



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2016 – 12:13 AM GMT

PDB ID : 4Y28
Title : The structure of plant photosystem I super-complex at 2.8 angstrom resolution.
Authors : Mazor, Y.; Brovikov, A.; Nelson, N.
Deposited on : 2015-02-09
Resolution : 2.80 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

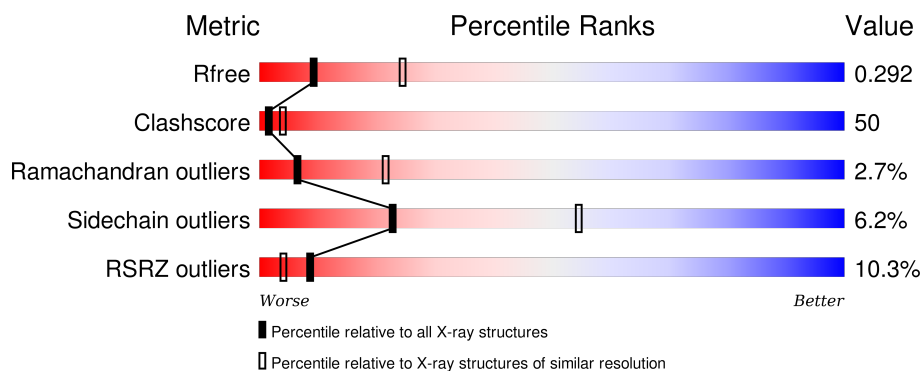
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	758	<div> <div>6%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
2	B	733	<div> <div>6%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
3	I	30	<div> <div>13%</div> <div>33%</div> <div>53%</div> <div>10%</div> <div>.</div> </div>
4	J	42	<div> <div>7%</div> <div>33%</div> <div>52%</div> <div>7%</div> <div>5%</div> <div>.</div> </div>
5	F	154	<div> <div>4%</div> <div>67%</div> <div>27%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
6	G	97	
7	L	167	
8	C	81	
9	D	147	
10	E	66	
11	H	90	
12	K	129	
13	2	269	
14	4	252	
15	1	202	
16	3	275	

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
17	CL0	A	1011	X	-	-	-
18	CLA	1	1001	X	-	X	-
18	CLA	1	1002	X	-	X	-
18	CLA	1	1003	X	-	X	-
18	CLA	1	1004	X	-	X	-
18	CLA	1	1005	X	-	-	-
18	CLA	1	1006	X	-	-	-
18	CLA	1	1007	X	-	-	-
18	CLA	1	1008	X	-	X	-
18	CLA	1	1011	X	-	-	-
18	CLA	1	1012	X	-	-	-
18	CLA	1	1013	X	-	-	-
18	CLA	1	1014	X	-	-	-
18	CLA	2	2001	X	-	X	-
18	CLA	2	2002	X	-	X	-
18	CLA	2	2003	X	-	X	-
18	CLA	2	2004	X	-	X	-
18	CLA	2	2005	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	2006	X	-	X	-
18	CLA	2	2007	X	-	X	-
18	CLA	2	2008	X	-	-	-
18	CLA	2	2009	X	-	-	-
18	CLA	2	2012	X	-	X	X
18	CLA	2	2016	X	-	X	-
18	CLA	2	2019	X	-	-	-
18	CLA	3	3001	X	-	X	-
18	CLA	3	3002	X	-	-	-
18	CLA	3	3003	X	-	X	-
18	CLA	3	3004	X	-	-	-
18	CLA	3	3005	X	-	-	-
18	CLA	3	3006	X	-	X	-
18	CLA	3	3007	X	-	-	-
18	CLA	3	3008	X	-	-	X
18	CLA	3	3010	X	-	X	-
18	CLA	3	3012	X	-	X	-
18	CLA	3	3013	X	-	X	-
18	CLA	3	3017	X	-	-	-
18	CLA	3	3018	X	-	-	-
18	CLA	3	3019	X	-	-	-
18	CLA	4	4001	X	-	X	-
18	CLA	4	4002	X	-	-	-
18	CLA	4	4003	X	-	-	-
18	CLA	4	4004	X	-	-	-
18	CLA	4	4005	X	-	-	-
18	CLA	4	4006	X	-	X	-
18	CLA	4	4007	X	-	-	-
18	CLA	4	4008	X	-	-	-
18	CLA	4	4009	X	-	-	-
18	CLA	4	4012	X	-	X	-
18	CLA	4	4016	X	-	X	-
18	CLA	4	4017	X	-	-	-
18	CLA	A	1013	X	-	-	-
18	CLA	A	1022	X	-	-	-
18	CLA	A	1101	X	-	-	-
18	CLA	A	1102	X	-	-	-
18	CLA	A	1103	X	-	-	-
18	CLA	A	1104	X	-	-	-
18	CLA	A	1105	X	-	-	-
18	CLA	A	1106	X	-	-	-
18	CLA	A	1107	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	1108	X	-	-	-
18	CLA	A	1109	X	-	-	-
18	CLA	A	1110	X	-	-	-
18	CLA	A	1111	X	-	-	-
18	CLA	A	1112	X	-	-	-
18	CLA	A	1113	X	-	-	-
18	CLA	A	1114	X	-	-	-
18	CLA	A	1115	X	-	-	-
18	CLA	A	1116	X	-	-	-
18	CLA	A	1117	X	-	-	X
18	CLA	A	1118	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1120	X	-	-	-
18	CLA	A	1121	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	-	-
18	CLA	A	1124	X	-	-	-
18	CLA	A	1125	X	-	-	-
18	CLA	A	1126	X	-	-	-
18	CLA	A	1127	X	-	-	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1130	X	-	-	-
18	CLA	A	1131	X	-	-	-
18	CLA	A	1132	X	-	-	-
18	CLA	A	1133	X	-	-	-
18	CLA	A	1134	X	-	-	-
18	CLA	A	1135	X	-	-	-
18	CLA	A	1136	X	-	-	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1138	X	-	-	-
18	CLA	A	1139	X	-	-	-
18	CLA	A	1140	X	-	-	X
18	CLA	A	1151	X	-	-	-
18	CLA	A	1237	X	-	-	-
18	CLA	B	1012	X	-	-	-
18	CLA	B	1021	X	-	-	-
18	CLA	B	1023	X	-	-	-
18	CLA	B	1201	X	-	-	-
18	CLA	B	1202	X	-	-	-
18	CLA	B	1203	X	-	-	-
18	CLA	B	1204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1205	X	-	-	-
18	CLA	B	1206	X	-	-	-
18	CLA	B	1207	X	-	-	-
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	-	-
18	CLA	B	1210	X	-	-	-
18	CLA	B	1211	X	-	-	-
18	CLA	B	1212	X	-	-	-
18	CLA	B	1213	X	-	-	-
18	CLA	B	1214	X	-	-	-
18	CLA	B	1215	X	-	-	-
18	CLA	B	1216	X	-	-	-
18	CLA	B	1217	X	-	-	-
18	CLA	B	1218	X	-	-	-
18	CLA	B	1219	X	-	-	-
18	CLA	B	1220	X	-	-	-
18	CLA	B	1221	X	-	-	-
18	CLA	B	1222	X	-	-	X
18	CLA	B	1223	X	-	-	-
18	CLA	B	1224	X	-	-	-
18	CLA	B	1225	X	-	-	-
18	CLA	B	1226	X	-	-	-
18	CLA	B	1227	X	-	-	-
18	CLA	B	1228	X	-	-	-
18	CLA	B	1229	X	-	-	-
18	CLA	B	1230	X	-	-	-
18	CLA	B	1231	X	-	-	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	X	-	-	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1236	X	-	-	-
18	CLA	B	1238	X	-	-	-
18	CLA	B	1239	X	-	-	-
18	CLA	B	1240	X	-	-	-
18	CLA	F	1301	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	G	1001	X	-	X	-
18	CLA	G	1002	X	-	X	-
18	CLA	G	1003	X	-	X	-
18	CLA	H	1000	X	-	-	-
18	CLA	J	1302	X	-	-	X
18	CLA	K	1001	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	L	1501	X	-	-	-
18	CLA	L	1502	X	-	-	-
18	CLA	L	1503	X	-	-	-
22	BCR	3	3503	-	-	X	-
22	BCR	A	6003	-	-	-	X
22	BCR	A	6007	-	-	-	X
22	BCR	B	6004	-	-	-	X
22	BCR	B	6005	-	-	-	X
22	BCR	B	6009	-	-	-	X
22	BCR	G	2011	-	-	X	-
22	BCR	J	6012	-	-	-	X
22	BCR	J	6013	-	-	-	X
22	BCR	L	6019	-	-	X	X
22	BCR	L	6020	-	-	-	X
27	LUT	1	1501	X	-	X	-
27	LUT	1	1502	X	-	-	-
27	LUT	2	2501	X	-	X	-
27	LUT	2	2502	X	-	X	X
27	LUT	3	3501	X	-	X	X
27	LUT	3	3502	X	-	X	X
27	LUT	4	4501	X	-	X	-
27	LUT	4	4502	X	-	X	-
27	LUT	4	4503	X	-	X	X
27	LUT	I	6018	X	-	-	-
28	CHL	1	1009	-	-	X	-
28	CHL	3	3011	-	-	X	X
29	ZEX	4	4505	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35653 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	742	5852	3833	997	1004	18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	LEU	engineered mutation	UNP P05310
A	22	LEU	VAL	engineered mutation	UNP P05310
A	117	ARG	GLY	engineered mutation	UNP P05310
A	220	GLY	ARG	engineered mutation	UNP P05310

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	732	5856	3851	995	996	14	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	LEU	ILE	engineered mutation	UNP P05311
B	115	ILE	ASN	engineered mutation	UNP P05311
B	273	MET	VAL	engineered mutation	UNP P05311
B	471	SER	THR	engineered mutation	UNP P05311
B	476	VAL	ILE	engineered mutation	UNP P05311
B	477	LEU	PRO	engineered mutation	UNP P05311
B	635	TYR	ILE	engineered mutation	UNP P05311

- Molecule 3 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	29	Total	C	N	O	S	0	0	0
			224	155	35	33	1			

- Molecule 4 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	41	Total	C	N	O	S	0	0	0
			321	217	50	54				

- Molecule 5 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	150	Total	C	N	O	S	0	0	0
			1187	770	207	208	2			

- Molecule 6 is a protein called photosystem I reaction center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	91	Total	C	N	O	S	0	0	0
			689	444	117	128				

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	160	Total	C	N	O	S	0	0	0
			1197	791	190	215	1			

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	0
			1116	720	192	201	3			

- Molecule 10 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	E	66	Total	C	N	O	0	0	0
			530	337	93	100			

- Molecule 11 is a protein called Photosystem I reaction center subunit VI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	H	84	Total	C	N	O	0	0	0
			642	425	97	120			

- Molecule 12 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	57	Total	C	N	O	S	0	0	0
			379	241	64	71	3			

- Molecule 13 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	2	207	Total	C	N	O	S	0	0	0
			1613	1057	263	289	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	133	LEU	ASN	engineered mutation	UNP Q41038

- Molecule 14 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	4	198	Total	C	N	O	S	0	0	0
			1544	1007	252	282	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	128	ASP	ALA	engineered mutation	UNP Q9SQL2

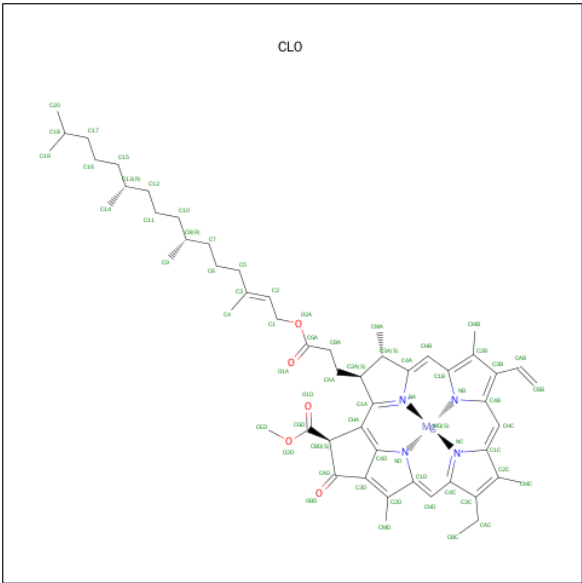
- Molecule 15 is a protein called Light-harvesting complex I chlorophyll A/B-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	194	Total	C	N	O	S	0	0	0
			1513	986	254	268	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

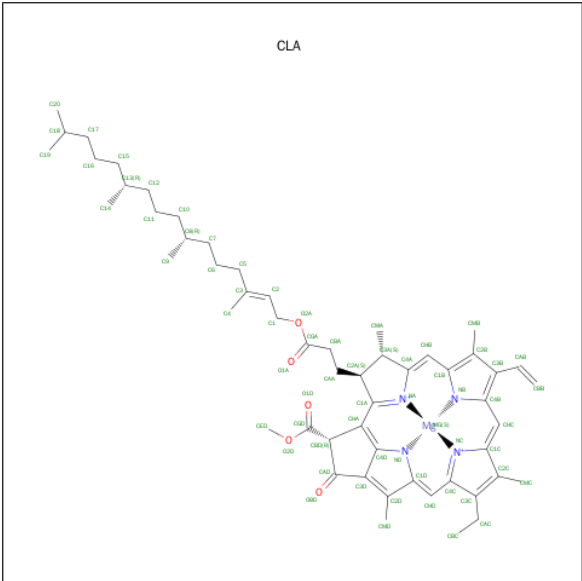
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	3	215	1619	1053	263	298	5	0	0	0

- Molecule 17 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	H	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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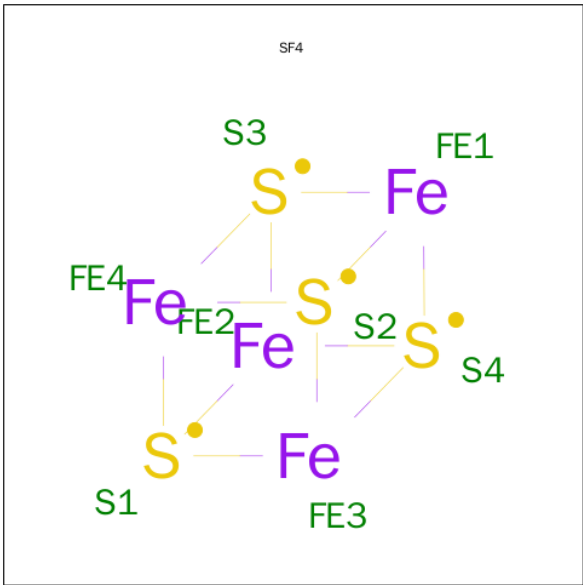
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	2	1	Total 27	C 22	Mg 1	N 4	0	0
18	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	4	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	1	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	1	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	1	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	1	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	1	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	1	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	1	1	Total 46	C 36	Mg 1	N 4 O 5	0	0

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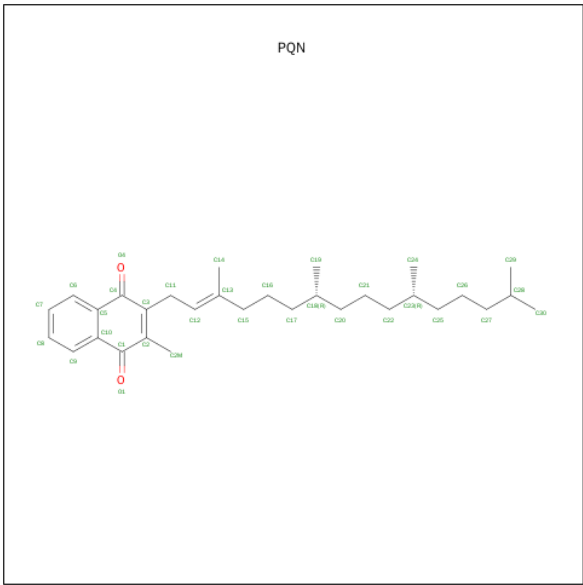
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N		0	0
			27	22	1	4			

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



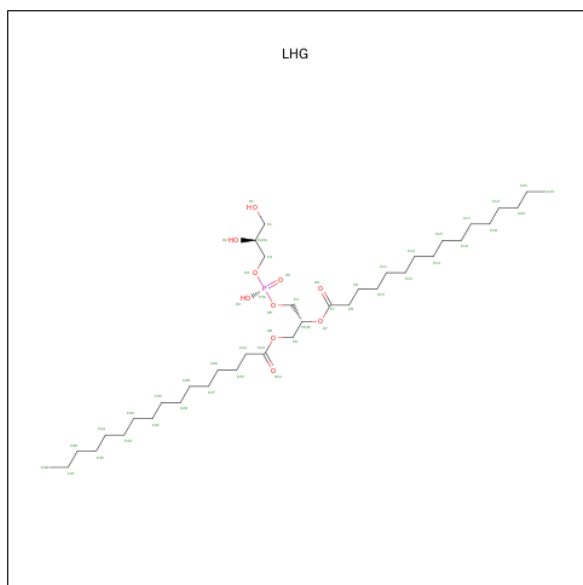
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			33	31	2		

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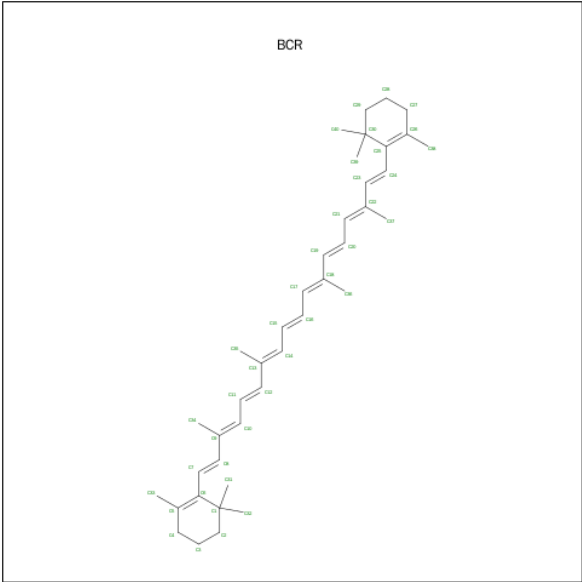
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	O	P	0	0
			40	29	10	1		
21	A	1	Total	C	O	P	0	0
			49	38	10	1		
21	B	1	Total	C	O	P	0	0
			21	10	10	1		
21	2	1	Total	C	O	P	0	0
			24	13	10	1		
21	1	1	Total	C	O	P	0	0
			49	38	10	1		

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



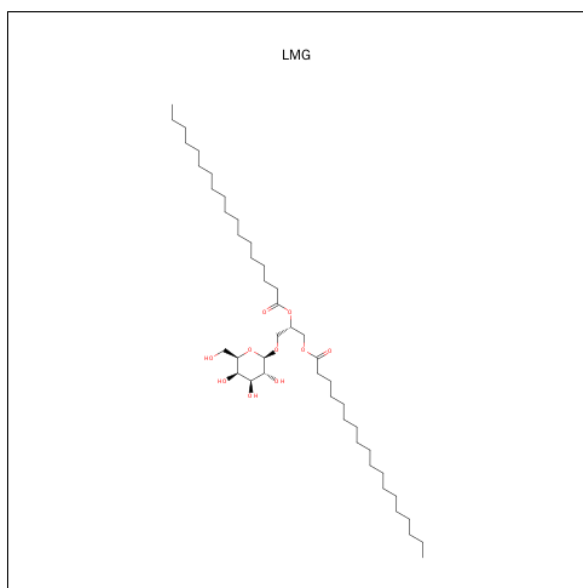
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	3	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 38 28 10	0	0
23	J	1	Total C O 55 45 10	0	0
23	F	1	Total C O 23 13 10	0	0
23	F	1	Total C O 37 27 10	0	0

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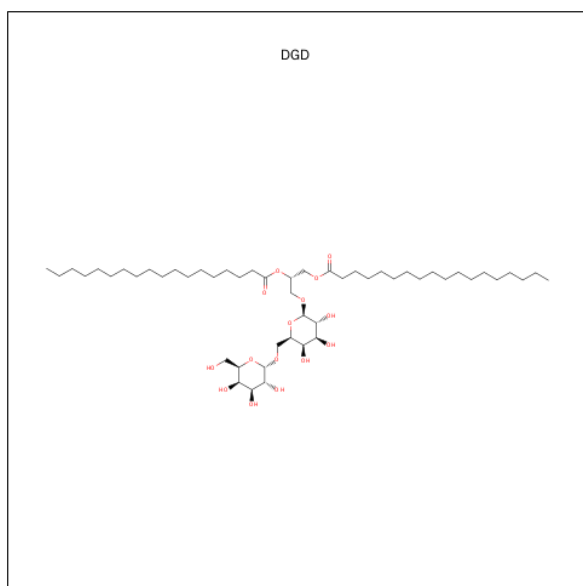
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	G	1	Total	C	O	0	0
			41	31	10		
23	2	1	Total	C	O	0	0
			35	25	10		
23	4	1	Total	C	O	0	0
			35	25	10		

- Molecule 24 is CALCIUM ION (three-letter code: CA) (formula: Ca).

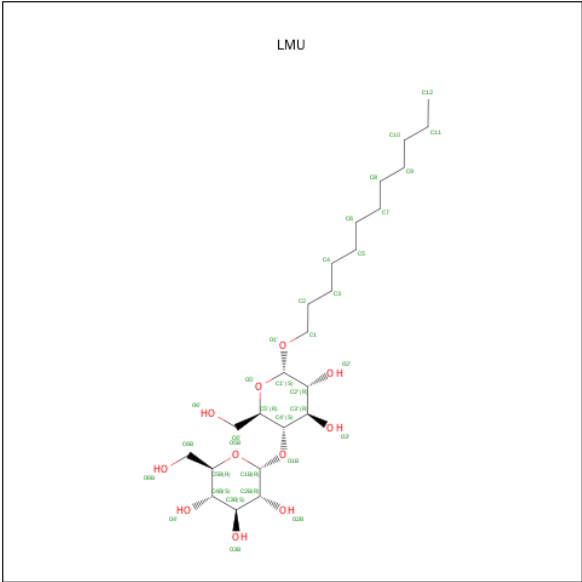
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	B	1	Total	Ca	0	0
			1	1		

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



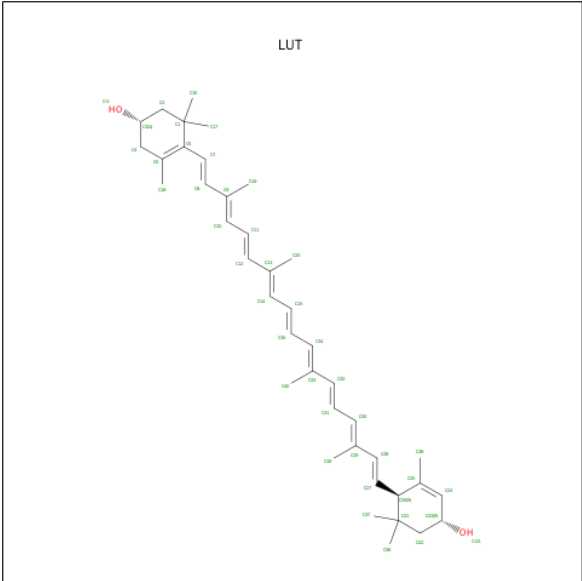
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			61	46	15		

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			35	24	11		
26	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



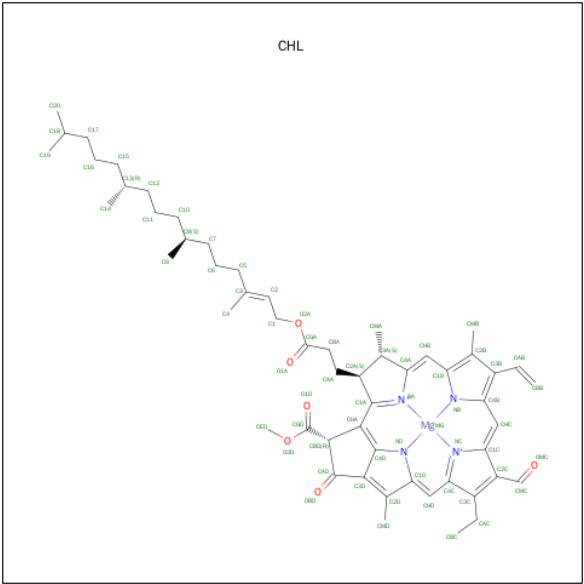
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	I	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	2	1	Total	C	O	0	0
			42	40	2		
27	2	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	1	1	Total	C	O	0	0
			42	40	2		
27	1	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		

- Molecule 28 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



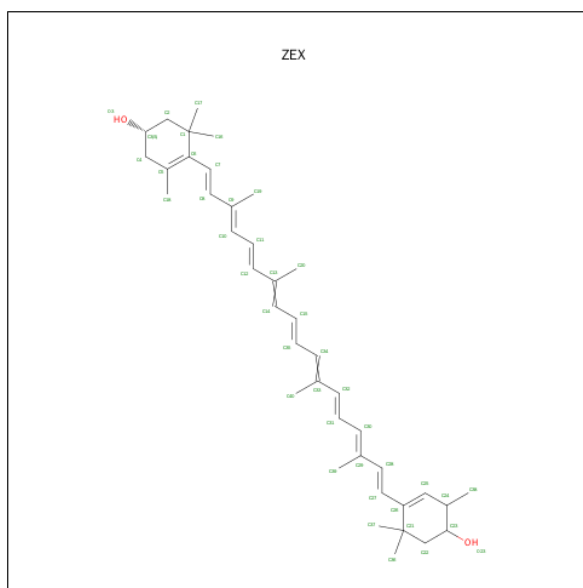
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	3	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 29 is (3S,5R,6S,3'S,5'R,6'S) BETA-CAROTENE-3,23-DIOL (three-letter code: ZEX) (formula: $C_{40}H_{56}O_2$).

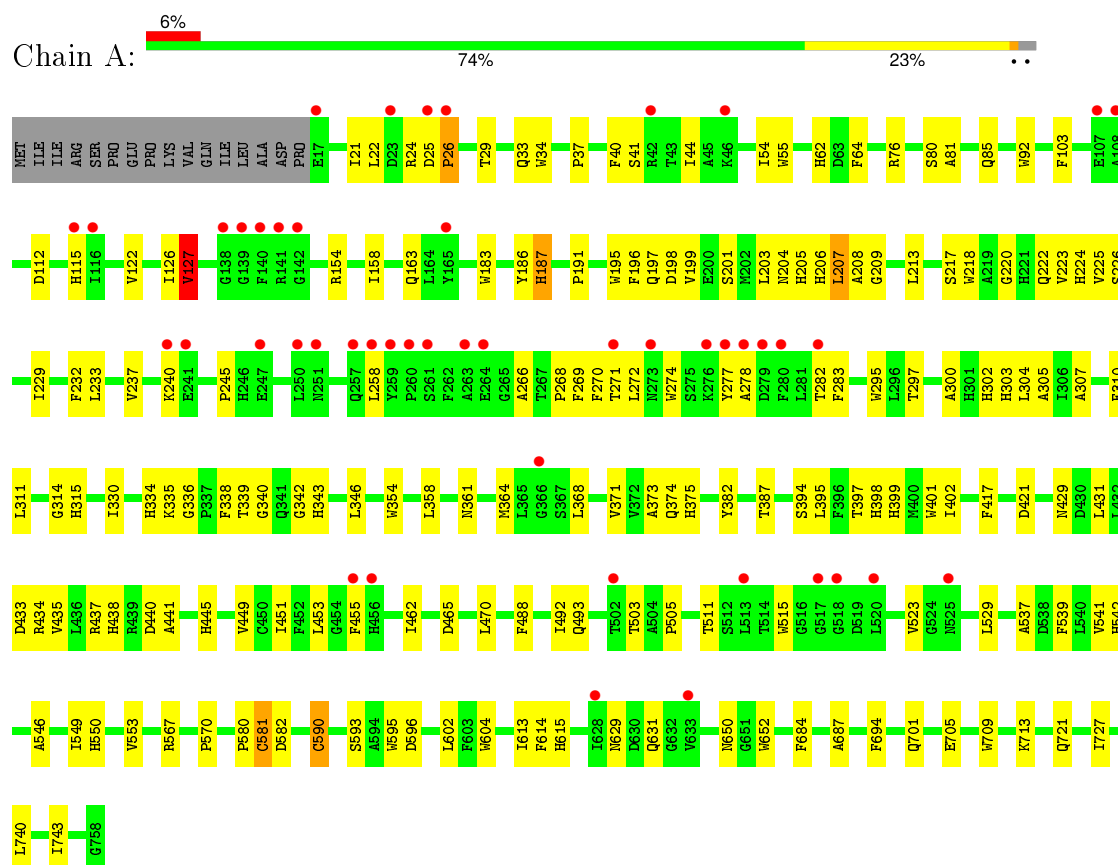


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	4	1	Total	C	O	0	0
			42	40	2		

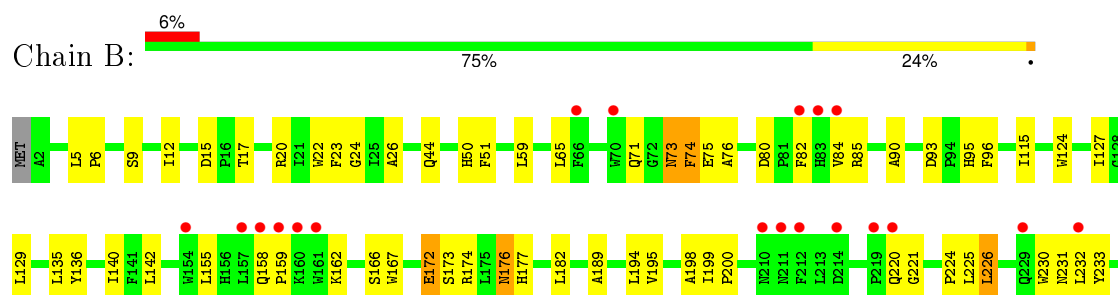
3 Residue-property plots

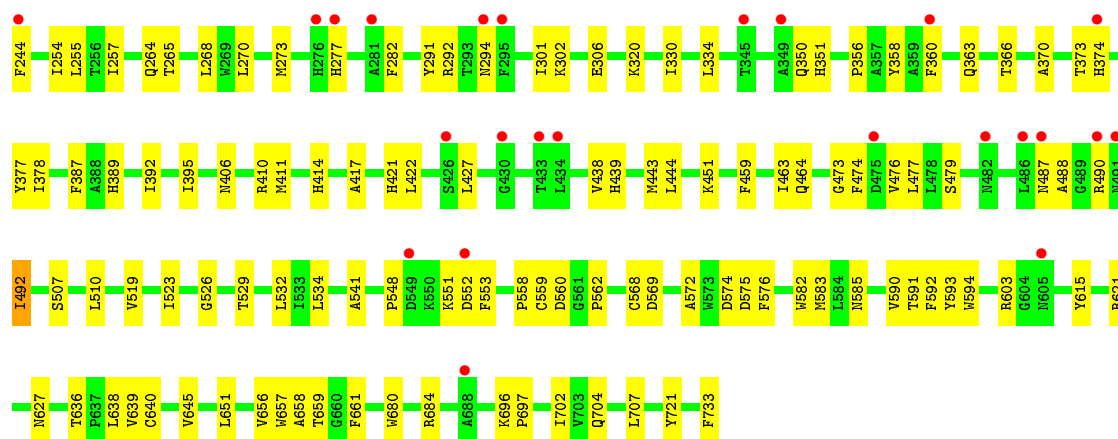
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Photosystem I P700 chlorophyll a apoprotein A1

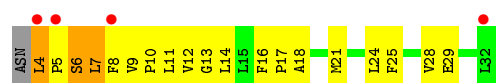


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





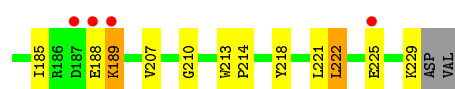
• Molecule 3: Photosystem I reaction center subunit VIII



• Molecule 4: Photosystem I reaction center subunit IX



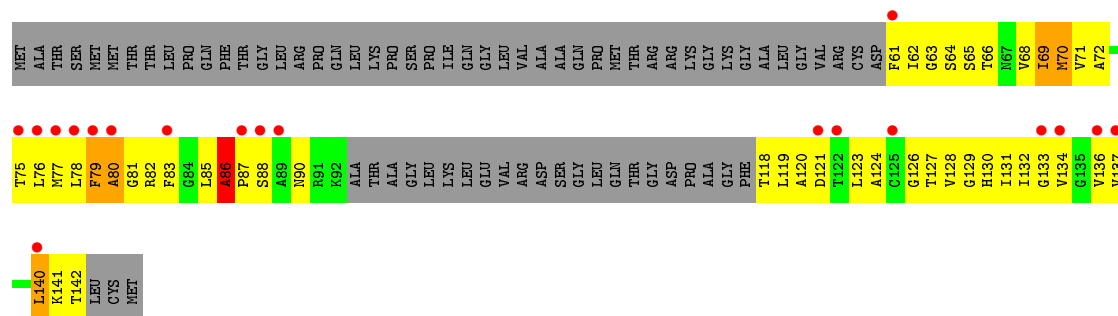
• Molecule 5: Photosystem I reaction center subunit III



