB-C4A-NA	2.95	128.59	124.51
20	A	7041	LMU	O1B-C1B-C2B	2.96	115.31	108.10
19	1	1307	CLA	C3D-C4D-ND	2.96	112.76	110.13
19	A	1781	CLA	CAC-C3C-C4C	2.96	129.13	124.83
23	B	1779	BCR	C33-C5-C4	2.97	119.06	113.43
19	A	1777	CLA	C4-C3-C5	2.97	119.05	115.68
19	B	1736	CLA	CHB-C4A-NA	2.98	128.63	124.51
19	B	1750	CLA	O2A-CGA-CBA	2.98	120.97	111.90
19	2	1221	CLA	O2A-CGA-CBA	2.98	120.99	111.90
23	B	1777	BCR	C38-C26-C27	2.98	119.08	113.43
24	B	1781	LMG	O8-C28-C29	2.99	121.00	111.90
19	H	1080	CLA	C4-C3-C5	2.99	119.97	115.41
19	A	1793	CLA	O2A-CGA-CBA	2.99	121.00	111.90
19	4	1199	CLA	O2A-CGA-CBA	2.99	121.00	111.90
19	F	1157	CLA	CHB-C4A-NA	2.99	128.65	124.51
19	1	1143	CLA	O2A-CGA-CBA	2.99	121.02	111.90
19	A	1796	CLA	CHB-C4A-NA	3.00	128.66	124.51
19	A	1801	CLA	CHC-C1C-NC	3.00	129.32	123.67
19	4	1210	CLA	C3D-C2D-C1D	3.00	108.94	106.30
19	4	1207	CLA	C3D-C4D-ND	3.00	112.79	110.13
19	3	1219	CLA	C3D-C4D-ND	3.00	112.80	110.13
19	A	1813	CLA	CHB-C4A-NA	3.00	128.67	124.51
19	A	1772	CLA	CHB-C4A-NA	3.00	128.67	124.51
19	A	1798	CLA	CHB-C4A-NA	3.01	128.67	124.51
19	3	3008	CLA	O2A-CGA-CBA	3.01	121.07	111.90
19	A	1795	CLA	C4-C3-C5	3.01	119.09	115.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1187	CLA	C4A-NA-C1A	3.01	110.25	106.36
19	4	1201	CLA	CMB-C2B-C3B	3.02	131.00	125.09
19	A	1801	CLA	O2A-CGA-CBA	3.02	121.11	111.90
19	A	1791	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	B	1760	CLA	CED-O2D-CGD	3.02	123.08	115.99
19	2	1213	CLA	O2A-CGA-CBA	3.02	121.11	111.90
19	3	1212	CLA	C3D-C4D-ND	3.03	112.81	110.13
19	A	1767	CLA	CHB-C4A-NA	3.03	128.70	124.51
20	A	7025	LMU	C1'-C2'-C3'	3.03	115.94	109.97
19	3	3001	CLA	C3D-C4D-ND	3.03	112.82	110.13
19	4	1206	CLA	CHB-C4A-NA	3.03	128.71	124.51
20	A	7037	LMU	O1B-C1B-O5B	3.03	118.36	110.68
19	F	1157	CLA	CHC-C1C-NC	3.04	129.39	123.67
19	A	1764	CLA	CHB-C4A-NA	3.04	128.71	124.51
19	1	1149	CLA	CED-O2D-CGD	3.04	123.12	115.99
20	A	7015	LMU	C4B-C3B-C2B	3.05	116.47	110.79
19	A	1765	CLA	C4-C3-C5	3.05	120.06	115.41
19	A	1815	CLA	CHB-C4A-NA	3.05	128.73	124.51
19	4	1201	CLA	CHB-C4A-NA	3.05	128.73	124.51
19	A	1763	CLA	CHC-C1C-NC	3.06	129.42	123.67
19	A	1781	CLA	O2A-CGA-CBA	3.06	121.22	111.90
20	A	7026	LMU	O5'-C1'-C2'	3.06	116.55	110.28
23	A	1809	BCR	C38-C26-C27	3.06	119.23	113.43
19	4	1200	CLA	CAC-C3C-C4C	3.06	129.27	124.83
19	3	1214	CLA	C3D-C2D-C1D	3.06	109.00	106.30
19	2	1223	CLA	CHB-C4A-NA	3.07	128.75	124.51
19	A	1789	CLA	CAC-C3C-C4C	3.07	129.29	124.83
23	B	1776	BCR	C38-C26-C27	3.07	119.25	113.43
19	1	1014	CLA	CHC-C1C-NC	3.07	129.46	123.67
23	A	1808	BCR	C1-C6-C7	3.07	124.43	115.82
19	B	1742	CLA	C5-C3-C2	3.08	126.89	121.05
19	A	1783	CLA	CHC-C1C-NC	3.08	129.47	123.67
20	A	7038	LMU	O5'-C1'-C2'	3.08	116.60	110.28
19	4	1199	CLA	CAC-C3C-C4C	3.09	129.31	124.83
19	1	1014	CLA	C4-C3-C5	3.09	119.18	115.68
19	4	1209	CLA	CHC-C1C-NC	3.09	129.48	123.67
21	B	8053	SUC	C3-C4-C5	3.09	114.93	109.72
19	2	1212	CLA	CHB-C4A-NA	3.09	128.78	124.51
19	B	1745	CLA	CHC-C1C-NC	3.09	129.49	123.67
19	B	1772	CLA	CHC-C1C-NC	3.09	129.49	123.67
19	A	1772	CLA	CHC-C1C-NC	3.10	129.50	123.67
20	A	7037	LMU	O5B-C5B-C6B	3.10	114.20	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1745	CLA	C4-C3-C5	3.11	120.16	115.41
19	F	1155	CLA	CHB-C4A-NA	3.12	128.83	124.51
19	H	1081	CLA	CHC-C1C-NC	3.12	129.55	123.67
19	B	1735	CLA	CED-O2D-CGD	3.12	123.31	115.99
19	B	1758	CLA	CHC-C1C-NC	3.12	129.55	123.67
20	2	1224	LMU	O1B-C4'-C5'	3.12	117.53	109.32
20	A	7027	LMU	C2'-C3'-C4'	3.13	116.48	109.60
19	J	1043	CLA	C4-C3-C5	3.13	120.19	115.41
23	L	1169	BCR	C38-C26-C27	3.13	119.37	113.43
19	3	1214	CLA	C3D-C4D-ND	3.13	112.91	110.13
20	A	7031	LMU	O1B-C1B-C2B	3.14	115.75	108.10
19	3	1216	CLA	C3D-C2D-C1D	3.14	109.07	106.30
19	B	1735	CLA	CMB-C2B-C3B	3.14	131.24	125.09
19	B	1747	CLA	O2A-CGA-CBA	3.15	121.48	111.90
20	A	7005	LMU	O1'-C1'-C2'	3.15	112.01	108.04
20	A	1811	LMU	C2'-C3'-C4'	3.15	116.51	109.60
19	A	1764	CLA	CHC-C1C-NC	3.15	129.60	123.67
19	A	1787	CLA	O2A-CGA-CBA	3.15	121.51	111.90
20	A	7024	LMU	C1'-C2'-C3'	3.16	116.19	109.97
19	1	1194	CLA	C3D-C4D-ND	3.16	112.93	110.13
19	G	1099	CLA	CHB-C4A-NA	3.16	128.88	124.51
19	B	1754	CLA	CHC-C1C-NC	3.16	129.61	123.67
19	3	3008	CLA	CHC-C1C-NC	3.16	129.61	123.67
19	4	1203	CLA	C3D-C2D-C1D	3.16	109.08	106.30
19	4	1204	CLA	C3D-C4D-ND	3.16	112.94	110.13
19	A	1772	CLA	O2A-CGA-CBA	3.17	121.55	111.90
20	A	7027	LMU	C1'-C2'-C3'	3.18	116.24	109.97
19	A	1789	CLA	O2A-CGA-CBA	3.18	121.59	111.90
19	A	1800	CLA	CHC-C1C-NC	3.18	129.66	123.67
19	1	1145	CLA	O2A-CGA-CBA	3.19	121.61	111.90
19	I	1031	CLA	CHC-C1C-NC	3.19	129.67	123.67
20	A	1811	LMU	C1B-O5B-C5B	3.19	119.93	113.75
19	4	1203	CLA	C3D-C4D-ND	3.19	112.96	110.13
19	1	1505	CLA	O2A-CGA-CBA	3.20	121.65	111.90
19	2	1223	CLA	CHC-C1C-NC	3.20	129.69	123.67
19	1	1198	CLA	C3D-C4D-ND	3.21	112.97	110.13
19	A	1797	CLA	C3A-C2A-C1A	3.21	106.94	101.50
19	2	1212	CLA	O2A-CGA-CBA	3.21	121.68	111.90
19	4	1199	CLA	CHB-C4A-NA	3.21	128.95	124.51
19	1	1192	CLA	O2A-CGA-CBA	3.21	121.69	111.90
19	B	1738	CLA	O2A-CGA-CBA	3.22	121.70	111.90
19	2	1222	CLA	CHB-C4A-NA	3.22	128.96	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1788	CLA	O2A-CGA-CBA	3.22	121.71	111.90
19	B	1754	CLA	CHB-C4A-NA	3.23	128.98	124.51
21	B	8062	SUC	O1-C2'-C3'	3.23	119.31	108.04
19	F	1155	CLA	CMB-C2B-C3B	3.23	131.75	125.14
20	A	7024	LMU	O1'-C1'-C2'	3.23	112.12	108.04
19	2	1222	CLA	O2A-CGA-CBA	3.24	121.76	111.90
19	B	1757	CLA	CHC-C1C-NC	3.24	129.76	123.67
19	B	1752	CLA	C4-C3-C5	3.24	120.35	115.41
19	A	1814	CLA	CHB-C4A-NA	3.24	128.99	124.51
23	A	1807	BCR	C33-C5-C4	3.24	119.57	113.43
19	1	1187	CLA	CAC-C3C-C4C	3.25	129.54	124.83
20	A	7024	LMU	C1B-O5B-C5B	3.25	120.04	113.75
19	2	1219	CLA	CHC-C1C-NC	3.25	129.78	123.67
19	1	1014	CLA	O2D-CGD-CBD	3.25	115.76	111.30
19	2	1213	CLA	CHB-C4A-NA	3.25	129.01	124.51
19	2	1220	CLA	C3D-C2D-C1D	3.26	109.17	106.30
19	B	1771	CLA	CHC-C1C-NC	3.26	129.80	123.67
19	A	1769	CLA	CHB-C4A-NA	3.26	129.02	124.51
19	R	1055	CLA	CHC-C1C-NC	3.26	129.80	123.67
19	4	1211	CLA	CHC-C1C-NC	3.26	129.81	123.67
19	B	1767	CLA	CHC-C1C-NC	3.27	129.82	123.67
19	1	1307	CLA	CHC-C1C-NC	3.27	129.62	123.78
19	3	1220	CLA	C3D-C2D-C1D	3.27	109.18	106.30
19	B	1756	CLA	CHC-C1C-NC	3.28	129.84	123.67
20	A	1810	LMU	C2'-C3'-C4'	3.28	116.80	109.60
19	A	1785	CLA	C4-C3-C5	3.28	120.41	115.41
19	B	1762	CLA	CHC-C1C-NC	3.28	129.84	123.67
19	2	1222	CLA	CHC-C1C-NC	3.28	129.85	123.67
19	B	1755	CLA	CHC-C1C-NC	3.28	129.85	123.67
19	R	1054	CLA	CED-O2D-CGD	3.28	123.69	115.99
19	4	1196	CLA	C4-C3-C5	3.29	120.43	115.41
19	1	1200	CLA	C3D-C2D-C1D	3.29	109.20	106.30
19	3	1222	CLA	C4-C3-C5	3.30	120.44	115.41
19	A	1786	CLA	O2A-CGA-CBA	3.30	121.95	111.90
19	1	1192	CLA	CHC-C1C-NC	3.30	129.88	123.67
23	B	1774	BCR	C33-C5-C4	3.30	119.68	113.43
20	A	7001	LMU	O5B-C5B-C6B	3.30	114.70	106.36
19	4	1197	CLA	CHC-C1C-NC	3.31	129.89	123.67
19	B	1753	CLA	CBA-CAA-C2A	3.31	123.07	113.73
19	B	1740	CLA	CHC-C1C-NC	3.31	129.70	123.78
19	1	1198	CLA	C3D-C2D-C1D	3.31	109.22	106.30
19	1	1196	CLA	CHC-C1C-NC	3.31	129.90	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1218	CLA	CAC-C3C-C4C	3.31	129.64	124.83
19	A	1777	CLA	CHC-C1C-NC	3.32	129.91	123.67
19	1	1190	CLA	CED-O2D-CGD	3.32	123.78	115.99
19	H	1081	CLA	CED-O2D-CGD	3.32	123.78	115.99
19	3	1222	CLA	O2A-CGA-CBA	3.33	122.04	111.90
19	A	1790	CLA	CHB-C4A-NA	3.33	129.12	124.51
19	A	1780	CLA	CHC-C1C-NC	3.33	129.95	123.67
19	1	1191	CLA	CHC-C1C-NC	3.34	129.95	123.67
19	B	1741	CLA	CHC-C1C-NC	3.34	129.95	123.67
19	4	1198	CLA	O2A-CGA-CBA	3.34	122.07	111.90
19	B	1735	CLA	CHC-C1C-NC	3.34	129.95	123.67
19	B	1770	CLA	O2A-CGA-CBA	3.34	122.07	111.90
20	A	7040	LMU	O1'-C1'-C2'	3.34	112.26	108.04
19	4	1205	CLA	O2A-CGA-CBA	3.34	122.08	111.90
19	A	1814	CLA	CHC-C1C-NC	3.34	129.96	123.67
19	A	1775	CLA	CHC-C1C-NC	3.35	129.97	123.67
19	2	1220	CLA	CHC-C1C-NC	3.35	129.76	123.78
20	A	7009	LMU	C2'-C3'-C4'	3.35	116.95	109.60
19	1	1194	CLA	C3D-C2D-C1D	3.35	109.25	106.30
19	1	1195	CLA	C3D-C4D-ND	3.35	113.10	110.13
19	1	1193	CLA	CHC-C1C-NC	3.35	129.97	123.67
23	A	1805	BCR	C33-C5-C4	3.35	119.78	113.43
20	A	7043	LMU	O5B-C1B-C2B	3.35	117.15	110.28
19	B	1750	CLA	CHC-C1C-NC	3.35	129.98	123.67
19	1	1505	CLA	CHC-C1C-NC	3.36	129.98	123.67
20	A	1810	LMU	C1B-O5B-C5B	3.36	120.26	113.75
19	B	1751	CLA	CHC-C1C-NC	3.36	129.99	123.67
19	B	1760	CLA	CHC-C1C-NC	3.36	129.99	123.67
20	A	7022	LMU	O1B-C4'-C3'	3.36	115.84	107.17
19	A	1774	CLA	O2A-CGA-CBA	3.36	122.14	111.90
19	1	1014	CLA	CED-O2D-CGD	3.36	123.88	115.99
19	3	1221	CLA	C4-C3-C5	3.37	120.55	115.41
19	A	1761	CLA	C4-C3-C5	3.37	120.55	115.41
19	B	1739	CLA	CHB-C4A-NA	3.37	129.17	124.51
19	B	1758	CLA	CHB-C4A-NA	3.37	129.17	124.51
19	1	1148	CLA	CHC-C1C-NC	3.38	130.02	123.67
20	A	7022	LMU	O1B-C1B-C2B	3.38	116.32	108.10
19	B	1743	CLA	CHC-C1C-NC	3.38	130.03	123.67
19	R	1054	CLA	O2A-CGA-CBA	3.38	122.20	111.90
19	2	2006	CLA	O2D-CGD-CBD	3.39	115.94	111.30
19	B	1751	CLA	CHB-C4A-NA	3.39	129.20	124.51
23	L	1169	BCR	C36-C18-C19	3.39	123.75	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	1079	CLA	CAA-C2A-C1A	3.40	124.45	112.47
19	A	1779	CLA	CHC-C1C-NC	3.40	130.07	123.67
19	B	1784	CLA	CHB-C4A-NA	3.41	129.22	124.51
19	4	1199	CLA	C4-C3-C5	3.41	120.61	115.41
19	2	1217	CLA	C4-C3-C5	3.41	120.61	115.41
20	A	7036	LMU	C1B-O5B-C5B	3.41	120.36	113.75
19	A	1798	CLA	CHC-C1C-NC	3.41	130.08	123.67
20	A	7043	LMU	C1'-C2'-C3'	3.41	116.69	109.97
19	A	1785	CLA	CHC-C1C-NC	3.41	130.09	123.67
19	4	1198	CLA	O2D-CGD-CBD	3.42	115.99	111.30
19	1	1142	CLA	CHC-C1C-NC	3.42	130.10	123.67
19	A	1796	CLA	O2A-CGA-CBA	3.42	122.32	111.90
19	A	1768	CLA	CHC-C1C-NC	3.42	130.11	123.67
19	2	1215	CLA	CHC-C1C-NC	3.42	130.11	123.67
19	A	1787	CLA	CHC-C1C-NC	3.43	130.12	123.67
20	A	7034	LMU	O1'-C1'-C2'	3.43	112.37	108.04
19	3	3015	CLA	C3D-C4D-ND	3.43	113.17	110.13
19	A	1770	CLA	C3D-C2D-C1D	3.43	109.32	106.30
19	H	1080	CLA	CHC-C1C-NC	3.43	130.13	123.67
20	A	7038	LMU	O1B-C4'-C3'	3.43	116.03	107.17
19	A	1773	CLA	CHC-C1C-NC	3.43	130.13	123.67
19	1	1192	CLA	C4-C3-C5	3.44	120.67	115.41
19	A	1771	CLA	O2A-CGA-CBA	3.44	122.39	111.90
19	I	1031	CLA	O2A-CGA-CBA	3.44	122.39	111.90
19	A	1815	CLA	CHC-C1C-NC	3.44	130.15	123.67
19	G	1099	CLA	CHC-C1C-NC	3.45	130.16	123.67
19	B	1737	CLA	O2A-CGA-CBA	3.45	122.41	111.90
19	R	1054	CLA	CHC-C1C-NC	3.45	130.16	123.67
19	B	1784	CLA	O2A-CGA-CBA	3.45	122.41	111.90
19	B	1744	CLA	CHC-C1C-NC	3.45	130.16	123.67
19	1	1188	CLA	CED-O2D-CGD	3.46	124.10	115.99
19	A	1816	CLA	CHC-C1C-NC	3.46	130.19	123.67
19	A	1816	CLA	CHB-C4A-NA	3.47	129.30	124.51
19	B	1765	CLA	CHC-C1C-NC	3.47	130.19	123.67
23	I	1032	BCR	C15-C14-C13	3.47	132.21	127.20
19	4	1202	CLA	CHC-C1C-NC	3.47	129.98	123.78
19	B	1764	CLA	CHC-C1C-NC	3.47	130.20	123.67
19	3	1219	CLA	C3D-C2D-C1D	3.47	109.36	106.30
23	B	1776	BCR	C8-C9-C10	3.47	124.58	118.98
19	A	1778	CLA	CAA-C2A-C1A	3.47	119.83	112.14
19	4	4014	CLA	CHB-C4A-NA	3.48	129.32	124.51
19	A	1765	CLA	O2A-CGA-CBA	3.48	122.49	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7030	LMU	O1B-C1B-C2B	3.48	116.57	108.10
20	A	7025	LMU	C1B-O5B-C5B	3.48	120.50	113.75
20	A	7026	LMU	O1B-C4'-C5'	3.48	118.47	109.32
20	A	7040	LMU	O1B-C1B-C2B	3.49	116.58	108.10
19	4	1208	CLA	C3D-C4D-ND	3.49	113.23	110.13
19	B	1758	CLA	O2A-CGA-CBA	3.49	122.54	111.90
21	B	8051	SUC	O5-C5-C4	3.49	116.24	109.68
19	A	1781	CLA	CHC-C1C-NC	3.49	130.25	123.67
19	L	1167	CLA	CHC-C1C-NC	3.49	130.25	123.67
19	A	1762	CLA	CHC-C1C-NC	3.50	130.25	123.67
19	A	1813	CLA	CED-O2D-CGD	3.50	124.19	115.99
20	A	7043	LMU	O5B-C5B-C4B	3.50	116.25	109.68
19	F	1157	CLA	CED-O2D-CGD	3.50	124.19	115.99
19	4	1210	CLA	CHC-C1C-NC	3.50	130.04	123.78
19	A	1792	CLA	CHC-C1C-NC	3.50	130.26	123.67
19	A	1783	CLA	O2A-CGA-CBA	3.50	122.57	111.90
19	B	1737	CLA	CHC-C1C-NC	3.51	130.27	123.67
20	4	1212	LMU	O1'-C1'-C2'	3.52	112.48	108.04
19	B	1739	CLA	O2A-CGA-CBA	3.52	122.61	111.90
19	1	1194	CLA	CHC-C1C-NC	3.52	130.07	123.78
19	4	1204	CLA	C3D-C2D-C1D	3.52	109.40	106.30
20	A	7030	LMU	O2B-C2B-C1B	3.52	117.74	110.02
19	A	1797	CLA	O2A-CGA-CBA	3.52	122.63	111.90
19	1	1014	CLA	CHB-C4A-NA	3.52	129.38	124.51
19	A	1771	CLA	CHC-C1C-NC	3.52	130.30	123.67
19	4	1200	CLA	CHC-C1C-NC	3.53	130.32	123.67
19	A	1814	CLA	CAA-C2A-C1A	3.54	124.94	112.47
20	A	7024	LMU	C2'-C3'-C4'	3.54	117.37	109.60
19	1	1146	CLA	O2A-CGA-CBA	3.54	122.69	111.90
19	B	1735	CLA	C4-C3-C5	3.54	120.82	115.41
19	R	1054	CLA	C4-C3-C5	3.55	120.83	115.41
19	3	3001	CLA	CHC-C1C-NC	3.55	130.13	123.78
19	B	1763	CLA	CHC-C1C-NC	3.56	130.37	123.67
19	B	1754	CLA	O2A-CGA-CBA	3.56	122.75	111.90
23	A	1804	BCR	C33-C5-C4	3.56	120.18	113.43
19	4	1196	CLA	CHC-C1C-NC	3.57	130.38	123.67
19	3	1222	CLA	CHC-C1C-NC	3.57	130.39	123.67
23	A	1808	BCR	C33-C5-C4	3.57	120.20	113.43
19	A	1790	CLA	CHC-C1C-NC	3.57	130.40	123.67
19	A	1817	CLA	CGD-CBD-CAD	3.57	122.74	110.62
19	B	1752	CLA	CHC-C1C-NC	3.58	130.40	123.67
20	A	7043	LMU	C1B-C2B-C3B	3.58	117.02	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1746	CLA	CHC-C1C-NC	3.58	130.41	123.67
19	1	1308	CLA	CHC-C1C-NC	3.58	130.41	123.67
20	A	7009	LMU	C1'-C2'-C3'	3.58	117.04	109.97
19	L	1167	CLA	CHB-C4A-NA	3.59	129.47	124.51
20	A	7020	LMU	C1B-C2B-C3B	3.59	117.05	109.97
20	A	7016	LMU	C2'-C3'-C4'	3.59	117.49	109.60
23	A	1803	BCR	C33-C5-C4	3.60	120.25	113.43
19	1	1193	CLA	CAA-CBA-CGA	3.60	123.85	113.32
19	A	1782	CLA	CHC-C1C-NC	3.60	130.44	123.67
20	A	7016	LMU	C1B-C2B-C3B	3.60	117.07	109.97
20	A	7034	LMU	C4B-C3B-C2B	3.61	117.53	110.79
19	4	1203	CLA	CHC-C1C-NC	3.61	130.23	123.78
20	A	7028	LMU	O1'-C1'-C2'	3.61	112.61	108.04
19	B	1746	CLA	CAC-C3C-C4C	3.62	130.08	124.83
19	B	1747	CLA	CHC-C1C-NC	3.62	130.48	123.67
20	A	1811	LMU	O5B-C1B-C2B	3.62	117.71	110.28
19	4	4007	CLA	O2D-CGD-CBD	3.62	116.27	111.30
19	B	1770	CLA	CHC-C1C-NC	3.62	130.49	123.67
19	A	1766	CLA	CHC-C1C-NC	3.63	130.49	123.67
19	B	1736	CLA	CHC-C1C-NC	3.63	130.50	123.67
19	1	1192	CLA	CAC-C3C-C4C	3.63	130.10	124.83
20	A	7001	LMU	C1B-C2B-C3B	3.63	117.14	109.97
19	4	1198	CLA	CED-O2D-CGD	3.64	124.53	115.99
19	B	1740	CLA	C3D-C2D-C1D	3.64	109.51	106.30
19	H	1079	CLA	CMB-C2B-C3B	3.65	132.22	125.09
19	4	1208	CLA	CHC-C1C-NC	3.65	130.30	123.78
19	3	1219	CLA	CHC-C1C-NC	3.65	130.31	123.78
19	1	1197	CLA	CHC-C1C-NC	3.66	130.56	123.67
19	B	1759	CLA	CHC-C1C-NC	3.66	130.56	123.67
20	A	7017	LMU	C4B-C3B-C2B	3.66	117.63	110.79
19	A	1788	CLA	CHC-C1C-NC	3.67	130.57	123.67
19	A	1770	CLA	CHC-C1C-NC	3.67	130.34	123.78
19	1	1195	CLA	C3D-C2D-C1D	3.67	109.53	106.30
19	3	3011	CLA	C4-C3-C5	3.69	121.04	115.41
19	A	1784	CLA	CHC-C1C-NC	3.69	130.61	123.67
19	B	1742	CLA	CHC-C1C-NC	3.69	130.61	123.67
19	B	1768	CLA	CHC-C1C-NC	3.69	130.61	123.67
19	4	1202	CLA	C3D-C4D-ND	3.69	113.41	110.13
19	A	1773	CLA	O2A-CGA-CBA	3.69	123.15	111.90
19	1	1145	CLA	CHC-C1C-NC	3.70	130.63	123.67
19	J	1043	CLA	O2A-CGA-CBA	3.71	123.19	111.90
19	2	1214	CLA	C3D-C4D-ND	3.71	113.42	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	1155	CLA	CHC-C1C-NC	3.71	130.65	123.67
19	A	1760	CLA	CHC-C1C-NC	3.72	130.67	123.67
20	A	7023	LMU	O1'-C1'-C2'	3.72	112.74	108.04
19	A	1814	CLA	O2A-CGA-CBA	3.72	123.25	111.90
19	A	1759	CLA	CHB-C4A-NA	3.73	129.67	124.51
20	A	7020	LMU	C1B-O5B-C5B	3.74	121.00	113.75
19	B	1740	CLA	C3D-C4D-ND	3.74	113.45	110.13
19	1	1146	CLA	CHB-C4A-NA	3.75	129.69	124.51
19	A	1786	CLA	CHC-C1C-NC	3.75	130.72	123.67
19	B	1739	CLA	CHC-C1C-NC	3.75	130.73	123.67
19	3	3001	CLA	C3D-C2D-C1D	3.75	109.61	106.30
20	4	1212	LMU	C1B-O5B-C5B	3.76	121.03	113.75
19	A	1794	CLA	CHC-C1C-NC	3.76	130.74	123.67
19	J	1043	CLA	CHB-C4A-NA	3.76	129.71	124.51
20	A	7017	LMU	C1'-O5'-C5'	3.77	121.05	113.75
19	B	1784	CLA	CHC-C1C-NC	3.77	130.76	123.67
20	A	7038	LMU	C1'-O5'-C5'	3.78	121.08	113.75
19	1	1309	CLA	CHC-C1C-NC	3.78	130.54	123.78
19	1	1149	CLA	O2A-CGA-CBA	3.78	123.42	111.90
19	A	1776	CLA	CHC-C1C-NC	3.79	130.80	123.67
19	A	1778	CLA	CHC-C1C-NC	3.80	130.82	123.67
19	B	1748	CLA	CHC-C1C-NC	3.80	130.82	123.67
20	A	7032	LMU	C2'-C3'-C4'	3.81	117.96	109.60
19	2	1212	CLA	CHC-C1C-NC	3.81	130.85	123.67
20	A	7021	LMU	O1'-C1'-C2'	3.83	112.87	108.04
20	A	7026	LMU	O1B-C4'-C3'	3.83	117.05	107.17
19	3	1218	CLA	CHC-C1C-NC	3.83	130.88	123.67
20	A	7015	LMU	C1B-C2B-C3B	3.83	117.52	109.97
19	2	1213	CLA	CHC-C1C-NC	3.84	130.89	123.67
19	B	1762	CLA	C4-C3-C5	3.84	121.27	115.41
19	1	1149	CLA	CBA-CAA-C2A	3.84	124.57	113.73
19	4	1202	CLA	C3D-C2D-C1D	3.85	109.69	106.30
19	1	1143	CLA	CHC-C1C-NC	3.85	130.92	123.67
20	B	1782	LMU	O1'-C1'-C2'	3.86	112.91	108.04
19	1	1188	CLA	CHC-C1C-NC	3.86	130.93	123.67
19	A	1780	CLA	C4-C3-C5	3.86	121.30	115.41
19	2	1216	CLA	CHC-C1C-NC	3.86	130.68	123.78
19	A	1799	CLA	C3D-C2D-C1D	3.86	109.70	106.30
19	1	1189	CLA	CHC-C1C-NC	3.87	130.95	123.67
20	A	7033	LMU	O5'-C1'-C2'	3.87	118.22	110.28
23	I	1032	BCR	C15-C16-C17	3.87	131.95	123.39
19	1	1198	CLA	CHC-C1C-NC	3.87	130.71	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1772	CLA	C4-C3-C5	3.87	121.32	115.41
19	3	1216	CLA	CHC-C1C-NC	3.88	130.71	123.78
23	B	1779	BCR	C34-C9-C8	3.88	124.55	118.10
19	B	1761	CLA	CHC-C1C-NC	3.88	130.98	123.67
19	H	1079	CLA	O2A-CGA-CBA	3.88	123.74	111.90
20	A	7024	LMU	O5B-C1B-C2B	3.89	118.25	110.28
19	3	1212	CLA	CHC-C1C-NC	3.89	130.74	123.78
19	B	1738	CLA	CHB-C4A-NA	3.91	129.91	124.51
19	H	1079	CLA	CHB-C4A-NA	3.92	129.93	124.51
19	3	3015	CLA	CHC-C1C-NC	3.92	130.79	123.78
19	A	1817	CLA	CHB-C4A-NA	3.92	129.94	124.51
20	A	7014	LMU	O1'-C1'-C2'	3.92	113.00	108.04
23	A	1807	BCR	C38-C26-C27	3.92	120.87	113.43
19	4	1205	CLA	CED-O2D-CGD	3.93	125.21	115.99
20	A	7033	LMU	C3B-C4B-C5B	3.94	117.06	110.20
20	A	7023	LMU	C2'-C3'-C4'	3.94	118.25	109.60
19	2	2010	CLA	CHC-C1C-NC	3.94	130.82	123.78
19	4	4014	CLA	CHC-C1C-NC	3.94	131.08	123.67
19	3	3014	CLA	C3D-C4D-ND	3.94	113.62	110.13
19	4	1207	CLA	CHC-C1C-NC	3.95	130.84	123.78
19	4	1204	CLA	CHC-C1C-NC	3.96	130.85	123.78
20	A	7047	LMU	O1B-C4'-C5'	3.96	119.74	109.32
22	A	1802	PQN	C14-C13-C15	3.98	121.49	115.41
19	1	1307	CLA	C3D-C2D-C1D	3.99	109.81	106.30
19	1	1200	CLA	CHC-C1C-NC	3.99	130.92	123.78
19	A	1774	CLA	CHC-C1C-NC	3.99	131.18	123.67
20	A	7009	LMU	O5B-C5B-C4B	3.99	117.18	109.68
19	4	4007	CLA	CHB-C4A-NA	4.00	130.04	124.51
19	B	1766	CLA	CHC-C1C-NC	4.00	131.21	123.67
19	1	1149	CLA	CHC-C1C-NC	4.00	131.21	123.67
19	A	1767	CLA	CHC-C1C-NC	4.01	131.21	123.67
19	2	1217	CLA	O2A-CGA-CBA	4.01	124.13	111.90
19	1	1145	CLA	CHB-C4A-NA	4.02	130.07	124.51
19	3	3014	CLA	CHC-C1C-NC	4.03	130.98	123.78
19	A	1799	CLA	CHC-C1C-NC	4.03	130.99	123.78
19	J	1043	CLA	CHC-C1C-NC	4.04	131.27	123.67
19	3	1217	CLA	CAC-C3C-C4C	4.04	130.69	124.83
20	A	7004	LMU	O1'-C1'-C2'	4.04	113.15	108.04
19	3	1220	CLA	CHC-C1C-NC	4.04	131.01	123.78
20	A	7013	LMU	O1B-C4'-C3'	4.05	117.62	107.17
20	A	7039	LMU	O1B-C1B-C2B	4.06	117.97	108.10
19	B	1756	CLA	C4-C3-C5	4.06	121.60	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	7021	LMU	C1B-O5B-C5B	4.06	121.62	113.75
19	B	1768	CLA	C4-C3-C5	4.06	121.61	115.41
19	A	1817	CLA	CHC-C1C-NC	4.06	131.31	123.67
19	A	1798	CLA	C4-C3-C5	4.06	121.61	115.41
19	4	1196	CLA	CED-O2D-CGD	4.07	125.53	115.99
19	2	1214	CLA	CHC-C1C-NC	4.07	131.06	123.78
19	1	1200	CLA	C3D-C4D-ND	4.07	113.74	110.13
20	A	7043	LMU	C1B-O5B-C5B	4.07	121.65	113.75
19	A	1793	CLA	CHC-C1C-NC	4.08	131.34	123.67
19	B	1757	CLA	O2A-CGA-CBA	4.09	124.36	111.90
20	A	7027	LMU	O1'-C1'-C2'	4.10	113.21	108.04
19	2	1218	CLA	CHC-C1C-NC	4.10	131.11	123.78
19	3	3014	CLA	C3D-C2D-C1D	4.11	109.92	106.30
20	A	1811	LMU	O1'-C1'-C2'	4.12	113.24	108.04
19	A	1799	CLA	C3D-C4D-ND	4.12	113.78	110.13
19	3	1215	CLA	CHC-C1C-NC	4.12	131.14	123.78
19	A	1787	CLA	C4-C3-C5	4.13	121.72	115.41
19	B	1738	CLA	CHC-C1C-NC	4.14	131.47	123.67
19	A	1791	CLA	CHC-C1C-NC	4.16	131.50	123.67
19	2	2006	CLA	CHC-C1C-NC	4.17	131.52	123.67
19	1	1199	CLA	CHC-C1C-NC	4.17	131.52	123.67
19	A	1759	CLA	CHC-C1C-NC	4.17	131.52	123.67
19	A	1761	CLA	CHC-C1C-NC	4.17	131.52	123.67
19	A	1795	CLA	CHC-C1C-NC	4.17	131.52	123.67
19	1	1187	CLA	CHC-C1C-NC	4.17	131.53	123.67
19	1	1309	CLA	C3D-C2D-C1D	4.18	109.98	106.30
20	A	7038	LMU	C1B-O5B-C5B	4.18	121.86	113.75
19	1	1197	CLA	CBA-CAA-C2A	4.18	125.53	113.73
20	A	7019	LMU	C2'-C3'-C4'	4.19	118.80	109.60
19	4	1199	CLA	CHC-C1C-NC	4.20	131.57	123.67
19	B	1771	CLA	O2D-CGD-CBD	4.20	117.07	111.30
19	B	1769	CLA	CHC-C1C-NC	4.21	131.59	123.67
19	1	1190	CLA	CHC-C1C-NC	4.21	131.60	123.67
19	1	1146	CLA	CHC-C1C-NC	4.22	131.60	123.67
19	2	1223	CLA	C4-C3-C5	4.22	121.85	115.41
19	B	1771	CLA	O2A-CGA-CBA	4.26	124.87	111.90
19	4	4007	CLA	CHC-C1C-NC	4.26	131.68	123.67
21	2	1225	SUC	C1-C2-C3	4.26	118.38	109.97
19	2	1212	CLA	CGD-CBD-CAD	4.28	125.13	110.62
19	A	1769	CLA	CHC-C1C-NC	4.31	131.78	123.67
19	1	1193	CLA	CAA-C2A-C3A	4.31	125.61	113.22
19	1	1149	CLA	C3A-C2A-C1A	4.31	108.81	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1781	LMG	O7-C10-C11	4.33	120.93	111.53
19	4	1200	CLA	O2A-CGA-CBA	4.35	125.15	111.90
19	1	1187	CLA	CHB-C4A-NA	4.35	130.53	124.51
19	4	1210	CLA	C2B-C1B-NB	4.35	114.00	110.09
19	R	1055	CLA	O2A-CGA-CBA	4.36	125.17	111.90
19	H	1079	CLA	CHC-C1C-NC	4.36	131.87	123.67
19	4	1208	CLA	C3D-C2D-C1D	4.36	110.14	106.30
19	2	1217	CLA	CHC-C1C-NC	4.36	131.88	123.67
20	A	7009	LMU	C3B-C4B-C5B	4.37	117.82	110.20
19	A	1765	CLA	CHC-C1C-NC	4.38	131.92	123.67
23	A	1808	BCR	C36-C18-C19	4.40	125.41	118.10
23	B	1775	BCR	C38-C26-C27	4.40	121.77	113.43
20	A	7016	LMU	O1'-C1'-C2'	4.41	113.61	108.04
19	4	1201	CLA	O2A-CGA-CBA	4.41	125.34	111.90
19	1	1505	CLA	C4-C3-C5	4.41	122.15	115.41
19	4	1201	CLA	C3A-C2A-C1A	4.42	109.00	101.50
19	2	1221	CLA	CHC-C1C-NC	4.44	132.02	123.67
20	L	1170	LMU	C3B-C4B-C5B	4.44	117.94	110.20
19	A	1770	CLA	C3D-C4D-ND	4.48	114.11	110.13
19	3	1214	CLA	CHC-C1C-NC	4.49	131.81	123.78
23	A	1808	BCR	C8-C9-C10	4.50	126.23	118.98
19	4	1201	CLA	O2D-CGD-CBD	4.53	117.52	111.30
19	A	1789	CLA	CHC-C1C-NC	4.56	132.24	123.67
19	A	1797	CLA	CHC-C1C-NC	4.58	132.28	123.67
21	B	8061	SUC	C1-O5-C5	4.59	122.65	113.75
19	1	1309	CLA	C3D-C4D-ND	4.60	114.21	110.13
19	B	1752	CLA	O2D-CGD-CBD	4.60	117.61	111.30
19	4	4014	CLA	CAA-C2A-C1A	4.63	128.81	112.47
23	I	1032	BCR	C7-C8-C9	4.63	133.28	126.22
19	2	1216	CLA	C2B-C1B-NB	4.67	114.28	110.09
19	A	1760	CLA	O2A-CGA-CBA	4.67	126.14	111.90
21	B	8051	SUC	C1-O5-C5	4.68	122.82	113.75
19	1	1145	CLA	O2D-CGD-CBD	4.70	117.75	111.30
19	3	3011	CLA	CHC-C1C-NC	4.71	132.53	123.67
19	4	1201	CLA	CHC-C1C-NC	4.71	132.54	123.67
19	A	1767	CLA	O2D-CGD-CBD	4.73	117.79	111.30
19	4	1205	CLA	CHC-C1C-NC	4.74	132.59	123.67
19	2	2010	CLA	C2B-C1B-NB	4.74	114.35	110.09
19	B	1737	CLA	O2D-CGD-CBD	4.76	117.83	111.30
19	3	1220	CLA	C3D-C4D-ND	4.82	114.41	110.13
19	4	1198	CLA	CHC-C1C-NC	4.84	132.78	123.67
19	A	1761	CLA	O2D-CGD-CBD	4.85	117.95	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1779	CLA	O2D-CGD-CBD	4.85	117.96	111.30
23	I	1032	BCR	C38-C26-C27	4.86	122.64	113.43
20	A	7026	LMU	O1B-C1B-C2B	4.87	119.95	108.10
20	A	7021	LMU	O1B-C4'-C3'	4.88	119.75	107.17
23	A	1807	BCR	C23-C22-C21	4.91	126.89	118.98
19	1	1188	CLA	O2D-CGD-CBD	4.92	118.05	111.30
21	B	8062	SUC	O1-C1-C2	5.03	125.14	108.36
20	A	7035	LMU	O1B-C4'-C3'	5.05	120.22	107.17
20	A	7015	LMU	O1'-C1'-C2'	5.07	114.44	108.04
20	A	7032	LMU	C1B-O5B-C5B	5.07	123.58	113.75
20	A	7026	LMU	O5'-C5'-C6'	5.09	119.22	106.36
19	1	1197	CLA	O2A-CGA-CBA	5.14	127.55	111.90
19	1	1199	CLA	C4-C3-C5	5.15	121.51	115.68
19	4	1197	CLA	CBD-CHA-C1A	5.15	130.95	128.59
23	I	1032	BCR	C8-C9-C10	5.15	127.29	118.98
19	2	1220	CLA	C2B-C1B-NB	5.20	114.75	110.09
19	B	1784	CLA	O2D-CGD-CBD	5.20	118.44	111.30
19	4	1206	CLA	O2D-CGD-CBD	5.20	118.44	111.30
19	B	1740	CLA	C2B-C1B-NB	5.25	114.80	110.09
19	B	1766	CLA	C4-C3-C5	5.30	121.68	115.68
19	2	1215	CLA	O2D-CGD-CBD	5.32	118.59	111.30
19	3	1217	CLA	CHC-C1C-NC	5.33	133.69	123.67
19	3	1216	CLA	C2B-C1B-NB	5.33	114.88	110.09
19	A	1817	CLA	O2D-CGD-CBD	5.33	118.62	111.30
19	4	1208	CLA	C2B-C1B-NB	5.37	114.91	110.09
19	3	1218	CLA	C4-C3-C5	5.43	123.69	115.41
19	3	1215	CLA	C2B-C1B-NB	5.46	114.99	110.09
19	R	1055	CLA	O2D-CGD-CBD	5.46	118.79	111.30
19	3	1217	CLA	O2D-CGD-CBD	5.46	118.80	111.30
20	A	7014	LMU	O2B-C2B-C3B	5.48	122.67	110.34
19	B	1743	CLA	O2D-CGD-CBD	5.49	118.83	111.30
20	A	7030	LMU	C1B-O5B-C5B	5.49	124.41	113.75
19	A	1783	CLA	O2D-CGD-CBD	5.51	118.85	111.30
19	4	1201	CLA	CAA-C2A-C1A	5.52	131.93	112.47
20	A	7014	LMU	O1B-C1B-C2B	5.53	121.55	108.10
19	J	1043	CLA	O2D-CGD-CBD	5.56	118.92	111.30
19	A	1789	CLA	C4-C3-C5	5.56	123.90	115.41
20	A	7001	LMU	O1'-C1'-C2'	5.57	115.08	108.04
19	1	1198	CLA	C2B-C1B-NB	5.60	115.12	110.09
19	3	1212	CLA	C2B-C1B-NB	5.61	115.12	110.09
19	1	1149	CLA	CAA-C2A-C3A	5.61	129.36	113.22
19	4	1204	CLA	C2B-C1B-NB	5.62	115.13	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1207	CLA	C2B-C1B-NB	5.63	115.14	110.09
19	1	1307	CLA	C2B-C1B-NB	5.66	115.17	110.09
21	B	8062	SUC	C6-C5-C4	5.67	127.01	113.02
19	2	1214	CLA	C2B-C1B-NB	5.68	115.19	110.09
19	3	3015	CLA	C2B-C1B-NB	5.69	115.19	110.09
19	A	1771	CLA	O2D-CGD-CBD	5.69	119.11	111.30
19	1	1194	CLA	C2B-C1B-NB	5.73	115.23	110.09
19	B	1755	CLA	O2D-CGD-CBD	5.75	119.19	111.30
19	A	1788	CLA	O2D-CGD-CBD	5.75	119.19	111.30
19	F	1156	CLA	O2D-CGD-CBD	5.77	119.21	111.30
19	3	3014	CLA	C2B-C1B-NB	5.77	115.27	110.09
19	B	1744	CLA	O2D-CGD-CBD	5.77	119.22	111.30
19	1	1505	CLA	O2D-CGD-CBD	5.78	119.23	111.30
19	A	1816	CLA	C4-C3-C5	5.82	124.30	115.41
19	1	1190	CLA	O2D-CGD-CBD	5.82	119.28	111.30
19	A	1768	CLA	O2D-CGD-CBD	5.83	119.30	111.30
19	B	1764	CLA	O2D-CGD-CBD	5.86	119.34	111.30
20	2	1224	LMU	O1'-C1'-C2'	5.87	115.45	108.04
19	3	1214	CLA	C2B-C1B-NB	5.89	115.37	110.09
19	A	1780	CLA	O2D-CGD-CBD	5.90	119.39	111.30
19	A	1760	CLA	O2D-CGD-CBD	5.91	119.41	111.30
19	A	1795	CLA	O2D-CGD-CBD	5.92	119.43	111.30
19	A	1769	CLA	O2D-CGD-CBD	5.93	119.44	111.30
20	A	7011	LMU	O1'-C1'-C2'	5.95	115.56	108.04
19	1	1143	CLA	O2D-CGD-CBD	5.96	119.47	111.30
19	3	3001	CLA	C2B-C1B-NB	5.96	115.44	110.09
19	4	1200	CLA	O2D-CGD-CBD	5.97	119.50	111.30
19	B	1742	CLA	O2D-CGD-CBD	5.98	119.50	111.30
19	A	1776	CLA	O2D-CGD-CBD	6.01	119.54	111.30
19	B	1753	CLA	O2D-CGD-CBD	6.03	119.58	111.30
19	1	1197	CLA	O2D-CGD-CBD	6.07	119.63	111.30
19	1	1193	CLA	O2D-CGD-CBD	6.10	119.67	111.30
19	4	1202	CLA	C2B-C1B-NB	6.13	115.59	110.09
19	A	1814	CLA	O2D-CGD-CBD	6.15	119.74	111.30
19	1	1189	CLA	O2D-CGD-CBD	6.20	119.81	111.30
19	R	1054	CLA	O2D-CGD-CBD	6.22	119.84	111.30
19	2	1218	CLA	C2B-C1B-NB	6.23	115.68	110.09
19	B	1750	CLA	O2D-CGD-CBD	6.23	119.85	111.30
19	A	1790	CLA	O2D-CGD-CBD	6.33	119.98	111.30
19	B	1745	CLA	O2D-CGD-CBD	6.34	119.99	111.30
19	1	1309	CLA	C2B-C1B-NB	6.37	115.80	110.09
19	2	1221	CLA	O2D-CGD-CBD	6.38	120.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1770	CLA	O2D-CGD-CBD	6.44	120.13	111.30
19	4	1198	CLA	CGD-CBD-CAD	6.48	132.57	110.62
19	1	1195	CLA	C2B-C1B-NB	6.48	115.91	110.09
19	1	1200	CLA	C2B-C1B-NB	6.52	115.94	110.09
19	3	1219	CLA	C2B-C1B-NB	6.55	115.96	110.09
19	A	1799	CLA	C2B-C1B-NB	6.58	115.99	110.09
19	A	1815	CLA	O2D-CGD-CBD	6.59	120.34	111.30
19	1	1142	CLA	O2D-CGD-CBD	6.61	120.37	111.30
19	B	1735	CLA	O2D-CGD-CBD	6.62	120.39	111.30
19	3	1220	CLA	C2B-C1B-NB	6.63	116.04	110.09
19	A	1764	CLA	O2D-CGD-CBD	6.65	120.43	111.30
19	3	3011	CLA	O2D-CGD-CBD	6.66	120.43	111.30
19	I	1031	CLA	O2D-CGD-CBD	6.67	120.45	111.30
19	B	1747	CLA	O2D-CGD-CBD	6.68	120.47	111.30
19	B	1751	CLA	O2D-CGD-CBD	6.70	120.49	111.30
19	1	1146	CLA	O2D-CGD-CBD	6.71	120.51	111.30
19	B	1760	CLA	O2D-CGD-CBD	6.72	120.51	111.30
19	A	1770	CLA	C2B-C1B-NB	6.72	116.12	110.09
19	2	1222	CLA	O2D-CGD-CBD	6.76	120.57	111.30
19	1	1199	CLA	CAA-C2A-C1A	6.76	136.32	112.47
19	1	1308	CLA	O2D-CGD-CBD	6.77	120.58	111.30
19	B	1756	CLA	O2D-CGD-CBD	6.78	120.60	111.30
19	A	1772	CLA	O2D-CGD-CBD	6.78	120.61	111.30
19	3	3008	CLA	O2D-CGD-CBD	6.80	120.63	111.30
19	A	1796	CLA	O2D-CGD-CBD	6.81	120.65	111.30
19	A	1792	CLA	O2D-CGD-CBD	6.86	120.72	111.30
19	1	1192	CLA	O2D-CGD-CBD	6.89	120.75	111.30
19	A	1762	CLA	O2D-CGD-CBD	6.90	120.77	111.30
19	A	1782	CLA	O2D-CGD-CBD	6.91	120.79	111.30
19	1	1193	CLA	C3A-C2A-C1A	6.92	113.24	101.50
19	A	1791	CLA	O2D-CGD-CBD	6.96	120.85	111.30
19	4	1203	CLA	C2B-C1B-NB	6.96	116.34	110.09
19	B	1748	CLA	O2D-CGD-CBD	6.97	120.86	111.30
19	A	1787	CLA	O2D-CGD-CBD	7.01	120.91	111.30
19	A	1816	CLA	O2D-CGD-CBD	7.03	120.94	111.30
19	B	1765	CLA	O2D-CGD-CBD	7.04	120.96	111.30
19	A	1773	CLA	O2D-CGD-CBD	7.09	121.03	111.30
19	A	1800	CLA	O2D-CGD-CBD	7.10	121.05	111.30
19	1	1148	CLA	O2D-CGD-CBD	7.13	121.08	111.30
19	A	1781	CLA	O2D-CGD-CBD	7.14	121.09	111.30
19	3	1222	CLA	O2D-CGD-CBD	7.22	121.21	111.30
19	A	1801	CLA	O2D-CGD-CBD	7.35	121.38	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1763	CLA	O2D-CGD-CBD	7.39	121.43	111.30
19	2	1212	CLA	O2D-CGD-CBD	7.39	121.44	111.30
19	F	1155	CLA	CBD-CHA-C1A	7.43	131.99	128.59
19	4	1211	CLA	O2D-CGD-CBD	7.44	121.51	111.30
19	B	1741	CLA	O2D-CGD-CBD	7.45	121.51	111.30
19	A	1789	CLA	O2D-CGD-CBD	7.45	121.52	111.30
19	A	1765	CLA	O2D-CGD-CBD	7.49	121.58	111.30
19	A	1766	CLA	O2D-CGD-CBD	7.55	121.65	111.30
19	B	1763	CLA	O2D-CGD-CBD	7.60	121.72	111.30
19	1	1199	CLA	O2D-CGD-CBD	7.62	121.76	111.30
19	B	1746	CLA	O2D-CGD-CBD	7.62	121.76	111.30
19	H	1080	CLA	O2D-CGD-CBD	7.67	121.83	111.30
19	1	1187	CLA	O2D-CGD-CBD	7.72	121.89	111.30
19	A	1777	CLA	O2D-CGD-CBD	7.75	121.94	111.30
19	1	1149	CLA	O2D-CGD-CBD	7.76	121.94	111.30
19	L	1167	CLA	O2D-CGD-CBD	7.80	122.00	111.30
19	2	1223	CLA	O2D-CGD-CBD	7.81	122.02	111.30
19	F	1157	CLA	O2D-CGD-CBD	7.81	122.02	111.30
19	B	1762	CLA	O2D-CGD-CBD	7.85	122.08	111.30
19	B	1757	CLA	O2D-CGD-CBD	7.86	122.09	111.30
19	H	1079	CLA	O2D-CGD-CBD	7.92	122.16	111.30
19	4	1205	CLA	O2D-CGD-CBD	7.92	122.17	111.30
19	A	1774	CLA	O2D-CGD-CBD	7.97	122.23	111.30
19	H	1081	CLA	O2D-CGD-CBD	8.06	122.36	111.30
19	B	1749	CLA	O2D-CGD-CBD	8.12	122.44	111.30
19	A	1785	CLA	O2D-CGD-CBD	8.12	122.45	111.30
19	A	1786	CLA	O2D-CGD-CBD	8.18	122.53	111.30
19	A	1798	CLA	O2D-CGD-CBD	8.22	122.58	111.30
19	B	1736	CLA	O2D-CGD-CBD	8.33	122.73	111.30
19	A	1797	CLA	O2D-CGD-CBD	8.39	122.80	111.30
19	A	1775	CLA	CBD-CHA-C1A	8.41	132.44	128.59
19	B	1754	CLA	O2D-CGD-CBD	8.47	122.92	111.30
19	1	1196	CLA	CBD-CHA-C1A	8.48	132.47	128.59
19	4	1199	CLA	O2D-CGD-CBD	8.49	122.95	111.30
19	B	1738	CLA	O2D-CGD-CBD	8.53	123.01	111.30
19	A	1794	CLA	O2D-CGD-CBD	8.57	123.06	111.30
19	B	1768	CLA	O2D-CGD-CBD	8.59	123.09	111.30
19	2	1217	CLA	O2D-CGD-CBD	8.69	123.22	111.30
19	2	1213	CLA	O2D-CGD-CBD	8.71	123.25	111.30
19	B	1759	CLA	O2D-CGD-CBD	8.71	123.25	111.30
19	A	1793	CLA	O2D-CGD-CBD	8.72	123.26	111.30
19	B	1767	CLA	O2D-CGD-CBD	8.81	123.39	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	1213	CLA	CBD-CHA-C1A	8.96	132.69	128.59
19	B	1758	CLA	O2D-CGD-CBD	8.97	123.60	111.30
19	G	1099	CLA	O2D-CGD-CBD	8.98	123.62	111.30
20	A	7008	LMU	O1'-C1'-C2'	9.00	119.41	108.04
19	3	1221	CLA	O2D-CGD-CBD	9.04	123.70	111.30
19	B	1761	CLA	O2D-CGD-CBD	9.04	123.70	111.30
19	B	1766	CLA	O2D-CGD-CBD	9.05	123.72	111.30
19	3	1218	CLA	O2D-CGD-CBD	9.28	124.03	111.30
19	B	1769	CLA	O2D-CGD-CBD	9.53	124.38	111.30
19	A	1778	CLA	O2D-CGD-CBD	9.70	124.60	111.30
19	A	1784	CLA	O2D-CGD-CBD	9.73	124.65	111.30
19	B	1739	CLA	O2D-CGD-CBD	9.88	124.86	111.30
19	4	4014	CLA	O2D-CGD-CBD	9.89	124.87	111.30
23	A	1807	BCR	C21-C20-C19	9.94	153.42	123.13
19	B	1772	CLA	CBD-CHA-C1A	10.15	133.24	128.59
19	A	1759	CLA	O2D-CGD-CBD	10.21	125.31	111.30
19	1	1191	CLA	CBD-CHA-C1A	10.23	133.28	128.59
19	L	1168	CLA	O2D-CGD-CBD	11.15	126.60	111.30
19	2	1219	CLA	CBD-CHA-C1A	11.20	133.72	128.59
19	4	1209	CLA	CBD-CHA-C1A	11.29	133.76	128.59
19	A	1774	CLA	C3B-CAB-CBB	14.12	155.21	126.32
23	B	1775	BCR	C21-C20-C19	14.82	168.29	123.13
23	B	1776	BCR	C21-C20-C19	14.89	168.52	123.13
19	4	1205	CLA	C3B-CAB-CBB	15.15	157.31	126.32
19	3	1221	CLA	C3B-CAB-CBB	15.50	158.04	126.32
23	A	1804	BCR	C21-C20-C19	16.02	171.97	123.13
19	1	1014	CLA	C3B-CAB-CBB	16.06	159.18	126.32
23	A	1803	BCR	C21-C20-C19	16.87	174.54	123.13
19	G	1099	CLA	C3B-CAB-CBB	17.15	161.41	126.32
23	B	1779	BCR	C21-C20-C19	17.28	175.80	123.13
23	A	1806	BCR	C21-C20-C19	17.31	175.90	123.13
23	B	1777	BCR	C21-C20-C19	17.34	175.98	123.13
23	B	1778	BCR	C21-C20-C19	17.54	176.60	123.13
19	A	1761	CLA	C3B-CAB-CBB	17.63	162.39	126.32
23	A	1808	BCR	C21-C20-C19	17.65	176.93	123.13
23	A	1809	BCR	C21-C20-C19	17.80	177.39	123.13
23	I	1032	BCR	C21-C20-C19	17.92	177.76	123.13
23	B	1774	BCR	C21-C20-C19	17.95	177.84	123.13
23	L	1169	BCR	C21-C20-C19	17.97	177.89	123.13
23	B	1780	BCR	C21-C20-C19	18.07	178.22	123.13
23	A	1805	BCR	C21-C20-C19	18.12	178.37	123.13
19	4	1201	CLA	C3B-CAB-CBB	18.44	164.05	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1782	CLA	C3B-CAB-CBB	18.87	164.94	126.32
19	A	1785	CLA	C3B-CAB-CBB	19.35	165.90	126.32
19	F	1157	CLA	C3B-CAB-CBB	19.99	167.22	126.32
19	B	1768	CLA	C3B-CAB-CBB	20.21	167.67	126.32
19	B	1746	CLA	C3B-CAB-CBB	20.25	167.75	126.32
23	A	1807	BCR	C20-C21-C22	20.27	156.47	127.20
19	B	1770	CLA	C3B-CAB-CBB	20.28	167.81	126.32
19	A	1764	CLA	C3B-CAB-CBB	20.33	167.91	126.32
19	A	1789	CLA	C3B-CAB-CBB	20.34	167.94	126.32
19	4	1199	CLA	C3B-CAB-CBB	20.45	168.16	126.32
19	B	1763	CLA	C3B-CAB-CBB	20.66	168.59	126.32
19	A	1797	CLA	C3B-CAB-CBB	20.69	168.65	126.32
19	A	1760	CLA	C3B-CAB-CBB	20.79	168.85	126.32
19	B	1784	CLA	C3B-CAB-CBB	20.84	168.96	126.32
19	2	1217	CLA	C3B-CAB-CBB	20.87	169.02	126.32
19	B	1771	CLA	C3B-CAB-CBB	21.24	169.78	126.32
19	A	1780	CLA	C3B-CAB-CBB	21.26	169.82	126.32
19	3	1218	CLA	C3B-CAB-CBB	21.34	169.98	126.32
19	A	1779	CLA	C3B-CAB-CBB	21.36	170.02	126.32
19	4	1198	CLA	C3B-CAB-CBB	21.39	170.08	126.32
19	A	1772	CLA	C3B-CAB-CBB	21.39	170.08	126.32
19	A	1765	CLA	C3B-CAB-CBB	21.49	170.28	126.32
19	B	1737	CLA	C3B-CAB-CBB	21.65	170.61	126.32
19	A	1796	CLA	C3B-CAB-CBB	21.77	170.87	126.32
19	1	1192	CLA	C3B-CAB-CBB	21.82	170.96	126.32
19	B	1736	CLA	C3B-CAB-CBB	21.82	170.97	126.32
19	A	1778	CLA	C3B-CAB-CBB	21.83	170.99	126.32
19	B	1758	CLA	C3B-CAB-CBB	21.84	171.00	126.32
19	B	1759	CLA	C3B-CAB-CBB	21.84	171.01	126.32
19	A	1759	CLA	C3B-CAB-CBB	21.88	171.08	126.32
19	B	1743	CLA	C3B-CAB-CBB	21.99	171.30	126.32
19	B	1745	CLA	C3B-CAB-CBB	21.99	171.31	126.32
19	A	1776	CLA	C3B-CAB-CBB	22.00	171.32	126.32
19	2	1215	CLA	C3B-CAB-CBB	22.01	171.34	126.32
19	H	1079	CLA	C3B-CAB-CBB	22.15	171.65	126.32
19	B	1757	CLA	C3B-CAB-CBB	22.20	171.74	126.32
19	A	1767	CLA	C3B-CAB-CBB	22.21	171.75	126.32
19	A	1768	CLA	C3B-CAB-CBB	22.24	171.83	126.32
19	2	1213	CLA	C3B-CAB-CBB	22.31	171.96	126.32
19	B	1762	CLA	C3B-CAB-CBB	22.32	171.99	126.32
19	A	1784	CLA	C3B-CAB-CBB	22.38	172.10	126.32
19	3	3011	CLA	C3B-CAB-CBB	22.41	172.18	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1765	CLA	C3B-CAB-CBB	22.42	172.20	126.32
19	4	4014	CLA	C3B-CAB-CBB	22.43	172.22	126.32
19	2	1222	CLA	C3B-CAB-CBB	22.54	172.43	126.32
19	A	1777	CLA	C3B-CAB-CBB	22.64	172.65	126.32
19	A	1781	CLA	C3B-CAB-CBB	22.65	172.66	126.32
19	1	1199	CLA	C3B-CAB-CBB	22.72	172.81	126.32
19	B	1748	CLA	C3B-CAB-CBB	22.74	172.84	126.32
19	2	1221	CLA	C3B-CAB-CBB	22.76	172.88	126.32
19	1	1188	CLA	C3B-CAB-CBB	22.79	172.95	126.32
19	B	1760	CLA	C3B-CAB-CBB	22.80	172.97	126.32
19	A	1769	CLA	C3B-CAB-CBB	22.91	173.20	126.32
19	1	1146	CLA	C3B-CAB-CBB	22.93	173.23	126.32
19	B	1742	CLA	C3B-CAB-CBB	22.94	173.26	126.32
19	1	1193	CLA	C3B-CAB-CBB	22.95	173.27	126.32
19	2	1212	CLA	C3B-CAB-CBB	23.02	173.43	126.32
19	A	1763	CLA	C3B-CAB-CBB	23.14	173.66	126.32
19	B	1756	CLA	C3B-CAB-CBB	23.14	173.66	126.32
19	A	1800	CLA	C3B-CAB-CBB	23.17	173.72	126.32
19	B	1766	CLA	C3B-CAB-CBB	23.28	173.95	126.32
19	4	1211	CLA	C3B-CAB-CBB	23.29	173.97	126.32
19	A	1793	CLA	C3B-CAB-CBB	23.32	174.03	126.32
19	B	1735	CLA	C3B-CAB-CBB	23.33	174.04	126.32
19	A	1816	CLA	C3B-CAB-CBB	23.33	174.04	126.32
19	H	1080	CLA	C3B-CAB-CBB	23.42	174.25	126.32
19	B	1744	CLA	C3B-CAB-CBB	23.54	174.47	126.32
19	A	1795	CLA	C3B-CAB-CBB	23.56	174.52	126.32
19	B	1769	CLA	C3B-CAB-CBB	23.60	174.60	126.32
19	A	1801	CLA	C3B-CAB-CBB	23.67	174.76	126.32
19	L	1167	CLA	C3B-CAB-CBB	23.69	174.78	126.32
19	4	1206	CLA	C3B-CAB-CBB	23.70	174.82	126.32
19	1	1197	CLA	C3B-CAB-CBB	23.71	174.82	126.32
19	A	1792	CLA	C3B-CAB-CBB	23.71	174.83	126.32
19	A	1766	CLA	C3B-CAB-CBB	23.73	174.86	126.32
19	B	1739	CLA	C3B-CAB-CBB	23.76	174.94	126.32
19	A	1787	CLA	C3B-CAB-CBB	23.82	175.05	126.32
19	1	1505	CLA	C3B-CAB-CBB	23.86	175.14	126.32
19	B	1767	CLA	C3B-CAB-CBB	23.91	175.25	126.32
19	B	1738	CLA	C3B-CAB-CBB	23.95	175.31	126.32
19	B	1747	CLA	C3B-CAB-CBB	23.96	175.35	126.32
19	A	1762	CLA	C3B-CAB-CBB	23.98	175.37	126.32
19	B	1750	CLA	C3B-CAB-CBB	24.13	175.70	126.32
19	1	1190	CLA	C3B-CAB-CBB	24.16	175.75	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	1755	CLA	C3B-CAB-CBB	24.18	175.80	126.32
19	1	1189	CLA	C3B-CAB-CBB	24.19	175.82	126.32
19	F	1156	CLA	C3B-CAB-CBB	24.25	175.94	126.32
19	B	1754	CLA	C3B-CAB-CBB	24.28	175.99	126.32
19	A	1791	CLA	C3B-CAB-CBB	24.28	176.00	126.32
19	A	1794	CLA	C3B-CAB-CBB	24.29	176.01	126.32
19	1	1148	CLA	C3B-CAB-CBB	24.33	176.10	126.32
19	H	1081	CLA	C3B-CAB-CBB	24.35	176.13	126.32
19	1	1143	CLA	C3B-CAB-CBB	24.38	176.21	126.32
19	B	1764	CLA	C3B-CAB-CBB	24.40	176.24	126.32
19	A	1783	CLA	C3B-CAB-CBB	24.43	176.29	126.32
19	1	1308	CLA	C3B-CAB-CBB	24.50	176.45	126.32
19	2	2006	CLA	C3B-CAB-CBB	24.50	176.46	126.32
19	A	1790	CLA	C3B-CAB-CBB	24.54	176.52	126.32
19	R	1054	CLA	C3B-CAB-CBB	24.54	176.54	126.32
19	A	1814	CLA	C3B-CAB-CBB	24.63	176.71	126.32
19	B	1761	CLA	C3B-CAB-CBB	24.67	176.80	126.32
19	A	1786	CLA	C3B-CAB-CBB	24.70	176.86	126.32
19	A	1817	CLA	C3B-CAB-CBB	24.71	176.88	126.32
19	A	1815	CLA	C3B-CAB-CBB	24.74	176.94	126.32
19	4	1200	CLA	C3B-CAB-CBB	24.74	176.95	126.32
19	B	1749	CLA	C3B-CAB-CBB	24.79	177.03	126.32
19	3	3008	CLA	C3B-CAB-CBB	24.83	177.12	126.32
19	R	1055	CLA	C3B-CAB-CBB	24.86	177.18	126.32
19	B	1753	CLA	C3B-CAB-CBB	24.86	177.18	126.32
19	B	1751	CLA	C3B-CAB-CBB	24.89	177.24	126.32
19	4	1196	CLA	C3B-CAB-CBB	24.90	177.26	126.32
19	A	1771	CLA	C3B-CAB-CBB	24.95	177.36	126.32
19	A	1813	CLA	C3B-CAB-CBB	24.96	177.40	126.32
19	1	1142	CLA	C3B-CAB-CBB	25.07	177.61	126.32
19	1	1187	CLA	C3B-CAB-CBB	25.11	177.69	126.32
19	2	1223	CLA	C3B-CAB-CBB	25.12	177.71	126.32
19	3	1222	CLA	C3B-CAB-CBB	25.16	177.79	126.32
19	4	4007	CLA	C3B-CAB-CBB	25.17	177.81	126.32
19	1	1145	CLA	C3B-CAB-CBB	25.18	177.83	126.32
19	A	1788	CLA	C3B-CAB-CBB	25.20	177.87	126.32
19	A	1773	CLA	C3B-CAB-CBB	25.24	177.95	126.32
19	J	1043	CLA	C3B-CAB-CBB	25.28	178.03	126.32
19	L	1168	CLA	C3B-CAB-CBB	25.32	178.12	126.32
19	I	1031	CLA	C3B-CAB-CBB	25.40	178.29	126.32
19	B	1752	CLA	C3B-CAB-CBB	25.50	178.50	126.32
19	3	1217	CLA	C3B-CAB-CBB	25.74	178.97	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1798	CLA	C3B-CAB-CBB	25.77	179.06	126.32
23	B	1776	BCR	C20-C21-C22	29.10	169.23	127.20
23	B	1775	BCR	C20-C21-C22	30.78	171.65	127.20
23	B	1780	BCR	C20-C21-C22	33.93	176.20	127.20
23	B	1778	BCR	C20-C21-C22	34.05	176.38	127.20
23	A	1808	BCR	C20-C21-C22	34.14	176.50	127.20
23	A	1809	BCR	C20-C21-C22	34.27	176.70	127.20
23	A	1803	BCR	C20-C21-C22	34.44	176.95	127.20
23	I	1032	BCR	C20-C21-C22	34.85	177.54	127.20
23	B	1779	BCR	C20-C21-C22	34.89	177.59	127.20
23	A	1804	BCR	C20-C21-C22	35.00	177.74	127.20
23	B	1777	BCR	C20-C21-C22	35.05	177.82	127.20
23	A	1806	BCR	C20-C21-C22	35.12	177.93	127.20
23	A	1805	BCR	C20-C21-C22	35.20	178.03	127.20
23	L	1169	BCR	C20-C21-C22	35.44	178.38	127.20
23	B	1774	BCR	C20-C21-C22	35.91	179.07	127.20