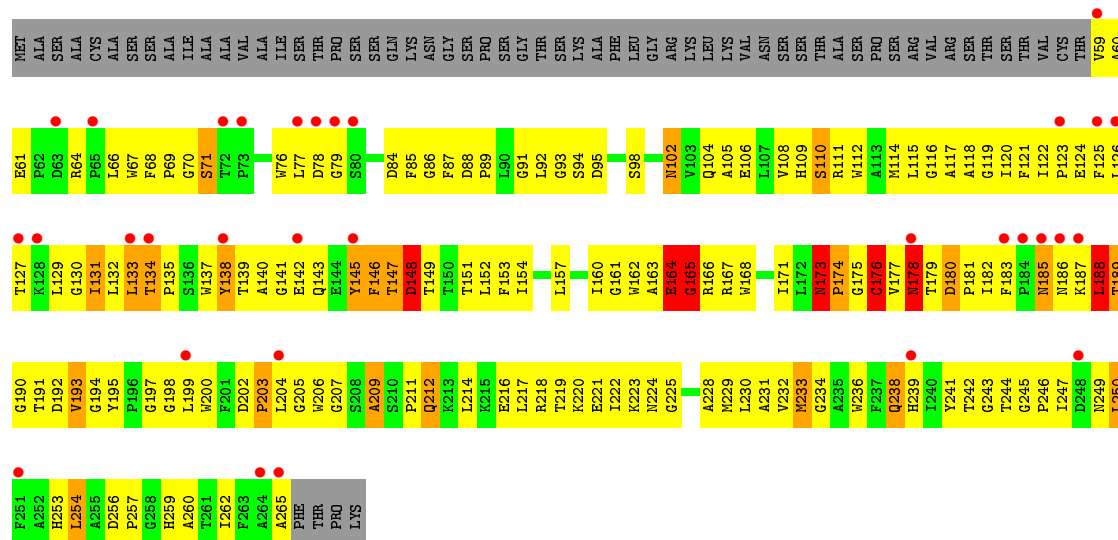
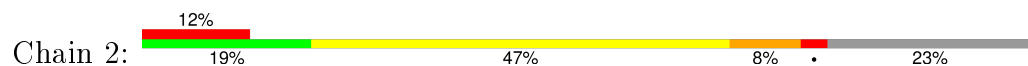
• Molecule 6: photosystem I reaction center



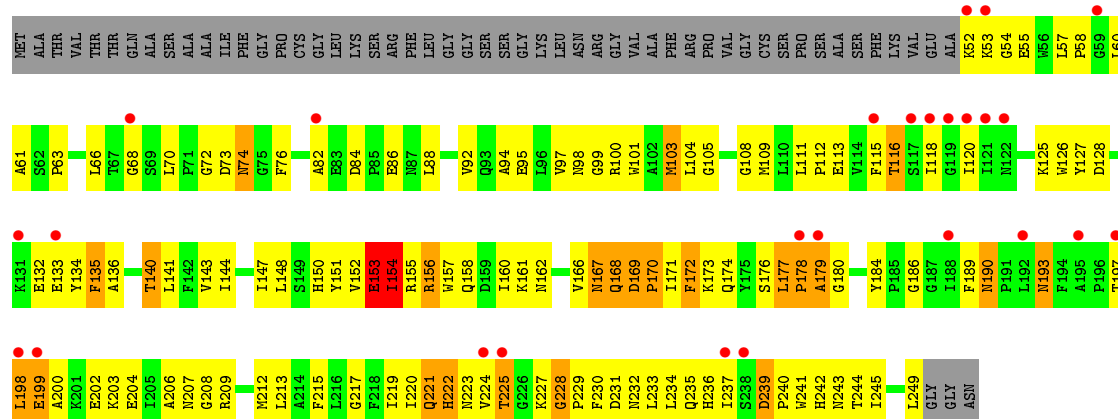
• Molecule 7: Putative uncharacterized protein



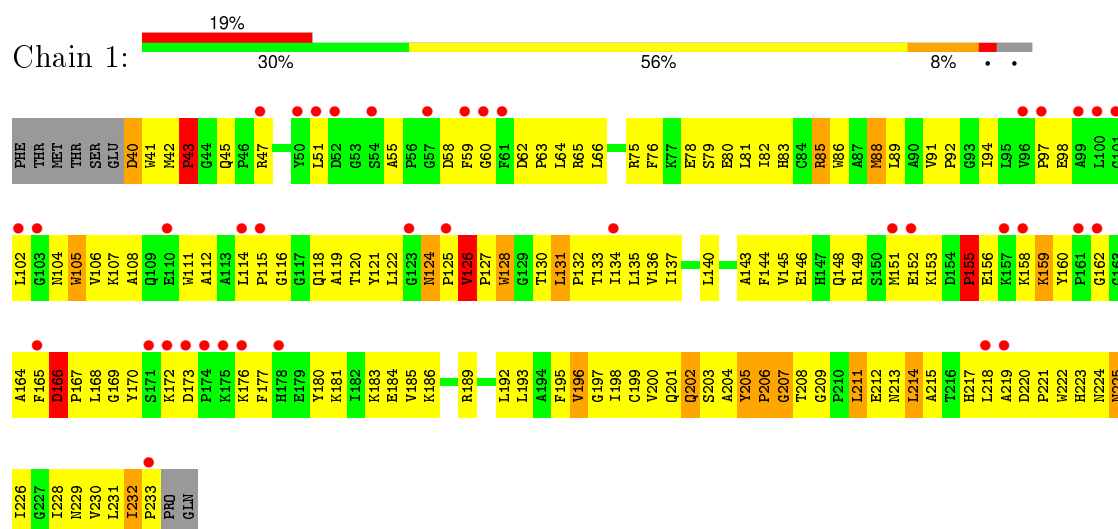
- Molecule 13: Type II chlorophyll a/b binding protein from photosystem I



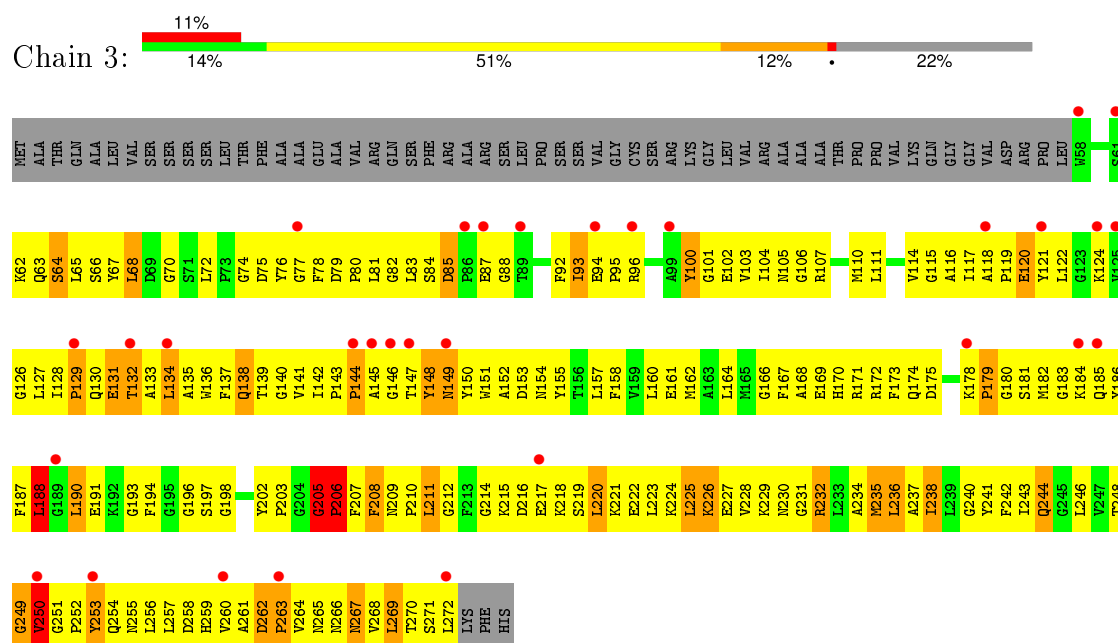
- Molecule 14: Chlorophyll a-b binding protein P4, chloroplastic



- Molecule 15: Light-harvesting complex I chlorophyll A/B-binding protein



- Molecule 16: Chlorophyll a-b binding protein 3, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	189.00Å 201.90Å 213.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.80 39.89 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.65-2.80) 88.8 (39.89-2.79)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.268 0.280 , 0.292	Depositor DCC
R_{free} test set	3970 reflections (2.27%)	DCC
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 199903 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	35653	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LUT, DGD, SF4, CHL, CLA, PQN, LMU, ZEX, CL0, CA, 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	A	0.23	0/6049	0.40	0/8253
2	B	0.24	0/6067	0.40	0/8287
3	I	0.92	0/230	1.02	2/313 (0.6%)
4	J	0.76	0/330	0.90	2/452 (0.4%)
5	F	0.62	0/1214	0.64	0/1638
6	G	0.78	0/705	1.01	3/956 (0.3%)
7	L	0.76	0/1233	0.94	7/1690 (0.4%)
8	C	0.82	0/625	0.81	1/846 (0.1%)
9	D	1.00	0/1146	1.06	7/1550 (0.5%)
10	E	0.89	0/542	0.90	3/737 (0.4%)
11	H	0.62	0/662	0.85	4/902 (0.4%)
12	K	0.48	0/381	0.87	1/517 (0.2%)
13	2	0.94	2/1672 (0.1%)	1.09	11/2292 (0.5%)
14	4	0.93	2/1592 (0.1%)	0.99	10/2174 (0.5%)
15	1	0.86	0/1563	1.04	6/2132 (0.3%)
16	3	0.86	2/1666 (0.1%)	1.08	11/2265 (0.5%)
All	All	0.63	6/25677 (0.0%)	0.76	68/35004 (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
6	G	0	1
7	L	0	1
13	2	0	1
14	4	0	1
16	3	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	153	GLU	C-O	-10.68	1.03	1.23
13	2	164	GLU	C-O	-10.38	1.03	1.23
16	3	205	GLY	C-N	7.70	1.48	1.34
16	3	205	GLY	C-O	-7.23	1.12	1.23
13	2	164	GLU	C-N	6.29	1.44	1.33
14	4	154	ILE	C-N	5.62	1.47	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	101	PHE	C-N-CA	11.02	149.25	121.70
6	G	100	HIS	N-CA-C	-10.25	83.33	111.00
13	2	165	GLY	N-CA-C	-9.45	89.48	113.10
11	H	120	GLY	N-CA-C	-8.68	91.41	113.10
16	3	206	PRO	CA-N-CD	-8.59	99.47	111.50
13	2	164	GLU	CA-C-N	-8.50	99.19	116.20
13	2	190	GLY	N-CA-C	-8.41	92.06	113.10
15	1	155	PRO	CA-N-CD	-8.14	100.10	111.50
16	3	205	GLY	CA-C-N	-8.10	94.42	117.10
14	4	153	GLU	CA-C-N	-8.02	99.56	117.20
7	L	174	ASP	N-CA-C	7.89	132.29	111.00
16	3	205	GLY	CA-C-O	7.72	134.49	120.60
14	4	153	GLU	O-C-N	-7.71	110.37	122.70
13	2	180	ASP	N-CA-C	-7.57	90.56	111.00
13	2	165	GLY	CA-C-N	-7.52	100.66	117.20
13	2	165	GLY	C-N-CA	-7.50	102.95	121.70
15	1	43	PRO	CA-N-CD	-7.31	101.27	111.50
15	1	207	GLY	N-CA-C	-7.10	95.35	113.10
10	E	113	ALA	N-CA-C	-6.98	92.17	111.00
13	2	165	GLY	O-C-N	6.97	133.86	122.70
9	D	173	VAL	CB-CA-C	-6.87	98.35	111.40
14	4	154	ILE	N-CA-C	-6.82	92.60	111.00
16	3	249	GLY	N-CA-C	-6.78	96.14	113.10
13	2	164	GLU	O-C-N	-6.70	111.81	123.20
16	3	205	GLY	O-C-N	-6.50	108.74	121.10
15	1	43	PRO	N-CA-C	6.32	128.52	112.10
16	3	134	LEU	N-CA-C	-6.24	94.14	111.00
13	2	148	ASP	N-CA-C	6.19	127.72	111.00
7	L	55	GLN	N-CA-C	5.95	127.07	111.00
11	H	132	PRO	C-N-CD	5.95	140.89	128.40
16	3	208	PHE	C-N-CA	-5.79	107.23	121.70
13	2	147	THR	N-CA-C	5.77	126.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	190	ARG	N-CA-C	-5.72	95.56	111.00
7	L	176	LEU	N-CA-C	-5.71	95.60	111.00
14	4	154	ILE	C-N-CA	-5.70	107.45	121.70
11	H	133	PRO	CA-N-CD	-5.67	103.56	111.50
7	L	175	GLN	N-CA-C	5.61	126.14	111.00
10	E	66	ILE	N-CA-C	5.57	126.04	111.00
9	D	193	GLY	N-CA-C	-5.55	99.23	113.10
9	D	77	PRO	CA-N-CD	-5.55	103.73	111.50
14	4	198	LEU	N-CA-C	-5.55	96.02	111.00
11	H	132	PRO	CA-N-CD	-5.54	103.74	111.50
8	C	17	CYS	CA-CB-SG	-5.45	104.19	114.00
15	1	166	ASP	C-N-CD	5.39	139.72	128.40
15	1	232	ILE	C-N-CD	5.39	139.72	128.40
9	D	159	PHE	C-N-CD	5.36	139.66	128.40
7	L	178	THR	N-CA-C	-5.29	96.72	111.00
14	4	177	LEU	C-N-CD	5.28	139.50	128.40
16	3	64	SER	N-CA-C	5.27	125.24	111.00
14	4	180	GLY	N-CA-C	5.27	126.28	113.10
4	J	39	PHE	C-N-CD	5.27	139.46	128.40
16	3	262	ASP	C-N-CD	5.25	139.42	128.40
7	L	172	GLN	C-N-CD	5.25	139.41	128.40
7	L	161	ALA	C-N-CD	5.24	139.41	128.40
16	3	85	ASP	C-N-CD	5.23	139.39	128.40
9	D	158	VAL	N-CA-C	5.20	125.03	111.00
9	D	134	ARG	N-CA-C	5.16	124.93	111.00
13	2	61	GLU	C-N-CD	5.14	139.19	128.40
12	K	86	ALA	C-N-CD	5.14	139.19	128.40
16	3	118	ALA	C-N-CD	5.13	139.18	128.40
14	4	190	ASN	C-N-CD	5.11	139.13	128.40
14	4	228	GLY	C-N-CD	5.10	139.10	128.40
3	I	16	PHE	C-N-CD	5.09	139.09	128.40
6	G	98	VAL	N-CA-C	5.07	124.69	111.00
3	I	7	LEU	CA-CB-CG	-5.06	103.65	115.30
14	4	239	ASP	C-N-CD	5.06	139.02	128.40
10	E	67	GLY	C-N-CD	5.03	138.95	128.40
4	J	11	ALA	C-N-CD	5.00	138.91	128.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	2	164	GLU	Mainchain

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Mol	Chain	Res	Type	Group
16	3	205	GLY	Mainchain
14	4	153	GLU	Mainchain
6	G	101	PHE	Peptide
7	L	98	ARG	Sidechain

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	A	5852	0	5710	169	0
2	B	5856	0	5666	146	0
3	I	224	0	247	34	0
4	J	321	0	328	48	0
5	F	1187	0	1226	39	3
6	G	689	0	675	112	0
7	L	1197	0	1187	165	3
8	C	612	0	594	36	0
9	D	1116	0	1126	103	0
10	E	530	0	530	44	0
11	H	642	0	637	48	0
12	K	379	0	386	92	0
13	2	1613	0	1554	371	0
14	4	1544	0	1489	230	0
15	1	1513	0	1495	379	0
16	3	1619	0	1554	472	0
17	A	65	0	72	6	0
18	1	615	0	511	235	0
18	2	628	0	538	255	0
18	3	698	0	559	265	0
18	4	677	0	635	195	0
18	A	2583	0	2555	197	0
18	B	2519	0	2617	217	0
18	F	95	0	72	20	0
18	G	161	0	141	92	0
18	H	46	0	33	4	0
18	J	50	0	39	7	0
18	K	46	0	33	12	0
18	L	160	0	137	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	8	0	0	1	0
19	C	16	0	0	0	0
20	A	33	0	46	3	0
20	B	33	0	46	5	0
21	1	49	0	74	15	0
21	2	24	0	18	6	0
21	A	89	0	127	12	0
21	B	21	0	12	1	0
22	3	40	0	48	21	0
22	A	240	0	292	21	0
22	B	200	0	245	24	0
22	F	80	0	98	19	0
22	G	40	0	49	29	0
22	I	40	0	49	3	0
22	J	80	0	98	15	0
22	K	40	0	49	17	0
22	L	80	0	98	28	0
23	2	35	0	40	9	0
23	4	35	0	40	6	0
23	B	38	0	46	3	0
23	F	60	0	60	13	0
23	G	41	0	52	20	0
23	J	55	0	86	9	0
24	B	1	0	0	0	0
25	B	61	0	83	4	0
26	B	70	0	92	4	0
27	1	84	0	110	48	0
27	2	84	0	110	55	0
27	3	84	0	110	62	0
27	4	126	0	165	84	0
27	I	42	0	55	14	0
28	1	103	0	78	35	0
28	2	141	0	95	39	0
28	3	56	0	47	22	0
28	4	145	0	99	44	0
29	4	42	0	56	12	0
All	All	35653	0	35119	3560	3

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 50.