All (617) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	1194	CLA	NC
19	1	1194	CLA	ND
19	1	1194	CLA	NA
19	1	1308	CLA	NC
19	1	1308	CLA	ND
19	1	1308	CLA	NA
19	A	1763	CLA	NC
19	A	1763	CLA	ND
19	A	1763	CLA	NA
19	B	1751	CLA	NC
19	B	1751	CLA	ND
19	B	1751	CLA	NA
19	A	1785	CLA	C8
19	A	1785	CLA	NC
19	A	1785	CLA	ND
19	A	1785	CLA	NA
19	A	1773	CLA	NC
19	A	1773	CLA	ND
19	A	1773	CLA	NA
19	B	1739	CLA	C8
19	B	1739	CLA	NC
19	B	1739	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	1739	CLA	NA
19	4	1210	CLA	NC
19	4	1210	CLA	ND
19	4	1210	CLA	NA
19	F	1155	CLA	NC
19	F	1155	CLA	ND
19	F	1155	CLA	NA
19	B	1770	CLA	C8
19	B	1770	CLA	NC
19	B	1770	CLA	ND
19	B	1770	CLA	NA
19	4	1211	CLA	NC
19	4	1211	CLA	ND
19	4	1211	CLA	NA
19	B	1765	CLA	NC
19	B	1765	CLA	ND
19	B	1765	CLA	NA
19	A	1760	CLA	C8
19	A	1760	CLA	NC
19	A	1760	CLA	ND
19	A	1760	CLA	NA
19	2	1216	CLA	NC
19	2	1216	CLA	ND
19	2	1216	CLA	NA
19	A	1778	CLA	NC
19	A	1778	CLA	ND
19	A	1778	CLA	NA
19	B	1750	CLA	NC
19	B	1750	CLA	ND
19	B	1750	CLA	NA
19	A	1791	CLA	NC
19	A	1791	CLA	ND
19	A	1791	CLA	NA
19	3	3014	CLA	NC
19	3	3014	CLA	ND
19	3	3014	CLA	NA
19	3	1212	CLA	NC
19	3	1212	CLA	ND
19	3	1212	CLA	NA
19	3	1218	CLA	C8
19	3	1218	CLA	NC
19	3	1218	CLA	ND

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Mol	Chain	Res	Type	Atom
19	3	1218	CLA	NA
21	B	8056	SUC	C2'
19	B	1757	CLA	C8
19	B	1757	CLA	NC
19	B	1757	CLA	ND
19	B	1757	CLA	NA
19	A	1794	CLA	NC
19	A	1794	CLA	ND
19	A	1794	CLA	NA
19	B	1756	CLA	C8
19	B	1756	CLA	NC
19	B	1756	CLA	ND
19	B	1756	CLA	NA
19	H	1079	CLA	C8
19	H	1079	CLA	NC
19	H	1079	CLA	ND
19	H	1079	CLA	NA
19	1	1505	CLA	C8
19	1	1505	CLA	NC
19	1	1505	CLA	ND
19	1	1505	CLA	NA
19	1	1191	CLA	NC
19	1	1191	CLA	ND
19	1	1191	CLA	NA
19	B	1744	CLA	C8
19	B	1744	CLA	NC
19	B	1744	CLA	ND
19	B	1744	CLA	NA
22	B	1773	PQN	C23
19	1	1143	CLA	NC
19	1	1143	CLA	ND
19	1	1143	CLA	NA
19	B	1741	CLA	C8
19	B	1741	CLA	NC
19	B	1741	CLA	ND
19	B	1741	CLA	NA
19	G	1099	CLA	NC
19	G	1099	CLA	ND
19	G	1099	CLA	NA
19	A	1792	CLA	NC
19	A	1792	CLA	ND
19	A	1792	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B	1758	CLA	C8
19	B	1758	CLA	NC
19	B	1758	CLA	ND
19	B	1758	CLA	NA
19	A	1770	CLA	NC
19	A	1770	CLA	ND
19	A	1770	CLA	NA
19	1	1197	CLA	CBD
19	1	1197	CLA	NC
19	1	1197	CLA	ND
19	1	1197	CLA	NA
19	B	1760	CLA	NC
19	B	1760	CLA	ND
19	B	1760	CLA	NA
19	B	1738	CLA	C8
19	B	1738	CLA	NC
19	B	1738	CLA	ND
19	B	1738	CLA	NA
19	4	1199	CLA	C8
19	4	1199	CLA	NC
19	4	1199	CLA	ND
19	4	1199	CLA	NA
19	1	1188	CLA	NC
19	1	1188	CLA	ND
19	1	1188	CLA	NA
19	A	1790	CLA	NC
19	A	1790	CLA	ND
19	A	1790	CLA	NA
19	A	1766	CLA	NC
19	A	1766	CLA	ND
19	A	1766	CLA	NA
21	B	8054	SUC	C2'
19	B	1752	CLA	C8
19	B	1752	CLA	NC
19	B	1752	CLA	ND
19	B	1752	CLA	NA
19	4	1205	CLA	NC
19	4	1205	CLA	ND
19	4	1205	CLA	NA
19	A	1795	CLA	NC
19	A	1795	CLA	ND
19	A	1795	CLA	NA