All (3560) 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)
16:3:138:GLN:HB2	16:3:145:ALA:HB2	1.25	1.18
18:3:3012:CLA:HBB1	18:3:3012:CLA:HMB1	1.18	1.17
16:3:268:VAL:HG21	18:3:3003:CLA:H43	1.17	1.16
18:3:3004:CLA:HBB1	18:3:3004:CLA:HMB1	1.25	1.15
16:3:111:LEU:HD22	18:3:3006:CLA:CBB	1.74	1.15
16:3:127:LEU:HB2	18:3:3018:CLA:HBC1	1.29	1.15
7:L:85:ASN:HB3	18:L:1501:CLA:HAC1	1.26	1.14
18:4:4009:CLA:HHC	18:4:4009:CLA:HBB1	1.28	1.14
27:4:4502:LUT:H28	27:4:4502:LUT:H381	1.27	1.13
18:2:2012:CLA:HMB1	18:2:2012:CLA:HBB1	1.27	1.13
13:2:122:ILE:HG23	13:2:133:LEU:HB2	1.31	1.12
18:2:2002:CLA:HMC1	18:2:2002:CLA:HBC2	1.30	1.12
13:2:139:THR:H	28:2:2010:CHL:CED	1.61	1.12
18:2:2001:CLA:H42	18:2:2002:CLA:HBA1	1.30	1.12
12:K:69:ILE:HA	18:K:1001:CLA:O1A	1.50	1.12
18:4:4007:CLA:HBB1	18:4:4007:CLA:HHC	1.30	1.12
22:K:2011:BCR:HC8	22:K:2011:BCR:H321	1.31	1.12
14:4:118:ILE:HD13	14:4:120:ILE:HD11	1.33	1.11
13:2:126:LEU:HB3	13:2:133:LEU:HD13	1.32	1.11
7:L:113:PRO:HG3	18:L:1503:CLA:HBB1	1.21	1.11
18:2:2004:CLA:H52	27:2:2502:LUT:H383	1.32	1.10
13:2:131:ILE:HD12	13:2:133:LEU:HD21	1.15	1.10
18:4:4001:CLA:H12	27:4:4501:LUT:H373	1.24	1.10
16:3:206:PRO:HD2	16:3:207:PHE:HB2	1.17	1.10
18:3:3010:CLA:HMB1	18:3:3013:CLA:HAB	1.16	1.10
7:L:58:GLN:HG3	7:L:59:PRO:HD2	1.35	1.09
18:1:1003:CLA:HBB1	18:1:1003:CLA:H92	1.11	1.09
18:2:2016:CLA:HBB1	18:2:2016:CLA:HHC	1.33	1.08
7:L:145:LEU:HD11	22:L:6019:BCR:H392	1.34	1.08
4:J:2:ARG:HE	4:J:4:LEU:HD12	1.17	1.08
27:4:4503:LUT:H8	27:4:4503:LUT:H181	1.31	1.08
18:G:1001:CLA:H62	22:G:2011:BCR:H343	1.28	1.08
18:G:1001:CLA:HHC	18:G:1001:CLA:HBB1	1.31	1.07
15:1:114:LEU:HD23	15:1:115:PRO:HD2	1.25	1.07
18:4:4002:CLA:H12	18:4:4002:CLA:HMA2	1.13	1.07
18:2:2009:CLA:HHC	18:2:2009:CLA:HBB1	1.27	1.07
13:2:223:LYS:NZ	21:2:2801:LHG:O5	1.88	1.07
16:3:94:GLU:OE2	16:3:96:ARG:N	1.86	1.07
13:2:87:PHE:CZ	27:2:2502:LUT:H372	1.89	1.06
11:H:96:ARG:HG2	11:H:97:GLY:H	1.19	1.06
13:2:70:GLY:O	16:3:178:LYS:NZ	1.88	1.06
13:2:166:ARG:NH1	18:4:4009:CLA:OBD	1.88	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:149:ARG:NH2	18:1:1012:CLA:O1D	1.87	1.06
6:G:92:LEU:H	6:G:92:LEU:HD12	1.19	1.06
18:2:2006:CLA:HBD	18:2:2006:CLA:H43	1.35	1.05
28:1:1010:CHL:HMC	28:1:1010:CHL:HBC3	1.38	1.05
16:3:111:LEU:CD2	18:3:3006:CLA:HBB2	1.84	1.05
16:3:111:LEU:CD2	18:3:3006:CLA:CBB	2.34	1.05
12:K:137:VAL:HA	12:K:140:LEU:HD22	1.35	1.05
12:K:78:LEU:HD22	12:K:82:ARG:HG2	1.06	1.05
18:F:1302:CLA:HHD	18:F:1302:CLA:HBC2	1.35	1.04
7:L:94:ASN:HB2	7:L:97:LEU:HD12	1.34	1.04
14:4:170:PRO:HB2	18:4:4016:CLA:HMA3	1.06	1.04
18:2:2008:CLA:HHD	18:2:2008:CLA:HBC3	1.38	1.03
18:2:2001:CLA:C4	18:2:2002:CLA:HBA1	1.89	1.03
13:2:188:LEU:HD23	13:2:198:GLY:HA3	1.39	1.03
18:3:3003:CLA:H42	18:3:3003:CLA:C1D	1.88	1.03
15:1:97:PRO:HB2	15:1:102:LEU:HB2	1.35	1.03
18:4:4007:CLA:HBC2	18:4:4007:CLA:HHD	1.37	1.03
7:L:176:LEU:HD12	7:L:177:GLN:H	1.23	1.03
13:2:186:ASN:ND2	18:2:2016:CLA:O1D	1.90	1.03
16:3:164:LEU:HB3	22:3:3503:BCR:H351	1.41	1.02
12:K:72:ALA:HB3	18:K:1001:CLA:O2A	1.60	1.02
14:4:150:HIS:HA	18:4:4012:CLA:HAB	1.40	1.02
18:3:3002:CLA:HHC	18:3:3002:CLA:HBB1	1.42	1.02
13:2:186:ASN:HB3	18:2:2016:CLA:HMA3	1.40	1.02
18:3:3008:CLA:HHC	18:3:3008:CLA:HBB1	1.42	1.01
15:1:114:LEU:CD2	15:1:115:PRO:HD2	1.90	1.01
15:1:85:ARG:HB3	18:1:1001:CLA:HBC3	1.04	1.01
27:3:3501:LUT:H8	27:3:3501:LUT:H161	1.35	1.01
14:4:169:ASP:HB3	18:4:4016:CLA:C3D	1.90	1.01
13:2:114:MET:HE3	18:2:2001:CLA:HMC3	1.04	1.01
13:2:188:LEU:HD23	13:2:198:GLY:CA	1.89	1.01
21:1:1801:LHG:C38	21:1:1801:LHG:H223	1.90	1.00
10:E:66:ILE:HG22	10:E:95:GLN:HE22	1.25	1.00
14:4:63:PRO:HD2	14:4:66:LEU:HD12	1.40	1.00
13:2:200:TRP:NE1	18:2:2016:CLA:HAA2	1.76	1.00
7:L:94:ASN:CB	7:L:97:LEU:HD12	1.91	1.00
13:2:244:THR:HG22	13:2:245:GLY:H	1.25	1.00
8:C:8:TYR:HB3	9:D:191:SER:CB	1.90	1.00
13:2:122:ILE:CG2	13:2:133:LEU:HB2	1.90	1.00
15:1:209:GLY:HA3	15:1:212:GLU:HB3	1.44	1.00
18:G:1003:CLA:H51	23:G:2021:LMG:H311	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:65:LEU:HD13	16:3:67:TYR:CE1	1.96	1.00
18:3:3008:CLA:HBC2	18:3:3008:CLA:HHD	1.41	0.99
18:2:2001:CLA:H11	27:2:2501:LUT:H173	1.44	0.99
28:4:4010:CHL:HHD	28:4:4010:CHL:HBC2	1.42	0.99
12:K:78:LEU:HD22	12:K:82:ARG:CG	1.91	0.99
16:3:205:GLY:HA3	16:3:208:PHE:CA	1.89	0.99
15:1:183:LYS:HG3	18:1:1007:CLA:HED2	1.41	0.99
15:1:183:LYS:HD3	18:1:1002:CLA:HAA2	1.40	0.99
16:3:241:TYR:CE1	27:3:3501:LUT:H162	1.97	0.99
18:2:2016:CLA:HBA2	18:2:2016:CLA:HBD	1.43	0.99
18:3:3005:CLA:H93	18:3:3012:CLA:H43	1.44	0.99
15:1:85:ARG:CB	18:1:1001:CLA:HBC3	1.93	0.99
15:1:183:LYS:HD3	18:1:1002:CLA:CAA	1.92	0.99
6:G:108:ALA:HB1	6:G:111:TYR:CD1	1.98	0.98
13:2:262:ILE:HD11	18:2:2003:CLA:H11	1.45	0.98
16:3:268:VAL:HG23	18:3:3003:CLA:H12	1.41	0.98
18:3:3018:CLA:HBB1	18:3:3018:CLA:HMB1	1.45	0.98
15:1:88:MET:HB2	18:1:1001:CLA:HMC3	1.45	0.98
10:E:122:LEU:H	10:E:122:LEU:HD12	1.25	0.98
13:2:139:THR:H	28:2:2010:CHL:HED1	1.29	0.97
13:2:219:THR:HG22	18:2:2007:CLA:HED3	1.43	0.97
12:K:124:ALA:HB1	22:K:2011:BCR:HC7	1.46	0.97
15:1:97:PRO:CB	15:1:102:LEU:HB2	1.93	0.97
15:1:221:PRO:HG2	15:1:222:TRP:CE3	1.98	0.97
22:G:2011:BCR:H23C	22:G:2011:BCR:H403	1.43	0.97
16:3:138:GLN:CB	16:3:145:ALA:HB2	1.94	0.97
13:2:114:MET:HE3	18:2:2001:CLA:CMC	1.93	0.97
18:4:4003:CLA:HHC	18:4:4003:CLA:HBB1	1.46	0.97
13:2:220:LYS:HD3	18:2:2002:CLA:HED2	1.44	0.97
7:L:145:LEU:HD21	22:L:6019:BCR:H403	1.44	0.97
7:L:87:PRO:CD	18:L:1502:CLA:HED2	1.94	0.97
18:1:1008:CLA:HBB1	18:1:1008:CLA:HHC	1.47	0.96
16:3:205:GLY:HA3	16:3:208:PHE:CB	1.95	0.96
29:4:4505:ZEX:H362	29:4:4505:ZEX:H382	1.46	0.96
15:1:98:GLU:CB	15:1:211:LEU:HD21	1.94	0.96
14:4:153:GLU:OE2	14:4:156:ARG:NH1	1.98	0.96
7:L:138:VAL:O	7:L:142:SER:OG	1.84	0.96
13:2:126:LEU:HB3	13:2:133:LEU:CD1	1.96	0.95
18:2:2006:CLA:CBD	18:2:2006:CLA:H43	1.96	0.95
16:3:111:LEU:HD22	18:3:3006:CLA:HBB2	0.97	0.95
2:B:50:HIS:HB3	18:B:1210:CLA:HED3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2001:CLA:HMB1	18:2:2001:CLA:HBB1	1.47	0.95
3:I:4:LEU:HD11	3:I:6:SER:HB2	1.48	0.95
18:4:4008:CLA:HAA1	18:4:4008:CLA:C1	1.96	0.95
9:D:192:ILE:HG22	9:D:193:GLY:H	1.29	0.95
13:2:230:LEU:HD21	18:2:2004:CLA:HMC1	1.44	0.95
16:3:205:GLY:HA3	16:3:208:PHE:HB2	1.47	0.95
13:2:116:GLY:HA2	27:2:2502:LUT:H181	1.48	0.95
18:4:4002:CLA:C1	18:4:4002:CLA:HMA2	1.96	0.94
13:2:126:LEU:HD12	13:2:127:THR:N	1.82	0.94
13:2:87:PHE:CE2	27:2:2502:LUT:H363	2.03	0.94
15:1:222:TRP:CH2	18:1:1008:CLA:HMB3	2.03	0.94
13:2:188:LEU:HD22	13:2:189:THR:N	1.82	0.94
18:4:4001:CLA:C1	27:4:4501:LUT:H373	1.97	0.94
18:4:4007:CLA:CED	18:4:4007:CLA:H2A	1.98	0.93
13:2:106:GLU:O	13:2:110:SER:OG	1.85	0.93
18:3:3010:CLA:CMB	18:3:3013:CLA:HAB	1.97	0.93
12:K:137:VAL:HA	12:K:140:LEU:CD2	1.97	0.93
13:2:220:LYS:N	18:2:2007:CLA:HED1	1.83	0.93
15:1:232:ILE:HG23	15:1:233:PRO:HD2	1.46	0.93
13:2:193:VAL:HG23	13:2:194:GLY:H	1.30	0.93
15:1:202:GLN:NE2	15:1:208:THR:HB	1.84	0.93
13:2:115:LEU:HB3	18:2:2006:CLA:HBB2	1.51	0.93
28:4:4011:CHL:HBC2	28:4:4011:CHL:HHD	1.48	0.93
16:3:136:TRP:O	27:3:3502:LUT:O3	1.85	0.92
14:4:103:MET:HE1	14:4:207:ASN:HB3	1.51	0.92
16:3:209:ASN:OD1	27:3:3501:LUT:O23	1.85	0.92
6:G:77:PHE:HE1	18:G:1002:CLA:HAB	1.33	0.92
14:4:118:ILE:HD13	14:4:120:ILE:CD1	2.00	0.92
16:3:241:TYR:HE1	27:3:3501:LUT:H162	1.28	0.92
4:J:28:GLU:OE1	18:J:1302:CLA:C4D	2.17	0.92
15:1:121:TYR:CD2	15:1:122:LEU:HG	2.04	0.92
13:2:186:ASN:CB	18:2:2016:CLA:HMA3	2.00	0.92
18:2:2003:CLA:HHB	18:2:2008:CLA:HBC3	1.53	0.91
18:1:1011:CLA:C3	27:1:1501:LUT:H23	2.00	0.91
12:K:71:VAL:HG11	12:K:129:GLY:O	1.70	0.91
16:3:206:PRO:HD2	16:3:207:PHE:CB	2.00	0.91
27:4:4501:LUT:H28	27:4:4501:LUT:H371	1.53	0.91
18:3:3010:CLA:HBB1	18:3:3010:CLA:HHC	1.51	0.91
18:2:2007:CLA:H92	18:2:2007:CLA:H51	1.53	0.91
14:4:103:MET:HE3	14:4:207:ASN:C	1.90	0.91
9:D:76:ASP:HB3	9:D:77:PRO:HB3	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:131:ILE:CD1	13:2:133:LEU:HD21	2.00	0.91
18:1:1004:CLA:CBB	27:1:1502:LUT:H12	2.01	0.91
18:1:1003:CLA:CBB	18:1:1003:CLA:H92	2.00	0.90
15:1:126:VAL:HG23	15:1:127:PRO:HA	1.53	0.90
14:4:170:PRO:CB	18:4:4016:CLA:HMA3	1.99	0.90
16:3:184:LYS:HG2	16:3:185:GLN:HG2	1.54	0.90
18:2:2005:CLA:HBC1	18:2:2012:CLA:HBC1	1.52	0.90
18:1:1008:CLA:HED2	18:1:1008:CLA:C3D	2.00	0.90
13:2:163:ALA:O	13:2:166:ARG:HB3	1.72	0.90
18:1:1003:CLA:CGA	18:1:1008:CLA:HED1	2.00	0.90
15:1:127:PRO:HG2	15:1:128:TRP:CD1	2.07	0.90
14:4:125:LYS:NZ	14:4:231:ASP:OD1	2.03	0.90
22:J:6012:BCR:H23C	22:J:6012:BCR:H383	1.51	0.90
13:2:211:PRO:O	13:2:212:GLN:HG3	1.70	0.90
16:3:102:GLU:OE2	16:3:232:ARG:NH2	2.04	0.90
18:B:1229:CLA:HAB	18:B:1230:CLA:HMB2	1.54	0.90
18:2:2004:CLA:H8	27:2:2502:LUT:C38	2.00	0.90
18:1:1001:CLA:HHC	27:1:1501:LUT:H32	1.54	0.90
18:2:2004:CLA:H8	27:2:2502:LUT:H381	1.53	0.90
13:2:115:LEU:CB	18:2:2006:CLA:HBB2	2.02	0.89
27:4:4503:LUT:H363	28:1:1009:CHL:H8	1.53	0.89
16:3:225:LEU:HB3	16:3:226:LYS:NZ	1.87	0.89
15:1:146:GLU:HG2	15:1:149:ARG:HH11	1.35	0.89
18:4:4017:CLA:HED1	21:1:1801:LHG:H151	1.54	0.89
16:3:105:ASN:ND2	18:3:3012:CLA:HMD1	1.88	0.89
28:4:4013:CHL:HHD	28:4:4013:CHL:HBC2	1.54	0.89
16:3:248:THR:HG22	16:3:250:VAL:HG23	1.54	0.89
14:4:158:GLN:HE22	14:4:161:LYS:HE3	1.36	0.89
13:2:70:GLY:HA3	16:3:174:GLN:HE21	1.36	0.89
11:H:96:ARG:O	11:H:98:LEU:N	2.05	0.89
6:G:103:ALA:O	6:G:105:ASP:N	2.04	0.89
16:3:268:VAL:CG2	18:3:3003:CLA:H43	2.03	0.89
15:1:230:VAL:C	15:1:231:LEU:HD23	1.93	0.89
14:4:170:PRO:HB2	18:4:4016:CLA:CMA	1.99	0.89
13:2:120:ILE:HG21	27:2:2501:LUT:C37	2.03	0.89
18:3:3004:CLA:C2	27:3:3502:LUT:H363	2.02	0.89
18:G:1001:CLA:C6	22:G:2011:BCR:H343	2.03	0.88
5:F:221:LEU:C	5:F:222:LEU:HD23	1.94	0.88
18:2:2004:CLA:H52	27:2:2502:LUT:C38	2.03	0.88
14:4:220:ILE:HD12	18:4:4003:CLA:HAC2	1.52	0.88
16:3:203:PRO:HD3	28:3:3011:CHL:HMD2	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:13:GLY:O	3:I:14:LEU:HD23	1.73	0.88
12:K:124:ALA:HB1	22:K:2011:BCR:H331	1.54	0.88
12:K:141:LYS:O	12:K:142:THR:OG1	1.91	0.88
13:2:220:LYS:CD	18:2:2002:CLA:HED2	2.02	0.88
15:1:183:LYS:CG	18:1:1007:CLA:HED2	2.03	0.88
14:4:94:ALA:CA	18:4:4012:CLA:HED2	2.03	0.88
12:K:128:VAL:O	12:K:132:ILE:HG13	1.74	0.88
18:1:1008:CLA:HED2	18:1:1008:CLA:C4D	2.03	0.88
13:2:139:THR:N	28:2:2010:CHL:CED	2.37	0.88
16:3:110:MET:CE	16:3:230:ASN:HB3	2.02	0.88
15:1:232:ILE:HG23	15:1:233:PRO:CD	2.02	0.88
27:3:3502:LUT:H8	27:3:3502:LUT:H161	1.55	0.88
15:1:183:LYS:HD3	18:1:1002:CLA:CBA	2.04	0.88
18:2:2003:CLA:C2B	27:2:2501:LUT:H383	2.03	0.88
18:4:4017:CLA:HMC2	29:4:4505:ZEX:H393	1.54	0.88
16:3:127:LEU:HB2	18:3:3018:CLA:CBC	2.02	0.88
18:3:3003:CLA:H42	18:3:3003:CLA:C2D	2.04	0.88
7:L:121:ARG:CG	7:L:127:GLY:HA2	2.04	0.88
18:1:1005:CLA:HMD2	18:1:1012:CLA:C1D	2.04	0.87
15:1:130:THR:HG22	15:1:132:PRO:CD	2.03	0.87
13:2:219:THR:HG22	18:2:2007:CLA:CED	2.03	0.87
16:3:65:LEU:CB	16:3:68:LEU:HD21	2.03	0.87
10:E:66:ILE:HG22	10:E:95:GLN:NE2	1.88	0.87
18:2:2001:CLA:C1	27:2:2501:LUT:H173	2.04	0.87
18:3:3003:CLA:H11	18:3:3003:CLA:C4D	2.03	0.87
15:1:186:LYS:NZ	21:1:1801:LHG:O5	2.06	0.87
18:2:2005:CLA:H41	18:2:2005:CLA:H72	1.56	0.87
28:2:2013:CHL:HHC	28:2:2013:CHL:HBB1	1.57	0.87
4:J:2:ARG:HE	4:J:4:LEU:CD1	1.88	0.87
9:D:134:ARG:NH2	9:D:136:GLU:OE2	2.05	0.87
13:2:124:GLU:O	13:2:127:THR:HG22	1.75	0.87
18:L:1502:CLA:C4C	22:L:6019:BCR:H282	2.04	0.87
15:1:183:LYS:HG3	18:1:1007:CLA:CED	2.04	0.87
15:1:111:TRP:CZ3	18:1:1006:CLA:HED1	2.10	0.87
13:2:70:GLY:HA3	16:3:174:GLN:NE2	1.90	0.86
14:4:115:PHE:O	14:4:118:ILE:HG22	1.73	0.86
18:2:2005:CLA:H41	18:2:2005:CLA:C7	2.03	0.86
14:4:94:ALA:HA	18:4:4012:CLA:HED2	1.57	0.86
5:F:138:LEU:HD23	5:F:159:GLU:OE2	1.74	0.86
15:1:226:ILE:HG21	18:1:1003:CLA:H42	1.56	0.86
15:1:152:GLU:O	15:1:153:LYS:HD3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:120:ILE:O	13:2:123:PRO:HD2	1.74	0.86
18:1:1001:CLA:H61	27:1:1501:LUT:C30	2.06	0.86
28:4:4011:CHL:HBD	28:4:4011:CHL:HAA1	1.57	0.86
28:3:3011:CHL:HBA2	28:3:3011:CHL:HBD	1.58	0.86
13:2:114:MET:CE	18:2:2001:CLA:HMC3	2.00	0.86
16:3:140:GLY:HA2	18:3:3013:CLA:HBC2	1.57	0.86
12:K:65:SER:O	12:K:69:ILE:HG22	1.74	0.86
18:A:1104:CLA:HED1	18:A:1128:CLA:H2	1.58	0.86
1:A:220:GLY:HA3	18:A:1113:CLA:HBB1	1.55	0.86
15:1:88:MET:HE3	18:1:1001:CLA:HHC	1.57	0.86
15:1:132:PRO:O	15:1:136:VAL:HG23	1.75	0.86
15:1:230:VAL:HG13	18:1:1014:CLA:C1B	2.05	0.85
16:3:220:LEU:HD23	16:3:221:LYS:N	1.91	0.85
27:2:2501:LUT:H28	27:2:2501:LUT:H371	1.55	0.85
16:3:236:LEU:HD23	18:3:3004:CLA:HMC1	1.57	0.85
16:3:131:GLU:OE2	18:3:3018:CLA:HMA3	1.76	0.85
2:B:733:PHE:HB3	11:H:134:LYS:HE2	1.58	0.85
18:1:1005:CLA:HBB1	18:1:1005:CLA:HMB1	1.58	0.85
15:1:152:GLU:C	15:1:153:LYS:HD3	1.96	0.85
7:L:146:THR:O	7:L:150:ILE:HG13	1.76	0.85
18:3:3017:CLA:CGA	18:3:3017:CLA:H3A	2.03	0.85
9:D:76:ASP:HB3	9:D:77:PRO:CB	2.07	0.85
28:2:2010:CHL:CBB	28:2:2013:CHL:HBB2	2.05	0.85
6:G:65:SER:OG	18:G:1001:CLA:HBA1	1.75	0.85
13:2:148:ASP:O	13:2:149:THR:HB	1.74	0.85
18:3:3003:CLA:CMB	27:3:3501:LUT:H173	2.05	0.85
18:G:1003:CLA:C9	18:G:1003:CLA:H13	2.06	0.85
13:2:109:HIS:CD2	18:2:2012:CLA:HMD1	2.11	0.85
16:3:226:LYS:H	16:3:226:LYS:HZ2	1.20	0.85
13:2:143:GLN:HB2	13:2:145:TYR:CE1	2.11	0.85
16:3:110:MET:HE2	16:3:230:ASN:HB3	1.59	0.85
7:L:85:ASN:HB3	18:L:1501:CLA:CAC	2.06	0.85
15:1:111:TRP:CH2	18:1:1006:CLA:HED1	2.12	0.85
18:G:1003:CLA:H13	18:G:1003:CLA:H8	1.56	0.85
16:3:248:THR:HG21	16:3:255:ASN:ND2	1.92	0.85
16:3:135:ALA:N	16:3:138:GLN:HG2	1.91	0.84
16:3:256:LEU:O	16:3:260:VAL:HG23	1.77	0.84
14:4:233:LEU:O	14:4:237:ILE:HG13	1.77	0.84
13:2:127:THR:HG21	13:2:247:ILE:CD1	2.07	0.84
12:K:86:ALA:HB1	12:K:87:PRO:HD3	1.55	0.84
3:I:6:SER:O	3:I:7:LEU:HD22	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:137:VAL:CA	12:K:140:LEU:HD22	2.07	0.84
14:4:217:GLY:O	14:4:221:GLN:HB2	1.77	0.84
16:3:267:ASN:O	16:3:270:THR:OG1	1.93	0.84
15:1:85:ARG:HB3	18:1:1001:CLA:CBC	1.99	0.84
12:K:71:VAL:CG1	12:K:129:GLY:O	2.25	0.84
13:2:116:GLY:HA2	27:2:2502:LUT:C18	2.07	0.84
27:1:1501:LUT:C8	27:1:1501:LUT:H181	2.05	0.84
18:4:4001:CLA:H52	27:4:4501:LUT:H371	1.58	0.84
6:G:149:LYS:NZ	6:G:149:LYS:HB2	1.91	0.84
15:1:148:GLN:O	15:1:151:MET:HG2	1.78	0.84
16:3:146:GLY:O	16:3:147:THR:OG1	1.94	0.84
7:L:121:ARG:HG3	7:L:127:GLY:HA2	1.58	0.84
15:1:126:VAL:CG2	15:1:127:PRO:HA	2.07	0.84
18:4:4006:CLA:C1B	27:4:4503:LUT:H172	2.07	0.84
7:L:120:LEU:HB3	7:L:126:ALA:CB	2.08	0.84
13:2:200:TRP:HE1	18:2:2016:CLA:HAA2	1.41	0.83
18:G:1003:CLA:H13	18:G:1003:CLA:C8	2.08	0.83
8:C:8:TYR:HD2	9:D:191:SER:HA	1.40	0.83
16:3:164:LEU:HB3	22:3:3503:BCR:C35	2.09	0.83
28:4:4013:CHL:CHB	27:4:4503:LUT:H192	2.08	0.83
9:D:192:ILE:HG23	10:E:80:GLU:OE2	1.77	0.83
18:4:4002:CLA:HHC	18:4:4002:CLA:HBB1	1.60	0.83
12:K:64:SER:O	12:K:68:VAL:HG23	1.79	0.83
16:3:208:PHE:HB3	18:3:3001:CLA:HMD1	1.61	0.83
16:3:269:LEU:HD11	18:3:3008:CLA:HED1	1.58	0.83
22:A:6003:BCR:H23C	18:A:1103:CLA:H61	1.61	0.83
18:2:2002:CLA:C1	18:2:2002:CLA:HED1	2.09	0.83
18:2:2004:CLA:HMB1	18:2:2004:CLA:HBB1	1.58	0.83
18:2:2016:CLA:HHD	18:2:2016:CLA:HBC2	1.59	0.83
18:3:3013:CLA:HMA2	22:3:3503:BCR:C35	2.08	0.83
15:1:230:VAL:O	15:1:231:LEU:HD23	1.78	0.83
18:4:4005:CLA:OBD	18:4:4012:CLA:HBA2	1.78	0.83
6:G:116:LYS:HG3	18:G:1002:CLA:ND	1.93	0.83
13:2:186:ASN:HD21	18:2:2016:CLA:CGD	1.91	0.82
13:2:220:LYS:CE	18:2:2002:CLA:HED2	2.09	0.82
16:3:190:LEU:HB2	16:3:207:PHE:CZ	2.14	0.82
15:1:88:MET:HB2	18:1:1001:CLA:CMC	2.09	0.82
13:2:233:MET:HA	13:2:233:MET:CE	2.08	0.82
7:L:85:ASN:CB	18:L:1501:CLA:HAC1	2.07	0.82
18:2:2016:CLA:CBA	18:2:2016:CLA:HBD	2.09	0.82
18:2:2009:CLA:HED3	16:3:171:ARG:CG	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:120:THR:HG22	15:1:124:ASN:C	1.98	0.82
15:1:164:ALA:O	15:1:167:PRO:HD3	1.80	0.82
18:4:4005:CLA:HMD2	18:4:4012:CLA:CHD	2.09	0.82
18:4:4007:CLA:HBB1	18:4:4007:CLA:CHC	2.09	0.82
13:2:151:THR:O	13:2:154:ILE:HG22	1.78	0.82
16:3:226:LYS:CE	18:3:3007:CLA:HED2	2.09	0.82
13:2:239:HIS:O	13:2:243:GLY:N	2.11	0.82
13:2:87:PHE:CE2	27:2:2502:LUT:H372	2.15	0.82
28:4:4010:CHL:CBB	28:4:4013:CHL:HBB2	2.10	0.82
3:I:14:LEU:C	3:I:17:PRO:HD2	2.00	0.82
7:L:87:PRO:HD2	18:L:1502:CLA:HED2	1.61	0.82
18:3:3001:CLA:CGA	27:3:3501:LUT:H382	2.09	0.82
18:3:3001:CLA:HBA1	27:3:3501:LUT:H382	1.62	0.82
18:3:3006:CLA:HED2	18:3:3006:CLA:C1A	2.09	0.82
13:2:131:ILE:HG22	13:2:132:LEU:H	1.45	0.82
6:G:65:SER:CB	18:G:1001:CLA:HBA1	2.09	0.82
6:G:139:LEU:O	6:G:142:SER:OG	1.98	0.82
27:3:3502:LUT:H361	27:3:3502:LUT:H28	1.61	0.82
4:J:36:ALA:HB1	23:J:5001:LMG:H111	1.60	0.82
18:3:3004:CLA:O1A	18:3:3004:CLA:H3A	1.80	0.81
27:4:4503:LUT:H363	28:1:1009:CHL:C9	2.10	0.81
18:2:2002:CLA:HMB1	18:2:2002:CLA:HBB1	1.62	0.81
13:2:87:PHE:HE2	27:2:2502:LUT:H363	1.43	0.81
18:G:1001:CLA:H41	22:G:2011:BCR:H342	1.60	0.81
13:2:139:THR:HG23	13:2:142:GLU:OE2	1.80	0.81
18:2:2007:CLA:HBC2	18:2:2007:CLA:HMC1	1.63	0.81
18:3:3002:CLA:HBC2	18:3:3002:CLA:HMC1	1.62	0.81
14:4:152:VAL:O	14:4:155:ARG:HB3	1.79	0.81
18:L:1501:CLA:HBA1	18:L:1501:CLA:CHA	2.08	0.81
15:1:226:ILE:HA	18:1:1003:CLA:OBD	1.80	0.81
15:1:106:VAL:CG2	15:1:208:THR:HG21	2.11	0.81
7:L:199:TRP:O	7:L:203:LEU:HD13	1.80	0.81
16:3:248:THR:HG21	16:3:255:ASN:HD22	1.42	0.81
13:2:139:THR:H	28:2:2010:CHL:HED3	1.44	0.81
14:4:103:MET:CE	14:4:207:ASN:HB3	2.09	0.81
13:2:188:LEU:HD13	13:2:188:LEU:O	1.80	0.81
16:3:206:PRO:HA	16:3:209:ASN:C	2.01	0.81
7:L:87:PRO:O	7:L:98:ARG:HD2	1.80	0.81
6:G:61:SER:HB2	18:G:1001:CLA:OBD	1.81	0.81
2:B:166:SER:HB3	6:G:102:GLU:HB2	1.63	0.81
13:2:131:ILE:HB	13:2:133:LEU:CD1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:111:TRP:CD1	15:1:119:ALA:HB2	2.16	0.81
15:1:85:ARG:HH21	18:1:1001:CLA:C4D	1.93	0.81
18:K:1001:CLA:HBB1	18:K:1001:CLA:HHC	1.62	0.81
18:G:1001:CLA:CAB	22:G:2011:BCR:H363	2.11	0.81
18:2:2009:CLA:CHC	18:2:2009:CLA:HBB1	2.09	0.81
16:3:258:ASP:CB	16:3:266:ASN:HD21	1.93	0.81
4:J:6:THR:HG21	23:F:5001:LMG:HC72	1.62	0.81
15:1:202:GLN:NE2	15:1:202:GLN:O	2.12	0.80
7:L:176:LEU:O	7:L:178:THR:HG22	1.80	0.80
9:D:204:THR:HG22	9:D:206:LYS:HG2	1.62	0.80
13:2:66:LEU:H	16:3:186:TYR:HE2	1.25	0.80
15:1:106:VAL:HG21	15:1:208:THR:HG21	1.60	0.80
13:2:123:PRO:HA	13:2:126:LEU:HD21	1.62	0.80
18:3:3018:CLA:HBC2	18:3:3018:CLA:HMC1	1.63	0.80
3:I:6:SER:C	3:I:7:LEU:HD22	2.02	0.80
12:K:63:GLY:O	12:K:66:THR:HG22	1.82	0.80
13:2:68:PHE:HB3	13:2:71:SER:OG	1.81	0.80
16:3:142:ILE:HD11	18:3:3010:CLA:HBC3	1.60	0.80
18:2:2008:CLA:HBC3	18:2:2008:CLA:CHD	2.11	0.80
16:3:269:LEU:HD11	18:3:3008:CLA:CED	2.11	0.80
6:G:137:TYR:O	6:G:141:THR:HG23	1.81	0.80
13:2:219:THR:C	18:2:2007:CLA:HED1	2.01	0.80
27:3:3502:LUT:H371	27:3:3502:LUT:C28	2.11	0.80
18:3:3006:CLA:HBB1	18:3:3006:CLA:HHC	1.63	0.80
18:4:4008:CLA:HHD	18:4:4008:CLA:HBC2	1.63	0.80
18:3:3003:CLA:C3B	27:3:3501:LUT:H172	2.12	0.80
15:1:130:THR:HG22	15:1:132:PRO:HD2	1.63	0.80
18:1:1004:CLA:HMD2	28:1:1009:CHL:CBB	2.10	0.80
14:4:152:VAL:C	14:4:155:ARG:HB3	2.03	0.80
9:D:76:ASP:HB3	9:D:77:PRO:CA	2.12	0.80
4:J:10:VAL:HG11	23:F:5001:LMG:O2	1.82	0.80
13:2:137:TRP:HH2	13:2:236:TRP:HA	1.46	0.80
16:3:107:ARG:HB2	28:3:3011:CHL:HED1	1.63	0.80
18:1:1004:CLA:O1A	18:1:1004:CLA:H3A	1.80	0.80
15:1:126:VAL:CB	15:1:127:PRO:HA	2.12	0.80
23:J:5001:LMG:O3	5:F:128:ARG:NH2	2.15	0.80
16:3:206:PRO:CD	16:3:207:PHE:HB2	2.07	0.79
13:2:68:PHE:HD2	13:2:71:SER:HB3	1.47	0.79
13:2:230:LEU:CD2	18:2:2004:CLA:HMC1	2.12	0.79
13:2:127:THR:HG21	13:2:247:ILE:HD13	1.63	0.79
16:3:106:GLY:O	16:3:110:MET:HB2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:111:TRP:CZ2	18:1:1013:CLA:HBC1	2.17	0.79
6:G:144:ASN:ND2	18:G:1003:CLA:HED2	1.96	0.79
6:G:76:ARG:HE	6:G:116:LYS:HE2	1.46	0.79
5:F:132:ASN:O	5:F:136:GLN:HG2	1.81	0.79
13:2:126:LEU:HA	13:2:130:GLY:O	1.81	0.79
13:2:120:ILE:HG21	27:2:2501:LUT:H373	1.63	0.79
18:3:3005:CLA:HMD2	18:3:3012:CLA:C1D	2.13	0.79
6:G:76:ARG:HG3	6:G:77:PHE:CE1	2.17	0.79