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Mol	Chain	Res	Type	Atom
19	1	1198	CLA	NC
19	1	1198	CLA	ND
19	1	1198	CLA	NA
19	A	1797	CLA	C2A
19	A	1797	CLA	NC
19	A	1797	CLA	ND
19	A	1797	CLA	NA
19	A	1787	CLA	C8
19	A	1787	CLA	NC
19	A	1787	CLA	ND
19	A	1787	CLA	NA
19	1	1187	CLA	NC
19	1	1187	CLA	ND
19	1	1187	CLA	NA
19	A	1768	CLA	NC
19	A	1768	CLA	ND
19	A	1768	CLA	NA
19	B	1740	CLA	NC
19	B	1740	CLA	ND
19	B	1740	CLA	NA
19	B	1749	CLA	C8
19	B	1749	CLA	NC
19	B	1749	CLA	ND
19	B	1749	CLA	NA
19	3	1216	CLA	NC
19	3	1216	CLA	ND
19	3	1216	CLA	NA
19	B	1755	CLA	C8
19	B	1755	CLA	NC
19	B	1755	CLA	ND
19	B	1755	CLA	NA
19	2	1220	CLA	NC
19	2	1220	CLA	ND
19	2	1220	CLA	NA
19	A	1781	CLA	C8
19	A	1781	CLA	NC
19	A	1781	CLA	ND
19	A	1781	CLA	NA
19	1	1189	CLA	NC
19	1	1189	CLA	ND
19	1	1189	CLA	NA
19	A	1764	CLA	C8