18:K:1001:CLA:HHO	18:K:1001:CLA:HBC2	1.62	0.79
18:4:4012:CLA:H122	18:4:4012:CLA:H91	1.65	0.79
18:2:2004:CLA:HMD2	18:2:2009:CLA:CBB	2.12	0.79
16:3:138:GLN:HB2	16:3:145:ALA:CB	2.09	0.79
18:3:3008:CLA:HBC2	18:3:3008:CLA:CHD	2.10	0.79
15:1:225:ASN:O	15:1:228:ILE:HG22	1.83	0.79
12:K:133:GLY:O	12:K:137:VAL:HG23	1.82	0.79
14:4:170:PRO:HB3	18:4:4016:CLA:C4A	2.13	0.79
28:1:1010:CHL:CBB	18:1:1013:CLA:HBB2	2.11	0.79
6:G:144:ASN:HD22	18:G:1003:CLA:HED2	1.46	0.79
9:D:82:PRO:HG3	9:D:128:ASN:ND2	1.98	0.79
27:3:3501:LUT:H171	27:3:3501:LUT:C8	2.12	0.79
16:3:78:PHE:N	18:3:3004:CLA:OBD	2.16	0.79
7:L:120:LEU:HB3	7:L:126:ALA:HB3	1.63	0.79
15:1:133:THR:O	15:1:137:ILE:HG13	1.82	0.79
15:1:85:ARG:HB2	18:1:1011:CLA:HED2	1.65	0.78
12:K:70:MET:HE2	12:K:71:VAL:CA	2.12	0.78
13:2:87:PHE:HZ	27:2:2502:LUT:H372	1.42	0.78
18:1:1003:CLA:HBA1	18:1:1008:CLA:CED	2.13	0.78
1:A:401:TRP:CD1	18:A:1126:CLA:HAB	2.19	0.78
13:2:187:LYS:O	13:2:188:LEU:HB3	1.83	0.78
15:1:88:MET:CB	18:1:1001:CLA:HMC3	2.13	0.78
6:G:114:VAL:HG11	18:G:1002:CLA:HAA2	1.66	0.78
18:3:3013:CLA:HMA2	22:3:3503:BCR:H353	1.66	0.78
18:1:1003:CLA:HBA1	18:1:1008:CLA:HED1	1.65	0.78
18:B:1238:CLA:HAB	20:B:5002:PQN:H162	1.66	0.78
12:K:70:MET:HE2	12:K:71:VAL:N	1.98	0.78
14:4:169:ASP:HB3	18:4:4016:CLA:C2D	2.12	0.78
18:4:4016:CLA:HBD	18:4:4016:CLA:HBA1	1.65	0.78
18:2:2001:CLA:OBD	18:2:2001:CLA:HED2	1.82	0.78
8:C:75:ARG:NH2	9:D:99:GLU:OE2	2.14	0.78
16:3:138:GLN:O	16:3:145:ALA:HB3	1.82	0.78
15:1:97:PRO:HB2	15:1:102:LEU:CB	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:123:PRO:HA	13:2:126:LEU:CD2	2.14	0.78
18:3:3001:CLA:H43	18:3:3002:CLA:HBA1	1.65	0.78
15:1:202:GLN:HE22	15:1:208:THR:HB	1.48	0.78
14:4:208:GLY:O	14:4:212:MET:HG3	1.83	0.78
9:D:100:PHE:CE1	9:D:158:VAL:HB	2.19	0.78
13:2:262:ILE:HD11	18:2:2003:CLA:C1	2.14	0.78
15:1:146:GLU:HG2	15:1:149:ARG:NH1	1.98	0.78
7:L:132:LEU:O	7:L:132:LEU:HD12	1.82	0.78
18:2:2003:CLA:H42	18:2:2003:CLA:C1D	2.14	0.78
16:3:182:MET:CE	16:3:182:MET:HA	2.14	0.78
15:1:83:HIS:CE1	18:1:1012:CLA:HMD1	2.19	0.78
15:1:114:LEU:HD23	15:1:115:PRO:CD	2.11	0.78
12:K:71:VAL:HG21	12:K:133:GLY:HA2	1.66	0.78
2:B:73:ASN:HD22	2:B:74:PHE:H	1.28	0.78
13:2:139:THR:CA	28:2:2010:CHL:HED3	2.14	0.77
13:2:139:THR:N	28:2:2010:CHL:HED3	2.00	0.77
18:F:1302:CLA:CHD	18:F:1302:CLA:HBC2	2.14	0.77
11:H:96:ARG:HG2	11:H:97:GLY:N	1.97	0.77
16:3:139:THR:HG23	16:3:140:GLY:H	1.49	0.77
13:2:182:ILE:CD1	18:4:4007:CLA:HAB	2.14	0.77
12:K:70:MET:HE2	12:K:71:VAL:CG2	2.15	0.77
18:1:1005:CLA:H12	18:1:1005:CLA:HED1	1.64	0.77
14:4:143:VAL:O	14:4:147:ILE:HG12	1.85	0.77
18:B:1220:CLA:H42	18:B:1221:CLA:H13	1.65	0.77
7:L:139:VAL:O	7:L:143:ILE:HG13	1.85	0.77
6:G:121:LEU:HD23	6:G:121:LEU:O	1.83	0.77
27:2:2502:LUT:H28	27:2:2502:LUT:H361	1.67	0.77
16:3:222:GLU:C	16:3:226:LYS:HZ3	1.87	0.77
14:4:150:HIS:CA	18:4:4012:CLA:HAB	2.14	0.77
6:G:77:PHE:CE1	18:G:1002:CLA:HAB	2.19	0.77
16:3:158:PHE:HB2	18:3:3010:CLA:HMC2	1.67	0.77
16:3:101:GLY:HA2	18:3:3012:CLA:HED2	1.64	0.77
18:1:1003:CLA:CBA	18:1:1008:CLA:HED1	2.14	0.77
18:2:2012:CLA:CBB	18:2:2012:CLA:HMB1	2.14	0.77
16:3:205:GLY:CA	16:3:208:PHE:HB2	2.14	0.77
12:K:71:VAL:HG12	12:K:129:GLY:HA2	1.67	0.77
16:3:152:ALA:HB3	16:3:157:LEU:HD21	1.65	0.77
18:4:4012:CLA:C12	18:4:4012:CLA:H91	2.15	0.77
6:G:149:LYS:HZ2	6:G:149:LYS:HB2	1.48	0.77
13:2:131:ILE:HD12	13:2:133:LEU:CD2	2.08	0.77
16:3:110:MET:SD	16:3:231:GLY:HA2	2.25	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:4503:LUT:H363	28:1:1009:CHL:C8	2.14	0.77
7:L:87:PRO:HB3	7:L:101:GLU:OE1	1.85	0.77
12:K:124:ALA:CB	22:K:2011:BCR:H331	2.15	0.77
6:G:64:ILE:O	6:G:68:THR:HG22	1.85	0.77
6:G:115:SER:HB2	18:G:1002:CLA:OBD	1.84	0.77
16:3:162:MET:HA	16:3:162:MET:CE	2.14	0.77
13:2:233:MET:HA	13:2:233:MET:HE2	1.66	0.76
16:3:110:MET:HE1	16:3:230:ASN:O	1.85	0.76
15:1:232:ILE:HG22	15:1:233:PRO:O	1.85	0.76
3:I:4:LEU:HD12	3:I:6:SER:H	1.50	0.76
16:3:120:GLU:CD	16:3:253:TYR:HB3	2.04	0.76
18:3:3002:CLA:CHC	18:3:3002:CLA:HBB1	2.13	0.76
4:J:2:ARG:HD3	4:J:4:LEU:HB2	1.65	0.76
13:2:131:ILE:HB	13:2:133:LEU:HG	1.67	0.76
15:1:222:TRP:NE1	18:1:1008:CLA:HMA1	1.99	0.76
3:I:14:LEU:O	3:I:17:PRO:HD2	1.86	0.76
12:K:72:ALA:CB	18:K:1001:CLA:O2A	2.32	0.76
18:G:1001:CLA:HBB1	18:G:1001:CLA:CHC	2.09	0.76
16:3:68:LEU:N	16:3:68:LEU:HD13	2.00	0.76
13:2:262:ILE:HD11	18:2:2003:CLA:H43	1.65	0.76
18:3:3003:CLA:H92	18:3:3003:CLA:C1C	2.14	0.76
16:3:155:TYR:CZ	18:3:3010:CLA:HAC1	2.20	0.76
15:1:209:GLY:CA	15:1:212:GLU:HB3	2.14	0.76
7:L:178:THR:HG23	7:L:181:GLY:H	1.49	0.76
13:2:125:PHE:HB3	13:2:131:ILE:CD1	2.16	0.76
16:3:139:THR:HG23	16:3:140:GLY:N	2.01	0.76
18:2:2012:CLA:HBB1	18:2:2012:CLA:CMB	2.08	0.76
16:3:65:LEU:HD13	16:3:67:TYR:HE1	1.49	0.76
1:A:539:PHE:HA	18:A:1136:CLA:HED1	1.65	0.76
13:2:191:THR:HG22	13:2:192:ASP:H	1.51	0.76
13:2:115:LEU:HB3	18:2:2006:CLA:CBB	2.15	0.76
18:2:2003:CLA:H42	18:2:2003:CLA:CHD	2.15	0.76
13:2:246:PRO:HA	13:2:249:ASN:OD1	1.84	0.76
15:1:85:ARG:CB	18:1:1011:CLA:HED2	2.15	0.76
18:A:1123:CLA:HMA3	18:A:1119:CLA:HMB2	1.67	0.76
7:L:176:LEU:HD12	7:L:177:GLN:N	2.00	0.76
1:A:269:PHE:HA	1:A:274:TRP:HE1	1.50	0.76
13:2:178:ASN:O	13:2:187:LYS:HD2	1.85	0.76
16:3:172:ARG:NH2	18:3:3012:CLA:O1D	2.12	0.76
16:3:205:GLY:HA3	16:3:208:PHE:N	2.00	0.76
15:1:192:LEU:O	15:1:196:VAL:HG23	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:3011:CHL:CBA	28:3:3011:CHL:HBD	2.16	0.76
18:3:3006:CLA:HMB3	27:3:3502:LUT:H182	1.68	0.76
18:4:4007:CLA:CBB	18:4:4007:CLA:HHC	2.15	0.76
14:4:221:GLN:O	14:4:225:THR:HB	1.86	0.76
6:G:94:GLU:HB2	6:G:98:VAL:H	1.51	0.76
16:3:161:GLU:OE1	18:3:3010:CLA:HAB	1.86	0.75
15:1:121:TYR:HD2	15:1:122:LEU:HG	1.50	0.75
15:1:126:VAL:HG23	15:1:127:PRO:CA	2.15	0.75
11:H:130:GLN:HB3	11:H:132:PRO:HB3	1.68	0.75
16:3:119:PRO:CB	16:3:133:ALA:HB2	2.17	0.75
27:2:2501:LUT:H371	27:2:2501:LUT:C28	2.17	0.75
16:3:226:LYS:HE3	18:3:3007:CLA:HED2	1.67	0.75
27:1:1502:LUT:H28	27:1:1502:LUT:H371	1.68	0.75
16:3:137:PHE:O	16:3:141:VAL:HG12	1.86	0.75
18:4:4005:CLA:HMD2	18:4:4012:CLA:C4C	2.16	0.75
7:L:176:LEU:CD1	7:L:177:GLN:H	1.97	0.75
6:G:149:LYS:O	6:G:149:LYS:HE3	1.86	0.75
16:3:131:GLU:O	16:3:131:GLU:HG3	1.87	0.75
16:3:185:GLN:HB2	16:3:186:TYR:CD1	2.20	0.75
11:H:133:PRO:HD2	11:H:135:LEU:H	1.52	0.75
18:2:2003:CLA:HHB	18:2:2008:CLA:CBC	2.15	0.75
23:2:2802:LMG:HO5	23:2:2802:LMG:HO4	1.33	0.75
18:3:3010:CLA:CBB	18:3:3010:CLA:HHC	2.16	0.75
14:4:156:ARG:NH2	18:4:4012:CLA:O1D	2.19	0.75
2:B:704:GLN:HG3	25:B:7101:DGD:HA22	1.67	0.75
7:L:130:GLY:O	7:L:133:ALA:N	2.19	0.75
16:3:79:ASP:OD1	16:3:82:GLY:N	2.19	0.75
13:2:199:LEU:O	13:2:199:LEU:HD23	1.87	0.75
13:2:139:THR:HA	28:2:2010:CHL:HED3	1.68	0.75
15:1:58:ASP:HA	18:1:1004:CLA:HED2	1.69	0.75
13:2:130:GLY:O	13:2:133:LEU:HD11	1.87	0.75
16:3:120:GLU:OE1	16:3:252:PRO:HG2	1.87	0.75
18:3:3010:CLA:H93	18:3:3010:CLA:C2C	2.17	0.75
27:4:4503:LUT:C28	27:4:4503:LUT:H371	2.16	0.75
1:A:440:ASP:HB2	9:D:88:THR:HG21	1.68	0.75
16:3:65:LEU:HB3	16:3:68:LEU:HD21	1.67	0.75
16:3:225:LEU:HB3	16:3:226:LYS:CE	2.16	0.75
13:2:129:LEU:HD22	13:2:131:ILE:CG1	2.17	0.74
14:4:158:GLN:NE2	14:4:161:LYS:HE3	2.02	0.74
6:G:84:ARG:NH2	6:G:123:ASP:OD2	2.19	0.74
1:A:503:THR:HG21	18:A:1133:CLA:HMD1	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3003:CLA:H92	18:3:3003:CLA:CHC	2.18	0.74
18:3:3006:CLA:HMD2	18:3:3018:CLA:CAB	2.17	0.74
7:L:113:PRO:CG	18:L:1503:CLA:HBB1	2.12	0.74
14:4:82:ALA:HB1	14:4:88:LEU:HD13	1.68	0.74
16:3:267:ASN:CG	16:3:270:THR:HG23	2.07	0.74
15:1:160:TYR:HB3	18:1:1001:CLA:HED3	1.69	0.74
22:F:6016:BCR:C8	22:F:6016:BCR:H331	2.16	0.74
12:K:130:HIS:O	12:K:134:VAL:HG23	1.86	0.74
14:4:168:GLN:O	18:4:4016:CLA:HED3	1.87	0.74
16:3:101:GLY:HA2	18:3:3012:CLA:CED	2.18	0.74
18:3:3001:CLA:HBA1	27:3:3501:LUT:C38	2.17	0.74
15:1:226:ILE:N	18:1:1003:CLA:O1A	2.20	0.74
18:L:1501:CLA:HBA2	18:H:1000:CLA:HHB	1.69	0.74
6:G:76:ARG:HD2	6:G:76:ARG:O	1.86	0.74
18:2:2002:CLA:HBC2	18:2:2002:CLA:CMC	2.12	0.74
16:3:266:ASN:O	16:3:270:THR:HG21	1.87	0.74
27:3:3502:LUT:C8	27:3:3502:LUT:H161	2.12	0.74
18:1:1003:CLA:C9	18:1:1003:CLA:HBB1	2.04	0.74
15:1:131:LEU:HD23	15:1:131:LEU:N	2.03	0.74
15:1:165:PHE:O	15:1:167:PRO:HD2	1.88	0.74
27:4:4501:LUT:C28	27:4:4501:LUT:H371	2.11	0.74
1:A:24:ARG:HH11	1:A:76:ARG:HH12	1.34	0.74
14:4:235:GLN:HB3	14:4:243:ASN:HD22	1.51	0.74
16:3:225:LEU:HB3	16:3:226:LYS:HZ1	1.51	0.74
28:1:1010:CHL:CMC	28:1:1010:CHL:HBC3	2.17	0.74
18:2:2005:CLA:H71	23:2:2802:LMG:H132	1.70	0.74
9:D:115:MET:HE1	9:D:130:LEU:HD11	1.68	0.74
14:4:213:LEU:HD12	23:4:4801:LMG:H302	1.68	0.74
2:B:488:ALA:O	6:G:146:TYR:OH	2.06	0.74
18:3:3002:CLA:CBB	18:3:3002:CLA:HHC	2.17	0.74
13:2:105:ALA:HB2	18:2:2012:CLA:HED2	1.68	0.74
13:2:174:PRO:HD2	13:2:175:GLY:H	1.52	0.74
16:3:259:HIS:NE2	18:3:3008:CLA:NC	2.36	0.74
18:B:1236:CLA:HED1	18:B:1234:CLA:HMB2	1.69	0.74
9:D:191:SER:C	9:D:192:ILE:HD12	2.07	0.74
13:2:254:LEU:HD23	13:2:254:LEU:N	2.01	0.74
18:3:3013:CLA:CBB	27:3:3502:LUT:H181	2.17	0.74
21:1:1801:LHG:HC61	21:1:1801:LHG:HC81	1.70	0.74
28:4:4013:CHL:HHD	28:4:4013:CHL:CBC	2.18	0.74
14:4:215:PHE:CD2	27:4:4502:LUT:H14	2.22	0.74
18:G:1003:CLA:C5	23:G:2021:LMG:H311	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:116:LYS:HE3	18:G:1002:CLA:NC	2.02	0.74
1:A:217:SER:HA	18:A:1113:CLA:HBB2	1.70	0.74
18:G:1003:CLA:H93	23:G:2021:LMG:H162	1.70	0.73
8:C:10:THR:HG23	8:C:64:SER:OG	1.88	0.73
13:2:250:LEU:CD2	13:2:254:LEU:HD21	2.18	0.73
18:2:2001:CLA:C4	18:2:2002:CLA:H3A	2.17	0.73
15:1:88:MET:HE3	18:1:1001:CLA:CHC	2.17	0.73
14:4:151:TYR:HB2	28:1:1009:CHL:H11	1.69	0.73
21:1:1801:LHG:H383	21:1:1801:LHG:H223	1.70	0.73
18:L:1501:CLA:CBD	18:L:1501:CLA:HBA1	2.18	0.73
12:K:75:THR:HG21	12:K:129:GLY:CA	2.18	0.73
16:3:65:LEU:HD13	16:3:67:TYR:CZ	2.23	0.73
18:2:2003:CLA:HMA1	18:2:2008:CLA:HBC2	1.70	0.73
28:1:1010:CHL:OMC	18:1:1013:CLA:HAB	1.89	0.73
12:K:71:VAL:HG12	12:K:129:GLY:CA	2.18	0.73
12:K:76:LEU:O	12:K:79:PHE:HB2	1.89	0.73
8:C:61:ASP:HB2	10:E:118:ASN:ND2	2.03	0.73
13:2:162:TRP:O	13:2:166:ARG:HB2	1.87	0.73
28:2:2010:CHL:HBB1	28:2:2013:CHL:HBB2	1.68	0.73
12:K:72:ALA:O	12:K:76:LEU:HG	1.89	0.73
10:E:66:ILE:HG23	10:E:67:GLY:N	2.03	0.73
13:2:122:ILE:HG23	13:2:133:LEU:CB	2.16	0.73
18:2:2016:CLA:HBA2	18:2:2016:CLA:CBD	2.17	0.73
18:4:4003:CLA:H93	18:4:4003:CLA:C4B	2.18	0.73
18:4:4017:CLA:HED2	28:1:1009:CHL:HMB2	1.69	0.73
16:3:103:VAL:O	16:3:107:ARG:HG3	1.89	0.73
18:L:1501:CLA:HBA1	18:L:1501:CLA:HBD	1.71	0.73
18:4:4002:CLA:CBB	18:4:4002:CLA:HHC	2.19	0.73
4:J:2:ARG:O	4:J:4:LEU:N	2.20	0.73
4:J:6:THR:CG2	23:F:5001:LMG:HC1	2.19	0.73
11:H:59:ASP:OD1	11:H:59:ASP:N	2.22	0.73
18:1:1003:CLA:C2B	27:1:1501:LUT:H173	2.18	0.73
18:B:1219:CLA:HBB2	22:B:6009:BCR:H343	1.70	0.73
7:L:121:ARG:HG2	7:L:127:GLY:H	1.53	0.73
18:3:3008:CLA:HHC	18:3:3008:CLA:CBB	2.15	0.73
7:L:91:THR:HG22	7:L:175:GLN:NE2	2.03	0.73
18:2:2002:CLA:HED1	18:2:2002:CLA:O2A	1.89	0.73
14:4:169:ASP:HB3	18:4:4016:CLA:C4D	2.19	0.73
23:J:5001:LMG:O10	23:J:5001:LMG:HC8	1.87	0.73
13:2:219:THR:CG2	18:2:2007:CLA:HED3	2.19	0.72
18:3:3001:CLA:CBA	27:3:3501:LUT:H382	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1005:CLA:HMD2	18:1:1012:CLA:ND	2.03	0.72
18:B:1216:CLA:HMB2	18:B:1221:CLA:HMA3	1.71	0.72
5:F:222:LEU:HD23	5:F:222:LEU:N	2.03	0.72
13:2:120:ILE:HD13	27:2:2501:LUT:H373	1.71	0.72
28:2:2011:CHL:HAA1	28:2:2011:CHL:HBD	1.69	0.72
16:3:187:PHE:O	16:3:188:LEU:HB2	1.88	0.72
13:2:131:ILE:HB	13:2:133:LEU:CG	2.20	0.72
27:1:1501:LUT:H8	27:1:1501:LUT:H181	1.69	0.72
7:L:87:PRO:HD3	18:L:1502:CLA:HED2	1.69	0.72
7:L:116:LYS:HD3	18:L:1503:CLA:HMB2	1.71	0.72
18:4:4016:CLA:OBD	18:4:4016:CLA:HED2	1.89	0.72
13:2:118:ALA:CB	18:2:2006:CLA:HMC3	2.19	0.72
14:4:236:HIS:NE2	18:4:4008:CLA:NC	2.38	0.72
2:B:684:ARG:HH21	7:L:67:GLY:HA3	1.55	0.72
18:G:1001:CLA:HAB	22:G:2011:BCR:H363	1.71	0.72
11:H:132:PRO:CD	11:H:133:PRO:HD3	2.19	0.72
7:L:166:LEU:HD23	7:L:166:LEU:O	1.90	0.72
13:2:177:VAL:O	13:2:179:THR:N	2.22	0.72
16:3:166:GLY:HA2	18:3:3012:CLA:CBB	2.19	0.72
18:K:1001:CLA:CBB	18:K:1001:CLA:HHC	2.19	0.72
14:4:225:THR:CG2	14:4:227:LYS:H	2.00	0.72
16:3:184:LYS:CG	16:3:185:GLN:HE21	2.02	0.72
18:3:3004:CLA:CBB	18:3:3004:CLA:HMB1	2.14	0.72
7:L:128:GLN:CB	7:L:204:LEU:HG	2.19	0.72
11:H:112:ALA:O	11:H:115:SER:HB3	1.88	0.72
16:3:244:GLN:O	16:3:248:THR:HB	1.90	0.72
9:D:195:ASN:HD22	9:D:195:ASN:H	1.37	0.72
18:2:2006:CLA:CAD	18:2:2006:CLA:H43	2.18	0.72
18:2:2009:CLA:HED3	16:3:171:ARG:HG3	1.70	0.72
16:3:268:VAL:CG2	18:3:3003:CLA:H12	2.19	0.72
16:3:122:LEU:O	16:3:126:GLY:N	2.23	0.72
7:L:121:ARG:HA	7:L:124:GLU:O	1.89	0.72
13:2:191:THR:HG22	13:2:192:ASP:N	2.03	0.72
18:2:2001:CLA:H42	18:2:2002:CLA:CBA	2.15	0.72
18:2:2016:CLA:CHC	18:2:2016:CLA:HBB1	2.12	0.72
16:3:169:GLU:CD	16:3:172:ARG:HH11	1.92	0.72
15:1:82:ILE:HD12	15:1:149:ARG:NH2	2.05	0.72
27:1:1502:LUT:H371	27:1:1502:LUT:C28	2.18	0.72
22:L:6020:BCR:H19C	18:L:1501:CLA:HMB2	1.72	0.72
16:3:206:PRO:HA	16:3:209:ASN:O	1.90	0.71
16:3:202:TYR:HB3	18:3:3001:CLA:O1D	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1001:CLA:O1A	18:1:1001:CLA:H3A	1.88	0.71
15:1:211:LEU:HD12	15:1:212:GLU:H	1.55	0.71
14:4:151:TYR:O	14:4:155:ARG:HB2	1.89	0.71
16:3:263:PRO:CG	18:3:3008:CLA:HMB3	2.20	0.71
15:1:200:VAL:HG11	18:1:1003:CLA:HAC2	1.71	0.71
18:A:1102:CLA:HBA2	18:A:1109:CLA:H51	1.72	0.71
21:2:2801:LHG:O4	21:2:2801:LHG:O2	2.07	0.71
14:4:140:THR:HB	15:1:225:ASN:OD1	1.90	0.71
13:2:163:ALA:C	13:2:166:ARG:HB3	2.10	0.71
16:3:223:LEU:CA	16:3:226:LYS:HG2	2.20	0.71
1:A:37:PRO:HA	18:A:1101:CLA:HBC1	1.72	0.71
18:F:1301:CLA:HHC	18:F:1301:CLA:HBB1	1.72	0.71
10:E:122:LEU:HD12	10:E:122:LEU:N	2.02	0.71
6:G:149:LYS:C	6:G:149:LYS:HE3	2.11	0.71
9:D:112:ILE:N	9:D:112:ILE:HD12	2.04	0.71
13:2:148:ASP:O	13:2:149:THR:CB	2.38	0.71
13:2:193:VAL:HG23	13:2:194:GLY:N	2.04	0.71
18:3:3003:CLA:CAB	27:3:3501:LUT:H172	2.20	0.71
18:B:1204:CLA:H2	3:I:8:PHE:HD2	1.53	0.71
18:G:1001:CLA:HED2	18:G:1001:CLA:C3D	2.21	0.71
14:4:168:GLN:OE1	14:4:171:ILE:HA	1.89	0.71
22:J:6013:BCR:H392	22:J:6013:BCR:H23C	1.71	0.71
13:2:177:VAL:HG23	13:2:178:ASN:N	2.05	0.71
16:3:169:GLU:OE2	16:3:172:ARG:NH1	2.22	0.71
16:3:141:VAL:HG22	16:3:143:PRO:HD2	1.72	0.71
18:1:1011:CLA:C5	27:1:1501:LUT:H23	2.18	0.71
14:4:118:ILE:CD1	14:4:120:ILE:HD11	2.06	0.71
15:1:186:LYS:HD3	18:1:1007:CLA:O1D	1.90	0.71
15:1:88:MET:HE3	18:1:1001:CLA:CAB	2.20	0.71
18:B:1220:CLA:HAB	18:B:1227:CLA:HMD2	1.73	0.71
18:B:1235:CLA:H72	18:B:1235:CLA:HBB1	1.71	0.71
7:L:102:VAL:HG13	7:L:106:HIS:CE1	2.26	0.71
15:1:125:PRO:O	15:1:126:VAL:HG22	1.89	0.71
23:G:2021:LMG:HC61	15:1:115:PRO:HA	1.71	0.71
16:3:223:LEU:HA	16:3:226:LYS:HG2	1.73	0.71
18:L:1502:CLA:HAC2	22:L:6019:BCR:H292	1.72	0.71
14:4:60:LEU:HG	14:4:61:ALA:N	2.06	0.71
16:3:142:ILE:O	16:3:146:GLY:HA2	1.90	0.70
16:3:265:ASN:O	16:3:270:THR:HB	1.91	0.70
18:3:3006:CLA:H43	18:3:3018:CLA:O2A	1.90	0.70
14:4:152:VAL:HG13	28:4:4011:CHL:NB	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:67:TYR:HE2	16:3:84:SER:CB	2.04	0.70
4:J:28:GLU:OE1	18:J:1302:CLA:CHA	2.39	0.70
18:2:2005:CLA:C7	23:2:2802:LMG:H132	2.21	0.70
22:L:6019:BCR:H393	22:L:6019:BCR:C27	2.21	0.70
22:K:2011:BCR:HC8	22:K:2011:BCR:C32	2.16	0.70
18:A:1114:CLA:HBB1	18:A:1114:CLA:HHC	1.73	0.70
18:2:2016:CLA:CBB	18:2:2016:CLA:HHC	2.14	0.70
16:3:226:LYS:HZ2	16:3:226:LYS:N	1.89	0.70
18:3:3001:CLA:C4	18:3:3002:CLA:HBA1	2.20	0.70
15:1:202:GLN:HE21	15:1:202:GLN:C	1.94	0.70
18:L:1501:CLA:HAA1	18:H:1000:CLA:HMB2	1.73	0.70
18:4:4016:CLA:HBC2	18:4:4016:CLA:HMC1	1.73	0.70
9:D:192:ILE:HG22	9:D:193:GLY:N	2.03	0.70
13:2:200:TRP:CD1	18:2:2016:CLA:HAA2	2.25	0.70
28:2:2010:CHL:HHC	28:2:2010:CHL:HBB1	1.71	0.70
16:3:226:LYS:NZ	16:3:226:LYS:H	1.88	0.70
18:4:4003:CLA:HBB1	18:4:4003:CLA:CHC	2.19	0.70
18:1:1001:CLA:ND	27:1:1501:LUT:H383	2.06	0.70
18:1:1008:CLA:CBB	18:1:1008:CLA:HHC	2.22	0.70
6:G:75:GLY:O	6:G:80:PHE:HB2	1.90	0.70
18:3:3006:CLA:CHA	18:3:3006:CLA:HED2	2.21	0.70
15:1:41:TRP:CD1	15:1:59:PHE:HA	2.26	0.70
18:4:4002:CLA:OBD	18:4:4007:CLA:HBD	1.92	0.70
18:3:3012:CLA:H12	18:3:3017:CLA:CBB	2.22	0.70
15:1:121:TYR:O	15:1:122:LEU:HD23	1.91	0.70
28:4:4013:CHL:HHB	27:4:4503:LUT:H192	1.72	0.70
13:2:77:LEU:CD1	13:2:86:GLY:HA2	2.22	0.70
18:2:2003:CLA:C3B	27:2:2501:LUT:H383	2.21	0.70
28:4:4013:CHL:HHB	27:4:4503:LUT:C19	2.22	0.70
2:B:582:TRP:CH2	18:B:1012:CLA:HAB	2.27	0.70
27:I:6018:LUT:C8	27:I:6018:LUT:H181	2.21	0.70
16:3:120:GLU:CD	16:3:253:TYR:H	1.95	0.70
18:1:1008:CLA:CHC	18:1:1008:CLA:HBB1	2.19	0.70
4:J:38:THR:C	23:J:5001:LMG:H122	2.11	0.70
10:E:111:ASN:ND2	10:E:113:ALA:O	2.24	0.70
9:D:169:PRO:O	9:D:170:LYS:HB3	1.90	0.70
28:2:2013:CHL:HBC2	28:2:2013:CHL:OMC	1.92	0.70
16:3:107:ARG:CB	28:3:3011:CHL:HED1	2.21	0.70
14:4:150:HIS:O	14:4:154:ILE:HG22	1.91	0.70
11:H:72:SER:OG	11:H:73:ASP:N	2.25	0.70
13:2:141:GLY:HA2	28:2:2013:CHL:HBC1	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1004:CLA:HMD2	28:1:1009:CHL:HBB1	1.73	0.69
15:1:126:VAL:HB	15:1:127:PRO:HA	1.73	0.69
15:1:104:ASN:CG	15:1:208:THR:HG23	2.11	0.69
7:L:91:THR:HA	7:L:175:GLN:NE2	2.05	0.69
18:2:2003:CLA:CHB	18:2:2008:CLA:HMD3	2.22	0.69
15:1:167:PRO:HD2	27:1:1501:LUT:O23	1.91	0.69
18:A:1131:CLA:HMA1	27:I:6018:LUT:H22	1.74	0.69
7:L:83:LEU:O	7:L:89:TYR:HD2	1.75	0.69
2:B:294:ASN:HB3	6:G:107:ARG:HA	1.74	0.69
1:A:593:SER:OG	1:A:596:ASP:OD2	2.10	0.69
27:2:2501:LUT:H28	27:2:2501:LUT:C37	2.22	0.69
16:3:135:ALA:H	16:3:138:GLN:HG2	1.55	0.69
16:3:166:GLY:O	16:3:170:HIS:ND1	2.23	0.69
27:3:3502:LUT:H371	27:3:3502:LUT:H28	1.73	0.69
18:3:3008:CLA:CHC	18:3:3008:CLA:HBB1	2.16	0.69
15:1:89:LEU:O	15:1:92:PRO:HD2	1.92	0.69
18:2:2002:CLA:HED1	18:2:2002:CLA:CGA	2.22	0.69
18:2:2016:CLA:HBD	18:2:2016:CLA:CGA	2.22	0.69
16:3:155:TYR:CE1	18:3:3010:CLA:HAC1	2.27	0.69
16:3:259:HIS:CG	18:3:3003:CLA:HAA2	2.28	0.69
14:4:94:ALA:N	18:4:4012:CLA:HED2	2.07	0.69
10:E:111:ASN:HD22	10:E:113:ALA:H	1.40	0.69
11:H:68:ASP:OD1	11:H:71:GLY:HA3	1.92	0.69
14:4:120:ILE:N	14:4:120:ILE:HD12	2.07	0.69
16:3:117:ILE:HD11	16:3:252:PRO:HB2	1.73	0.69
5:F:106:LEU:HD13	5:F:106:LEU:O	1.91	0.69
18:3:3003:CLA:H122	18:3:3003:CLA:C9	2.23	0.69
15:1:202:GLN:CD	15:1:208:THR:HB	2.12	0.69
14:4:136:ALA:HB1	14:4:140:THR:HG21	1.75	0.69
17:A:1011:CL0:H2	17:A:1011:CL0:H15	1.75	0.69
14:4:197:THR:OG1	14:4:200:ALA:HB2	1.93	0.69
13:2:123:PRO:HA	13:2:126:LEU:CG	2.22	0.69
18:3:3004:CLA:CGA	18:3:3004:CLA:H3A	2.22	0.69
28:4:4011:CHL:HAA1	28:4:4011:CHL:CBD	2.21	0.69
18:G:1001:CLA:HHC	18:G:1001:CLA:CBB	2.15	0.69
18:2:2005:CLA:HBC1	18:2:2012:CLA:CBC	2.23	0.69
18:2:2008:CLA:HAA2	16:3:160:LEU:HB2	1.74	0.69
16:3:110:MET:HA	16:3:234:ALA:CB	2.23	0.69
15:1:232:ILE:HD11	18:1:1014:CLA:HMD2	1.74	0.69
15:1:75:ARG:NH1	18:1:1005:CLA:O1A	2.26	0.69
18:A:1013:CLA:H203	18:A:1140:CLA:H51	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:2502:LUT:H361	27:2:2502:LUT:C28	2.22	0.69
16:3:259:HIS:HA	16:3:266:ASN:CB	2.23	0.69
15:1:209:GLY:O	15:1:213:ASN:N	2.19	0.69
14:4:212:MET:HE3	18:4:4004:CLA:HMC3	1.74	0.69
18:4:4007:CLA:H2A	18:4:4007:CLA:O2D	1.93	0.69
13:2:77:LEU:HD12	13:2:86:GLY:HA2	1.75	0.69
16:3:258:ASP:HB2	16:3:266:ASN:HD21	1.58	0.68
18:1:1004:CLA:H2	27:1:1502:LUT:H182	1.74	0.68
6:G:76:ARG:HE	6:G:116:LYS:CE	2.04	0.68
15:1:193:LEU:O	15:1:193:LEU:HD23	1.93	0.68
18:3:3006:CLA:CBB	18:3:3006:CLA:HHC	2.22	0.68
16:3:155:TYR:CE1	18:3:3010:CLA:CAC	2.76	0.68
18:4:4002:CLA:CHC	18:4:4002:CLA:HBB1	2.23	0.68
18:4:4007:CLA:HBC2	18:4:4007:CLA:CHD	2.13	0.68
18:4:4017:CLA:CED	28:1:1009:CHL:HMB2	2.23	0.68
22:A:6017:BCR:H362	18:B:1023:CLA:H112	1.75	0.68
12:K:124:ALA:O	12:K:128:VAL:HG23	1.94	0.68
15:1:144:PHE:O	15:1:148:GLN:HG2	1.93	0.68
13:2:117:ALA:HB1	27:2:2501:LUT:H32	1.75	0.68
13:2:131:ILE:CG2	13:2:133:LEU:HG	2.23	0.68
13:2:186:ASN:OD1	18:2:2016:CLA:H2A	1.93	0.68
27:3:3501:LUT:C8	27:3:3501:LUT:H161	2.17	0.68
18:4:4006:CLA:C3B	27:4:4502:LUT:H183	2.23	0.68
7:L:98:ARG:HH22	7:L:175:GLN:HE22	1.41	0.68
12:K:71:VAL:HG21	12:K:133:GLY:CA	2.23	0.68
6:G:76:ARG:HG2	6:G:116:LYS:HZ1	1.58	0.68
13:2:125:PHE:HB3	13:2:131:ILE:HD11	1.75	0.68
18:3:3004:CLA:HBB1	18:3:3004:CLA:CMB	2.08	0.68
18:3:3012:CLA:HBB1	18:3:3012:CLA:CMB	2.03	0.68
18:1:1002:CLA:HED2	18:1:1002:CLA:O1A	1.94	0.68
22:L:6019:BCR:H23C	22:L:6019:BCR:C38	2.23	0.68
13:2:69:PRO:HD2	18:2:2009:CLA:O1D	1.93	0.68
18:3:3010:CLA:HBB1	18:3:3010:CLA:CHC	2.20	0.68
15:1:177:PHE:CE2	15:1:181:LYS:HE2	2.28	0.68
27:4:4502:LUT:C28	27:4:4502:LUT:H381	2.06	0.68
18:A:1022:CLA:H122	22:A:6017:BCR:H352	1.75	0.68
7:L:91:THR:HA	7:L:98:ARG:NH2	2.08	0.68
12:K:66:THR:O	12:K:69:ILE:HG23	1.94	0.68
13:2:68:PHE:CD2	13:2:71:SER:HB3	2.29	0.68
14:4:132:GLU:HB2	14:4:133:GLU:OE2	1.94	0.68
16:3:246:LEU:HD23	16:3:246:LEU:C	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2008:CLA:HBB1	18:2:2008:CLA:HHC	1.75	0.68
13:2:186:ASN:CG	18:2:2016:CLA:HMA3	2.14	0.68
18:1:1002:CLA:HMC1	18:1:1002:CLA:HBC2	1.75	0.68
15:1:58:ASP:HA	18:1:1004:CLA:CED	2.23	0.68
11:H:132:PRO:HD2	11:H:133:PRO:CD	2.23	0.68
18:3:3005:CLA:HMD2	18:3:3012:CLA:CHD	2.23	0.68
16:3:155:TYR:HA	18:3:3010:CLA:HMC1	1.74	0.68
29:4:4505:ZEX:H362	29:4:4505:ZEX:C38	2.22	0.68
4:J:2:ARG:NE	4:J:4:LEU:HD12	2.01	0.68
13:2:211:PRO:O	13:2:212:GLN:CG	2.42	0.68
14:4:213:LEU:CD1	23:4:4801:LMG:H302	2.24	0.68
7:L:162:PRO:HG2	11:H:68:ASP:HB2	1.75	0.68
28:2:2013:CHL:O2A	28:2:2013:CHL:HMA2	1.94	0.68
18:3:3007:CLA:HBC2	18:3:3007:CLA:HMC1	1.76	0.68
3:I:4:LEU:HD12	3:I:4:LEU:C	2.14	0.68
7:L:109:PHE:HE1	18:L:1503:CLA:C2C	2.06	0.68
5:F:139:LEU:HD23	5:F:139:LEU:N	2.07	0.68
10:E:111:ASN:ND2	10:E:113:ALA:H	1.91	0.68
15:1:106:VAL:HG21	15:1:202:GLN:OE1	1.94	0.68
14:4:203:LYS:HA	18:4:4007:CLA:O1D	1.92	0.68
18:G:1001:CLA:H41	22:G:2011:BCR:C34	2.22	0.68
13:2:130:GLY:C	13:2:131:ILE:HG13	2.14	0.68
13:2:177:VAL:HG23	13:2:178:ASN:H	1.59	0.68
18:3:3013:CLA:CMA	22:3:3503:BCR:H353	2.23	0.68
16:3:237:ALA:HB1	27:3:3501:LUT:H161	1.76	0.68
22:L:6019:BCR:H271	22:L:6019:BCR:H393	1.76	0.68
1:A:387:THR:HG21	1:A:523:VAL:HB	1.75	0.68
18:2:2009:CLA:HED3	16:3:171:ARG:HG2	1.76	0.67
15:1:130:THR:HG22	15:1:132:PRO:HD3	1.76	0.67
15:1:80:GLU:HG3	18:1:1004:CLA:C1B	2.24	0.67
7:L:161:ALA:HB3	7:L:174:ASP:OD1	1.94	0.67
18:K:1001:CLA:CHC	18:K:1001:CLA:HBB1	2.24	0.67
12:K:78:LEU:HB3	12:K:82:ARG:HB2	1.75	0.67
9:D:195:ASN:ND2	9:D:195:ASN:H	1.92	0.67
11:H:106:GLY:O	11:H:110:THR:HG22	1.94	0.67
13:2:129:LEU:HD23	13:2:129:LEU:C	2.15	0.67
13:2:175:GLY:O	13:2:176:CYS:HB3	1.92	0.67
15:1:221:PRO:HG2	15:1:222:TRP:CZ3	2.30	0.67
14:4:209:ARG:HD3	18:4:4004:CLA:CHD	2.24	0.67
18:G:1003:CLA:H91	18:G:1003:CLA:H13	1.73	0.67
9:D:160:PRO:HD2	9:D:161:SER:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:131:ILE:HG22	13:2:132:LEU:N	2.09	0.67
18:K:1001:CLA:H2A	18:K:1001:CLA:O2D	1.93	0.67
2:B:15:ASP:HB3	2:B:20:ARG:HB3	1.76	0.67
16:3:183:GLY:HA2	16:3:194:PHE:CB	2.23	0.67
18:2:2001:CLA:H11	27:2:2501:LUT:C17	2.24	0.67
15:1:85:ARG:HH11	15:1:85:ARG:CG	2.08	0.67
14:4:197:THR:O	14:4:200:ALA:HB3	1.95	0.67
14:4:198:LEU:O	14:4:199:GLU:HB2	1.94	0.67
18:2:2005:CLA:HMD2	18:2:2012:CLA:C1D	2.24	0.67
16:3:218:LYS:HD3	16:3:218:LYS:C	2.15	0.67
15:1:131:LEU:HD23	15:1:131:LEU:H	1.58	0.67
22:G:2011:BCR:C23	22:G:2011:BCR:H403	2.19	0.67
16:3:249:GLY:O	16:3:250:VAL:HG23	1.94	0.67
16:3:119:PRO:HB2	16:3:133:ALA:CB	2.25	0.67
6:G:120:ALA:HB3	6:G:123:ASP:OD1	1.95	0.67
7:L:166:LEU:HD23	7:L:166:LEU:C	2.15	0.67
13:2:188:LEU:C	13:2:188:LEU:HD22	2.15	0.67
16:3:138:GLN:CG	16:3:145:ALA:HB2	2.24	0.67
18:4:4003:CLA:HBC2	18:4:4003:CLA:HHD	1.77	0.67
18:4:4001:CLA:H52	27:4:4501:LUT:H28	1.75	0.67
7:L:90:ARG:O	7:L:98:ARG:NH2	2.27	0.67
14:4:170:PRO:HA	18:4:4016:CLA:O1D	1.95	0.67
15:1:152:GLU:CG	15:1:156:GLU:HA	2.25	0.67
12:K:86:ALA:CB	12:K:87:PRO:HD3	2.25	0.67
13:2:64:ARG:NH2	13:2:77:LEU:O	2.28	0.67
9:D:129:LEU:HD23	9:D:129:LEU:C	2.14	0.67
14:4:220:ILE:HD12	18:4:4003:CLA:CAC	2.23	0.67
16:3:251:GLY:O	16:3:255:ASN:N	2.24	0.67
14:4:229:PRO:HA	14:4:232:ASN:HD22	1.59	0.67
15:1:195:PHE:O	15:1:198:ILE:HB	1.95	0.67
13:2:203:PRO:HD2	27:2:2501:LUT:O3	1.95	0.67
18:3:3004:CLA:H2	27:3:3502:LUT:H363	1.77	0.67
18:4:4003:CLA:H11	18:4:4008:CLA:OBD	1.94	0.67
18:1:1001:CLA:CHC	27:1:1501:LUT:H32	2.25	0.67
15:1:130:THR:HG22	15:1:131:LEU:N	2.10	0.67
12:K:66:THR:HA	12:K:69:ILE:CG2	2.23	0.67
12:K:76:LEU:N	12:K:76:LEU:HD23	2.10	0.67
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.76	0.67
18:2:2009:CLA:CED	16:3:171:ARG:HG3	2.25	0.66
13:2:262:ILE:HA	18:2:2003:CLA:OBD	1.94	0.66
16:3:220:LEU:HD23	16:3:220:LEU:C	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:267:ASN:O	16:3:271:SER:N	2.28	0.66
12:K:136:VAL:O	12:K:140:LEU:HD22	1.94	0.66
6:G:116:LYS:HE3	18:G:1002:CLA:C1C	2.23	0.66
14:4:112:PRO:O	14:4:116:THR:OG1	2.13	0.66
18:B:1210:CLA:HBB1	18:B:1210:CLA:HHC	1.76	0.66
18:B:1204:CLA:H2	3:I:8:PHE:CD2	2.31	0.66
9:D:192:ILE:CG2	9:D:193:GLY:H	2.07	0.66
18:3:3001:CLA:HBB2	27:3:3501:LUT:H34	1.77	0.66
15:1:85:ARG:HB2	18:1:1011:CLA:CED	2.25	0.66
18:1:1011:CLA:HMB1	18:1:1011:CLA:HBB1	1.77	0.66
13:2:70:GLY:CA	16:3:174:GLN:HE21	2.05	0.66
18:1:1003:CLA:C3B	27:1:1501:LUT:H173	2.26	0.66
1:A:34:TRP:CE3	4:J:8:LEU:HD22	2.30	0.66
7:L:102:VAL:HG22	18:L:1502:CLA:O1D	1.94	0.66
18:4:4003:CLA:HHC	18:4:4003:CLA:CBB	2.23	0.66
14:4:105:GLY:O	14:4:109:MET:HE2	1.95	0.66
7:L:96:LEU:C	7:L:96:LEU:HD23	2.15	0.66
6:G:132:HIS:CE1	22:G:2011:BCR:H19C	2.29	0.66
9:D:157:ARG:HB2	9:D:167:LEU:HD11	1.76	0.66
13:2:222:ILE:N	13:2:222:ILE:HD12	2.09	0.66
18:1:1005:CLA:HMD2	18:1:1012:CLA:CHD	2.26	0.66
1:A:462:ILE:HG22	18:A:1132:CLA:HBC2	1.78	0.66
4:J:6:THR:HG22	23:F:5001:LMG:HC1	1.76	0.66
7:L:204:LEU:HD13	7:L:204:LEU:O	1.95	0.66
13:2:188:LEU:HD23	13:2:198:GLY:N	2.09	0.66
16:3:223:LEU:N	16:3:226:LYS:HZ3	1.93	0.66
16:3:258:ASP:HB3	16:3:266:ASN:HD21	1.61	0.66
16:3:268:VAL:HG23	18:3:3003:CLA:C1	2.21	0.66
21:1:1801:LHG:O3	21:1:1801:LHG:O1	2.10	0.66
15:1:226:ILE:HG13	18:1:1003:CLA:HMD2	1.76	0.66
14:4:105:GLY:HA2	18:4:4006:CLA:CBB	2.25	0.66
7:L:129:ALA:O	7:L:132:LEU:HB3	1.96	0.66
11:H:131:LEU:HB2	11:H:132:PRO:HA	1.78	0.66
13:2:119:GLY:O	13:2:123:PRO:HD3	1.96	0.66
13:2:160:ILE:CD1	28:2:2013:CHL:HMB3	2.25	0.66
16:3:268:VAL:HG21	18:3:3003:CLA:C4	2.11	0.66
16:3:155:TYR:CD1	18:3:3010:CLA:HAC2	2.31	0.66
15:1:94:ILE:HG13	27:1:1502:LUT:H382	1.78	0.66
14:4:235:GLN:HB3	14:4:243:ASN:ND2	2.10	0.66
5:F:94:ARG:NH1	5:F:143:ASP:O	2.26	0.66
16:3:223:LEU:HA	16:3:226:LYS:CG	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1004:CLA:H3A	18:1:1004:CLA:CGA	2.26	0.66
28:1:1009:CHL:O2D	28:1:1009:CHL:H2A	1.96	0.66
15:1:120:THR:HG22	15:1:124:ASN:O	1.94	0.66
15:1:43:PRO:HB2	28:1:1009:CHL:O1D	1.96	0.66
18:4:4001:CLA:HBC2	28:4:4011:CHL:O1A	1.96	0.66
14:4:212:MET:HB3	27:4:4502:LUT:C34	2.26	0.66
2:B:12:ILE:HD11	2:B:23:PHE:HB3	1.77	0.66
13:2:244:THR:HG22	13:2:245:GLY:N	2.03	0.66
8:C:8:TYR:CD2	9:D:191:SER:HA	2.27	0.66
15:1:204:ALA:C	15:1:206:PRO:HD3	2.16	0.66
16:3:267:ASN:OD1	16:3:270:THR:HG23	1.94	0.66
18:3:3008:CLA:HBA1	18:3:3008:CLA:HBD	1.77	0.66
18:1:1006:CLA:HMA2	18:1:1013:CLA:HBC2	1.76	0.66
15:1:98:GLU:HA	15:1:102:LEU:HB3	1.77	0.66
18:4:4001:CLA:H52	27:4:4501:LUT:C37	2.26	0.66
18:4:4005:CLA:HMD2	18:4:4012:CLA:C1D	2.25	0.66
6:G:76:ARG:NE	6:G:116:LYS:HE2	2.11	0.66
8:C:14:CYS:C	8:C:15:THR:HG23	2.16	0.66
8:C:25:VAL:HG21	8:C:48:CYS:HB2	1.77	0.66
18:G:1003:CLA:H91	18:G:1003:CLA:C13	2.26	0.65
7:L:91:THR:HG22	7:L:175:GLN:HE21	1.61	0.65
5:F:138:LEU:CD2	5:F:159:GLU:OE2	2.44	0.65
16:3:178:LYS:HB2	16:3:181:SER:OG	1.96	0.65
16:3:184:LYS:HG2	16:3:185:GLN:HE21	1.59	0.65
18:1:1014:CLA:O2D	18:1:1014:CLA:HBA2	1.94	0.65
16:3:94:GLU:OE2	16:3:95:PRO:HD2	1.96	0.65
1:A:453:LEU:HD21	18:A:1136:CLA:HAB	1.78	0.65
13:2:174:PRO:CD	13:2:175:GLY:H	2.08	0.65
16:3:267:ASN:OD1	16:3:269:LEU:HG	1.95	0.65
16:3:78:PHE:HB3	18:3:3004:CLA:OBD	1.96	0.65
10:E:111:ASN:HD21	10:E:113:ALA:HB3	1.60	0.65
2:B:603:ARG:HH22	2:B:627:ASN:HD21	1.43	0.65
13:2:256:ASP:OD1	13:2:259:HIS:HD2	1.79	0.65
13:2:111:ARG:NH1	28:2:2011:CHL:OBD	2.27	0.65
18:2:2016:CLA:HBC2	18:2:2016:CLA:CHD	2.25	0.65
1:A:567:ARG:NH2	9:D:88:THR:O	2.29	0.65
2:B:487:ASN:HB3	6:G:149:LYS:HB3	1.77	0.65
23:2:2802:LMG:O4	23:2:2802:LMG:O5	2.10	0.65
22:B:6006:BCR:H362	18:B:1211:CLA:H2	1.79	0.65
3:I:5:PRO:O	3:I:7:LEU:N	2.29	0.65
18:2:2002:CLA:O1D	18:2:2007:CLA:H42	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3002:CLA:HMD2	18:3:3007:CLA:C4D	2.27	0.65
18:3:3001:CLA:HBA2	27:3:3501:LUT:H24	1.78	0.65
2:B:176:ASN:HD21	2:B:291:TYR:H	1.43	0.65
18:3:3013:CLA:HMA2	22:3:3503:BCR:H352	1.77	0.65
15:1:85:ARG:HD2	18:1:1001:CLA:C3C	2.26	0.65
18:1:1003:CLA:O1A	18:1:1003:CLA:HBD	1.97	0.65
15:1:146:GLU:OE2	15:1:149:ARG:NH1	2.29	0.65
22:A:6011:BCR:H24C	18:B:1230:CLA:HMC2	1.79	0.65
22:B:6004:BCR:H24C	18:B:1218:CLA:HMD2	1.78	0.65
12:K:72:ALA:HB3	18:K:1001:CLA:CGA	2.26	0.65
13:2:191:THR:O	13:2:192:ASP:HB2	1.96	0.65
14:4:140:THR:O	14:4:144:ILE:HG13	1.96	0.65
12:K:70:MET:CE	12:K:71:VAL:HA	2.26	0.65
13:2:239:HIS:ND1	13:2:244:THR:O	2.29	0.65
16:3:65:LEU:O	16:3:68:LEU:HD22	1.97	0.65
1:A:441:ALA:O	1:A:445:HIS:ND1	2.30	0.65
18:2:2004:CLA:H13	27:2:2502:LUT:H393	1.78	0.65
18:3:3005:CLA:H93	18:3:3012:CLA:C4	2.25	0.65
14:4:104:LEU:C	18:4:4006:CLA:HBB2	2.17	0.65
22:L:6019:BCR:H311	22:L:6019:BCR:HC8	1.79	0.65
12:K:75:THR:HG21	12:K:129:GLY:N	2.12	0.65
13:2:262:ILE:CD1	18:2:2003:CLA:H43	2.27	0.65
16:3:234:ALA:O	16:3:238:ILE:HG22	1.97	0.65
18:4:4002:CLA:HMC2	27:4:4501:LUT:C11	2.26	0.65
27:4:4503:LUT:H28	27:4:4503:LUT:H361	1.79	0.65
3:I:6:SER:O	3:I:9:VAL:HG23	1.97	0.65
16:3:231:GLY:O	16:3:235:MET:HG3	1.97	0.64
18:3:3005:CLA:H12	18:3:3005:CLA:HED1	1.79	0.64
16:3:74:GLY:HA2	16:3:225:LEU:CD2	2.27	0.64
16:3:63:GLN:OE1	16:3:78:PHE:HD2	1.80	0.64
18:4:4009:CLA:H2A	18:4:4009:CLA:O2D	1.98	0.64
18:F:1302:CLA:HBB1	18:F:1302:CLA:HHC	1.79	0.64
14:4:223:ASN:O	14:4:225:THR:N	2.30	0.64
15:1:98:GLU:CA	15:1:102:LEU:HB3	2.26	0.64
16:3:121:TYR:O	16:3:124:LYS:HB2	1.96	0.64
28:4:4010:CHL:HBB1	28:4:4013:CHL:HBB2	1.79	0.64
1:A:629:ASN:ND2	1:A:631:GLN:OE1	2.30	0.64
18:2:2002:CLA:H2A	18:2:2002:CLA:O1A	1.96	0.64
28:2:2010:CHL:O2D	28:2:2010:CHL:H2A	1.96	0.64
16:3:184:LYS:C	16:3:185:GLN:HG2	2.18	0.64
15:1:202:GLN:HE21	15:1:202:GLN:CA	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:114:VAL:HG11	18:G:1002:CLA:CAA	2.26	0.64
18:4:4006:CLA:NB	27:4:4503:LUT:H172	2.13	0.64
18:B:1229:CLA:H61	22:F:6016:BCR:H393	1.79	0.64
16:3:117:ILE:HD13	16:3:252:PRO:HG2	1.78	0.64
16:3:75:ASP:OD1	16:3:77:GLY:N	2.30	0.64
16:3:216:ASP:OD1	16:3:216:ASP:N	2.27	0.64
18:2:2007:CLA:O1D	18:2:2007:CLA:H2A	1.98	0.64
16:3:105:ASN:ND2	18:3:3012:CLA:OBD	2.30	0.64
16:3:225:LEU:N	16:3:226:LYS:HZ2	1.94	0.64
18:4:4008:CLA:HBB1	18:4:4008:CLA:HHC	1.78	0.64
28:4:4010:CHL:HBB1	28:4:4013:CHL:CBB	2.27	0.64
2:B:656:VAL:HG22	18:B:1239:CLA:HMB3	1.79	0.64
13:2:218:ARG:O	13:2:222:ILE:HD13	1.98	0.64
7:L:169:ARG:HD2	7:L:171:LYS:CB	2.28	0.64
16:3:144:PRO:HG2	16:3:145:ALA:H	1.61	0.64
18:3:3006:CLA:HMB2	18:3:3013:CLA:C4B	2.27	0.64
15:1:98:GLU:N	15:1:102:LEU:HB3	2.12	0.64
5:F:207:VAL:HB	18:F:1301:CLA:HED2	1.79	0.64
22:L:6019:BCR:H23C	22:L:6019:BCR:H382	1.79	0.64
21:2:2801:LHG:HC42	22:3:3503:BCR:H281	1.80	0.64
18:1:1002:CLA:O2D	18:1:1002:CLA:H2A	1.98	0.64
11:H:132:PRO:HD2	11:H:133:PRO:HD3	1.79	0.64
14:4:225:THR:HG22	14:4:227:LYS:H	1.61	0.64
14:4:72:GLY:HA2	23:4:4801:LMG:O5	1.97	0.64
16:3:158:PHE:CB	18:3:3010:CLA:HMC2	2.28	0.64
18:4:4005:CLA:HMC2	27:4:4502:LUT:C12	2.28	0.64
29:4:4505:ZEX:H41	18:1:1014:CLA:O1A	1.98	0.64
6:G:95:GLN:O	6:G:95:GLN:HG3	1.98	0.64
1:A:24:ARG:HD3	1:A:76:ARG:HH22	1.63	0.64
13:2:135:PRO:HG2	18:2:2006:CLA:CED	2.27	0.64
16:3:259:HIS:HA	16:3:266:ASN:HB2	1.80	0.64
18:3:3003:CLA:H122	18:3:3003:CLA:H91	1.80	0.64
18:3:3003:CLA:HMB3	27:3:3501:LUT:H173	1.80	0.64
18:A:1131:CLA:HAB	18:A:1132:CLA:HHB	1.79	0.64
18:A:1151:CLA:HAB	18:A:1122:CLA:HHB	1.80	0.64
13:2:131:ILE:HB	13:2:133:LEU:HD11	1.78	0.63
7:L:211:TYR:HE2	18:L:1503:CLA:C2	2.12	0.63
4:J:10:VAL:HA	4:J:14:ALA:HB2	1.79	0.63
16:3:111:LEU:CD2	18:3:3006:CLA:HBB1	2.27	0.63
18:3:3001:CLA:HBB1	27:3:3501:LUT:H32	1.79	0.63
15:1:79:SER:HB2	18:1:1012:CLA:HED2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:4501:LUT:H28	27:4:4501:LUT:C37	2.28	0.63
1:A:34:TRP:HE3	4:J:8:LEU:HD22	1.63	0.63
18:4:4009:CLA:HBB1	18:4:4009:CLA:CHC	2.11	0.63
7:L:211:TYR:HE2	18:L:1503:CLA:C3	2.12	0.63
28:1:1010:CHL:HHC	28:1:1010:CHL:HBB1	1.78	0.63
15:1:130:THR:CG2	15:1:132:PRO:HD2	2.26	0.63
13:2:202:ASP:OD2	13:2:205:GLY:HA2	1.99	0.63
16:3:136:TRP:CG	16:3:137:PHE:N	2.66	0.63
15:1:97:PRO:HB2	15:1:102:LEU:HD22	1.79	0.63
27:1:1502:LUT:H28	27:1:1502:LUT:C37	2.28	0.63
7:L:96:LEU:HD12	11:H:94:THR:HG21	1.81	0.63
15:1:146:GLU:CG	15:1:149:ARG:HH11	2.10	0.63
15:1:169:GLY:O	15:1:172:LYS:HG3	1.99	0.63
18:B:1204:CLA:H51	27:I:6018:LUT:O23	1.99	0.63
13:2:204:LEU:HB3	13:2:206:TRP:NE1	2.14	0.63
13:2:131:ILE:CB	13:2:133:LEU:HG	2.28	0.63
18:L:1502:CLA:HBA1	18:L:1502:CLA:CHA	2.27	0.63
12:K:71:VAL:CG1	12:K:132:ILE:HB	2.29	0.63
18:3:3003:CLA:H92	18:3:3003:CLA:C2C	2.29	0.63
18:A:1139:CLA:H43	18:A:1138:CLA:H171	1.80	0.63
16:3:65:LEU:HD23	16:3:66:SER:H	1.63	0.63
6:G:94:GLU:HB2	6:G:98:VAL:N	2.13	0.63
15:1:193:LEU:C	15:1:193:LEU:HD23	2.18	0.63
8:C:54:CYS:SG	8:C:55:GLU:N	2.72	0.63
18:1:1007:CLA:HBC2	18:1:1007:CLA:HMC1	1.81	0.63
15:1:211:LEU:CD1	15:1:212:GLU:H	2.12	0.63
7:L:133:ALA:O	7:L:136:GLY:N	2.30	0.63
7:L:145:LEU:CD2	22:L:6019:BCR:H403	2.26	0.63
4:J:16:THR:HG21	22:J:6013:BCR:C40	2.29	0.63
7:L:163:SER:O	7:L:172:GLN:HG2	1.99	0.63
2:B:351:HIS:HB3	18:B:1214:CLA:HED2	1.80	0.63
18:3:3006:CLA:CHC	18:3:3006:CLA:HBB1	2.27	0.62
15:1:158:LYS:C	15:1:159:LYS:HD3	2.19	0.62
14:4:105:GLY:N	18:4:4006:CLA:HBB2	2.14	0.62
1:A:604:TRP:CH2	18:A:1022:CLA:HAB	2.34	0.62
14:4:170:PRO:HB3	18:4:4016:CLA:NA	2.12	0.62
16:3:257:LEU:O	16:3:261:ALA:N	2.30	0.62
15:1:151:MET:HG3	15:1:151:MET:O	1.97	0.62
1:A:546:ALA:HB1	18:A:1136:CLA:HMB3	1.79	0.62
18:2:2003:CLA:C1B	27:2:2501:LUT:H383	2.28	0.62
18:2:2006:CLA:C4	18:2:2006:CLA:H71	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:2:2802:LMG:O2	23:2:2802:LMG:H292	1.98	0.62
16:3:193:GLY:HA3	16:3:207:PHE:CD2	2.33	0.62
12:K:85:LEU:CB	12:K:118:THR:HG21	2.29	0.62
9:D:139:LEU:O	9:D:139:LEU:HD23	1.99	0.62
16:3:190:LEU:HB2	16:3:207:PHE:HZ	1.63	0.62
15:1:143:ALA:HA	18:1:1012:CLA:HAB	1.79	0.62
15:1:111:TRP:NE1	15:1:119:ALA:HB2	2.14	0.62
15:1:127:PRO:HG2	15:1:128:TRP:NE1	2.14	0.62
18:L:1501:CLA:CBA	18:L:1501:CLA:HBD	2.29	0.62
6:G:76:ARG:HG3	6:G:77:PHE:CD1	2.34	0.62
13:2:197:GLY:CA	18:2:2001:CLA:HED1	2.29	0.62
15:1:146:GLU:O	15:1:149:ARG:HB2	1.98	0.62
28:4:4013:CHL:HBB1	28:4:4013:CHL:HHC	1.80	0.62
6:G:116:LYS:HB2	18:G:1002:CLA:C4D	2.29	0.62
13:2:104:GLN:NE2	13:2:193:VAL:HB	2.15	0.62
18:2:2005:CLA:H41	18:2:2005:CLA:H92	1.79	0.62
13:2:88:ASP:OD1	27:2:2502:LUT:O23	2.16	0.62
16:3:225:LEU:O	16:3:225:LEU:HD13	1.99	0.62
16:3:262:ASP:HB3	16:3:265:ASN:ND2	2.15	0.62
18:3:3003:CLA:H11	18:3:3003:CLA:C3D	2.27	0.62
15:1:162:GLY:N	18:1:1001:CLA:HED2	2.14	0.62
15:1:183:LYS:CD	18:1:1002:CLA:HAA2	2.23	0.62
15:1:155:PRO:O	15:1:158:LYS:N	2.33	0.62
2:B:5:LEU:HD22	3:I:28:VAL:HG22	1.82	0.62
18:A:1110:CLA:HBC3	18:A:1111:CLA:HAB	1.81	0.62
16:3:134:LEU:CB	16:3:138:GLN:HG3	2.30	0.62
18:3:3003:CLA:HAB	27:3:3501:LUT:H172	1.82	0.62
18:3:3017:CLA:HBB1	18:3:3017:CLA:HHC	1.82	0.62
6:G:133:ILE:HA	22:G:2011:BCR:H401	1.81	0.62
13:2:87:PHE:HB3	18:2:2004:CLA:CAD	2.29	0.62
18:1:1005:CLA:HMB1	18:1:1005:CLA:CBB	2.28	0.62
18:4:4016:CLA:CBD	18:4:4016:CLA:HBA1	2.29	0.62
9:D:173:VAL:HG12	9:D:174:TYR:N	2.14	0.62
14:4:177:LEU:HD13	18:4:4016:CLA:HMD3	1.81	0.62
18:A:1110:CLA:CBC	18:A:1111:CLA:HAB	2.29	0.62
14:4:239:ASP:OD2	14:4:242:HIS:HD2	1.82	0.62
13:2:220:LYS:HG2	18:2:2007:CLA:O2D	1.99	0.62
18:3:3001:CLA:O1A	18:3:3001:CLA:H3A	1.99	0.62
28:3:3011:CHL:CGD	28:3:3011:CHL:HAA1	2.29	0.62
22:B:6006:BCR:H311	18:B:1212:CLA:HMB2	1.82	0.62
13:2:104:GLN:HE22	13:2:193:VAL:CG2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:220:LYS:HA	18:2:2007:CLA:CED	2.30	0.62
13:2:220:LYS:CA	18:2:2007:CLA:HED1	2.30	0.62
16:3:169:GLU:HA	16:3:169:GLU:OE2	1.99	0.62
18:A:1138:CLA:H111	18:A:1138:CLA:HAB	1.82	0.62
2:B:85:ARG:HD2	2:B:115:ILE:HD13	1.82	0.62
7:L:109:PHE:CE1	18:L:1503:CLA:C2C	2.83	0.62
10:E:66:ILE:HG23	10:E:93:VAL:HG11	1.81	0.62
5:F:163:PRO:O	5:F:166:LEU:HB3	1.99	0.62
13:2:123:PRO:HA	13:2:126:LEU:HG	1.82	0.61
13:2:109:HIS:NE2	18:2:2012:CLA:HMD1	2.15	0.61
16:3:164:LEU:HD13	22:3:3503:BCR:C35	2.30	0.61
16:3:164:LEU:CB	22:3:3503:BCR:H351	2.26	0.61
18:4:4003:CLA:H93	18:4:4003:CLA:CHC	2.30	0.61
13:2:165:GLY:O	18:4:4009:CLA:HED2	1.99	0.61
18:A:1130:CLA:HMB1	18:A:1130:CLA:HBB1	1.81	0.61
9:D:75:LEU:O	9:D:76:ASP:HB2	1.98	0.61
9:D:158:VAL:O	9:D:159:PHE:HB2	1.99	0.61
9:D:111:GLN:O	9:D:123:MET:N	2.31	0.61
11:H:123:LEU:HD12	11:H:123:LEU:H	1.64	0.61
18:2:2001:CLA:H41	18:2:2002:CLA:H3A	1.81	0.61
13:2:89:PRO:HD2	27:2:2502:LUT:H221	1.82	0.61
15:1:158:LYS:HD3	15:1:159:LYS:NZ	2.15	0.61
7:L:90:ARG:C	7:L:98:ARG:HH21	2.04	0.61
18:2:2005:CLA:C4	18:2:2005:CLA:H72	2.29	0.61
18:B:1222:CLA:H41	18:B:1234:CLA:H43	1.82	0.61
1:A:354:TRP:HB3	18:A:1103:CLA:HAC1	1.81	0.61
22:B:6005:BCR:H311	18:B:1202:CLA:H42	1.83	0.61
18:B:1206:CLA:H18	27:I:6018:LUT:H403	1.82	0.61
10:E:95:GLN:HA	10:E:95:GLN:OE1	2.00	0.61
1:A:361:ASN:ND2	18:A:1103:CLA:OBD	2.29	0.61
1:A:590:CYS:HB3	19:A:3001:SF4:S2	2.41	0.61
15:1:85:ARG:HD2	18:1:1001:CLA:C4C	2.30	0.61
18:B:1205:CLA:H2	18:B:1205:CLA:H102	1.83	0.61
10:E:76:ILE:C	10:E:77:LEU:HD12	2.20	0.61
11:H:122:ILE:HG22	11:H:122:ILE:O	1.99	0.61
18:2:2009:CLA:HED1	16:3:167:PHE:O	2.01	0.61
13:2:105:ALA:CB	18:2:2012:CLA:HED2	2.31	0.61
15:1:230:VAL:HG12	15:1:231:LEU:HD23	1.82	0.61
18:B:1229:CLA:HAB	18:B:1230:CLA:CMB	2.27	0.61
3:I:13:GLY:C	3:I:14:LEU:HD23	2.21	0.61
6:G:98:VAL:O	6:G:99:THR:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2012:CLA:H12	23:2:2802:LMG:C36	2.30	0.61
18:3:3003:CLA:C2B	27:3:3501:LUT:H173	2.29	0.61
9:D:134:ARG:O	9:D:135:LYS:HB3	2.01	0.61
1:A:222:GLN:HA	1:A:226:SER:HB2	1.83	0.61
13:2:127:THR:HG21	13:2:247:ILE:HD11	1.83	0.61
18:2:2002:CLA:HMC1	18:2:2002:CLA:CBC	2.19	0.61
18:2:2006:CLA:HMA2	28:2:2013:CHL:HAC2	1.83	0.61
16:3:182:MET:HE1	16:3:182:MET:HA	1.81	0.61
16:3:184:LYS:HG2	16:3:185:GLN:CG	2.29	0.61
2:B:173:SER:O	2:B:177:HIS:ND1	2.20	0.61
15:1:111:TRP:CE2	15:1:119:ALA:CB	2.84	0.61
1:A:358:LEU:HD11	18:A:1128:CLA:HBB1	1.82	0.61
12:K:81:GLY:O	12:K:82:ARG:HD3	1.99	0.61
4:J:7:TYR:CZ	23:F:5001:LMG:HC4	2.36	0.61
6:G:121:LEU:HD23	6:G:121:LEU:C	2.22	0.61
9:D:140:ALA:O	9:D:143:THR:HG22	2.00	0.61
13:2:115:LEU:HB2	18:2:2006:CLA:HBB2	1.82	0.60
16:3:155:TYR:CZ	18:3:3010:CLA:CAC	2.83	0.60
16:3:110:MET:HE1	16:3:230:ASN:C	2.22	0.60
18:3:3004:CLA:H93	18:3:3005:CLA:HMB3	1.83	0.60
15:1:211:LEU:HD12	15:1:211:LEU:N	2.16	0.60
18:L:1502:CLA:CHD	22:L:6019:BCR:H282	2.31	0.60
16:3:67:TYR:HE2	16:3:84:SER:HB2	1.66	0.60
18:2:2004:CLA:CMB	18:2:2004:CLA:HBB1	2.31	0.60
16:3:175:ASP:HB2	28:3:3011:CHL:HAC2	1.82	0.60
18:3:3005:CLA:HBA2	18:3:3005:CLA:O2D	2.00	0.60
2:B:451:LYS:NZ	18:B:1230:CLA:O1D	2.35	0.60
18:G:1001:CLA:HED2	18:G:1001:CLA:CAD	2.31	0.60
16:3:120:GLU:OE2	16:3:253:TYR:N	2.33	0.60
18:3:3010:CLA:HMB1	18:3:3013:CLA:CAB	2.10	0.60
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.83	0.60
22:F:6016:BCR:H382	22:F:6016:BCR:C23	2.32	0.60
12:K:83:PHE:HB2	22:K:2011:BCR:C4	2.31	0.60
14:4:167:ASN:CG	14:4:168:GLN:H	2.03	0.60
13:2:105:ALA:CA	18:2:2012:CLA:HED2	2.31	0.60
15:1:217:HIS:CE1	15:1:221:PRO:CB	2.85	0.60
14:4:103:MET:CG	18:4:4001:CLA:HMC3	2.31	0.60
18:A:1104:CLA:HAB	18:A:1127:CLA:HMC2	1.83	0.60