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Mol	Chain	Res	Type	Atom
19	A	1764	CLA	NC
19	A	1764	CLA	ND
19	A	1764	CLA	NA
19	B	1742	CLA	C8
19	B	1742	CLA	NC
19	B	1742	CLA	ND
19	B	1742	CLA	NA
19	A	1769	CLA	NC
19	A	1769	CLA	ND
19	A	1769	CLA	NA
19	3	1221	CLA	C8
19	3	1221	CLA	NC
19	3	1221	CLA	ND
19	3	1221	CLA	NA
19	2	1218	CLA	NC
19	2	1218	CLA	ND
19	2	1218	CLA	NA
19	R	1054	CLA	C8
19	R	1054	CLA	NC
19	R	1054	CLA	ND
19	R	1054	CLA	NA
19	3	3008	CLA	NC
19	3	3008	CLA	ND
19	3	3008	CLA	NA
19	A	1783	CLA	C8
19	A	1783	CLA	NC
19	A	1783	CLA	ND
19	A	1783	CLA	NA
19	1	1195	CLA	NC
19	1	1195	CLA	ND
19	1	1195	CLA	NA
19	L	1168	CLA	CBD
19	L	1168	CLA	NC
19	L	1168	CLA	ND
19	L	1168	CLA	NA
19	A	1813	CLA	C8
19	A	1813	CLA	NC
19	A	1813	CLA	ND
19	A	1813	CLA	NA
19	A	1798	CLA	C8
19	A	1798	CLA	NC
19	A	1798	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1798	CLA	NA
19	A	1784	CLA	C8
19	A	1784	CLA	NC
19	A	1784	CLA	ND
19	A	1784	CLA	NA
19	3	1219	CLA	NC
19	3	1219	CLA	ND
19	3	1219	CLA	NA
19	1	1307	CLA	NC
19	1	1307	CLA	ND
19	1	1307	CLA	NA
19	A	1775	CLA	NC
19	A	1775	CLA	ND
19	A	1775	CLA	NA
19	1	1148	CLA	C8
19	1	1148	CLA	NC
19	1	1148	CLA	ND
19	1	1148	CLA	NA
21	B	8051	SUC	C2'
19	2	1212	CLA	NC
19	2	1212	CLA	ND
19	2	1212	CLA	NA
19	4	1208	CLA	NC
19	4	1208	CLA	ND
19	4	1208	CLA	NA
21	B	8060	SUC	C2'
19	B	1762	CLA	C8
19	B	1762	CLA	NC
19	B	1762	CLA	ND
19	B	1762	CLA	NA
19	1	1146	CLA	NC
19	1	1146	CLA	ND
19	1	1146	CLA	NA
21	B	8059	SUC	C2'
19	B	1767	CLA	C8
19	B	1767	CLA	NC
19	B	1767	CLA	ND
19	B	1767	CLA	NA
19	2	1215	CLA	NC
19	2	1215	CLA	ND
19	2	1215	CLA	NA
19	4	1207	CLA	NC

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Mol	Chain	Res	Type	Atom
19	4	1207	CLA	ND
19	4	1207	CLA	NA
19	3	1215	CLA	NC
19	3	1215	CLA	ND
19	3	1215	CLA	NA
19	4	4007	CLA	NC
19	4	4007	CLA	ND
19	4	4007	CLA	NA
21	3	1223	SUC	C2'
19	B	1737	CLA	C8
19	B	1737	CLA	NC
19	B	1737	CLA	ND
19	B	1737	CLA	NA
19	4	1204	CLA	NC
19	4	1204	CLA	ND
19	4	1204	CLA	NA
19	4	1201	CLA	NC
19	4	1201	CLA	C2A
19	4	1201	CLA	ND
19	4	1201	CLA	NA
19	1	1196	CLA	NC
19	1	1196	CLA	ND
19	1	1196	CLA	NA
19	A	1779	CLA	NC
19	A	1779	CLA	ND
19	A	1779	CLA	NA
19	B	1768	CLA	C8
19	B	1768	CLA	NC
19	B	1768	CLA	ND
19	B	1768	CLA	NA
19	B	1745	CLA	C8
19	B	1745	CLA	NC
19	B	1745	CLA	ND
19	B	1745	CLA	NA
19	A	1789	CLA	C8
19	A	1789	CLA	NC
19	A	1789	CLA	ND
19	A	1789	CLA	NA
19	4	1198	CLA	C8
19	4	1198	CLA	CBD
19	4	1198	CLA	NC
19	4	1198	CLA	ND

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Mol	Chain	Res	Type	Atom
19	4	1198	CLA	NA
19	B	1766	CLA	NC
19	B	1766	CLA	ND
19	B	1766	CLA	NA
19	A	1762	CLA	C8
19	A	1762	CLA	NC
19	A	1762	CLA	ND
19	A	1762	CLA	NA
19	2	1222	CLA	NC
19	2	1222	CLA	ND
19	2	1222	CLA	NA
19	A	1776	CLA	C8
19	A	1776	CLA	NC
19	A	1776	CLA	ND
19	A	1776	CLA	NA
19	1	1192	CLA	C8
19	1	1192	CLA	NC
19	1	1192	CLA	ND
19	1	1192	CLA	NA
19	A	1780	CLA	C8
19	A	1780	CLA	NC
19	A	1780	CLA	ND
19	A	1780	CLA	NA
19	B	1764	CLA	NC
19	B	1764	CLA	ND
19	B	1764	CLA	NA
19	I	1031	CLA	C8
19	I	1031	CLA	NC
19	I	1031	CLA	ND
19	I	1031	CLA	NA
19	A	1815	CLA	C8
19	A	1815	CLA	NC
19	A	1815	CLA	ND
19	A	1815	CLA	NA
19	2	1219	CLA	NC
19	2	1219	CLA	ND
19	2	1219	CLA	NA
19	A	1759	CLA	NC
19	A	1759	CLA	ND
19	A	1759	CLA	NA
19	4	1196	CLA	C8
19	4	1196	CLA	NC

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Mol	Chain	Res	Type	Atom
19	4	1196	CLA	ND
19	4	1196	CLA	NA
19	J	1043	CLA	C8
19	J	1043	CLA	NC
19	J	1043	CLA	ND
19	J	1043	CLA	NA
19	F	1156	CLA	NC
19	F	1156	CLA	ND
19	F	1156	CLA	NA
19	3	3015	CLA	NC
19	3	3015	CLA	ND
19	3	3015	CLA	NA
19	1	1145	CLA	C8
19	1	1145	CLA	CBD
19	1	1145	CLA	NC
19	1	1145	CLA	ND
19	1	1145	CLA	NA
19	1	1014	CLA	CBD
19	1	1014	CLA	NC
19	1	1014	CLA	ND
19	1	1014	CLA	NA
19	A	1817	CLA	C8
19	A	1817	CLA	NC
19	A	1817	CLA	ND
19	A	1817	CLA	NA
19	A	1816	CLA	NC
19	A	1816	CLA	ND
19	A	1816	CLA	NA
21	2	1225	SUC	C2'
19	1	1190	CLA	NC
19	1	1190	CLA	ND
19	1	1190	CLA	NA
19	4	1202	CLA	NC
19	4	1202	CLA	ND
19	4	1202	CLA	NA
19	A	1772	CLA	NC
19	A	1772	CLA	ND
19	A	1772	CLA	NA
19	2	1217	CLA	C8
19	2	1217	CLA	NC
19	2	1217	CLA	ND
19	2	1217	CLA	NA

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Mol	Chain	Res	Type	Atom
19	2	2006	CLA	NC
19	2	2006	CLA	ND
19	2	2006	CLA	NA
22	A	1802	PQN	C23
19	A	1801	CLA	C8
19	A	1801	CLA	NC
19	A	1801	CLA	ND
19	A	1801	CLA	NA
19	B	1754	CLA	NC
19	B	1754	CLA	ND
19	B	1754	CLA	NA
19	B	1735	CLA	C8
19	B	1735	CLA	NC
19	B	1735	CLA	ND
19	B	1735	CLA	NA
19	4	1203	CLA	NC
19	4	1203	CLA	ND
19	4	1203	CLA	NA
19	A	1771	CLA	NC
19	A	1771	CLA	ND
19	A	1771	CLA	NA
19	1	1193	CLA	C2A
19	1	1193	CLA	NC
19	1	1193	CLA	ND
19	1	1193	CLA	NA
19	B	1748	CLA	NC
19	B	1748	CLA	ND
19	B	1748	CLA	NA
19	B	1747	CLA	NC
19	B	1747	CLA	ND
19	B	1747	CLA	NA
19	1	1309	CLA	NC
19	1	1309	CLA	ND
19	1	1309	CLA	NA
19	H	1080	CLA	C8
19	H	1080	CLA	NC
19	H	1080	CLA	ND
19	H	1080	CLA	NA
19	B	1736	CLA	NC
19	B	1736	CLA	ND
19	B	1736	CLA	NA
19	A	1782	CLA	C8