18:B:1218:CLA:H41	18:B:1218:CLA:H92	1.84	0.60
18:F:1302:CLA:HHD	18:F:1302:CLA:CBC	2.23	0.60
12:K:136:VAL:C	12:K:140:LEU:HD22	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:116:LYS:HG3	18:G:1002:CLA:C1D	2.30	0.60
1:A:205:HIS:CD2	18:A:1111:CLA:HMC2	2.36	0.60
7:L:172:GLN:HG3	7:L:172:GLN:O	2.00	0.60
5:F:150:VAL:HG12	5:F:160:PHE:HB2	1.84	0.60
27:4:4503:LUT:C36	28:1:1009:CHL:H93	2.32	0.60
2:B:273:MET:O	2:B:277:HIS:ND1	2.34	0.60
16:3:137:PHE:CE1	16:3:138:GLN:HB3	2.37	0.60
18:1:1002:CLA:HMD2	18:1:1007:CLA:ND	2.16	0.60
15:1:41:TRP:HD1	15:1:59:PHE:C	2.04	0.60
2:B:422:LEU:HG	18:B:1236:CLA:HAB	1.82	0.60
1:A:274:TRP:O	12:K:141:LYS:HD2	2.01	0.60
13:2:199:LEU:C	13:2:199:LEU:HD23	2.22	0.60
13:2:154:ILE:HG21	18:4:4008:CLA:HED1	1.83	0.60
28:2:2011:CHL:HAA1	28:2:2011:CHL:CB D	2.30	0.60
27:3:3501:LUT:H171	27:3:3501:LUT:H8	1.82	0.60
16:3:74:GLY:CA	16:3:225:LEU:HD22	2.31	0.60
28:1:1009:CHL:HBB1	28:1:1009:CHL:HHC	1.83	0.60
27:4:4503:LUT:H8	27:4:4503:LUT:C18	2.19	0.60
18:B:1205:CLA:HAB	18:B:1206:CLA:HAA2	1.83	0.60
12:K:70:MET:CE	12:K:71:VAL:HG22	2.31	0.60
22:J:6013:BCR:H403	22:J:6013:BCR:C23	2.31	0.60
13:2:139:THR:HG22	13:2:139:THR:O	2.01	0.60
18:3:3001:CLA:O2A	27:3:3501:LUT:H382	2.01	0.60
18:3:3017:CLA:H2A	18:3:3017:CLA:O2D	2.02	0.60
15:1:166:ASP:CG	15:1:169:GLY:HA2	2.21	0.60
15:1:55:ALA:HB3	15:1:58:ASP:HB2	1.84	0.60
14:4:154:ILE:HG13	28:1:1009:CHL:HED1	1.82	0.60
15:1:120:THR:HG22	15:1:125:PRO:HA	1.84	0.60
28:4:4011:CHL:CBC	28:4:4011:CHL:HHD	2.28	0.60
22:A:6008:BCR:C23	18:A:1124:CLA:HAB	2.31	0.60
20:A:5001:PQN:H141	18:A:1139:CLA:HBB2	1.83	0.60
22:B:6004:BCR:H14C	18:B:1217:CLA:HBB1	1.83	0.60
3:I:24:LEU:HD22	22:L:6019:BCR:H333	1.82	0.60
2:B:560:ASP:CG	8:C:66:ARG:HH12	2.05	0.60
16:3:107:ARG:NH1	16:3:227:GLU:OE1	2.35	0.60
2:B:73:ASN:O	2:B:75:GLU:N	2.35	0.60
2:B:172:GLU:HG3	6:G:93:PRO:HG2	1.84	0.60
13:2:181:PRO:HD2	18:2:2016:CLA:CBB	2.32	0.59
18:3:3003:CLA:HMB2	18:3:3008:CLA:HBC1	1.84	0.59
27:3:3502:LUT:H361	27:3:3502:LUT:C28	2.32	0.59
15:1:41:TRP:CD1	15:1:59:PHE:CA	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:80:GLU:HG3	18:1:1004:CLA:NB	2.17	0.59
28:4:4010:CHL:HHD	28:4:4010:CHL:CBC	2.23	0.59
18:B:1206:CLA:HMB1	18:B:1206:CLA:HBB1	1.83	0.59
16:3:74:GLY:O	16:3:232:ARG:NH1	2.35	0.59
22:3:3503:BCR:C23	22:3:3503:BCR:H403	2.32	0.59
15:1:226:ILE:HG13	18:1:1003:CLA:CMD	2.32	0.59
18:A:1106:CLA:HAB	18:A:1126:CLA:H13	1.83	0.59
2:B:51:PHE:CE1	18:B:1208:CLA:HBB1	2.36	0.59
9:D:100:PHE:CE1	9:D:158:VAL:CB	2.85	0.59
13:2:85:PHE:HZ	13:2:223:LYS:HE3	1.66	0.59
15:1:58:ASP:CA	18:1:1004:CLA:HED2	2.32	0.59
2:B:174:ARG:HE	18:B:1221:CLA:HMD1	1.67	0.59
14:4:158:GLN:NE2	14:4:158:GLN:HA	2.17	0.59
16:3:162:MET:HA	16:3:162:MET:HE1	1.83	0.59
9:D:176:GLU:H	9:D:176:GLU:CD	2.06	0.59
28:2:2013:CHL:HBD	28:2:2013:CHL:HAA2	1.85	0.59
15:1:111:TRP:HZ3	18:1:1006:CLA:HED1	1.66	0.59
18:4:4004:CLA:H3A	18:4:4004:CLA:O1A	2.01	0.59
22:B:6004:BCR:H311	18:B:1212:CLA:H8	1.84	0.59
14:4:170:PRO:HD2	14:4:172:PHE:O	2.02	0.59
1:A:546:ALA:O	1:A:550:HIS:ND1	2.34	0.59
14:4:84:ASP:OD1	14:4:86:GLU:N	2.35	0.59
18:4:4001:CLA:C5	27:4:4501:LUT:H28	2.31	0.59
11:H:72:SER:O	11:H:73:ASP:HB3	2.01	0.59
18:2:2004:CLA:HMB1	18:2:2004:CLA:CBB	2.32	0.59
18:2:2016:CLA:O2A	18:2:2016:CLA:H2A	2.01	0.59
16:3:135:ALA:H	16:3:138:GLN:CG	2.15	0.59
16:3:268:VAL:HA	16:3:271:SER:HB3	1.84	0.59
18:3:3005:CLA:HMD2	18:3:3012:CLA:ND	2.16	0.59
16:3:67:TYR:CE2	16:3:84:SER:CB	2.86	0.59
6:G:114:VAL:HG12	6:G:116:LYS:H	1.68	0.59
16:3:137:PHE:CD1	16:3:138:GLN:N	2.71	0.59
16:3:155:TYR:CE1	18:3:3010:CLA:HAC2	2.38	0.59
2:B:377:TYR:CD2	18:B:1224:CLA:HAB	2.37	0.59
7:L:176:LEU:C	7:L:178:THR:HG22	2.23	0.59
16:3:104:ILE:HD12	16:3:172:ARG:CZ	2.33	0.59
15:1:183:LYS:HD3	18:1:1002:CLA:HBA2	1.83	0.59
15:1:80:GLU:OE2	15:1:189:ARG:NE	2.35	0.59
9:D:100:PHE:CE1	9:D:158:VAL:CG1	2.85	0.59
4:J:25:LEU:O	4:J:29:ILE:HG12	2.02	0.59
16:3:100:TYR:OH	16:3:172:ARG:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:263:PRO:HG2	18:3:3008:CLA:HMB3	1.84	0.59
18:3:3006:CLA:HMA1	18:3:3013:CLA:C3C	2.32	0.59
18:1:1003:CLA:C2	18:1:1008:CLA:HMD1	2.32	0.59
15:1:160:TYR:CZ	15:1:181:LYS:HD3	2.38	0.59
15:1:85:ARG:O	18:1:1001:CLA:HBC2	2.03	0.59
18:B:1240:CLA:HED3	18:B:1220:CLA:HMA1	1.85	0.59
18:B:1222:CLA:HAA2	18:B:1223:CLA:OBD	2.03	0.59
2:B:334:LEU:HD11	18:B:1226:CLA:HBB1	1.85	0.59
18:K:1001:CLA:HBC2	18:K:1001:CLA:CHD	2.30	0.59
12:K:70:MET:HE2	12:K:71:VAL:HA	1.82	0.59
16:3:243:ILE:CG2	18:3:3003:CLA:HMD3	2.33	0.59
16:3:127:LEU:O	18:3:3018:CLA:HBC3	2.02	0.59
15:1:111:TRP:CZ2	18:1:1013:CLA:CBC	2.85	0.59
6:G:129:SER:O	6:G:133:ILE:HG13	2.03	0.59
7:L:124:GLU:O	7:L:126:ALA:N	2.36	0.59
10:E:111:ASN:OD1	10:E:115:VAL:HG22	2.02	0.59
16:3:246:LEU:HD23	16:3:246:LEU:O	2.03	0.59
9:D:91:LEU:N	9:D:91:LEU:HD23	2.18	0.59
13:2:110:SER:HB3	13:2:225:GLY:HA3	1.85	0.58
16:3:134:LEU:HB3	16:3:138:GLN:HG3	1.85	0.58
18:1:1001:CLA:HBA1	27:1:1501:LUT:H382	1.85	0.58
15:1:221:PRO:CG	15:1:222:TRP:CZ3	2.86	0.58
18:B:1211:CLA:CMC	18:B:1212:CLA:HAB	2.33	0.58
7:L:211:TYR:CE2	18:L:1503:CLA:C2	2.85	0.58
14:4:225:THR:HG23	14:4:227:LYS:H	1.68	0.58
18:2:2007:CLA:H51	18:2:2007:CLA:C9	2.31	0.58
16:3:141:VAL:HG22	16:3:143:PRO:CD	2.32	0.58
16:3:267:ASN:ND2	16:3:270:THR:HG23	2.18	0.58
18:1:1001:CLA:H61	27:1:1501:LUT:H30	1.82	0.58
2:B:582:TRP:HH2	18:B:1012:CLA:HAB	1.68	0.58
5:F:82:LEU:HB3	5:F:140:CYS:O	2.02	0.58
15:1:186:LYS:CE	21:1:1801:LHG:HC41	2.33	0.58
12:K:83:PHE:HB2	22:K:2011:BCR:HC42	1.84	0.58
6:G:76:ARG:CG	6:G:77:PHE:CE1	2.86	0.58
16:3:248:THR:HG22	16:3:249:GLY:O	2.03	0.58
12:K:86:ALA:HB1	12:K:87:PRO:CD	2.28	0.58
23:4:4801:LMG:O5	23:4:4801:LMG:O4	2.14	0.58
13:2:125:PHE:O	13:2:130:GLY:N	2.30	0.58
14:4:95:GLU:HG3	18:4:4004:CLA:C4B	2.33	0.58
18:B:1207:CLA:HMC3	27:I:6018:LUT:C14	2.32	0.58
12:K:71:VAL:HG11	12:K:132:ILE:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:1001:CLA:H51	22:G:2011:BCR:H341	1.85	0.58
6:G:123:ASP:N	6:G:123:ASP:OD1	2.31	0.58
1:A:41:SER:HB3	1:A:44:ILE:HG22	1.84	0.58
13:2:126:LEU:HD23	13:2:133:LEU:O	2.04	0.58
6:G:111:TYR:N	6:G:111:TYR:CD1	2.71	0.58
18:A:1129:CLA:HMA2	7:L:71:THR:HG21	1.84	0.58
8:C:26:LEU:H	8:C:26:LEU:HD22	1.68	0.58
27:4:4501:LUT:C8	27:4:4501:LUT:H171	2.34	0.58
18:B:1209:CLA:HBB1	18:B:1209:CLA:HMB1	1.85	0.58
3:I:5:PRO:C	3:I:7:LEU:H	2.07	0.58
14:4:120:ILE:H	14:4:120:ILE:HD12	1.68	0.58
1:A:218:TRP:HD1	1:A:303:HIS:CD2	2.21	0.58
18:B:1203:CLA:HHB	18:B:1226:CLA:HAB	1.86	0.58
2:B:492:ILE:HD11	6:G:146:TYR:CE1	2.38	0.58
13:2:145:TYR:CB	18:2:2006:CLA:H92	2.34	0.58
16:3:142:ILE:HD11	18:3:3010:CLA:CBC	2.33	0.58
16:3:203:PRO:HD3	28:3:3011:CHL:CMD	2.29	0.58
28:3:3011:CHL:HHC	28:3:3011:CHL:HBB1	1.84	0.58
15:1:41:TRP:CE3	28:1:1009:CHL:HBC3	2.38	0.58
18:G:1003:CLA:C4B	23:G:2021:LMG:H151	2.33	0.58
14:4:223:ASN:O	14:4:224:VAL:HB	2.03	0.58
13:2:135:PRO:HG2	18:2:2006:CLA:HED1	1.86	0.58
22:3:3503:BCR:H323	22:3:3503:BCR:HC8	1.85	0.58
16:3:76:TYR:HB2	18:3:3004:CLA:HMD1	1.85	0.58
15:1:134:ILE:HD11	18:1:1013:CLA:C2D	2.34	0.58
18:A:1022:CLA:CAD	18:B:1021:CLA:HMB3	2.33	0.58
18:3:3001:CLA:CBA	27:3:3501:LUT:H24	2.34	0.58
16:3:62:LYS:O	16:3:63:GLN:HB2	2.04	0.58
15:1:165:PHE:O	27:1:1501:LUT:H24	2.04	0.58
15:1:177:PHE:CD2	15:1:181:LYS:HE2	2.38	0.58
14:4:153:GLU:CG	14:4:156:ARG:HH11	2.17	0.58
2:B:659:THR:HA	18:B:1023:CLA:HAB	1.85	0.58
12:K:72:ALA:CB	18:K:1001:CLA:CGA	2.81	0.58
6:G:92:LEU:N	6:G:92:LEU:HD12	2.02	0.58
7:L:121:ARG:C	7:L:124:GLU:H	2.07	0.58
7:L:143:ILE:O	7:L:146:THR:HG22	2.04	0.58
5:F:160:PHE:O	5:F:163:PRO:HD2	2.04	0.58
5:F:109:TYR:O	5:F:110:ALA:HB3	2.04	0.58
16:3:197:SER:OG	16:3:198:GLY:N	2.37	0.57
16:3:210:PRO:HB2	16:3:211:LEU:CD1	2.34	0.57
15:1:85:ARG:HE	18:1:1001:CLA:C4C	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4:4011:CHL:HHC	28:4:4011:CHL:HBB1	1.85	0.57
18:2:2008:CLA:CBB	18:2:2008:CLA:HHC	2.34	0.57
2:B:707:LEU:HD23	25:B:7101:DGD:HA21	1.85	0.57
9:D:88:THR:O	9:D:88:THR:HG22	2.04	0.57
7:L:91:THR:HA	7:L:175:GLN:HE22	1.69	0.57
16:3:94:GLU:OE1	16:3:96:ARG:HB2	2.04	0.57
16:3:119:PRO:HB2	16:3:133:ALA:HB2	1.86	0.57
14:4:178:PRO:O	14:4:179:ALA:HB2	2.04	0.57
13:2:110:SER:O	13:2:114:MET:HG3	2.04	0.57
13:2:224:ASN:OD1	18:2:2007:CLA:HMD1	2.04	0.57
16:3:62:LYS:HB2	16:3:63:GLN:OE1	2.04	0.57
14:4:57:LEU:HD11	18:4:4009:CLA:CED	2.35	0.57
14:4:103:MET:HB2	18:4:4001:CLA:CMC	2.34	0.57
18:B:1204:CLA:H3A	18:B:1205:CLA:HMB3	1.86	0.57
18:G:1003:CLA:C14	18:G:1003:CLA:H91	2.35	0.57
4:J:36:ALA:CB	23:J:5001:LMG:H111	2.30	0.57
12:K:90:ASN:O	16:3:64:SER:HB3	2.04	0.57
10:E:104:VAL:HG12	10:E:119:ASN:OD1	2.03	0.57
16:3:267:ASN:HA	18:3:3003:CLA:O1A	2.05	0.57
15:1:58:ASP:CB	18:1:1004:CLA:HED2	2.35	0.57
18:B:1216:CLA:HAA2	18:B:1221:CLA:HBB1	1.86	0.57
22:J:6012:BCR:C23	22:J:6012:BCR:H383	2.28	0.57
18:L:1502:CLA:HHD	22:L:6019:BCR:H292	1.87	0.57
12:K:136:VAL:HG12	12:K:140:LEU:HD21	1.86	0.57
7:L:121:ARG:HG2	7:L:127:GLY:N	2.20	0.57
11:H:132:PRO:N	11:H:133:PRO:HD3	2.18	0.57
9:D:155:PHE:CZ	9:D:168:HIS:HB3	2.39	0.57
16:3:263:PRO:HG3	18:3:3008:CLA:HMB3	1.85	0.57
16:3:110:MET:CE	27:3:3501:LUT:H201	2.35	0.57
18:G:1003:CLA:H62	23:G:2021:LMG:H132	1.84	0.57
9:D:76:ASP:CB	9:D:77:PRO:HB3	2.30	0.57
13:2:87:PHE:HE2	27:2:2502:LUT:C36	2.14	0.57
16:3:100:TYR:HD1	16:3:100:TYR:O	1.87	0.57
16:3:136:TRP:CD2	16:3:137:PHE:N	2.72	0.57
18:3:3010:CLA:C3C	18:3:3010:CLA:H93	2.35	0.57
15:1:124:ASN:OD1	15:1:124:ASN:N	2.38	0.57
14:4:184:TYR:O	18:4:4001:CLA:HED2	2.04	0.57
18:4:4006:CLA:C1B	27:4:4503:LUT:C17	2.83	0.57
14:4:101:TRP:CE2	28:4:4011:CHL:HED3	2.39	0.57
3:I:4:LEU:CD1	3:I:6:SER:H	2.15	0.57
1:A:24:ARG:NH1	1:A:76:ARG:HH12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2005:CLA:O1D	18:2:2012:CLA:H61	2.05	0.57
16:3:101:GLY:CA	18:3:3012:CLA:HED2	2.35	0.57
18:4:4003:CLA:H121	18:4:4003:CLA:H91	1.85	0.57
18:4:4008:CLA:CHD	18:4:4008:CLA:HBC2	2.34	0.57
15:1:127:PRO:CG	15:1:128:TRP:CD1	2.85	0.57
28:4:4013:CHL:HBB1	27:4:4502:LUT:H161	1.86	0.57
18:A:1127:CLA:H91	18:A:1117:CLA:H92	1.86	0.57
1:A:338:PHE:HB2	21:A:5003:LHG:HC42	1.86	0.57
18:B:1211:CLA:HBB1	18:B:1211:CLA:HHC	1.85	0.57
16:3:270:THR:HG1	16:3:271:SER:N	2.01	0.57
15:1:111:TRP:CD1	15:1:112:ALA:N	2.72	0.57
18:1:1011:CLA:H43	27:1:1501:LUT:O23	2.04	0.57
16:3:65:LEU:HB3	16:3:68:LEU:CD2	2.34	0.57
16:3:253:TYR:O	16:3:256:LEU:HB3	2.04	0.57
9:D:167:LEU:O	9:D:170:LYS:HB2	2.04	0.57
13:2:197:GLY:HA2	18:2:2001:CLA:HED1	1.86	0.57
13:2:114:MET:HE1	18:2:2001:CLA:CHC	2.34	0.57
18:2:2005:CLA:HED2	18:2:2012:CLA:O1A	2.05	0.57
15:1:205:TYR:HE2	18:1:1003:CLA:O1D	1.88	0.57
15:1:223:HIS:CD2	15:1:223:HIS:N	2.73	0.57
18:B:1240:CLA:HED3	18:B:1220:CLA:HHB	1.86	0.57
18:G:1003:CLA:H51	23:G:2021:LMG:C31	2.25	0.57
6:G:102:GLU:O	6:G:103:ALA:HB3	2.05	0.57
7:L:115:VAL:HG13	7:L:127:GLY:O	2.05	0.57
18:2:2001:CLA:CGA	18:2:2001:CLA:H3A	2.35	0.56
16:3:136:TRP:CE2	16:3:137:PHE:HB3	2.38	0.56
14:4:240:PRO:HG2	18:4:4008:CLA:C2B	2.34	0.56
15:1:167:PRO:HD2	27:1:1501:LUT:H1	1.70	0.56
14:4:147:ILE:HD11	21:1:1801:LHG:C36	2.35	0.56
18:L:1501:CLA:HED2	11:H:82:GLN:NE2	2.20	0.56
15:1:133:THR:HG22	15:1:137:ILE:HD11	1.87	0.56
7:L:171:LYS:O	7:L:172:GLN:HB3	2.04	0.56
13:2:143:GLN:CB	13:2:145:TYR:CE1	2.85	0.56
13:2:164:GLU:HA	13:2:167:ARG:H	1.70	0.56
16:3:185:GLN:HB2	16:3:186:TYR:CE1	2.39	0.56
18:1:1002:CLA:HMD2	18:1:1007:CLA:C4D	2.35	0.56
28:4:4013:CHL:CBB	27:4:4502:LUT:H161	2.34	0.56
13:2:211:PRO:O	13:2:212:GLN:CB	2.52	0.56
1:A:493:GLN:HG3	1:A:515:TRP:HD1	1.68	0.56
13:2:186:ASN:CG	18:2:2016:CLA:H2A	2.24	0.56
16:3:110:MET:SD	16:3:231:GLY:CA	2.92	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:259:HIS:ND1	18:3:3003:CLA:HAA2	2.20	0.56
16:3:105:ASN:CG	18:3:3012:CLA:HMD1	2.25	0.56
18:2:2009:CLA:HHC	18:2:2009:CLA:CBB	2.18	0.56
16:3:173:PHE:HD2	18:3:3012:CLA:HMA2	1.70	0.56
15:1:41:TRP:HD1	15:1:59:PHE:O	1.87	0.56
18:4:4005:CLA:HAB	27:4:4502:LUT:H35	1.86	0.56
18:G:1003:CLA:C3	23:G:2021:LMG:H331	2.35	0.56
27:I:6018:LUT:H162	22:I:6020:BCR:H353	1.87	0.56
15:1:83:HIS:HD2	27:1:1502:LUT:H35	1.69	0.56
1:A:310:PHE:HZ	18:A:1117:CLA:H121	1.70	0.56
22:B:6004:BCR:H371	18:B:1218:CLA:HMD2	1.87	0.56
18:G:1003:CLA:C4	23:G:2021:LMG:H332	2.36	0.56
18:G:1003:CLA:H52	23:G:2021:LMG:C33	2.35	0.56
14:4:88:LEU:O	14:4:92:VAL:HG23	2.05	0.56
9:D:97:VAL:O	9:D:97:VAL:HG12	2.05	0.56
13:2:125:PHE:HB3	13:2:131:ILE:HD12	1.88	0.56
13:2:160:ILE:HD11	28:2:2013:CHL:HMB3	1.86	0.56
1:A:40:PHE:HB3	18:A:1102:CLA:HED2	1.87	0.56
16:3:65:LEU:HB2	16:3:68:LEU:HD21	1.83	0.56
13:2:129:LEU:HD22	13:2:131:ILE:HG13	1.87	0.56
15:1:111:TRP:CE2	15:1:119:ALA:HB1	2.40	0.56
15:1:170:TYR:HE2	27:1:1501:LUT:H372	1.70	0.56
1:A:183:TRP:HB2	18:A:1109:CLA:HMC3	1.86	0.56
1:A:394:SER:HB3	18:A:1126:CLA:HMA1	1.88	0.56
18:G:1001:CLA:C4	22:G:2011:BCR:H342	2.35	0.56
11:H:133:PRO:HD2	11:H:135:LEU:N	2.21	0.56
18:3:3003:CLA:H42	18:3:3003:CLA:CHD	2.35	0.56
16:3:226:LYS:HE2	18:3:3007:CLA:HED2	1.84	0.56
15:1:180:TYR:HB3	18:1:1001:CLA:HMA1	1.86	0.56
18:4:4017:CLA:H3A	29:4:4505:ZEX:H202	1.88	0.56
10:E:102:PRO:HG2	10:E:103:VAL:HG23	1.88	0.56
2:B:476:VAL:HG12	2:B:477:LEU:H	1.71	0.56
13:2:141:GLY:HA2	28:2:2013:CHL:CBC	2.35	0.56
28:1:1010:CHL:HBB2	18:1:1013:CLA:HBB2	1.88	0.56
15:1:160:TYR:CE2	15:1:181:LYS:HD3	2.40	0.56
18:4:4005:CLA:CMD	18:4:4012:CLA:C1D	2.83	0.56
14:4:215:PHE:CE1	27:4:4502:LUT:H10	2.40	0.56
27:4:4503:LUT:H28	27:4:4503:LUT:H371	1.86	0.56
15:1:203:SER:O	15:1:204:ALA:HB3	2.05	0.56
14:4:52:LYS:O	14:4:53:LYS:HB3	2.06	0.56
18:2:2003:CLA:C1B	18:2:2008:CLA:HMD3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:167:PHE:O	16:3:171:ARG:HG3	2.05	0.56
14:4:97:VAL:HG21	14:4:156:ARG:NH2	2.21	0.56
18:B:1238:CLA:H13	27:I:6018:LUT:C19	2.36	0.56
18:G:1002:CLA:HBC3	18:G:1002:CLA:HMC1	1.86	0.56
9:D:202:LYS:O	9:D:203:PHE:HB2	2.04	0.56
1:A:373:ALA:HB2	1:A:399:HIS:HB2	1.88	0.56
18:2:2005:CLA:OBD	18:2:2012:CLA:HBA2	2.05	0.56
16:3:225:LEU:HB3	16:3:226:LYS:HE3	1.88	0.56
15:1:222:TRP:CH2	18:1:1008:CLA:CMB	2.85	0.56
22:B:6004:BCR:H292	18:B:1218:CLA:C4D	2.36	0.56
12:K:86:ALA:CB	12:K:87:PRO:CD	2.84	0.56
11:H:107:GLY:HA2	11:H:110:THR:CG2	2.36	0.56
18:2:2001:CLA:C3A	18:2:2001:CLA:CGA	2.83	0.56
16:3:190:LEU:O	16:3:194:PHE:N	2.38	0.56
10:E:78:ARG:O	10:E:79:GLN:HB2	2.05	0.56
13:2:126:LEU:HB2	13:2:134:THR:HA	1.87	0.55
18:2:2004:CLA:HHC	27:2:2502:LUT:H32	1.88	0.55
16:3:235:MET:O	16:3:238:ILE:HG23	2.06	0.55
16:3:263:PRO:HG3	18:3:3008:CLA:CMB	2.36	0.55
18:3:3003:CLA:C3B	27:3:3501:LUT:C17	2.84	0.55
18:B:1204:CLA:O2A	3:I:12:VAL:HG21	2.05	0.55
7:L:145:LEU:HD11	22:L:6019:BCR:C39	2.20	0.55
18:G:1001:CLA:HED3	18:G:1001:CLA:CHA	2.35	0.55
14:4:169:ASP:HA	18:4:4016:CLA:O1D	2.06	0.55
13:2:174:PRO:CD	13:2:175:GLY:N	2.70	0.55
28:4:4011:CHL:CHD	28:4:4011:CHL:HBC2	2.29	0.55
21:A:5003:LHG:H302	18:A:1122:CLA:H152	1.89	0.55
18:B:1021:CLA:HBB1	18:B:1021:CLA:HMB1	1.88	0.55
7:L:90:ARG:O	7:L:98:ARG:HD3	2.06	0.55
11:H:95:LYS:O	11:H:96:ARG:HB3	2.06	0.55
1:A:21:ILE:HD13	18:A:1108:CLA:HAA2	1.87	0.55
22:F:6014:BCR:C40	22:F:6014:BCR:H23C	2.36	0.55
18:1:1001:CLA:CGA	18:1:1001:CLA:H3A	2.35	0.55
15:1:118:GLN:O	15:1:119:ALA:HB3	2.06	0.55
18:4:4007:CLA:H2A	18:4:4007:CLA:HED2	1.87	0.55
2:B:26:ALA:HB2	25:B:7101:DGD:HA32	1.89	0.55
22:K:2011:BCR:H321	22:K:2011:BCR:C8	2.15	0.55
18:A:1105:CLA:HBB1	18:A:1105:CLA:HHC	1.89	0.55
2:B:292:ARG:HH21	6:G:107:ARG:NH1	2.04	0.55
18:A:1134:CLA:H92	18:A:1134:CLA:H2	1.87	0.55
13:2:142:GLU:O	13:2:142:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:134:LEU:CB	16:3:138:GLN:CG	2.84	0.55
16:3:236:LEU:CD2	18:3:3004:CLA:HMC1	2.33	0.55
15:1:112:ALA:HB3	28:1:1010:CHL:HMD3	1.89	0.55
18:A:1022:CLA:H161	22:A:6017:BCR:H321	1.89	0.55
1:A:92:TRP:HE1	18:A:1106:CLA:HBA1	1.72	0.55
22:A:6017:BCR:H292	20:B:5002:PQN:H142	1.89	0.55
4:J:38:THR:O	23:J:5001:LMG:H122	2.05	0.55
13:2:197:GLY:HA2	18:2:2001:CLA:CED	2.36	0.55
18:2:2016:CLA:CAD	18:2:2016:CLA:HED2	2.36	0.55
18:3:3006:CLA:C1D	18:3:3018:CLA:CBB	2.84	0.55
18:3:3010:CLA:H93	18:3:3010:CLA:C1C	2.37	0.55
16:3:74:GLY:HA2	16:3:225:LEU:HD22	1.87	0.55
18:4:4001:CLA:H51	27:4:4501:LUT:H30	1.89	0.55
18:G:1003:CLA:H91	18:G:1003:CLA:H142	1.88	0.55
16:3:65:LEU:CD2	16:3:66:SER:H	2.19	0.55
7:L:169:ARG:CZ	7:L:171:LYS:CB	2.85	0.55
1:A:223:VAL:HG23	1:A:224:HIS:CD2	2.42	0.55
13:2:139:THR:HA	28:2:2010:CHL:CED	2.35	0.55
16:3:140:GLY:HA2	18:3:3013:CLA:CBC	2.32	0.55
18:1:1001:CLA:HMC1	18:1:1001:CLA:HBC2	1.89	0.55
14:4:98:ASN:ND2	18:4:4012:CLA:HMD1	2.22	0.55
11:H:134:LYS:O	11:H:135:LEU:HG	2.06	0.55
9:D:100:PHE:CE1	9:D:158:VAL:HG11	2.41	0.55
9:D:109:LYS:HG2	9:D:110:GLU:N	2.22	0.55
18:2:2004:CLA:HHD	18:2:2004:CLA:HBC2	1.88	0.55
16:3:267:ASN:HB2	18:3:3003:CLA:O1A	2.07	0.55
16:3:110:MET:CE	27:3:3501:LUT:C20	2.85	0.55
27:4:4503:LUT:H361	28:1:1009:CHL:H62	1.89	0.55
15:1:126:VAL:CB	15:1:127:PRO:CA	2.83	0.55
18:B:1204:CLA:H11	27:I:6018:LUT:O23	2.07	0.55
22:J:6012:BCR:H23C	22:J:6012:BCR:C38	2.30	0.55
18:4:4017:CLA:OBD	28:1:1009:CHL:HMA1	2.06	0.55
18:4:4004:CLA:CBB	27:4:4502:LUT:H32	2.36	0.55
18:A:1102:CLA:HMA2	18:A:1109:CLA:HMD2	1.87	0.55
12:K:132:ILE:O	12:K:136:VAL:HG23	2.07	0.55
18:2:2003:CLA:C3B	27:2:2501:LUT:C38	2.85	0.55
18:3:3005:CLA:CMD	18:3:3012:CLA:C1D	2.84	0.55
18:3:3006:CLA:CHA	18:3:3006:CLA:CED	2.85	0.55
18:3:3003:CLA:C2B	27:3:3501:LUT:C17	2.84	0.55
18:1:1001:CLA:CBB	27:1:1501:LUT:C32	2.85	0.55
14:4:104:LEU:C	18:4:4006:CLA:CBB	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:4501:LUT:C17	27:4:4501:LUT:C8	2.85	0.55
22:G:2011:BCR:C40	22:G:2011:BCR:C23	2.85	0.55
16:3:65:LEU:CD1	16:3:67:TYR:HE1	2.20	0.55
11:H:110:THR:HG23	11:H:111:LEU:N	2.20	0.55
18:2:2001:CLA:O1A	18:2:2001:CLA:H3A	2.06	0.55
16:3:134:LEU:HB3	16:3:138:GLN:CG	2.36	0.55
7:L:94:ASN:HB3	7:L:97:LEU:HD12	1.83	0.55
9:D:100:PHE:CD1	9:D:158:VAL:HB	2.41	0.55
22:F:6014:BCR:C40	22:F:6014:BCR:C23	2.85	0.55
18:2:2002:CLA:CGA	18:2:2002:CLA:CED	2.84	0.54
18:3:3003:CLA:CHC	18:3:3003:CLA:C9	2.85	0.54
16:3:232:ARG:HD2	18:3:3004:CLA:C4C	2.37	0.54
15:1:134:ILE:CD1	18:1:1013:CLA:C2D	2.85	0.54
15:1:230:VAL:HG12	15:1:231:LEU:CD2	2.36	0.54
27:4:4502:LUT:C8	27:4:4502:LUT:C17	2.86	0.54
1:A:54:ILE:HD12	18:A:1139:CLA:HMB3	1.89	0.54
1:A:434:ARG:O	1:A:438:HIS:ND1	2.33	0.54
18:G:1001:CLA:CHA	18:G:1001:CLA:CED	2.85	0.54
7:L:121:ARG:O	7:L:124:GLU:N	2.38	0.54
14:4:186:GLY:O	14:4:189:PHE:HB2	2.07	0.54
13:2:118:ALA:CB	18:2:2006:CLA:CMC	2.85	0.54
16:3:104:ILE:HD12	16:3:172:ARG:NH2	2.21	0.54
16:3:129:PRO:O	16:3:132:THR:HG22	2.07	0.54
16:3:141:VAL:HG13	16:3:144:PRO:HD2	1.88	0.54
16:3:146:GLY:C	16:3:147:THR:HG1	2.02	0.54
16:3:196:GLY:O	16:3:197:SER:HB3	2.06	0.54
28:3:3011:CHL:CAA	28:3:3011:CHL:CBD	2.85	0.54
18:3:3017:CLA:O2A	18:3:3017:CLA:H3A	2.06	0.54
18:1:1001:CLA:C3A	18:1:1001:CLA:CGA	2.85	0.54
18:4:4006:CLA:C4B	27:4:4503:LUT:C17	2.86	0.54
17:A:1011:CL0:H13	18:B:1012:CLA:OBD	2.07	0.54
12:K:75:THR:HG21	12:K:129:GLY:HA2	1.88	0.54
14:4:118:ILE:HG23	14:4:120:ILE:H	1.72	0.54
8:C:14:CYS:SG	8:C:16:GLN:HG2	2.48	0.54
13:2:256:ASP:CG	13:2:259:HIS:HD2	2.10	0.54
10:E:78:ARG:NH1	10:E:124:GLU:OE1	2.40	0.54
13:2:125:PHE:CB	13:2:131:ILE:HD12	2.37	0.54
16:3:183:GLY:HA3	16:3:194:PHE:C	2.28	0.54
15:1:85:ARG:NE	18:1:1001:CLA:C4C	2.71	0.54
18:4:4007:CLA:CAA	18:4:4007:CLA:HED2	2.37	0.54
2:B:254:ILE:HG13	2:B:255:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:TRP:CH2	18:A:1115:CLA:HBB1	2.42	0.54
18:2:2016:CLA:CBD	18:2:2016:CLA:CGA	2.85	0.54
13:2:92:LEU:CD1	27:2:2502:LUT:C24	2.85	0.54
18:3:3003:CLA:C12	18:3:3003:CLA:C9	2.85	0.54
16:3:101:GLY:CA	18:3:3012:CLA:CED	2.85	0.54
18:4:4003:CLA:C1C	18:4:4003:CLA:H61	2.38	0.54
15:1:205:TYR:OH	18:1:1003:CLA:OBD	2.18	0.54
18:B:1207:CLA:H92	7:L:132:LEU:HG	1.90	0.54
22:L:6020:BCR:C19	18:L:1501:CLA:HMB2	2.37	0.54
7:L:116:LYS:HD3	18:L:1503:CLA:CMB	2.35	0.54
18:G:1001:CLA:C5	22:G:2011:BCR:C34	2.85	0.54
6:G:95:GLN:O	6:G:96:ASN:HB2	2.07	0.54