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Mol	Chain	Res	Type	Atom
19	A	1782	CLA	NC
19	A	1782	CLA	ND
19	A	1782	CLA	NA
19	1	1199	CLA	C2A
19	1	1199	CLA	NC
19	1	1199	CLA	ND
19	1	1199	CLA	NA
19	1	1199	CLA	C3A
19	2	1221	CLA	NC
19	2	1221	CLA	ND
19	2	1221	CLA	NA
19	1	1149	CLA	NC
19	1	1149	CLA	C2A
19	1	1149	CLA	ND
19	1	1149	CLA	NA
19	1	1149	CLA	CBD
19	B	1763	CLA	NC
19	B	1763	CLA	ND
19	B	1763	CLA	NA
19	B	1769	CLA	NC
19	B	1769	CLA	ND
19	B	1769	CLA	NA
19	3	3011	CLA	C8
19	3	3011	CLA	NC
19	3	3011	CLA	ND
19	3	3011	CLA	NA
19	A	1788	CLA	C8
19	A	1788	CLA	NC
19	A	1788	CLA	ND
19	A	1788	CLA	NA
19	L	1167	CLA	NC
19	L	1167	CLA	ND
19	L	1167	CLA	NA
19	3	1222	CLA	C8
19	3	1222	CLA	NC
19	3	1222	CLA	ND
19	3	1222	CLA	NA
21	H	1082	SUC	C2'
19	3	1213	CLA	NC
19	3	1213	CLA	ND
19	3	1213	CLA	NA
19	2	1213	CLA	C8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
19	2	1213	CLA	NC
19	2	1213	CLA	ND
19	2	1213	CLA	NA
19	B	1771	CLA	C8
19	B	1771	CLA	NC
19	B	1771	CLA	ND
19	B	1771	CLA	NA
19	H	1081	CLA	NC
19	H	1081	CLA	ND
19	H	1081	CLA	NA
19	3	1220	CLA	NC
19	3	1220	CLA	ND
19	3	1220	CLA	NA
19	B	1743	CLA	C8
19	B	1743	CLA	NC
19	B	1743	CLA	ND
19	B	1743	CLA	NA
19	A	1814	CLA	C8
19	A	1814	CLA	NC
19	A	1814	CLA	ND
19	A	1814	CLA	NA
19	4	1206	CLA	C8
19	4	1206	CLA	NC
19	4	1206	CLA	ND
19	4	1206	CLA	NA
19	B	1753	CLA	C8
19	B	1753	CLA	NC
19	B	1753	CLA	ND
19	B	1753	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	C3A
19	F	1157	CLA	ND
19	A	1774	CLA	C8
19	A	1774	CLA	NC
19	A	1774	CLA	ND
19	A	1774	CLA	NA
21	B	8061	SUC	C2'
19	A	1765	CLA	NC
19	A	1765	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	1765	CLA	NA
19	2	1214	CLA	NC
19	2	1214	CLA	ND
19	2	1214	CLA	NA
19	A	1777	CLA	NC
19	A	1777	CLA	ND
19	A	1777	CLA	NA
19	B	1784	CLA	C8
19	B	1784	CLA	NC
19	B	1784	CLA	ND
19	B	1784	CLA	NA
21	B	8062	SUC	C2'
19	4	1197	CLA	NC
19	4	1197	CLA	ND
19	4	1197	CLA	NA
19	A	1767	CLA	C8
19	A	1767	CLA	NC
19	A	1767	CLA	ND
19	A	1767	CLA	NA
19	2	2010	CLA	NC
19	2	2010	CLA	ND
19	2	2010	CLA	NA
19	4	1209	CLA	NC
19	4	1209	CLA	ND
19	4	1209	CLA	NA
19	3	1217	CLA	NC
19	3	1217	CLA	ND
19	3	1217	CLA	NA
19	R	1055	CLA	C8
19	R	1055	CLA	NC
19	R	1055	CLA	ND
19	R	1055	CLA	NA
19	1	1142	CLA	NC
19	1	1142	CLA	ND
19	1	1142	CLA	NA
19	A	1796	CLA	C8
19	A	1796	CLA	NC
19	A	1796	CLA	ND
19	A	1796	CLA	NA
19	A	1761	CLA	NC
19	A	1761	CLA	ND
19	A	1761	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B	1772	CLA	NC
19	B	1772	CLA	ND
19	B	1772	CLA	NA
19	A	1799	CLA	NC
19	A	1799	CLA	ND
19	A	1799	CLA	NA
19	A	1793	CLA	C8
19	A	1793	CLA	NC
19	A	1793	CLA	ND
19	A	1793	CLA	NA
19	3	1214	CLA	NC
19	3	1214	CLA	ND
19	3	1214	CLA	NA
19	B	1746	CLA	NC
19	B	1746	CLA	ND
19	B	1746	CLA	NA
19	2	1223	CLA	C8
19	2	1223	CLA	NC
19	2	1223	CLA	ND
19	2	1223	CLA	NA
19	B	1761	CLA	NC
19	B	1761	CLA	ND
19	B	1761	CLA	NA
19	1	1200	CLA	NC
19	1	1200	CLA	ND
19	1	1200	CLA	NA
19	3	3001	CLA	NC
19	3	3001	CLA	ND
19	3	3001	CLA	NA
21	B	8053	SUC	C2'
19	4	4014	CLA	NC
19	4	4014	CLA	ND
19	4	4014	CLA	NA
19	A	1800	CLA	C8
19	A	1800	CLA	NC
19	A	1800	CLA	ND
19	A	1800	CLA	NA
21	B	8055	SUC	C2'
19	4	1200	CLA	NC
19	4	1200	CLA	ND
19	4	1200	CLA	NA
19	B	1759	CLA	C8

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Mol	Chain	Res	Type	Atom
19	B	1759	CLA	NC
19	B	1759	CLA	ND
19	B	1759	CLA	NA
19	A	1786	CLA	NC
19	A	1786	CLA	ND
19	A	1786	CLA	NA
21	B	8052	SUC	C2'

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	1774	BCR	C20-C21-C22-C37
23	B	1774	BCR	C20-C21-C22-C23
23	B	1780	BCR	C20-C21-C22-C23
23	B	1780	BCR	C20-C21-C22-C37
23	A	1809	BCR	C21-C20-C19-C18
20	A	7027	LMU	C1-O1'-C1'-O5'
19	B	1769	CLA	CED-O2D-CGD-CBD
19	4	1205	CLA	CED-O2D-CGD-CBD
19	B	1755	CLA	CED-O2D-CGD-CBD
19	1	1197	CLA	CED-O2D-CGD-CBD
20	A	7030	LMU	C1'-O1'-C1-C2
19	A	1798	CLA	CED-O2D-CGD-CBD
19	B	1760	CLA	CED-O2D-CGD-CBD
19	A	1814	CLA	CED-O2D-CGD-CBD
19	F	1157	CLA	CED-O2D-CGD-CBD
19	A	1781	CLA	CED-O2D-CGD-CBD
19	2	2006	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

236 monomers are involved in 2765 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1014	CLA	1	0
19	1	1142	CLA	16	1
19	1	1143	CLA	27	0
19	1	1145	CLA	15	0
19	1	1146	CLA	9	0
19	1	1148	CLA	10	0
19	1	1149	CLA	9	0
19	1	1187	CLA	13	0
19	1	1188	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1189	CLA	8	0
19	1	1190	CLA	15	0
19	1	1191	CLA	6	0
19	1	1192	CLA	9	0
19	1	1193	CLA	6	1
19	1	1194	CLA	3	0
19	1	1195	CLA	1	0
19	1	1196	CLA	8	0
19	1	1197	CLA	7	0
19	1	1198	CLA	2	0
19	1	1199	CLA	16	0
19	1	1308	CLA	12	0
19	1	1505	CLA	2	0
19	2	1212	CLA	13	0
19	2	1213	CLA	25	0
19	2	1214	CLA	2	0
19	2	1215	CLA	16	0
19	2	1217	CLA	22	0
19	2	1218	CLA	1	0
19	2	1219	CLA	1	0
19	2	1221	CLA	21	0
19	2	1222	CLA	6	0
19	2	1223	CLA	19	0
20	2	1224	LMU	29	0
21	2	1225	SUC	10	0
19	2	2006	CLA	17	0
19	3	1213	CLA	4	0
19	3	1214	CLA	2	0
19	3	1215	CLA	3	0
19	3	1216	CLA	7	0
19	3	1217	CLA	14	0
19	3	1218	CLA	17	0
19	3	1219	CLA	2	0
19	3	1220	CLA	1	0
19	3	1221	CLA	17	0
19	3	1222	CLA	10	0
21	3	1223	SUC	6	0
19	3	3008	CLA	1	0
19	3	3011	CLA	13	0
19	4	1196	CLA	34	0
19	4	1197	CLA	3	0
19	4	1198	CLA	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	1199	CLA	21	0
19	4	1200	CLA	5	0
19	4	1201	CLA	18	0
19	4	1205	CLA	25	0
19	4	1206	CLA	11	0
19	4	1207	CLA	3	0
19	4	1208	CLA	4	0
19	4	1209	CLA	4	0
19	4	1210	CLA	10	0
19	4	1211	CLA	5	0
20	4	1212	LMU	1	0
19	4	4007	CLA	3	0
19	4	4014	CLA	14	0
19	A	1759	CLA	20	0
19	A	1760	CLA	36	0
19	A	1761	CLA	16	0
19	A	1762	CLA	13	0
19	A	1763	CLA	33	0
19	A	1764	CLA	21	0
19	A	1765	CLA	32	0
19	A	1766	CLA	4	0
19	A	1767	CLA	22	0
19	A	1768	CLA	4	0
19	A	1769	CLA	21	0
19	A	1770	CLA	14	0
19	A	1771	CLA	4	0
19	A	1772	CLA	21	0
19	A	1773	CLA	8	0
19	A	1774	CLA	46	0
19	A	1776	CLA	33	0
19	A	1777	CLA	8	0
19	A	1778	CLA	8	0
19	A	1779	CLA	20	0
19	A	1780	CLA	10	0
19	A	1781	CLA	43	0
19	A	1782	CLA	51	0
19	A	1783	CLA	49	0
19	A	1784	CLA	19	0
19	A	1785	CLA	18	0
19	A	1786	CLA	7	0
19	A	1787	CLA	23	0
19	A	1788	CLA	31	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1789	CLA	37	0
19	A	1790	CLA	19	0
19	A	1791	CLA	13	0
19	A	1792	CLA	7	0
19	A	1793	CLA	15	0
19	A	1794	CLA	6	0
19	A	1795	CLA	17	0
19	A	1796	CLA	33	0
19	A	1797	CLA	27	0
19	A	1798	CLA	6	0
19	A	1799	CLA	1	0
19	A	1800	CLA	29	0
19	A	1801	CLA	13	0
22	A	1802	PQN	7	0
23	A	1803	BCR	32	0
23	A	1804	BCR	23	0
23	A	1805	BCR	48	0
23	A	1806	BCR	36	0
23	A	1807	BCR	9	0
23	A	1808	BCR	24	0
23	A	1809	BCR	9	0
20	A	1810	LMU	5	0
20	A	1811	LMU	4	0
20	A	1812	LMU	4	0
19	A	1813	CLA	21	0
19	A	1814	CLA	30	0
19	A	1815	CLA	26	0
19	A	1816	CLA	17	0
19	A	1817	CLA	44	0
20	A	7001	LMU	13	0
20	A	7003	LMU	2	0
20	A	7004	LMU	3	0
20	A	7005	LMU	14	0
20	A	7006	LMU	6	0
20	A	7008	LMU	4	17
20	A	7009	LMU	8	1
20	A	7010	LMU	5	0
20	A	7011	LMU	3	0
20	A	7013	LMU	20	0
20	A	7014	LMU	3	0
20	A	7016	LMU	21	0
20	A	7017	LMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	7019	LMU	2	0
20	A	7020	LMU	8	0
20	A	7021	LMU	9	0
20	A	7022	LMU	5	0
20	A	7023	LMU	15	0
20	A	7025	LMU	9	0
20	A	7026	LMU	6	0
20	A	7027	LMU	5	0
20	A	7030	LMU	9	0
20	A	7031	LMU	5	0
20	A	7032	LMU	18	0
20	A	7033	LMU	9	0
20	A	7034	LMU	13	0
20	A	7036	LMU	8	0
20	A	7037	LMU	11	0
20	A	7038	LMU	7	0
20	A	7039	LMU	7	0
20	A	7040	LMU	3	0
20	A	7041	LMU	8	0
20	A	7042	LMU	21	0
20	A	7043	LMU	9	0
20	A	7049	LMU	16	0
19	B	1735	CLA	25	0
19	B	1736	CLA	9	0
19	B	1737	CLA	31	0
19	B	1738	CLA	22	0
19	B	1739	CLA	18	0
19	B	1740	CLA	4	0
19	B	1741	CLA	9	0
19	B	1742	CLA	8	0
19	B	1743	CLA	30	0
19	B	1744	CLA	17	0
19	B	1745	CLA	8	0
19	B	1746	CLA	19	0
19	B	1747	CLA	17	0
19	B	1748	CLA	7	0
19	B	1749	CLA	17	0
19	B	1750	CLA	7	0
19	B	1751	CLA	16	0
19	B	1752	CLA	15	0
19	B	1753	CLA	30	0
19	B	1754	CLA	24	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1755	CLA	39	0
19	B	1756	CLA	36	0
19	B	1757	CLA	13	0
19	B	1758	CLA	25	0
19	B	1759	CLA	24	0
19	B	1760	CLA	11	0
19	B	1761	CLA	29	0
19	B	1762	CLA	24	0
19	B	1763	CLA	18	0
19	B	1764	CLA	23	0
19	B	1765	CLA	30	0
19	B	1766	CLA	9	0
19	B	1767	CLA	12	0
19	B	1768	CLA	42	0
19	B	1769	CLA	47	0
19	B	1770	CLA	18	0
19	B	1771	CLA	17	0
19	B	1772	CLA	2	0
22	B	1773	PQN	28	0
23	B	1774	BCR	5	0
23	B	1775	BCR	8	0
23	B	1776	BCR	18	0
23	B	1777	BCR	32	0
23	B	1778	BCR	26	0
23	B	1779	BCR	34	0
23	B	1780	BCR	32	0
24	B	1781	LMG	17	0
20	B	1782	LMU	1	0
25	B	1783	SF4	17	0
19	B	1784	CLA	18	0
21	B	8052	SUC	6	0
21	B	8053	SUC	3	0
21	B	8054	SUC	2	0
21	B	8055	SUC	4	0
21	B	8056	SUC	4	0
21	B	8059	SUC	11	0
21	B	8060	SUC	3	0
21	B	8061	SUC	1	0
21	B	8062	SUC	1	17
25	C	1082	SF4	4	0
25	C	1083	SF4	1	0
19	F	1155	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	F	1156	CLA	5	0
19	F	1157	CLA	13	0
19	G	1099	CLA	4	0
19	H	1079	CLA	27	0
19	H	1080	CLA	13	0
19	H	1081	CLA	3	0
21	H	1082	SUC	14	0
19	I	1031	CLA	12	0
23	I	1032	BCR	38	0
19	J	1043	CLA	14	0
19	L	1167	CLA	27	0
19	L	1168	CLA	9	0
23	L	1169	BCR	36	0
20	L	1170	LMU	1	0
19	R	1054	CLA	10	0
19	R	1055	CLA	4	0
20	R	1056	LMU	9	1

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	165/241 (68%)	1.37	40 (24%) <b>1</b> <b>1</b>	21, 24, 25, 25	0
2	2	176/269 (65%)	0.93	38 (21%) <b>1</b> <b>1</b>	21, 23, 24, 25	0
3	3	153/276 (55%)	1.18	31 (20%) <b>1</b> <b>1</b>	49, 78, 110, 112	0
4	4	166/251 (66%)	0.56	13 (7%) <b>16</b> <b>13</b>	21, 23, 24, 25	0
5	A	730/758 (96%)	0.66	56 (7%) <b>16</b> <b>14</b>	20, 22, 23, 25	0
6	B	733/734 (99%)	0.71	64 (8%) <b>13</b> <b>12</b>	20, 22, 24, 25	0
7	C	81/81 (100%)	0.87	11 (13%) <b>4</b> <b>4</b>	21, 22, 23, 23	0
8	D	138/212 (65%)	0.99	30 (21%) <b>1</b> <b>1</b>	21, 23, 24, 25	0
9	E	65/143 (45%)	0.69	9 (13%) <b>4</b> <b>4</b>	21, 22, 24, 24	0
10	F	154/231 (66%)	0.65	12 (7%) <b>16</b> <b>13</b>	21, 22, 23, 24	0
11	G	95/167 (56%)	0.99	13 (13%) <b>4</b> <b>4</b>	21, 23, 24, 25	0
12	H	69/144 (47%)	0.92	10 (14%) <b>3</b> <b>3</b>	21, 23, 24, 25	0
13	I	30/40 (75%)	0.43	2 (6%) <b>21</b> <b>17</b>	21, 22, 23, 23	0
14	J	42/44 (95%)	0.54	3 (7%) <b>19</b> <b>16</b>	21, 23, 23, 24	0
15	K	84/131 (64%)	1.54	24 (28%) <b>1</b> <b>1</b>	21, 24, 24, 26	0
16	L	162/216 (75%)	0.63	18 (11%) <b>7</b> <b>7</b>	20, 23, 24, 25	0
17	N	85/170 (50%)	0.68	7 (8%) <b>14</b> <b>12</b>	22, 23, 24, 25	0
18	R	0/53	-	-	-	-
All	All	3128/4161 (75%)	0.80	381 (12%) <b>5</b> <b>6</b>	20, 23, 25, 112	0

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	10.6
3	3	40	SER	8.5
1	1	92	GLY	7.9

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Mol	Chain	Res	Type	RSRZ
1	1	87	ASN	7.5
15	K	64	GLY	6.9
11	G	74	TRP	6.9
1	1	88	PRO	6.9
11	G	4	PRO	6.8
6	B	566	GLY	6.6
4	4	114	SER	6.3
2	2	123	PRO	5.6
1	1	42	SER	5.5
3	3	77	ILE	5.3
6	B	258	LEU	5.3
16	L	116	PRO	5.2
2	2	118	CYS	5.2
10	F	38	PRO	5.1
15	K	17	LEU	5.1
5	A	124	TRP	5.1
3	3	58	GLU	5.1
6	B	210	ASN	5.1
3	3	55	ALA	5.0
6	B	491	ASN	5.0
5	A	32	GLU	5.0
5	A	33	GLN	5.0
15	K	63	CYS	5.0
8	D	141	VAL	5.0
6	B	204	GLY	5.0
1	1	17	SER	5.0
10	F	152	ASN	4.9
6	B	487	ASN	4.9
5	A	344	LYS	4.9
12	H	47	PHE	4.8
16	L	142	GLY	4.7
1	1	114	MET	4.7
8	D	61	PRO	4.7
6	B	263	PRO	4.6
5	A	34	TRP	4.6
6	B	486	LEU	4.6
8	D	108	GLU	4.6
3	3	123	PHE	4.6
15	K	65	ALA	4.5
10	F	37	ALA	4.5
16	L	141	GLY	4.4
15	K	77	GLY	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	J	6	THR	4.3
3	3	42	PRO	4.3
2	2	61	GLY	4.3
16	L	145	PHE	4.2
1	1	47	CYS	4.2
2	2	117	GLY	4.2
7	C	54	CYS	4.2
3	3	126	HIS	4.2
5	A	505	PRO	4.2
12	H	30	SER	4.2
2	2	200	PRO	4.2
1	1	39	TYR	4.2
2	2	152	SER	4.1
15	K	5	SER	4.1
16	L	115	ALA	4.1
16	L	117	ALA	4.1
1	1	113	SER	4.1
7	C	55	GLU	4.1
1	1	169	PRO	4.1
8	D	126	GLY	4.0
3	3	104	TYR	4.0
11	G	75	GLY	4.0
11	G	96	SER	4.0
1	1	80	GLY	3.9
4	4	135	GLY	3.9
5	A	236	GLY	3.9
16	L	81	GLY	3.9
8	D	50	TRP	3.9
8	D	140	ASN	3.9
5	A	101	ALA	3.9
5	A	659	ALA	3.9
10	F	124	PRO	3.8
8	D	24	THR	3.8
5	A	126	ILE	3.8
6	B	220	GLN	3.8
6	B	197	VAL	3.8
1	1	124	PRO	3.8
11	G	5	SER	3.8
15	K	68	HIS	3.8
4	4	86	SER	3.7
7	C	56	SER	3.7
7	C	34	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	1	111	GLN	3.7
6	B	249	GLY	3.7
10	F	110	ASP	3.7
9	E	79	THR	3.7
15	K	27	ALA	3.7
2	2	153	PRO	3.6
6	B	252	THR	3.6
1	1	184	PRO	3.6
1	1	134	SER	3.6
1	1	27	LEU	3.6
6	B	221	GLY	3.6
3	3	122	GLY	3.6
5	A	486	PRO	3.5
15	K	26	LEU	3.5
2	2	119	VAL	3.5
5	A	487	VAL	3.5
17	N	77	CYS	3.5
8	D	107	GLY	3.5
1	1	28	GLY	3.5
5	A	161	GLU	3.5
6	B	562	PRO	3.5
8	D	25	PRO	3.5
6	B	212	PHE	3.5
5	A	123	VAL	3.4
16	L	96	SER	3.4
2	2	43	TRP	3.4
6	B	92	TRP	3.4
5	A	388	ASP	3.4
6	B	213	LEU	3.3
6	B	251	GLY	3.3
8	D	99	GLN	3.3
2	2	110	TRP	3.3
1	1	93	THR	3.3
7	C	9	ASP	3.3
12	H	10	ASP	3.3
6	B	484	PRO	3.3
10	F	32	TYR	3.3
2	2	78	SER	3.3
17	N	48	GLY	3.3
15	K	21	ALA	3.3
1	1	164	GLN	3.3
9	E	84	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
4	4	134	PRO	3.3
12	H	26	SER	3.3
5	A	130	GLU	3.3
5	A	500	PRO	3.3
1	1	83	THR	3.2
5	A	125	PRO	3.2
15	K	49	THR	3.2
5	A	191	PRO	3.2
3	3	116	PHE	3.2
5	A	433	ASP	3.2
2	2	65	PRO	3.2
5	A	247	GLU	3.2
3	3	73	ILE	3.2
5	A	341	GLN	3.2
7	C	17	CYS	3.2
2	2	139	GLY	3.1
5	A	100	GLY	3.1
11	G	70	ASP	3.1
17	N	47	THR	3.1
5	A	718	PRO	3.1
12	H	46	PRO	3.1
6	B	214	ASP	3.1
2	2	140	GLY	3.1
2	2	158	GLU	3.0
17	N	49	CYS	3.0
2	2	77	PRO	3.0
2	2	156	LEU	3.0
6	B	242	HIS	3.0
4	4	131	VAL	3.0
6	B	259	GLY	3.0
3	3	204	THR	3.0
2	2	210	PRO	2.9
5	A	329	ASP	2.9
5	A	506	GLY	2.9
1	1	38	ARG	2.9
8	D	51	GLU	2.9
17	N	5	GLU	2.9
3	3	95	THR	2.9
8	D	125	PRO	2.9
1	1	185	TRP	2.9
8	D	135	ARG	2.9
5	A	232	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
7	C	15	THR	2.9
7	C	60	THR	2.9
5	A	429	ASN	2.9
6	B	209	TRP	2.8
1	1	123	TYR	2.8
8	D	21	ASP	2.8
5	A	724	ALA	2.8
8	D	116	ASP	2.8
10	F	76	ASP	2.8
16	L	42	ALA	2.8
15	K	54	GLY	2.8
15	K	56	THR	2.8
8	D	156	LEU	2.8
17	N	56	LYS	2.8
2	2	181	HIS	2.8
1	1	86	GLY	2.8
5	A	217	SER	2.8
5	A	575	LEU	2.8
7	C	57	ALA	2.8
15	K	78	LEU	2.7
2	2	104	TRP	2.7
6	B	170	ASN	2.7
4	4	38	ARG	2.7
3	3	80	LYS	2.7
3	3	113	LEU	2.7
15	K	59	ASP	2.7
5	A	485	GLN	2.7
2	2	122	ASP	2.7
5	A	286	GLY	2.7
9	E	64	PRO	2.7
6	B	319	HIS	2.7
16	L	69	VAL	2.7
2	2	121	THR	2.7
2	2	52	SER	2.7
2	2	157	LYS	2.6
3	3	43	GLU	2.6
5	A	742	GLY	2.6
8	D	41	GLN	2.6
13	I	5	PRO	2.6
8	D	139	LYS	2.6
12	H	29	PRO	2.6
8	D	152	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	2	186	THR	2.6
3	3	121	MET	2.6
6	B	565	GLY	2.6
5	A	266	ALA	2.6
5	A	582	ASP	2.6
16	L	98	CYS	2.6
5	A	635	THR	2.6
1	1	33	PRO	2.6
4	4	36	ASN	2.6
6	B	205	GLU	2.6
6	B	366	THR	2.6
1	1	104	ALA	2.6
12	H	12	GLU	2.6
4	4	77	ALA	2.6
16	L	101	MET	2.6
4	4	136	GLY	2.6
8	D	22	PRO	2.6
3	3	109	ASP	2.5
6	B	517	PHE	2.5
6	B	493	TRP	2.5
3	3	159	PRO	2.5
8	D	32	SER	2.5
16	L	134	ASP	2.5
3	3	72	ALA	2.5
4	4	141	LEU	2.5
5	A	501	GLY	2.5
1	1	34	ALA	2.5
2	2	76	THR	2.5
5	A	424	PRO	2.5
6	B	320	LYS	2.5
2	2	202	ALA	2.5
8	D	142	SER	2.5
8	D	151	LYS	2.5
5	A	249	ILE	2.5
11	G	59	LYS	2.5
1	1	79	GLY	2.4
15	K	50	GLY	2.4
9	E	56	ASP	2.4
8	D	136	SER	2.4
1	1	175	GLU	2.4
3	3	142	TYR	2.4
10	F	112	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
6	B	250	ALA	2.4
11	G	53	GLU	2.4
6	B	16	PRO	2.4
3	3	54	LEU	2.4
1	1	75	ALA	2.4
16	L	144	PHE	2.4
9	E	83	ALA	2.4
3	3	112	THR	2.4
2	2	92	THR	2.4
3	3	105	ASN	2.4
5	A	122	VAL	2.4
10	F	74	SER	2.4
4	4	67	ILE	2.4
6	B	73	ASN	2.3
11	G	39	ASN	2.3
6	B	492	ILE	2.3
1	1	163	VAL	2.3
3	3	120	LEU	2.3
5	A	31	PHE	2.3
5	A	278	ALA	2.3
11	G	56	SER	2.3
5	A	428	TYR	2.3
6	B	196	HIS	2.3
2	2	64	ILE	2.3
6	B	534	LEU	2.3
5	A	287	LEU	2.3
12	H	71	ASN	2.3
6	B	211	ASN	2.3
9	E	30	PRO	2.3
5	A	335	LYS	2.3
15	K	1	ASP	2.3
5	A	693	LEU	2.3
3	3	151	GLY	2.2
3	3	76	GLU	2.2
6	B	300	SER	2.2
12	H	28	ALA	2.2
1	1	172	GLY	2.2
6	B	473	GLY	2.2
6	B	690	LEU	2.2
12	H	43	PHE	2.2
6	B	217	PRO	2.2
8	D	134	MET	2.2