1:A:195:TRP:CZ2	18:A:1108:CLA:HMA1	2.42	0.54
18:2:2003:CLA:CHD	18:2:2003:CLA:C4	2.85	0.54
28:2:2011:CHL:CBB	18:2:2016:CLA:CAB	2.86	0.54
15:1:183:LYS:HG2	18:1:1007:CLA:HED2	1.89	0.54
15:1:80:GLU:OE2	15:1:189:ARG:NH2	2.39	0.54
18:A:1106:CLA:H62	18:A:1126:CLA:H92	1.89	0.54
18:B:1224:CLA:CGA	18:B:1224:CLA:H3A	2.37	0.54
23:F:5002:LMG:H292	18:1:1014:CLA:C1D	2.38	0.54
1:A:213:LEU:HD22	22:A:6002:BCR:H361	1.89	0.54
14:4:198:LEU:N	14:4:198:LEU:HD12	2.21	0.54
13:2:197:GLY:CA	18:2:2001:CLA:CED	2.85	0.54
18:1:1003:CLA:H12	18:1:1008:CLA:CMD	2.37	0.54
18:1:1006:CLA:HMA2	18:1:1013:CLA:CBC	2.38	0.54
15:1:134:ILE:HD11	18:1:1013:CLA:C3D	2.38	0.54
15:1:88:MET:CE	18:1:1001:CLA:CAB	2.85	0.54
14:4:152:VAL:CG1	28:4:4011:CHL:C1B	2.85	0.54
14:4:155:ARG:NH1	28:1:1009:CHL:OBD	2.41	0.54
18:4:4012:CLA:HMC1	18:4:4012:CLA:HBC3	1.90	0.54
18:G:1001:CLA:HMB2	22:G:2011:BCR:C15	2.37	0.54
16:3:117:ILE:CD1	16:3:252:PRO:HB2	2.38	0.54
13:2:178:ASN:HD22	13:2:179:THR:N	2.05	0.54
18:3:3010:CLA:C9	18:3:3010:CLA:C1C	2.85	0.54
15:1:88:MET:CE	18:1:1001:CLA:CHC	2.86	0.54
14:4:126:TRP:C	14:4:128:ASP:H	2.11	0.54
16:3:67:TYR:HE2	16:3:84:SER:HB3	1.72	0.54
16:3:120:GLU:OE2	16:3:254:GLN:N	2.31	0.54
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.90	0.54
16:3:179:PRO:HG2	16:3:180:GLY:H	1.71	0.54
2:B:225:LEU:O	2:B:230:TRP:NE1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2005:CLA:CBC	18:2:2012:CLA:CBC	2.85	0.54
18:2:2007:CLA:CBB	22:3:3503:BCR:C26	2.85	0.54
18:3:3013:CLA:CBB	27:3:3502:LUT:C18	2.86	0.54
22:3:3503:BCR:C8	22:3:3503:BCR:C32	2.86	0.54
15:1:120:THR:HG22	15:1:125:PRO:N	2.23	0.54
14:4:152:VAL:HG11	28:4:4011:CHL:CHB	2.38	0.54
18:G:1003:CLA:C5	23:G:2021:LMG:C33	2.85	0.54
3:I:4:LEU:HD11	3:I:6:SER:CB	2.29	0.54
18:4:4016:CLA:C1	18:4:4016:CLA:C4D	2.86	0.54
18:G:1002:CLA:HBA2	18:G:1002:CLA:HBD	1.89	0.54
1:A:268:PRO:HD2	1:A:277:TYR:CZ	2.43	0.54
13:2:125:PHE:CB	13:2:131:ILE:CD1	2.86	0.54
13:2:233:MET:HG2	18:2:2004:CLA:H193	1.89	0.54
18:2:2003:CLA:HMB3	18:2:2008:CLA:HBC1	1.89	0.54
28:2:2013:CHL:O2A	28:2:2013:CHL:H2A	2.07	0.54
13:2:225:GLY:O	13:2:229:MET:HG3	2.08	0.54
15:1:202:GLN:NE2	15:1:202:GLN:CA	2.71	0.54
18:4:4007:CLA:CBC	18:4:4007:CLA:CHD	2.86	0.54
22:J:6012:BCR:C38	22:J:6012:BCR:C23	2.85	0.54
12:K:79:PHE:O	12:K:80:ALA:HB2	2.07	0.54
18:G:1001:CLA:H51	22:G:2011:BCR:C34	2.38	0.54
14:4:170:PRO:CB	18:4:4016:CLA:C4A	2.85	0.54
14:4:169:ASP:CB	18:4:4016:CLA:C2D	2.85	0.54
15:1:40:ASP:N	15:1:47:ARG:HD2	2.23	0.54
28:2:2011:CHL:HBB2	18:2:2016:CLA:CBB	2.38	0.54
16:3:134:LEU:HB3	16:3:138:GLN:OE1	2.07	0.54
16:3:132:THR:O	16:3:134:LEU:HD23	2.07	0.54
18:1:1003:CLA:C2	18:1:1008:CLA:CMD	2.85	0.54
18:B:1240:CLA:HED1	22:B:6009:BCR:H353	1.89	0.54
1:A:266:ALA:HB3	16:3:272:LEU:HD13	1.90	0.54
22:F:6014:BCR:H23C	22:F:6014:BCR:H402	1.88	0.54
2:B:306:GLU:HA	2:B:320:LYS:HG2	1.90	0.54
18:4:4008:CLA:CBB	18:4:4008:CLA:HHC	2.37	0.53
18:4:4002:CLA:H12	18:4:4002:CLA:CMA	2.09	0.53
18:4:4006:CLA:C3B	27:4:4502:LUT:C18	2.85	0.53
2:B:523:ILE:HD13	18:B:1234:CLA:HAB	1.90	0.53
2:B:6:PRO:HG3	2:B:24:GLY:HA2	1.88	0.53
6:G:114:VAL:HG11	18:G:1002:CLA:CBA	2.38	0.53
13:2:104:GLN:NE2	13:2:193:VAL:CG2	2.72	0.53
28:1:1009:CHL:CED	28:1:1009:CHL:H2A	2.39	0.53
14:4:101:TRP:CZ2	28:4:4011:CHL:HED3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:4001:CLA:HHD	18:4:4001:CLA:HBC2	1.89	0.53
18:B:1240:CLA:H142	18:B:1227:CLA:HMC2	1.90	0.53
18:G:1003:CLA:C3	23:G:2021:LMG:C33	2.85	0.53
18:G:1002:CLA:HBB1	18:G:1002:CLA:HMB1	1.90	0.53
14:4:225:THR:HG21	14:4:232:ASN:OD1	2.09	0.53
7:L:169:ARG:HD2	7:L:171:LYS:H	1.72	0.53
18:2:2008:CLA:CBC	18:2:2008:CLA:CHD	2.85	0.53
16:3:161:GLU:CD	18:3:3010:CLA:HAB	2.29	0.53
18:3:3006:CLA:CMD	18:3:3018:CLA:CAB	2.87	0.53
18:3:3006:CLA:CMA	18:3:3013:CLA:C3C	2.85	0.53
15:1:58:ASP:CB	18:1:1004:CLA:CED	2.86	0.53
27:4:4503:LUT:H181	27:4:4503:LUT:C8	2.10	0.53
7:L:94:ASN:HB2	7:L:97:LEU:CD1	2.23	0.53
1:A:126:ILE:HB	22:J:6013:BCR:H322	1.90	0.53
13:2:67:TRP:NE1	13:2:86:GLY:O	2.41	0.53
13:2:188:LEU:CD2	13:2:198:GLY:HA3	2.24	0.53
28:3:3011:CHL:CBA	28:3:3011:CHL:CBD	2.85	0.53
21:A:7001:LHG:H252	18:A:1128:CLA:H42	1.89	0.53
18:B:1216:CLA:HMC2	18:B:1221:CLA:H18	1.91	0.53
7:L:91:THR:HA	7:L:98:ARG:HH21	1.71	0.53
18:2:2001:CLA:H43	18:2:2002:CLA:HBA1	1.85	0.53
18:3:3008:CLA:HBA1	18:3:3008:CLA:CBD	2.38	0.53
18:4:4004:CLA:CGA	18:4:4004:CLA:H3A	2.38	0.53
14:4:120:ILE:H	14:4:120:ILE:CD1	2.22	0.53
1:A:269:PHE:HD2	1:A:270:PHE:HD1	1.55	0.53
9:D:82:PRO:HG3	9:D:128:ASN:HD21	1.72	0.53
22:A:6002:BCR:H331	18:A:1112:CLA:HHB	1.90	0.53
14:4:199:GLU:HA	14:4:202:GLU:HG3	1.90	0.53
13:2:220:LYS:CE	18:2:2002:CLA:CED	2.85	0.53
13:2:246:PRO:O	13:2:249:ASN:HB2	2.09	0.53
16:3:110:MET:SD	16:3:231:GLY:N	2.82	0.53
15:1:58:ASP:CG	18:1:1004:CLA:HED2	2.29	0.53
14:4:135:PHE:O	14:4:136:ALA:HB3	2.09	0.53
18:4:4005:CLA:CMD	18:4:4012:CLA:ND	2.72	0.53
7:L:90:ARG:HA	11:H:72:SER:OG	2.09	0.53
18:4:4016:CLA:CHA	18:4:4016:CLA:HBA1	2.39	0.53
16:3:67:TYR:CE2	16:3:84:SER:HB2	2.43	0.53
9:D:76:ASP:HB3	9:D:77:PRO:HA	1.88	0.53
15:1:152:GLU:HG3	15:1:156:GLU:HA	1.91	0.53
23:4:4801:LMG:HC72	23:4:4801:LMG:O2	2.07	0.53
7:L:206:VAL:O	7:L:207:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:242:THR:HG22	13:2:242:THR:O	2.08	0.53
13:2:122:ILE:HG23	13:2:133:LEU:HD22	1.90	0.53
13:2:177:VAL:CG2	13:2:178:ASN:N	2.72	0.53
13:2:197:GLY:N	18:2:2001:CLA:CED	2.72	0.53
18:2:2005:CLA:H41	18:2:2005:CLA:C9	2.39	0.53
16:3:185:GLN:C	16:3:186:TYR:HD1	2.12	0.53
16:3:193:GLY:HA3	16:3:207:PHE:CE2	2.44	0.53
16:3:259:HIS:N	16:3:266:ASN:ND2	2.57	0.53
16:3:227:GLU:HB2	18:3:3001:CLA:C1B	2.39	0.53
15:1:221:PRO:CG	15:1:222:TRP:CE3	2.85	0.53
2:B:167:TRP:CZ2	18:B:1208:CLA:HMA1	2.44	0.53
27:I:6018:LUT:H181	27:I:6018:LUT:H8	1.90	0.53
16:3:119:PRO:HB2	16:3:133:ALA:HB1	1.89	0.53
1:A:209:GLY:HA2	18:A:1118:CLA:HBC1	1.91	0.53
1:A:493:GLN:HG3	1:A:515:TRP:CD1	2.43	0.53
18:2:2002:CLA:HMB1	18:2:2002:CLA:CBB	2.34	0.53
18:2:2003:CLA:CGA	18:2:2003:CLA:C1A	2.87	0.53
13:2:181:PRO:HD2	18:2:2016:CLA:HBB1	1.91	0.53
18:3:3012:CLA:HBC2	18:3:3012:CLA:HMC1	1.91	0.53
15:1:120:THR:HG22	15:1:125:PRO:CA	2.38	0.53
18:1:1001:CLA:C4D	27:1:1501:LUT:H383	2.39	0.53
18:1:1004:CLA:HBB2	27:1:1502:LUT:H12	1.86	0.53
15:1:104:ASN:ND2	15:1:208:THR:HG23	2.24	0.53
2:B:177:HIS:CG	18:B:1210:CLA:HMC2	2.44	0.53
14:4:245:ILE:HG12	14:4:249:LEU:HD12	1.89	0.53
16:3:226:LYS:N	16:3:226:LYS:CE	2.72	0.53
18:B:1238:CLA:H18	27:I:6018:LUT:H203	1.90	0.53
18:F:1301:CLA:HHC	18:F:1301:CLA:CBB	2.37	0.53
18:L:1502:CLA:C3C	22:L:6019:BCR:H282	2.39	0.53
22:L:6019:BCR:C38	22:L:6019:BCR:C23	2.85	0.53
18:A:1121:CLA:C2D	22:K:2011:BCR:H323	2.38	0.53
10:E:66:ILE:HB	10:E:95:GLN:OE1	2.08	0.53
8:C:26:LEU:N	8:C:26:LEU:HD22	2.23	0.53
2:B:389:HIS:HA	2:B:392:ILE:HD12	1.91	0.53
13:2:87:PHE:CE2	27:2:2502:LUT:C36	2.86	0.53
4:J:9:SER:O	4:J:10:VAL:HG22	2.09	0.53
13:2:250:LEU:HD23	13:2:254:LEU:HD21	1.89	0.53
9:D:173:VAL:HG12	9:D:174:TYR:H	1.72	0.53
3:I:29:GLU:HB2	7:L:151:SER:OG	2.08	0.53
18:3:3006:CLA:HMA2	18:3:3013:CLA:HAC2	1.91	0.52
14:4:212:MET:HB2	18:4:4004:CLA:HMC3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:145:VAL:O	15:1:148:GLN:HB2	2.08	0.52
7:L:204:LEU:HD13	7:L:204:LEU:C	2.28	0.52
18:A:1134:CLA:H3A	18:A:1116:CLA:H93	1.91	0.52
13:2:139:THR:CA	28:2:2010:CHL:CED	2.84	0.52
18:2:2002:CLA:HMD2	18:2:2007:CLA:ND	2.24	0.52
28:3:3011:CHL:O1D	28:3:3011:CHL:H2A	2.09	0.52
18:4:4004:CLA:HMC2	27:4:4502:LUT:C32	2.39	0.52
18:B:1221:CLA:HMA1	18:B:1221:CLA:H92	1.90	0.52
2:B:422:LEU:HG	18:B:1236:CLA:CAB	2.39	0.52
6:G:108:ALA:HB1	6:G:111:TYR:CE1	2.41	0.52
1:A:268:PRO:HA	1:A:271:THR:HG22	1.91	0.52
15:1:42:MET:SD	15:1:45:GLN:HG3	2.50	0.52
18:2:2012:CLA:C1	23:2:2802:LMG:C36	2.87	0.52
18:3:3004:CLA:CGA	18:3:3004:CLA:C3A	2.87	0.52
18:4:4003:CLA:O1A	18:4:4003:CLA:HBD	2.08	0.52
18:4:4001:CLA:CHD	18:4:4001:CLA:HBC2	2.40	0.52
1:A:401:TRP:NE1	18:A:1126:CLA:HAB	2.24	0.52
18:A:1101:CLA:ND	4:J:12:PRO:HG3	2.24	0.52
18:G:1001:CLA:CAB	22:G:2011:BCR:C36	2.86	0.52
2:B:636:THR:HG22	2:B:638:LEU:H	1.75	0.52
8:C:21:CYS:SG	8:C:24:ASP:N	2.83	0.52
2:B:373:THR:HG23	2:B:591:THR:HG21	1.91	0.52
13:2:186:ASN:ND2	18:2:2016:CLA:C1A	2.73	0.52
18:2:2006:CLA:C4	18:2:2006:CLA:CAD	2.85	0.52
18:2:2008:CLA:HBB1	18:2:2008:CLA:CHC	2.38	0.52
28:2:2010:CHL:HBB2	18:2:2012:CLA:HBC1	1.91	0.52
27:2:2501:LUT:C37	27:2:2501:LUT:C28	2.85	0.52
13:2:85:PHE:CD2	18:2:2009:CLA:HBC2	2.44	0.52
18:3:3008:CLA:HBA1	18:3:3008:CLA:CHA	2.38	0.52
16:3:171:ARG:HD3	28:3:3011:CHL:OMC	2.09	0.52
18:A:1138:CLA:H121	18:F:1301:CLA:HAC1	1.90	0.52
23:B:5005:LMG:H111	18:B:1227:CLA:HAA2	1.91	0.52
7:L:90:ARG:HB3	7:L:93:VAL:HG23	1.91	0.52
10:E:66:ILE:CG2	10:E:67:GLY:N	2.72	0.52
8:C:51:CYS:SG	8:C:53:ARG:HD3	2.49	0.52
18:3:3005:CLA:CMD	18:3:3012:CLA:ND	2.72	0.52
15:1:41:TRP:CE3	28:1:1009:CHL:CBC	2.91	0.52
15:1:94:ILE:HG23	15:1:105:TRP:HB3	1.91	0.52
14:4:94:ALA:HB2	18:4:4012:CLA:CED	2.40	0.52
1:A:595:TRP:CD1	18:A:1128:CLA:HMD1	2.45	0.52
16:3:121:TYR:HA	16:3:253:TYR:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:204:LEU:HB3	13:2:206:TRP:CD1	2.45	0.52
13:2:89:PRO:HD2	27:2:2502:LUT:C22	2.40	0.52
16:3:104:ILE:CD1	16:3:172:ARG:NH2	2.72	0.52
16:3:164:LEU:HD13	22:3:3503:BCR:H352	1.91	0.52
16:3:184:LYS:HG2	16:3:185:GLN:NE2	2.25	0.52
16:3:263:PRO:HD2	16:3:264:VAL:H	1.75	0.52
16:3:262:ASP:CB	16:3:265:ASN:ND2	2.73	0.52
16:3:267:ASN:ND2	16:3:270:THR:CG2	2.73	0.52
18:3:3006:CLA:CMB	18:3:3013:CLA:C4B	2.87	0.52
18:3:3017:CLA:HAA2	18:3:3017:CLA:CED	2.38	0.52
18:1:1006:CLA:HBC2	18:1:1006:CLA:HMC1	1.89	0.52
15:1:134:ILE:CD1	18:1:1013:CLA:C3D	2.88	0.52
15:1:211:LEU:H	15:1:211:LEU:HD12	1.75	0.52
15:1:226:ILE:O	15:1:229:ASN:N	2.43	0.52
14:4:94:ALA:N	18:4:4012:CLA:CED	2.73	0.52
18:B:1232:CLA:O1A	18:G:1003:CLA:HHB	2.09	0.52
2:B:182:LEU:HD13	18:B:1210:CLA:HHB	1.92	0.52
22:L:6020:BCR:H342	18:H:1000:CLA:HAB	1.92	0.52
4:J:38:THR:OG1	5:F:136:GLN:NE2	2.42	0.52
9:D:204:THR:O	9:D:206:LYS:N	2.42	0.52
10:E:79:GLN:HG3	10:E:84:TYR:CZ	2.45	0.52
13:2:134:THR:N	13:2:135:PRO:HD2	2.25	0.52
16:3:139:THR:CG2	16:3:140:GLY:N	2.73	0.52
15:1:130:THR:CG2	15:1:131:LEU:N	2.73	0.52
14:4:147:ILE:HD11	21:1:1801:LHG:H361	1.92	0.52
2:B:680:TRP:NE1	9:D:88:THR:HG23	2.25	0.52
12:K:120:ALA:HA	12:K:123:LEU:HD12	1.92	0.52
16:3:94:GLU:OE2	16:3:95:PRO:CD	2.57	0.52
9:D:135:LYS:O	9:D:138:CYS:N	2.43	0.52
9:D:155:PHE:CZ	9:D:168:HIS:CB	2.93	0.52
18:2:2003:CLA:H2	18:2:2008:CLA:OBD	2.09	0.52
18:2:2005:CLA:OBD	18:2:2012:CLA:H2	2.09	0.52
18:2:2007:CLA:C4C	21:2:2801:LHG:HC62	2.40	0.52
16:3:210:PRO:HB2	16:3:211:LEU:HD13	1.90	0.52
18:3:3010:CLA:HBD	18:3:3010:CLA:HAA1	1.92	0.52
18:1:1001:CLA:CBB	27:1:1501:LUT:H32	2.40	0.52
18:1:1011:CLA:CBB	18:1:1011:CLA:HMB1	2.38	0.52
18:1:1005:CLA:CMD	18:1:1012:CLA:ND	2.72	0.52
15:1:82:ILE:CD1	15:1:149:ARG:NH2	2.73	0.52
15:1:166:ASP:OD2	15:1:169:GLY:HA2	2.10	0.52
15:1:85:ARG:CB	18:1:1011:CLA:CED	2.85	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:100:ARG:HA	14:4:103:MET:HG3	1.91	0.52
18:G:1003:CLA:H52	23:G:2021:LMG:C32	2.39	0.52
7:L:176:LEU:CG	7:L:177:GLN:N	2.73	0.52
14:4:171:ILE:HD13	18:4:4016:CLA:HMA2	1.91	0.52
10:E:122:LEU:H	10:E:122:LEU:CD1	2.05	0.52
6:G:116:LYS:NZ	18:G:1002:CLA:C4B	2.73	0.52
6:G:77:PHE:CD1	6:G:77:PHE:N	2.78	0.52
26:B:8002:LMU:O2B	26:B:8002:LMU:O3'	2.19	0.52
1:A:342:GLY:O	1:A:343:HIS:HB2	2.09	0.52
13:2:122:ILE:HG21	13:2:133:LEU:HB2	1.89	0.52
13:2:177:VAL:CG2	13:2:178:ASN:H	2.22	0.52
13:2:220:LYS:HD3	18:2:2002:CLA:CED	2.29	0.52
13:2:234:GLY:O	13:2:238:GLN:HB2	2.10	0.52
16:3:223:LEU:HB3	18:3:3001:CLA:HMA1	1.92	0.52
18:3:3006:CLA:H12	22:3:3503:BCR:H313	1.91	0.52
18:3:3013:CLA:H2A	18:3:3013:CLA:O2D	2.09	0.52
18:1:1003:CLA:H11	18:1:1008:CLA:OBD	2.09	0.52
15:1:108:ALA:HA	15:1:111:TRP:CZ3	2.45	0.52
14:4:103:MET:CE	14:4:207:ASN:CB	2.85	0.52
1:A:397:THR:HG22	18:A:1126:CLA:HAB	1.91	0.52
18:B:1220:CLA:H13	22:B:6009:BCR:H312	1.92	0.52
3:I:9:VAL:O	3:I:13:GLY:N	2.34	0.52
16:3:115:GLY:O	16:3:119:PRO:CD	2.57	0.52
8:C:17:CYS:SG	8:C:18:VAL:N	2.83	0.52
13:2:188:LEU:HD22	13:2:189:THR:CA	2.39	0.52
13:2:216:GLU:O	13:2:220:LYS:HG3	2.09	0.52
18:3:3002:CLA:CMC	18:3:3002:CLA:HBC2	2.37	0.52
18:3:3003:CLA:CGA	18:3:3003:CLA:CHA	2.88	0.52
18:3:3006:CLA:C1A	18:3:3006:CLA:CED	2.85	0.52
16:3:164:LEU:CB	22:3:3503:BCR:C35	2.85	0.52
15:1:116:GLY:O	15:1:118:GLN:HG2	2.10	0.52
1:A:272:LEU:HD13	18:K:1001:CLA:HBC1	1.92	0.52
8:C:10:THR:HG23	8:C:64:SER:CB	2.40	0.52
4:J:36:ALA:CB	23:J:5001:LMG:HC72	2.40	0.52
16:3:174:GLN:HA	16:3:174:GLN:OE1	2.10	0.51
18:3:3003:CLA:C4	18:3:3003:CLA:C2D	2.85	0.51
18:3:3005:CLA:H12	18:3:3005:CLA:CED	2.39	0.51
27:3:3501:LUT:C16	27:3:3501:LUT:H8	2.13	0.51
15:1:104:ASN:ND2	15:1:208:THR:CG2	2.73	0.51
15:1:111:TRP:CE2	15:1:119:ALA:HB2	2.43	0.51
15:1:211:LEU:CD1	15:1:212:GLU:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:103:MET:HG3	18:4:4001:CLA:HMC3	1.92	0.51
28:4:4013:CHL:CHD	28:4:4013:CHL:HBC2	2.32	0.51
1:A:33:GLN:HB2	18:A:1109:CLA:HBA1	1.91	0.51
7:L:98:ARG:HH22	7:L:175:GLN:NE2	2.08	0.51
9:D:204:THR:HG22	9:D:206:LYS:CG	2.38	0.51
14:4:219:ILE:HG23	14:4:220:ILE:N	2.25	0.51
18:1:1011:CLA:HMC1	18:1:1011:CLA:HBC2	1.91	0.51
15:1:127:PRO:CG	15:1:128:TRP:NE1	2.73	0.51
15:1:196:VAL:O	15:1:199:CYS:N	2.43	0.51
18:A:1139:CLA:H61	4:J:18:TRP:CG	2.45	0.51
18:A:1022:CLA:OBD	18:B:1021:CLA:HMB3	2.10	0.51
18:G:1003:CLA:C5	23:G:2021:LMG:C31	2.85	0.51
7:L:121:ARG:CG	7:L:127:GLY:CA	2.84	0.51
11:H:107:GLY:C	11:H:110:THR:HG22	2.30	0.51
14:4:199:GLU:HG2	14:4:202:GLU:OE1	2.10	0.51
7:L:169:ARG:NH1	7:L:171:LYS:CB	2.73	0.51
9:D:163:GLU:OE2	9:D:164:VAL:N	2.42	0.51
13:2:131:ILE:CG2	13:2:132:LEU:H	2.20	0.51
13:2:178:ASN:O	13:2:179:THR:HG23	2.11	0.51
13:2:232:VAL:HG11	27:2:2502:LUT:H12	1.92	0.51
16:3:211:LEU:N	16:3:211:LEU:CD1	2.72	0.51
15:1:127:PRO:C	15:1:128:TRP:CD1	2.83	0.51
15:1:232:ILE:CG2	15:1:233:PRO:N	2.73	0.51
14:4:148:LEU:HB3	27:4:4503:LUT:H15	1.91	0.51
18:F:1302:CLA:HHC	18:F:1302:CLA:CBB	2.40	0.51
14:4:171:ILE:CD1	14:4:171:ILE:N	2.73	0.51
9:D:192:ILE:HG23	10:E:80:GLU:CD	2.31	0.51
9:D:211:LEU:N	9:D:211:LEU:CD1	2.72	0.51
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.39	0.51
13:2:220:LYS:NZ	18:2:2002:CLA:CED	2.73	0.51
18:2:2002:CLA:OBD	18:2:2007:CLA:HBD	2.10	0.51
27:2:2502:LUT:C8	27:2:2502:LUT:H181	2.40	0.51
14:4:147:ILE:HD13	21:1:1801:LHG:H351	1.92	0.51
27:4:4503:LUT:H363	28:1:1009:CHL:H93	1.86	0.51
7:L:91:THR:CB	7:L:175:GLN:NE2	2.73	0.51
14:4:120:ILE:N	14:4:120:ILE:CD1	2.72	0.51
6:G:92:LEU:H	6:G:92:LEU:CD1	1.98	0.51
13:2:222:ILE:N	13:2:222:ILE:CD1	2.73	0.51
16:3:153:ASP:OD1	16:3:154:ASN:N	2.44	0.51
13:2:129:LEU:CD2	13:2:131:ILE:CG1	2.86	0.51
13:2:262:ILE:CD1	18:2:2003:CLA:H11	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:2016:CLA:HBA2	18:2:2016:CLA:CHA	2.40	0.51
14:4:101:TRP:CE2	28:4:4011:CHL:CED	2.94	0.51
18:4:4005:CLA:HBC1	18:4:4012:CLA:HBC1	1.92	0.51
2:B:255:LEU:HD11	18:B:1212:CLA:HBC1	1.91	0.51
6:G:64:ILE:HD12	18:G:1001:CLA:C3D	2.40	0.51
14:4:171:ILE:HD12	14:4:171:ILE:N	2.25	0.51
13:2:241:TYR:CE1	13:2:265:ALA:HB3	2.46	0.51
18:2:2004:CLA:CHB	18:2:2004:CLA:H12	2.40	0.51
13:2:85:PHE:HD2	18:2:2009:CLA:HBC2	1.75	0.51
27:3:3501:LUT:H371	27:3:3501:LUT:H28	1.92	0.51
2:B:177:HIS:HB3	18:B:1210:CLA:HBB1	1.93	0.51
18:F:1301:CLA:HBB1	18:F:1301:CLA:CHC	2.39	0.51
9:D:191:SER:O	9:D:192:ILE:HB	2.11	0.51
16:3:65:LEU:HD13	16:3:67:TYR:OH	2.09	0.51
9:D:135:LYS:O	9:D:138:CYS:HB2	2.10	0.51
14:4:113:GLU:OE1	14:4:229:PRO:HG2	2.11	0.51
4:J:6:THR:CG2	23:F:5001:LMG:HC72	2.39	0.51
18:A:1110:CLA:HBD	18:A:1110:CLA:HBA1	1.93	0.51
1:A:208:ALA:HB1	18:A:1118:CLA:HBC3	1.93	0.51
1:A:346:LEU:HG	1:A:429:ASN:ND2	2.25	0.51
15:1:81:LEU:CD1	15:1:159:LYS:HG3	2.41	0.51
15:1:88:MET:CE	18:1:1001:CLA:HAB	2.41	0.51
17:A:1011:CL0:H13	18:B:1012:CLA:CAD	2.41	0.51
6:G:116:LYS:HE3	18:G:1002:CLA:CHC	2.40	0.51
14:4:206:ALA:HB2	23:4:4801:LMG:HC62	1.92	0.51
13:2:108:VAL:HG12	13:2:112:TRP:HD1	1.76	0.51
13:2:122:ILE:CD1	13:2:122:ILE:N	2.73	0.51
18:2:2005:CLA:C4	18:2:2005:CLA:H92	2.40	0.51
16:3:183:GLY:HA3	16:3:194:PHE:O	2.11	0.51
18:3:3005:CLA:HBC3	18:3:3005:CLA:HMC1	1.93	0.51
18:3:3012:CLA:C1	18:3:3017:CLA:CBB	2.89	0.51
27:3:3502:LUT:C16	27:3:3502:LUT:C8	2.86	0.51
18:1:1008:CLA:CHA	18:1:1008:CLA:CED	2.89	0.51
15:1:202:GLN:HA	15:1:202:GLN:HE21	1.75	0.51
15:1:222:TRP:NE1	18:1:1008:CLA:CMA	2.73	0.51
1:A:743:ILE:HG21	18:A:1126:CLA:HMC2	1.93	0.51
18:B:1230:CLA:H91	18:F:1301:CLA:HMA1	1.93	0.51
18:G:1001:CLA:HMB2	22:G:2011:BCR:C16	2.41	0.51
14:4:113:GLU:CD	14:4:230:PHE:HB3	2.30	0.51
1:A:629:ASN:HD21	1:A:631:GLN:HB2	1.75	0.51
10:E:91:VAL:HB	10:E:104:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:187:LYS:CG	13:2:188:LEU:H	2.23	0.51
18:2:2002:CLA:C1	18:2:2002:CLA:CED	2.85	0.51
16:3:134:LEU:HB2	16:3:138:GLN:HG3	1.92	0.51
16:3:197:SER:HB2	16:3:203:PRO:C	2.32	0.51
16:3:266:ASN:O	16:3:267:ASN:ND2	2.44	0.51
27:3:3502:LUT:C36	27:3:3502:LUT:H28	2.37	0.51
6:G:114:VAL:CG1	18:G:1002:CLA:HBA1	2.41	0.51
6:G:76:ARG:NE	6:G:116:LYS:NZ	2.59	0.51
16:3:248:THR:CG2	16:3:255:ASN:HD22	2.17	0.51
11:H:132:PRO:CD	11:H:133:PRO:CD	2.84	0.51
7:L:207:LEU:O	7:L:208:ASP:HB3	2.11	0.51
9:D:168:HIS:HA	9:D:169:PRO:C	2.30	0.51
13:2:120:ILE:C	13:2:123:PRO:HD2	2.31	0.51
13:2:130:GLY:O	13:2:131:ILE:HG13	2.10	0.51
18:2:2001:CLA:C4A	18:2:2001:CLA:CGA	2.89	0.51
18:2:2002:CLA:H2A	18:2:2002:CLA:O2D	2.11	0.51
16:3:171:ARG:HD3	28:3:3011:CHL:HBB1	1.93	0.51
16:3:184:LYS:CG	16:3:185:GLN:NE2	2.73	0.51
16:3:230:ASN:OD1	18:3:3007:CLA:HMD1	2.10	0.51
18:B:1216:CLA:CGA	18:B:1221:CLA:HBB1	2.41	0.51
15:1:152:GLU:OE1	15:1:152:GLU:HA	2.11	0.51
1:A:64:PHE:CD2	18:A:1103:CLA:HMC2	2.46	0.51
16:3:115:GLY:O	16:3:119:PRO:HD3	2.11	0.51
11:H:123:LEU:O	11:H:123:LEU:HD13	2.10	0.51
15:1:230:VAL:CG1	18:1:1014:CLA:C1B	2.86	0.50
12:K:127:THR:O	12:K:131:ILE:HG12	2.11	0.50
4:J:28:GLU:CD	18:J:1302:CLA:ND	2.64	0.50
14:4:228:GLY:O	14:4:232:ASN:ND2	2.45	0.50
18:A:1105:CLA:H12	22:J:6013:BCR:H14C	1.93	0.50
14:4:55:GLU:OE1	14:4:58:PRO:HA	2.11	0.50
13:2:85:PHE:CZ	13:2:223:LYS:HE3	2.47	0.50
14:4:152:VAL:HG13	28:4:4011:CHL:C1B	2.41	0.50
18:4:4001:CLA:CGA	18:4:4001:CLA:H3A	2.41	0.50
28:4:4013:CHL:HBA1	27:4:4503:LUT:C10	2.40	0.50
1:A:330:ILE:O	1:A:334:HIS:ND1	2.40	0.50
18:G:1003:CLA:C13	18:G:1003:CLA:H8	2.33	0.50
22:L:6019:BCR:C8	22:L:6019:BCR:H321	2.41	0.50
7:L:96:LEU:O	7:L:96:LEU:HD23	2.11	0.50
14:4:177:LEU:HD13	18:4:4016:CLA:CMD	2.41	0.50
16:3:182:MET:CA	16:3:182:MET:CE	2.88	0.50
16:3:232:ARG:NH2	18:3:3004:CLA:ND	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:1011:CLA:CHA	18:1:1011:CLA:HBA1	2.39	0.50
15:1:83:HIS:CE1	18:1:1012:CLA:CMD	2.94	0.50
28:4:4013:CHL:CBC	28:4:4013:CHL:CHD	2.85	0.50
18:B:1238:CLA:H191	3:I:18:ALA:HB2	1.93	0.50
12:K:137:VAL:N	12:K:140:LEU:HD22	2.26	0.50
1:A:25:ASP:HB3	1:A:26:PRO:HD2	1.94	0.50
18:2:2002:CLA:HMD2	18:2:2007:CLA:C1D	2.42	0.50
18:2:2009:CLA:HBD	18:2:2009:CLA:HAA1	1.92	0.50
13:2:92:LEU:HD12	27:2:2502:LUT:C24	2.41	0.50
16:3:224:LYS:O	16:3:228:VAL:HG23	2.10	0.50
16:3:182:MET:HB3	28:3:3011:CHL:HMC	1.94	0.50
18:1:1005:CLA:C3B	27:1:1502:LUT:C14	2.90	0.50
15:1:158:LYS:HD3	15:1:159:LYS:HZ1	1.73	0.50
1:A:604:TRP:HH2	18:A:1022:CLA:HAB	1.74	0.50
1:A:305:ALA:HA	18:A:1115:CLA:HMC3	1.93	0.50
14:4:60:LEU:HG	14:4:61:ALA:O	2.10	0.50
9:D:171:ASP:O	9:D:173:VAL:N	2.44	0.50
2:B:71:GLN:OE1	2:B:90:ALA:N	2.37	0.50
18:2:2002:CLA:CMB	18:2:2002:CLA:HBB1	2.34	0.50
16:3:135:ALA:H	16:3:138:GLN:CD	2.14	0.50
16:3:152:ALA:HB3	16:3:157:LEU:CD2	2.38	0.50
16:3:208:PHE:HB3	18:3:3001:CLA:CMD	2.37	0.50
16:3:205:GLY:CA	16:3:208:PHE:N	2.73	0.50
18:3:3003:CLA:C1A	18:3:3003:CLA:CGA	2.89	0.50
15:1:218:LEU:O	15:1:221:PRO:HD3	2.12	0.50
18:A:1013:CLA:H3A	18:A:1013:CLA:CGA	2.41	0.50
7:L:65:PHE:O	9:D:91:LEU:HG	2.11	0.50