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Mol	Chain	Res	Type	RSRZ
15	K	62	ALA	2.2
6	B	511	THR	2.2
8	D	106	SER	2.2
16	L	39	ASN	2.2
2	2	53	ARG	2.2
6	B	118	SER	2.2
6	B	208	ARG	2.2
6	B	346	SER	2.2
3	3	114	PHE	2.2
4	4	39	TRP	2.2
6	B	239	SER	2.2
9	E	28	ILE	2.2
1	1	115	GLU	2.2
9	E	73	ASN	2.2
8	D	127	ARG	2.2
8	D	115	LYS	2.2
11	G	76	SER	2.2
1	1	43	GLU	2.2
8	D	128	GLN	2.2
10	F	137	PRO	2.2
14	J	36	ALA	2.2
13	I	4	LEU	2.2
5	A	53	TRP	2.2
16	L	80	ALA	2.2
2	2	66	GLU	2.2
10	F	106	ILE	2.2
2	2	197	LEU	2.2
6	B	271	THR	2.2
1	1	46	HIS	2.2
1	1	52	LEU	2.1
14	J	4	PHE	2.1
1	1	95	PRO	2.1
2	2	138	PRO	2.1
3	3	168	GLY	2.1
5	A	516	GLY	2.1
2	2	182	ILE	2.1
16	L	140	THR	2.1
6	B	140	ILE	2.1
6	B	292	ARG	2.1
6	B	622	ASP	2.1
5	A	61	ALA	2.1
6	B	94	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
6	B	479	SER	2.1
2	2	171	MET	2.1
5	A	234	ASN	2.1
6	B	723	ALA	2.1
1	1	110	HIS	2.1
2	2	125	PHE	2.1
17	N	74	LYS	2.1
15	K	40	LEU	2.1
5	A	746	THR	2.1
7	C	10	THR	2.1
4	4	132	GLY	2.1
5	A	559	GLY	2.1
11	G	98	PHE	2.1
5	A	737	HIS	2.1
15	K	66	VAL	2.1
15	K	13	THR	2.1
6	B	183	PHE	2.1
6	B	237	PRO	2.1
10	F	109	ARG	2.1
3	3	108	ALA	2.1
7	C	50	GLY	2.1
1	1	78	PRO	2.1
5	A	371	VAL	2.1
9	E	92	ALA	2.1
6	B	264	GLN	2.0
1	1	96	THR	2.0
6	B	689	ASN	2.0
2	2	155	LYS	2.0
6	B	354	SER	2.0
6	B	625	TRP	2.0
16	L	77	THR	2.0
3	3	96	GLY	2.0
15	K	67	GLY	2.0
6	B	645	VAL	2.0
2	2	50	VAL	2.0
5	A	589	THR	2.0
6	B	131	THR	2.0
6	B	207	VAL	2.0
6	B	261	PHE	2.0
8	D	58	PHE	2.0
11	G	87	ALA	2.0
15	K	53	ALA	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
19	CLA	1	1197	51/65	0.59	0.53	4.78	2,42,60,60	0
19	CLA	4	1200	50/65	0.74	0.42	3.59	2,21,60,60	0
23	BCR	A	1803	40/40	0.63	0.44	2.48	2,45,60,60	0
19	CLA	A	1801	55/65	0.64	0.44	2.44	2,44,60,60	0
19	CLA	A	1776	58/65	0.81	0.36	2.11	2,20,60,60	0
23	BCR	I	1032	40/40	0.67	0.42	2.08	2,38,60,60	0
23	BCR	L	1169	40/40	0.72	0.48	2.03	2,18,60,60	0
23	BCR	A	1804	40/40	0.72	0.40	2.03	2,34,60,60	0
19	CLA	A	1792	46/65	0.80	0.41	1.97	2,20,60,60	0
23	BCR	B	1774	40/40	0.70	0.48	1.84	2,33,60,60	0
19	CLA	A	1780	58/65	0.78	0.36	1.83	2,18,60,60	0
23	BCR	A	1806	40/40	0.78	0.35	1.67	2,31,60,60	0
19	CLA	A	1775	36/65	0.66	0.40	1.63	2,51,60,60	0
23	BCR	A	1807	39/40	0.83	0.32	1.43	2,8,60,60	0
19	CLA	4	1199	55/65	0.68	0.39	1.21	4,39,60,60	0
19	CLA	4	1203	25/65	0.69	0.29	1.19	2,29,60,60	0
19	CLA	B	1746	46/65	0.64	0.42	0.96	2,28,60,60	0
20	LMU	A	7047	35/35	0.63	0.33	0.93	2,40,60,60	0
24	LMG	B	1781	49/55	0.77	0.35	0.93	2,20,60,60	0
19	CLA	A	1773	52/65	0.79	0.36	0.90	2,33,60,60	0
23	BCR	B	1775	40/40	0.84	0.30	0.84	2,5,60,60	0
19	CLA	G	1099	51/65	0.70	0.42	0.69	2,44,60,60	0
19	CLA	A	1782	65/65	0.81	0.33	0.68	2,16,60,60	0
19	CLA	A	1766	45/65	0.78	0.35	0.66	2,38,60,60	0
19	CLA	A	1774	60/65	0.84	0.33	0.64	2,11,52,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	A	1786	50/65	0.83	0.29	0.60	2,32,60,60	0
19	CLA	2	1222	50/65	0.75	0.31	0.58	2,25,60,60	0
19	CLA	H	1079	58/65	0.82	0.33	0.57	2,15,60,60	0
20	LMU	L	1170	35/35	0.75	0.29	0.56	2,22,60,60	0
23	BCR	B	1777	40/40	0.82	0.33	0.53	2,11,60,60	0
19	CLA	4	1196	55/65	0.74	0.36	0.52	2,33,60,60	0
19	CLA	4	1197	36/65	0.78	0.36	0.51	2,26,60,60	0
21	SUC	2	1225	22/23	0.74	0.28	0.51	2,35,60,60	0
23	BCR	A	1805	40/40	0.82	0.33	0.49	2,5,44,60	0
19	CLA	B	1749	61/65	0.82	0.30	0.45	2,16,60,60	0
23	BCR	B	1776	40/40	0.72	0.39	0.41	2,21,60,60	0
19	CLA	A	1764	60/65	0.90	0.30	0.40	2,10,60,60	0
19	CLA	A	1800	65/65	0.83	0.31	0.38	2,22,60,60	0
19	CLA	B	1771	65/65	0.86	0.32	0.34	2,2,55,60	0
23	BCR	B	1778	40/40	0.88	0.28	0.32	2,2,60,60	0
19	CLA	A	1787	60/65	0.82	0.28	0.29	2,18,60,60	0
19	CLA	B	1767	60/65	0.83	0.32	0.27	2,2,60,60	0
19	CLA	1	1192	61/65	0.72	0.31	0.26	2,35,60,60	0
23	BCR	B	1780	40/40	0.81	0.33	0.25	2,10,60,60	0
19	CLA	B	1762	59/65	0.85	0.28	0.22	2,6,60,60	0
19	CLA	4	1209	36/65	0.86	0.24	0.21	2,21,60,60	0
19	CLA	A	1777	51/65	0.74	0.30	0.19	2,44,60,60	0
19	CLA	B	1754	54/65	0.84	0.31	0.19	2,15,60,60	0
19	CLA	A	1781	59/65	0.82	0.29	0.15	2,25,60,60	0
19	CLA	B	1772	36/65	0.80	0.33	0.15	2,52,60,60	0
19	CLA	A	1790	50/65	0.84	0.27	0.14	2,18,56,60	0
19	CLA	A	1762	56/65	0.85	0.30	0.14	2,2,54,60	0
19	CLA	B	1736	45/65	0.84	0.27	0.13	2,14,56,60	0
19	CLA	3	1212	25/65	0.69	0.43	0.12	15,54,60,60	0
19	CLA	B	1784	65/65	0.88	0.28	0.12	2,2,55,60	0
19	CLA	B	1764	45/65	0.83	0.28	0.12	2,16,60,60	0
19	CLA	L	1167	47/65	0.84	0.26	0.08	2,13,45,60	0
19	CLA	B	1735	65/65	0.83	0.28	0.08	2,11,60,60	0
19	CLA	I	1031	60/65	0.84	0.30	0.08	2,18,60,60	0
19	CLA	B	1750	50/65	0.84	0.29	0.07	2,37,60,60	0
19	CLA	A	1760	55/65	0.83	0.31	0.07	2,11,60,60	0
19	CLA	B	1770	65/65	0.85	0.29	0.07	2,11,60,60	0
19	CLA	A	1783	65/65	0.88	0.29	0.06	2,2,50,60	0
19	CLA	B	1742	55/65	0.79	0.29	0.05	2,28,60,60	0
19	CLA	B	1744	60/65	0.78	0.35	0.04	2,19,60,60	0
19	CLA	2	1215	50/65	0.73	0.30	0.04	2,48,60,60	0
19	CLA	A	1767	65/65	0.76	0.39	0.04	2,15,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	H	1081	50/65	0.79	0.31	0.02	2,27,60,60	0
19	CLA	B	1745	60/65	0.71	0.35	0.00	2,40,60,60	0
19	CLA	A	1784	55/65	0.86	0.29	-0.01	2,12,60,60	0
19	CLA	A	1761	54/65	0.81	0.28	-0.01	2,10,60,60	0
19	CLA	A	1814	65/65	0.88	0.28	-0.01	2,4,48,60	0
19	CLA	B	1751	46/65	0.78	0.33	-0.02	2,34,60,60	0
19	CLA	B	1763	50/65	0.85	0.28	-0.06	2,11,53,60	0
19	CLA	A	1785	65/65	0.85	0.29	-0.09	2,12,60,60	0
19	CLA	L	1168	50/65	0.82	0.26	-0.10	2,18,60,60	0
19	CLA	A	1769	50/65	0.84	0.28	-0.11	2,29,60,60	0
19	CLA	A	1817	65/65	0.85	0.31	-0.14	2,14,56,60	0
19	CLA	B	1741	54/65	0.82	0.25	-0.14	2,17,60,60	0
19	CLA	B	1747	53/65	0.85	0.28	-0.20	2,14,60,60	0
19	CLA	1	1191	36/65	0.73	0.29	-0.20	2,52,60,60	0
22	PQN	A	1802	33/33	0.83	0.33	-0.20	2,4,59,60	0
19	CLA	F	1156	41/65	0.67	0.33	-0.24	2,41,60,60	0
23	BCR	A	1808	40/40	0.90	0.24	-0.25	2,4,50,60	0
19	CLA	A	1815	65/65	0.86	0.29	-0.28	2,2,60,60	0
19	CLA	B	1739	60/65	0.89	0.27	-0.29	2,2,60,60	0
19	CLA	A	1796	65/65	0.84	0.31	-0.29	2,8,60,60	0
19	CLA	2	1221	50/65	0.77	0.31	-0.33	2,18,60,60	0
19	CLA	B	1752	55/65	0.84	0.29	-0.34	2,30,60,60	0
19	CLA	A	1778	42/65	0.77	0.28	-0.35	2,46,60,60	0
19	CLA	B	1738	65/65	0.90	0.26	-0.36	2,2,53,60	0
19	CLA	B	1758	65/65	0.87	0.26	-0.36	2,11,46,60	0
19	CLA	B	1765	45/65	0.62	0.37	-0.36	12,37,60,60	0
19	CLA	A	1788	65/65	0.88	0.25	-0.37	2,9,59,60	0
19	CLA	B	1748	41/65	0.90	0.27	-0.38	2,5,40,60	0
19	CLA	B	1760	50/65	0.89	0.28	-0.39	2,12,60,60	0
19	CLA	B	1756	65/65	0.82	0.32	-0.42	2,15,60,60	0
19	CLA	A	1779	50/65	0.89	0.23	-0.42	2,7,60,60	0
19	CLA	B	1755	58/65	0.85	0.31	-0.42	2,13,60,60	0
19	CLA	B	1737	61/65	0.89	0.27	-0.45	2,9,48,60	0
20	LMU	A	1811	35/35	0.77	0.26	-0.47	2,27,60,60	0
19	CLA	A	1795	51/65	0.86	0.28	-0.49	2,12,60,60	0
20	LMU	A	1810	35/35	0.69	0.24	-0.51	2,26,60,60	0
19	CLA	A	1772	54/65	0.83	0.28	-0.51	2,31,60,60	0
19	CLA	B	1761	50/65	0.86	0.24	-0.51	2,7,51,60	0
19	CLA	F	1155	36/65	0.88	0.24	-0.51	2,17,60,60	0
19	CLA	A	1763	46/65	0.82	0.29	-0.52	2,20,60,60	0
19	CLA	B	1740	25/65	0.86	0.28	-0.53	2,2,60,60	0
19	CLA	A	1759	46/65	0.86	0.31	-0.54	2,14,49,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	A	1793	65/65	0.84	0.29	-0.55	2,6,60,60	0
19	CLA	B	1768	65/65	0.88	0.24	-0.56	2,7,60,60	0
19	CLA	A	1816	54/65	0.92	0.27	-0.57	2,6,45,60	0
19	CLA	1	1196	36/65	0.76	0.31	-0.61	2,35,60,60	0
19	CLA	A	1765	52/65	0.90	0.24	-0.67	2,10,60,60	0
19	CLA	A	1794	47/65	0.89	0.24	-0.68	2,8,50,60	0
19	CLA	A	1789	65/65	0.88	0.25	-0.68	2,14,60,60	0
19	CLA	B	1743	65/65	0.90	0.25	-0.69	2,13,60,60	0
19	CLA	B	1753	65/65	0.85	0.26	-0.69	2,17,60,60	0
19	CLA	A	1813	65/65	0.90	0.27	-0.70	2,2,48,60	0
19	CLA	B	1757	65/65	0.89	0.27	-0.71	2,10,56,60	0
19	CLA	3	1218	56/65	0.77	0.32	-0.71	2,36,60,60	0
19	CLA	4	1205	50/65	0.80	0.24	-0.75	2,20,60,60	0
19	CLA	1	1195	25/65	0.83	0.31	-0.78	11,37,60,60	0
19	CLA	B	1759	65/65	0.90	0.25	-0.83	2,6,53,60	0
19	CLA	A	1771	50/65	0.82	0.27	-0.84	2,21,60,60	0
19	CLA	1	1198	25/65	0.79	0.26	-0.91	2,42,60,60	0
22	PQN	B	1773	33/33	0.86	0.28	-0.92	2,2,46,51	0
19	CLA	4	1208	25/65	0.88	0.18	-0.92	2,2,26,32	0
19	CLA	1	1190	46/65	0.80	0.28	-0.96	2,35,60,60	0
19	CLA	B	1769	47/65	0.89	0.24	-0.96	2,5,55,60	0
23	BCR	B	1779	40/40	0.89	0.22	-0.97	2,6,60,60	0
19	CLA	1	1189	47/65	0.75	0.27	-1.03	2,17,60,60	0
19	CLA	3	1216	25/65	0.76	0.26	-1.04	2,56,60,60	0
19	CLA	3	1221	65/65	0.70	0.32	-1.14	2,26,60,60	0
25	SF4	C	1083	8/8	0.96	0.08	-2.02	12,19,20,24	0
25	SF4	C	1082	8/8	0.97	0.08	-2.30	18,22,26,32	0
25	SF4	B	1783	8/8	0.98	0.06	-2.71	23,24,24,25	0
19	CLA	4	1211	46/65	0.76	0.31	-	2,45,60,60	0
19	CLA	A	1770	25/65	0.80	0.28	-	2,31,60,60	0
20	LMU	A	7009	34/35	0.80	0.24	-	2,22,60,60	0
20	LMU	A	7037	35/35	0.68	0.29	-	2,30,60,60	0
21	SUC	B	8056	23/23	0.75	0.20	-	2,31,56,60	0
20	LMU	A	7033	35/35	0.81	0.20	-	2,46,60,60	0
20	LMU	A	7010	35/35	0.53	0.51	-	2,39,60,60	0
20	LMU	A	7038	35/35	0.58	0.32	-	2,34,60,60	0
19	CLA	1	1308	48/65	0.76	0.29	-	2,34,60,60	0
19	CLA	2	1218	25/65	0.86	0.19	-	2,12,60,60	0
19	CLA	2	1219	36/65	0.77	0.28	-	2,34,60,60	0
19	CLA	R	1054	57/65	0.72	0.29	-	2,38,60,60	0
19	CLA	3	3008	50/65	0.62	0.42	-	2,56,60,60	0
19	CLA	J	1043	61/65	0.78	0.24	-	2,19,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	LMU	A	7043	35/35	0.69	0.27	-	2,41,60,60	0
19	CLA	3	3015	25/65	0.74	0.30	-	2,42,60,60	0
20	LMU	A	7011	35/35	0.80	0.23	-	2,12,50,57	0
20	LMU	A	7030	35/35	0.77	0.23	-	2,16,60,60	0
19	CLA	1	1145	55/65	0.67	0.46	-	2,47,60,60	0
19	CLA	1	1014	51/65	0.62	0.43	-	2,51,60,60	0
20	LMU	4	1212	35/35	0.76	0.40	-	2,37,60,60	0
19	CLA	1	1188	41/65	0.86	0.22	-	2,41,60,60	0
19	CLA	2	1216	25/65	0.78	0.23	-	2,57,60,60	0
20	LMU	A	7036	34/35	0.79	0.23	-	2,23,60,60	0
21	SUC	B	8054	23/23	0.66	0.30	-	2,30,60,60	0
19	CLA	4	1202	25/65	0.68	0.37	-	2,39,60,60	0
19	CLA	A	1798	55/65	0.67	0.36	-	2,44,60,60	0
20	LMU	A	7001	35/35	0.75	0.25	-	2,37,60,60	0
19	CLA	2	1217	65/65	0.77	0.25	-	2,24,60,60	0
19	CLA	2	2006	50/65	0.77	0.41	-	2,33,60,60	0
20	LMU	A	7034	35/35	0.76	0.29	-	2,21,55,60	0
20	LMU	B	1782	25/35	0.81	0.21	-	2,36,60,60	0
19	CLA	4	1210	25/65	0.76	0.29	-	2,35,60,60	0
19	CLA	3	1219	25/65	0.79	0.26	-	2,37,60,60	0
20	LMU	2	1224	35/35	0.68	0.27	-	2,21,60,60	0
19	CLA	1	1505	55/65	0.56	0.41	-	2,49,60,60	0
19	CLA	1	1307	25/65	0.73	0.49	-	2,48,60,60	0
19	CLA	1	1193	51/65	0.71	0.32	-	2,36,60,60	0
19	CLA	1	1194	25/65	0.73	0.27	-	2,31,60,60	0
19	CLA	1	1148	55/65	0.72	0.46	-	2,46,60,60	0
19	CLA	1	1309	25/65	0.62	0.56	-	2,42,60,60	0
19	CLA	H	1080	55/65	0.67	0.35	-	2,33,60,60	0
20	LMU	A	7005	35/35	0.80	0.20	-	2,28,59,60	0
23	BCR	A	1809	40/40	0.59	0.41	-	2,32,60,60	0
21	SUC	B	8051	23/23	0.77	0.35	-	2,44,60,60	0
20	LMU	A	7013	35/35	0.69	0.23	-	2,44,60,60	0
20	LMU	A	7042	35/35	0.70	0.26	-	2,38,60,60	0
20	LMU	A	7022	35/35	0.67	0.23	-	2,36,60,60	0
19	CLA	2	1212	51/65	0.77	0.23	-	2,33,60,60	0
19	CLA	1	1199	51/65	0.76	0.38	-	2,39,60,60	0
20	LMU	A	7028	35/35	0.75	0.24	-	2,23,60,60	0
20	LMU	A	7040	35/35	0.69	0.30	-	2,37,60,60	0
19	CLA	1	1149	46/65	0.72	0.38	-	2,43,60,60	0
20	LMU	A	7026	35/35	0.61	0.34	-	2,15,60,60	0
21	SUC	B	8060	23/23	0.76	0.24	-	6,40,60,60	0
19	CLA	3	3011	65/65	0.79	0.31	-	2,33,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	A	1797	59/65	0.79	0.29	-	2,30,60,60	0
19	CLA	1	1146	50/65	0.65	0.32	-	2,60,60,60	0
21	SUC	B	8059	23/23	0.83	0.24	-	2,29,60,60	0
20	LMU	A	7021	35/35	0.72	0.37	-	2,35,60,60	0
20	LMU	A	7019	35/35	0.56	0.28	-	2,43,60,60	0
19	CLA	3	1222	65/65	0.66	0.42	-	2,46,60,60	0
20	LMU	A	7016	35/35	0.55	0.40	-	2,45,60,60	0
21	SUC	H	1082	23/23	0.73	0.28	-	3,33,60,60	0
20	LMU	A	7008	35/35	0.83	0.24	-	2,34,60,60	0
19	CLA	3	1213	36/65	0.70	0.26	-	2,53,60,60	0
19	CLA	2	1213	58/65	0.83	0.23	-	2,22,60,60	0
20	LMU	A	7006	35/35	0.79	0.20	-	2,25,60,60	0
19	CLA	A	1791	45/65	0.74	0.27	-	2,37,60,60	0
20	LMU	A	7015	35/35	0.73	0.38	-	2,35,60,60	0
19	CLA	3	1220	25/65	0.68	0.26	-	2,47,60,60	0
19	CLA	1	1143	50/65	0.75	0.33	-	2,28,60,60	0
20	LMU	A	7014	35/35	0.70	0.33	-	2,45,60,60	0
19	CLA	4	1207	25/65	0.84	0.26	-	2,15,60,60	0
19	CLA	4	1206	65/65	0.82	0.27	-	2,15,60,60	0
19	CLA	3	1215	25/65	0.64	0.31	-	17,42,60,60	0
19	CLA	F	1157	53/65	0.84	0.28	-	2,22,60,60	0
19	CLA	4	4007	52/65	0.61	0.44	-	2,34,60,60	0
21	SUC	B	8061	23/23	0.67	0.32	-	2,52,60,60	0
20	LMU	A	7031	35/35	0.60	0.39	-	2,40,60,60	0
21	SUC	3	1223	23/23	0.81	0.27	-	2,27,60,60	0
19	CLA	2	1214	25/65	0.72	0.48	-	2,27,60,60	0
20	LMU	A	7025	35/35	0.71	0.24	-	2,27,60,60	0
26	UNL	B	8057	23/-	0.80	0.22	-	2,31,60,60	0
21	SUC	B	8062	23/23	0.81	0.27	-	2,34,60,60	0
20	LMU	A	7004	35/35	0.83	0.25	-	2,11,50,60	0
19	CLA	4	1204	25/65	0.78	0.40	-	2,40,60,60	0
19	CLA	4	1201	52/65	0.82	0.26	-	2,26,60,60	0
19	CLA	2	2010	25/65	0.79	0.28	-	2,36,60,60	0
20	LMU	A	7027	35/35	0.75	0.25	-	2,29,60,60	0
19	CLA	3	1217	42/65	0.75	0.27	-	2,53,60,60	0
19	CLA	R	1055	65/65	0.70	0.34	-	2,35,60,60	0
19	CLA	1	1187	46/65	0.69	0.25	-	2,56,60,60	0
19	CLA	1	1142	46/65	0.71	0.25	-	2,51,60,60	0
19	CLA	A	1768	54/65	0.83	0.24	-	2,28,60,60	0
20	LMU	A	1812	35/35	0.65	0.29	-	2,45,60,60	0
20	LMU	R	1056	35/35	0.81	0.24	-	2,21,60,60	0
19	CLA	A	1799	25/65	0.71	0.30	-	2,43,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	LMU	A	7024	35/35	0.70	0.29	-	2,35,60,60	0
20	LMU	A	7003	35/35	0.72	0.31	-	2,44,60,60	0
20	LMU	A	7020	35/35	0.77	0.22	-	2,38,60,60	0
19	CLA	3	1214	25/65	0.82	0.19	-	2,28,60,60	0
19	CLA	3	3014	25/65	0.75	0.50	-	2,47,60,60	0
19	CLA	2	1223	61/65	0.70	0.25	-	2,34,60,60	0
20	LMU	A	7023	35/35	0.70	0.27	-	2,32,60,60	0
19	CLA	1	1200	25/65	0.80	0.28	-	5,42,60,60	0
19	CLA	3	3001	25/65	0.69	0.44	-	2,30,60,60	0
21	SUC	B	8053	22/23	0.66	0.44	-	6,52,60,60	0
19	CLA	4	4014	47/65	0.75	0.29	-	2,37,60,60	0
20	LMU	A	7049	35/35	0.58	0.30	-	2,51,60,60	0
21	SUC	B	8055	23/23	0.77	0.25	-	2,41,60,60	0
20	LMU	A	7041	35/35	0.68	0.24	-	2,38,60,60	0
19	CLA	2	1220	25/65	0.81	0.42	-	2,34,60,60	0
20	LMU	A	7035	35/35	0.82	0.23	-	2,29,60,60	0
19	CLA	4	1198	65/65	0.64	0.36	-	2,32,60,60	0
20	LMU	A	7039	35/35	0.73	0.26	-	2,33,60,60	0
19	CLA	B	1766	51/65	0.66	0.38	-	2,45,60,60	0
20	LMU	A	7032	35/35	0.85	0.21	-	2,31,60,60	0
21	SUC	B	8052	23/23	0.63	0.36	-	9,40,60,60	0
20	LMU	A	7017	35/35	0.61	0.22	-	2,31,60,60	0

## 6.5 Other polymers

There are no such residues in this entry.