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.92	0.50
13:2:220:LYS:HE2	18:2:2002:CLA:HED2	1.91	0.50
14:4:236:HIS:CE1	14:4:240:PRO:HB3	2.46	0.50
15:1:192:LEU:HD13	18:1:1004:CLA:HMC3	1.93	0.50
15:1:225:ASN:C	15:1:225:ASN:HD22	2.15	0.50
13:2:180:ASP:HB3	13:2:183:PHE:O	2.11	0.50
14:4:103:MET:HE3	14:4:208:GLY:N	2.26	0.50
28:4:4010:CHL:HHC	28:4:4010:CHL:HBB1	1.94	0.50
18:A:1101:CLA:C4D	4:J:12:PRO:HG3	2.41	0.50
2:B:377:TYR:HD2	18:B:1224:CLA:HAB	1.75	0.50
2:B:438:VAL:HG13	18:B:1012:CLA:H61	1.94	0.50
23:F:5002:LMG:H292	18:1:1014:CLA:C4D	2.42	0.50
12:K:118:THR:OG1	12:K:121:ASP:HB3	2.12	0.50
6:G:94:GLU:CB	6:G:98:VAL:H	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:572:ALA:HA	2:B:575:ASP:OD2	2.11	0.50
16:3:221:LYS:C	16:3:223:LEU:H	2.14	0.50
18:1:1003:CLA:H2	18:1:1008:CLA:HMD3	1.93	0.50
18:1:1003:CLA:HBA1	18:1:1008:CLA:HED2	1.93	0.50
15:1:76:PHE:HB3	18:1:1004:CLA:HMA1	1.92	0.50
18:4:4006:CLA:C2B	27:4:4502:LUT:H183	2.41	0.50
22:A:6008:BCR:H402	18:A:1119:CLA:H122	1.93	0.50
2:B:459:PHE:HD1	18:F:1302:CLA:HMC2	1.76	0.50
2:B:65:LEU:HD21	22:B:6006:BCR:H291	1.93	0.50
15:1:89:LEU:C	15:1:92:PRO:HD2	2.32	0.50
11:H:58:GLU:HA	11:H:58:GLU:OE1	2.10	0.50
13:2:126:LEU:CB	13:2:133:LEU:HD13	2.24	0.50
13:2:138:TYR:O	13:2:139:THR:HB	2.11	0.50
13:2:161:GLY:HA2	18:2:2012:CLA:CBB	2.42	0.50
16:3:269:LEU:HD11	18:3:3008:CLA:HED3	1.92	0.50
18:3:3003:CLA:HBD	18:3:3003:CLA:O1A	2.10	0.50
15:1:114:LEU:HD22	15:1:115:PRO:HD2	1.88	0.50
15:1:202:GLN:NE2	15:1:202:GLN:HA	2.27	0.50
18:B:1221:CLA:HBA2	18:B:1202:CLA:H8	1.92	0.50
23:B:5005:LMG:H172	18:B:1228:CLA:HBD	1.93	0.50
12:K:78:LEU:O	12:K:80:ALA:N	2.42	0.50
1:A:511:THR:HG23	18:A:1116:CLA:O1A	2.11	0.50
3:I:29:GLU:HA	3:I:29:GLU:OE2	2.11	0.50
14:4:74:ASN:ND2	14:4:74:ASN:N	2.60	0.50
18:2:2009:CLA:CED	16:3:171:ARG:CG	2.86	0.50
16:3:185:GLN:C	16:3:186:TYR:CD1	2.85	0.50
16:3:225:LEU:HD12	16:3:226:LYS:HE3	1.94	0.50
18:3:3003:CLA:C4D	18:3:3003:CLA:C1	2.85	0.50
16:3:127:LEU:CB	18:3:3018:CLA:CBC	2.85	0.50
15:1:102:LEU:O	15:1:104:ASN:N	2.41	0.50
28:4:4013:CHL:HBD	28:4:4013:CHL:HAA2	1.93	0.50
21:A:7001:LHG:H331	18:A:1104:CLA:H92	1.93	0.50
18:A:1123:CLA:HBB1	18:A:1119:CLA:H2	1.94	0.50
18:A:1122:CLA:H71	18:A:1122:CLA:H41	1.93	0.50
7:L:91:THR:CA	7:L:175:GLN:NE2	2.73	0.50
9:D:160:PRO:CD	9:D:161:SER:H	2.25	0.50
2:B:270:LEU:HD23	2:B:273:MET:HE3	1.93	0.50
13:2:118:ALA:HB3	18:2:2006:CLA:HMC3	1.92	0.49
18:4:4004:CLA:H111	27:4:4502:LUT:H393	1.94	0.49
18:A:1106:CLA:H2A	18:A:1106:CLA:HED2	1.94	0.49
1:A:740:LEU:HD22	18:A:1140:CLA:HMA1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:TYR:HB2	18:B:1021:CLA:HED3	1.94	0.49
2:B:529:THR:HG21	2:B:582:TRP:CE2	2.47	0.49
7:L:91:THR:CG2	7:L:175:GLN:NE2	2.73	0.49
6:G:76:ARG:NE	6:G:116:LYS:CE	2.73	0.49
12:K:61:PHE:O	12:K:64:SER:HB3	2.12	0.49
13:2:79:GLY:HA2	13:2:84:ASP:OD2	2.11	0.49
18:3:3006:CLA:HMA2	18:3:3013:CLA:CAC	2.41	0.49
2:B:592:PHE:HE2	18:B:1021:CLA:H62	1.76	0.49
22:B:6006:BCR:H392	18:B:1211:CLA:H3A	1.94	0.49
7:L:85:ASN:HB2	18:L:1501:CLA:HMC1	1.94	0.49
9:D:195:ASN:ND2	9:D:195:ASN:N	2.60	0.49
9:D:112:ILE:N	9:D:112:ILE:CD1	2.72	0.49
9:D:163:GLU:OE1	9:D:164:VAL:O	2.30	0.49
18:2:2002:CLA:O2D	18:2:2002:CLA:HAA2	2.13	0.49
2:B:657:TRP:CE3	18:B:1021:CLA:HMA1	2.48	0.49
22:F:6016:BCR:H382	22:F:6016:BCR:H23C	1.94	0.49
7:L:111:VAL:O	7:L:115:VAL:HG23	2.12	0.49
8:C:61:ASP:HB2	10:E:118:ASN:CG	2.32	0.49
13:2:77:LEU:HD13	13:2:86:GLY:HA2	1.93	0.49
18:2:2004:CLA:CGA	18:2:2004:CLA:H3A	2.42	0.49
18:2:2016:CLA:CBA	18:2:2016:CLA:CBD	2.85	0.49
18:4:4003:CLA:HBC2	18:4:4003:CLA:CHD	2.41	0.49
14:4:57:LEU:HD11	18:4:4009:CLA:HED1	1.95	0.49
18:1:1008:CLA:HED2	18:1:1008:CLA:CAD	2.43	0.49
15:1:202:GLN:OE1	15:1:208:THR:HB	2.11	0.49
18:B:1216:CLA:CMB	18:B:1221:CLA:HMA3	2.40	0.49
18:B:1238:CLA:H13	27:I:6018:LUT:H193	1.94	0.49
23:G:2021:LMG:O9	23:G:2021:LMG:HC92	2.13	0.49
7:L:90:ARG:HB2	7:L:98:ARG:HD3	1.95	0.49
22:K:2011:BCR:C32	22:K:2011:BCR:C8	2.85	0.49
12:K:70:MET:HE2	12:K:71:VAL:HG23	1.91	0.49
18:A:1110:CLA:H42	18:A:1110:CLA:C4C	2.42	0.49
11:H:123:LEU:HD12	11:H:123:LEU:N	2.26	0.49
13:2:238:GLN:NE2	18:2:2003:CLA:NA	2.60	0.49
15:1:183:LYS:NZ	18:1:1002:CLA:O1D	2.44	0.49
15:1:111:TRP:CG	15:1:119:ALA:HB2	2.47	0.49
22:L:6020:BCR:H342	18:H:1000:CLA:CAB	2.42	0.49
7:L:81:TRP:O	7:L:85:ASN:ND2	2.43	0.49
12:K:124:ALA:CB	22:K:2011:BCR:H343	2.42	0.49
12:K:70:MET:HE1	12:K:71:VAL:HG22	1.94	0.49
13:2:211:PRO:C	13:2:212:GLN:HG3	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:131:LEU:HB3	11:H:135:LEU:HD22	1.94	0.49
2:B:439:HIS:O	2:B:443:MET:HG2	2.12	0.49
13:2:66:LEU:N	16:3:186:TYR:HE2	2.03	0.49
14:4:241:TRP:CD2	18:4:4008:CLA:HMA1	2.47	0.49
13:2:147:THR:HG21	14:4:241:TRP:HE3	1.78	0.49
15:1:88:MET:CE	18:1:1001:CLA:HHC	2.38	0.49
15:1:226:ILE:HG12	15:1:230:VAL:HG23	1.94	0.49
1:A:336:GLY:N	21:A:5003:LHG:HC32	2.27	0.49
4:J:2:ARG:O	4:J:3:ASP:HB2	2.11	0.49
18:G:1002:CLA:CBB	18:G:1002:CLA:HMB1	2.42	0.49
4:J:36:ALA:HB1	23:J:5001:LMG:HC72	1.94	0.49
15:1:140:LEU:HD23	15:1:140:LEU:O	2.12	0.49
13:2:188:LEU:C	13:2:188:LEU:HD13	2.32	0.49
18:2:2005:CLA:H72	23:2:2802:LMG:H132	1.93	0.49
13:2:145:TYR:HB2	18:2:2006:CLA:H92	1.95	0.49
18:2:2007:CLA:C5	18:2:2007:CLA:C9	2.90	0.49
13:2:198:GLY:O	13:2:202:ASP:N	2.42	0.49
16:3:225:LEU:N	16:3:226:LYS:NZ	2.60	0.49
16:3:243:ILE:HG22	18:3:3003:CLA:HMD3	1.95	0.49
16:3:151:TRP:NE1	18:3:3013:CLA:OBD	2.37	0.49
15:1:158:LYS:O	15:1:159:LYS:HE2	2.13	0.49
15:1:217:HIS:ND1	15:1:221:PRO:HA	2.28	0.49
6:G:130:ILE:O	6:G:134:VAL:HG23	2.12	0.49
9:D:173:VAL:HG21	9:D:179:ASN:OD1	2.13	0.49
18:3:3018:CLA:HBC2	18:3:3018:CLA:CMC	2.39	0.49
18:3:3005:CLA:HMB2	27:3:3502:LUT:C32	2.43	0.49
14:4:147:ILE:CD1	21:1:1801:LHG:C36	2.91	0.49
28:4:4010:CHL:HBC2	28:4:4010:CHL:CHD	2.26	0.49
18:B:1213:CLA:HBB1	18:B:1213:CLA:HMB1	1.95	0.49
18:B:1222:CLA:CAD	18:B:1234:CLA:HBB1	2.43	0.49
16:3:187:PHE:CZ	18:3:3019:CLA:C4B	2.95	0.49
9:D:131:LYS:NZ	11:H:63:THR:O	2.46	0.49
28:2:2013:CHL:H2A	28:2:2013:CHL:O1D	2.12	0.49
13:2:232:VAL:HG11	27:2:2502:LUT:H10	1.94	0.49
14:4:151:TYR:C	14:4:151:TYR:CD1	2.85	0.49
18:4:4004:CLA:HBB1	27:4:4502:LUT:H30	1.95	0.49
28:4:4011:CHL:H11	27:4:4501:LUT:H383	1.93	0.49
14:4:94:ALA:CA	18:4:4012:CLA:CED	2.85	0.49
1:A:368:LEU:HD11	18:A:1117:CLA:H71	1.95	0.49
18:A:1123:CLA:HBA1	18:A:1127:CLA:H191	1.94	0.49
1:A:684:PHE:CG	22:A:6011:BCR:H363	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1205:CLA:O1A	18:B:1224:CLA:HBD	2.13	0.49
16:3:67:TYR:CE1	16:3:85:ASP:HA	2.48	0.49
1:A:80:SER:OG	1:A:186:TYR:HB2	2.12	0.49
7:L:125:ILE:HG22	7:L:125:ILE:O	2.12	0.49
1:A:713:LYS:NZ	5:F:229:LYS:O	2.40	0.49
13:2:118:ALA:O	13:2:121:PHE:N	2.46	0.49
16:3:169:GLU:HG3	18:3:3012:CLA:C4B	2.43	0.49
18:1:1008:CLA:C4D	18:1:1008:CLA:CED	2.85	0.49
18:B:1208:CLA:H12	18:B:1209:CLA:C4D	2.43	0.49
7:L:90:ARG:NH2	18:L:1501:CLA:HAC2	2.28	0.49
7:L:67:GLY:O	9:D:88:THR:HA	2.12	0.49
16:3:68:LEU:N	16:3:68:LEU:CD1	2.73	0.49
14:4:133:GLU:C	14:4:134:TYR:CD1	2.86	0.49
28:3:3011:CHL:CAA	28:3:3011:CHL:HBD	2.43	0.48
15:1:106:VAL:HG23	15:1:208:THR:HG21	1.89	0.48
15:1:222:TRP:CD1	18:1:1008:CLA:CMA	2.96	0.48
14:4:103:MET:HE1	27:4:4501:LUT:H15	1.95	0.48
1:A:438:HIS:HA	9:D:88:THR:OG1	2.13	0.48
18:B:1203:CLA:H8	25:B:7101:DGD:HBH2	1.95	0.48
22:B:6004:BCR:H351	22:B:6004:BCR:H15C	1.59	0.48
7:L:118:GLY:O	7:L:122:ASN:ND2	2.46	0.48
11:H:107:GLY:HA2	11:H:110:THR:HG21	1.94	0.48
10:E:76:ILE:HG22	10:E:78:ARG:H	1.78	0.48
2:B:224:PRO:HB3	2:B:232:LEU:HD22	1.93	0.48
28:2:2013:CHL:CBD	28:2:2013:CHL:HAA2	2.43	0.48
23:2:2802:LMG:HC92	23:2:2802:LMG:O9	2.14	0.48
18:3:3012:CLA:H12	18:3:3017:CLA:HBB2	1.94	0.48
29:4:4505:ZEX:H173	15:1:200:VAL:HG13	1.95	0.48
15:1:214:LEU:HA	18:1:1003:CLA:HMA2	1.94	0.48
18:B:1218:CLA:H61	18:B:1218:CLA:H41	1.67	0.48
18:L:1502:CLA:HAC2	22:L:6019:BCR:C29	2.42	0.48
7:L:90:ARG:HB3	7:L:93:VAL:CG2	2.43	0.48
16:3:119:PRO:C	16:3:133:ALA:CB	2.82	0.48
18:A:1110:CLA:O1A	16:3:81:LEU:HD22	2.13	0.48
13:2:220:LYS:HA	18:2:2007:CLA:HED2	1.94	0.48
18:3:3013:CLA:CMA	22:3:3503:BCR:C35	2.85	0.48
18:G:1001:CLA:C6	22:G:2011:BCR:C34	2.85	0.48
6:G:132:HIS:ND1	22:G:2011:BCR:H19C	2.27	0.48
16:3:270:THR:HG1	16:3:271:SER:H	1.60	0.48
18:3:3003:CLA:CAB	27:3:3501:LUT:C17	2.90	0.48
27:4:4503:LUT:C37	27:4:4503:LUT:C28	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1013:CLA:O2A	2:B:427:LEU:HA	2.12	0.48
2:B:350:GLN:HG3	18:B:1222:CLA:HED2	1.95	0.48
4:J:16:THR:HG21	22:J:6013:BCR:H401	1.95	0.48
9:D:166:TYR:CE2	9:D:170:LYS:HA	2.49	0.48
9:D:129:LEU:HD23	9:D:129:LEU:O	2.12	0.48
16:3:70:GLY:HA2	16:3:75:ASP:OD2	2.13	0.48
2:B:414:HIS:O	2:B:414:HIS:ND1	2.46	0.48
18:2:2005:CLA:H41	18:2:2005:CLA:C8	2.44	0.48
18:2:2004:CLA:C5	27:2:2502:LUT:C38	2.85	0.48
16:3:136:TRP:CZ2	16:3:137:PHE:HB3	2.49	0.48
18:3:3003:CLA:C12	18:3:3003:CLA:H93	2.44	0.48
18:3:3006:CLA:C2D	18:3:3018:CLA:CBB	2.91	0.48
15:1:88:MET:HB3	27:1:1501:LUT:C34	2.43	0.48
28:4:4011:CHL:CBC	28:4:4011:CHL:CHD	2.89	0.48
18:A:1106:CLA:H203	18:A:1101:CLA:HMA1	1.95	0.48
18:B:1230:CLA:O1D	4:J:35:ASP:HA	2.13	0.48
18:F:1302:CLA:CHD	18:F:1302:CLA:CBC	2.86	0.48
4:J:23:ALA:O	4:J:27:ILE:HG13	2.13	0.48
7:L:102:VAL:HG13	7:L:106:HIS:ND1	2.29	0.48
12:K:137:VAL:HA	12:K:140:LEU:HD23	1.89	0.48
16:3:94:GLU:CD	16:3:96:ARG:N	2.65	0.48
1:A:218:TRP:HA	18:A:1112:CLA:HBB1	1.94	0.48
1:A:581:CYS:SG	2:B:562:PRO:HG3	2.53	0.48
13:2:102:ASN:OD1	18:2:2004:CLA:H11	2.12	0.48
15:1:222:TRP:CE2	18:1:1008:CLA:HMA1	2.48	0.48
7:L:149:GLY:HA3	7:L:182:TRP:CD1	2.47	0.48
16:3:253:TYR:C	16:3:253:TYR:CD1	2.85	0.48
16:3:250:VAL:HG12	16:3:254:GLN:HG2	1.94	0.48
1:A:81:ALA:HB1	18:A:1103:CLA:HBB1	1.96	0.48
13:2:233:MET:CA	13:2:233:MET:CE	2.85	0.48
16:3:158:PHE:HB2	18:3:3010:CLA:CMC	2.42	0.48
16:3:197:SER:HB2	16:3:203:PRO:O	2.14	0.48
18:4:4001:CLA:HMB2	18:4:4002:CLA:HBA2	1.95	0.48
18:A:1022:CLA:H143	18:B:1207:CLA:HBC3	1.95	0.48
18:B:1240:CLA:C1D	18:B:1219:CLA:HMB3	2.44	0.48
2:B:387:PHE:HB3	2:B:534:LEU:HB3	1.96	0.48
3:I:17:PRO:O	3:I:21:MET:HG3	2.13	0.48
13:2:191:THR:CG2	13:2:192:ASP:H	2.24	0.48
18:A:1125:CLA:H11	18:A:1125:CLA:H51	1.69	0.48
2:B:44:GLN:NE2	2:B:162:LYS:HD2	2.29	0.48
13:2:238:GLN:NE2	18:2:2003:CLA:C4D	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:120:ILE:CG2	27:2:2501:LUT:H373	2.38	0.48
16:3:139:THR:O	16:3:147:THR:HG22	2.14	0.48
18:1:1005:CLA:HBB1	18:1:1005:CLA:CMB	2.30	0.48
15:1:181:LYS:O	15:1:185:VAL:HG23	2.13	0.48
15:1:218:LEU:CD2	18:1:1008:CLA:HBB1	2.44	0.48
14:4:108:GLY:O	14:4:112:PRO:HD2	2.14	0.48
2:B:59:LEU:HG	18:B:1204:CLA:HBB2	1.96	0.48
6:G:144:ASN:ND2	18:G:1003:CLA:CED	2.73	0.48
12:K:71:VAL:HG12	12:K:129:GLY:O	2.09	0.48
18:G:1001:CLA:C5	22:G:2011:BCR:H343	2.44	0.48
15:1:91:VAL:HB	15:1:92:PRO:HD3	1.96	0.48
6:G:109:LYS:HG3	6:G:110:GLU:HG3	1.96	0.48
10:E:107:PHE:N	10:E:107:PHE:CD1	2.82	0.48
13:2:117:ALA:O	13:2:120:ILE:HB	2.14	0.48
18:2:2002:CLA:HMC2	27:2:2501:LUT:H31	1.95	0.48
16:3:268:VAL:CG2	18:3:3003:CLA:C1	2.87	0.48
15:1:94:ILE:HG12	27:1:1502:LUT:H24	1.95	0.48
18:4:4006:CLA:CBB	27:4:4502:LUT:H181	2.44	0.48
18:G:1001:CLA:CAD	18:G:1001:CLA:CAD	2.92	0.48
8:C:8:TYR:C	8:C:10:THR:H	2.17	0.48
6:G:111:TYR:HD1	6:G:111:TYR:H	1.52	0.48
10:E:104:VAL:HG12	10:E:119:ASN:CG	2.34	0.48
9:D:211:LEU:N	9:D:211:LEU:HD12	2.28	0.48
14:4:193:ASN:N	14:4:193:ASN:OD1	2.46	0.48
13:2:176:CYS:HA	13:2:178:ASN:HD21	1.79	0.48
18:2:2002:CLA:CBC	18:2:2002:CLA:CMC	2.86	0.48
18:2:2005:CLA:HAB	27:2:2502:LUT:C40	2.43	0.48
16:3:223:LEU:C	16:3:226:LYS:HG2	2.34	0.48
16:3:236:LEU:HD21	18:3:3004:CLA:HBC3	1.96	0.48
15:1:97:PRO:C	15:1:102:LEU:HB2	2.34	0.48
15:1:41:TRP:HD1	15:1:59:PHE:CA	2.25	0.48
14:4:144:ILE:HD13	18:1:1008:CLA:HAA2	1.94	0.48
14:4:95:GLU:HG3	18:4:4004:CLA:NB	2.29	0.48
16:3:65:LEU:CB	16:3:68:LEU:CD2	2.85	0.48
14:4:239:ASP:CG	14:4:242:HIS:HD2	2.17	0.48
13:2:145:TYR:HB3	18:2:2006:CLA:C9	2.44	0.47
18:2:2016:CLA:HED2	18:2:2016:CLA:OBD	2.14	0.47
16:3:174:GLN:HB2	16:3:182:MET:HG2	1.96	0.47
22:3:3503:BCR:HC8	22:3:3503:BCR:C32	2.44	0.47
6:G:134:VAL:O	6:G:137:TYR:HB3	2.14	0.47
7:L:176:LEU:CG	7:L:177:GLN:H	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:1001:CLA:C2B	22:G:2011:BCR:C17	2.91	0.47
10:E:66:ILE:HG23	10:E:67:GLY:H	1.79	0.47
6:G:76:ARG:CD	6:G:116:LYS:HZ3	2.27	0.47
1:A:709:TRP:CD1	5:F:229:LYS:HD3	2.49	0.47
16:3:217:GLU:C	16:3:219:SER:H	2.17	0.47
18:2:2004:CLA:CHD	18:2:2004:CLA:HBC2	2.44	0.47
18:2:2005:CLA:HBA1	18:2:2005:CLA:H3A	1.70	0.47
16:3:271:SER:HB2	18:3:3003:CLA:CED	2.44	0.47
18:3:3010:CLA:H2A	18:3:3010:CLA:CED	2.44	0.47
15:1:111:TRP:HH2	18:1:1006:CLA:HED1	1.70	0.47
1:A:338:PHE:O	1:A:434:ARG:NH1	2.47	0.47
7:L:108:PHE:HZ	18:L:1503:CLA:OBD	1.97	0.47
7:L:165:THR:OG1	7:L:169:ARG:HB3	2.14	0.47
22:B:6010:BCR:H321	22:B:6010:BCR:HC8	1.95	0.47
13:2:246:PRO:HG2	13:2:247:ILE:H	1.80	0.47
16:3:106:GLY:O	16:3:110:MET:N	2.42	0.47
15:1:226:ILE:HG22	18:1:1003:CLA:O2A	2.14	0.47
18:1:1006:CLA:H43	18:1:1013:CLA:HBD	1.96	0.47
15:1:158:LYS:O	15:1:159:LYS:HG2	2.15	0.47
18:F:1302:CLA:HBB1	18:F:1302:CLA:CHC	2.44	0.47
22:F:6016:BCR:C8	22:F:6016:BCR:C33	2.85	0.47
11:H:113:TYR:C	11:H:115:SER:H	2.16	0.47
6:G:68:THR:HG23	18:G:1001:CLA:O2A	2.14	0.47
16:3:249:GLY:C	16:3:250:VAL:HG23	2.35	0.47
16:3:249:GLY:C	16:3:250:VAL:CG2	2.83	0.47
7:L:121:ARG:HG2	7:L:127:GLY:HA2	1.93	0.47
18:A:1125:CLA:HED1	18:A:1133:CLA:HAB	1.97	0.47
1:A:205:HIS:O	1:A:209:GLY:N	2.46	0.47
1:A:232:PHE:O	1:A:237:VAL:HG12	2.14	0.47
8:C:77:MET:HB3	8:C:79:LEU:HG	1.97	0.47
18:3:3002:CLA:HBD	18:3:3002:CLA:HAA2	1.94	0.47
18:1:1004:CLA:C3A	18:1:1004:CLA:CGA	2.92	0.47
14:4:190:ASN:OD1	27:4:4501:LUT:O23	2.23	0.47
18:A:1122:CLA:H202	18:A:1122:CLA:H101	1.96	0.47
20:A:5001:PQN:H201	18:A:1138:CLA:HBC1	1.95	0.47
18:G:1001:CLA:O1A	22:G:2011:BCR:H352	2.15	0.47
9:D:101:TYR:CE2	9:D:135:LYS:HB2	2.50	0.47
1:A:22:LEU:HA	16:3:88:GLY:HA3	1.96	0.47
13:2:168:TRP:CE3	18:2:2012:CLA:HMA1	2.48	0.47
13:2:177:VAL:C	13:2:179:THR:H	2.17	0.47
16:3:155:TYR:CE1	18:3:3010:CLA:H102	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3006:CLA:HAA1	18:3:3006:CLA:HBD	1.97	0.47
15:1:180:TYR:HB3	18:1:1001:CLA:CMA	2.45	0.47
15:1:166:ASP:OD1	15:1:169:GLY:N	2.48	0.47
18:4:4017:CLA:HAC2	29:4:4505:ZEX:H373	1.96	0.47
1:A:595:TRP:NE1	18:A:1128:CLA:HMD1	2.29	0.47
18:B:1220:CLA:CAB	18:B:1227:CLA:HMD2	2.44	0.47
14:4:158:GLN:CA	14:4:158:GLN:NE2	2.77	0.47
13:2:68:PHE:HD2	13:2:71:SER:CB	2.23	0.47
22:J:6013:BCR:H351	22:J:6013:BCR:H15C	1.67	0.47
16:3:110:MET:SD	16:3:230:ASN:C	2.93	0.47
16:3:139:THR:CG2	16:3:140:GLY:H	2.23	0.47
14:4:240:PRO:HG2	18:4:4008:CLA:C3B	2.44	0.47
15:1:43:PRO:HG2	28:1:1009:CHL:C3D	2.45	0.47
21:1:1801:LHG:H381	21:1:1801:LHG:H223	1.89	0.47
14:4:156:ARG:HB3	28:4:4011:CHL:CHD	2.45	0.47
18:B:1213:CLA:NC	18:B:1213:CLA:H52	2.29	0.47
18:F:1302:CLA:O1D	23:F:5002:LMG:HC91	2.14	0.47
7:L:116:LYS:HB3	18:L:1503:CLA:HMB3	1.97	0.47
13:2:87:PHE:CE2	27:2:2502:LUT:C37	2.94	0.47
16:3:136:TRP:HB2	27:3:3502:LUT:H22	1.97	0.47
16:3:62:LYS:NZ	16:3:76:TYR:CD2	2.83	0.47
18:1:1008:CLA:CHA	18:1:1008:CLA:HED2	2.45	0.47
28:4:4013:CHL:HBA1	28:4:4013:CHL:H3A	1.70	0.47
18:4:4001:CLA:C4D	27:4:4501:LUT:H382	2.45	0.47
18:B:1213:CLA:C3D	18:G:1003:CLA:HED1	2.44	0.47
18:B:1218:CLA:H192	18:1:1012:CLA:HMC2	1.96	0.47
18:A:1120:CLA:H112	18:A:1120:CLA:H91	1.73	0.47
18:B:1234:CLA:H41	18:B:1234:CLA:H101	1.95	0.47
18:B:1218:CLA:H151	18:G:1003:CLA:C15	2.45	0.47
22:I:6020:BCR:H15C	22:I:6020:BCR:H351	1.68	0.47
12:K:71:VAL:HG13	12:K:132:ILE:HB	1.97	0.47
14:4:118:ILE:CD1	14:4:120:ILE:CD1	2.76	0.47
6:G:65:SER:HB3	18:G:1001:CLA:HBA1	1.91	0.47
22:G:2011:BCR:H15C	22:G:2011:BCR:H351	1.69	0.47
14:4:172:PHE:HD1	14:4:173:LYS:H	1.63	0.47
16:3:217:GLU:C	16:3:219:SER:N	2.68	0.47
9:D:83:ILE:HG12	9:D:124:ARG:HH11	1.80	0.47
15:1:62:ASP:OD2	15:1:65:ARG:HA	2.15	0.47
2:B:417:ALA:O	2:B:421:HIS:ND1	2.46	0.47
13:2:129:LEU:HD22	13:2:131:ILE:HD11	1.96	0.47
18:2:2001:CLA:H41	18:2:2002:CLA:CMA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:214:GLY:O	16:3:220:LEU:CB	2.62	0.47
18:1:1001:CLA:C4D	27:1:1501:LUT:C38	2.93	0.47
18:B:1220:CLA:H101	18:B:1220:CLA:H62	1.64	0.47
18:F:1302:CLA:HMB2	22:F:6016:BCR:HC7	1.97	0.47
22:L:6019:BCR:H371	22:L:6019:BCR:H24C	1.68	0.47
2:B:73:ASN:HB2	2:B:76:ALA:HB3	1.96	0.47
9:D:171:ASP:OD1	9:D:179:ASN:ND2	2.48	0.47
15:1:222:TRP:CZ2	18:1:1008:CLA:HMB3	2.48	0.47
18:1:1011:CLA:HBD	18:1:1011:CLA:HBA2	1.95	0.47
15:1:85:ARG:HH11	15:1:85:ARG:HG2	1.79	0.47
15:1:85:ARG:NE	18:1:1001:CLA:CHD	2.78	0.47
18:4:4005:CLA:HMD2	18:4:4012:CLA:NC	2.30	0.47
21:A:7001:LHG:H191	18:A:1128:CLA:H111	1.97	0.47
1:A:371:VAL:HG12	18:A:1124:CLA:HED3	1.96	0.47
18:B:1239:CLA:HBA2	18:B:1239:CLA:H3A	1.47	0.47
2:B:576:PHE:CE1	18:B:1226:CLA:HAC2	2.49	0.47
4:J:7:TYR:CE2	23:F:5001:LMG:HC4	2.50	0.47
8:C:14:CYS:O	8:C:15:THR:OG1	2.15	0.47
13:2:256:ASP:O	13:2:260:ALA:HB3	2.14	0.47
1:A:582:ASP:OD1	8:C:53:ARG:HD2	2.15	0.47
13:2:114:MET:CE	18:2:2001:CLA:HHC	2.44	0.47
16:3:111:LEU:HD21	18:3:3006:CLA:HBB1	1.97	0.47
28:3:3011:CHL:CBA	28:3:3011:CHL:CHA	2.93	0.47
18:3:3006:CLA:NC	22:3:3503:BCR:HC31	2.29	0.47
16:3:80:PRO:CG	27:3:3502:LUT:H24	2.45	0.47
15:1:85:ARG:CD	18:1:1001:CLA:C4C	2.93	0.47
27:4:4502:LUT:H171	27:4:4502:LUT:C8	2.45	0.47
1:A:602:LEU:HD21	18:A:1128:CLA:HBC1	1.95	0.47
11:H:132:PRO:N	11:H:133:PRO:CD	2.78	0.47
18:A:1105:CLA:H3A	18:A:1105:CLA:HBA2	1.59	0.47
16:3:70:GLY:N	16:3:75:ASP:OD2	2.48	0.47
1:A:282:THR:OG1	1:A:283:PHE:N	2.48	0.47
2:B:82:PHE:CZ	2:B:363:GLN:HG2	2.49	0.47
9:D:151:ILE:HG22	9:D:152:LYS:N	2.29	0.47
13:2:207:GLY:HA2	18:2:2001:CLA:HAA2	1.97	0.46
13:2:69:PRO:HA	16:3:186:TYR:CZ	2.50	0.46
16:3:92:PHE:HB3	18:3:3005:CLA:H11	1.97	0.46
15:1:111:TRP:HZ2	18:1:1013:CLA:CBC	2.26	0.46
15:1:149:ARG:HA	18:1:1011:CLA:HBC3	1.96	0.46
18:1:1001:CLA:ND	27:1:1501:LUT:C38	2.75	0.46
15:1:232:ILE:CG2	15:1:233:PRO:CD	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:4006:CLA:C4B	27:4:4502:LUT:H183	2.45	0.46
18:A:1107:CLA:H151	18:A:1109:CLA:H142	1.95	0.46
1:A:335:LYS:O	18:A:1151:CLA:HBC3	2.15	0.46
1:A:203:LEU:O	1:A:207:LEU:HB2	2.15	0.46
2:B:576:PHE:HE1	18:B:1226:CLA:HAC2	1.79	0.46
18:B:1240:CLA:H161	18:B:1240:CLA:H143	1.76	0.46
2:B:282:PHE:HE2	22:G:2011:BCR:H281	1.79	0.46
14:4:176:SER:OG	14:4:177:LEU:N	2.49	0.46
7:L:61:ASN:OD1	7:L:166:LEU:HD21	2.14	0.46
11:H:107:GLY:O	11:H:110:THR:CG2	2.63	0.46
18:A:1110:CLA:H52	16:3:81:LEU:HD13	1.98	0.46
16:3:141:VAL:HG13	16:3:141:VAL:O	2.15	0.46
16:3:267:ASN:N	16:3:270:THR:OG1	2.48	0.46
18:3:3010:CLA:O2D	18:3:3010:CLA:H2A	2.15	0.46
28:3:3011:CHL:HBA1	28:3:3011:CHL:CHA	2.44	0.46
18:3:3018:CLA:CMB	18:3:3018:CLA:HBB1	2.29	0.46
14:4:103:MET:HE3	14:4:207:ASN:O	2.14	0.46
14:4:68:GLY:HA2	14:4:73:ASP:OD2	2.16	0.46
18:B:1208:CLA:HED2	18:B:1208:CLA:H2A	1.97	0.46
22:B:6004:BCR:H282	18:B:1218:CLA:HBA2	1.96	0.46
7:L:120:LEU:HD23	7:L:120:LEU:HA	1.72	0.46
18:2:2005:CLA:HMD2	18:2:2012:CLA:CHD	2.45	0.46
2:B:459:PHE:O	2:B:463:ILE:HG12	2.15	0.46
14:4:166:VAL:HB	14:4:177:LEU:HB2	1.97	0.46
13:2:137:TRP:CH2	13:2:236:TRP:HA	2.38	0.46
2:B:294:ASN:HA	6:G:107:ARG:HG2	1.98	0.46
18:2:2002:CLA:HAA2	18:2:2002:CLA:HBD	1.97	0.46
13:2:152:LEU:HD11	28:2:2013:CHL:HMD3	1.97	0.46
16:3:80:PRO:HG2	27:3:3502:LUT:H24	1.96	0.46
18:1:1002:CLA:HAA2	18:1:1002:CLA:HBD	1.98	0.46
14:4:125:LYS:O	14:4:128:ASP:HB2	2.16	0.46
18:4:4001:CLA:H41	18:4:4001:CLA:H61	1.60	0.46
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.50	0.46
18:B:1021:CLA:HBA2	18:B:1021:CLA:H3A	1.68	0.46
18:A:1121:CLA:H52	12:K:82:ARG:HG3	1.97	0.46
5:F:213:TRP:CD1	5:F:214:PRO:HD3	2.51	0.46
18:B:1215:CLA:CGA	18:B:1215:CLA:H3A	2.42	0.46
13:2:129:LEU:HD22	13:2:131:ILE:CD1	2.46	0.46
13:2:173:ASN:HB3	13:2:174:PRO:CD	2.44	0.46
27:2:2502:LUT:H15	27:2:2502:LUT:H201	1.81	0.46
18:3:3004:CLA:H61	27:3:3502:LUT:C36	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:143:ALA:CA	18:1:1012:CLA:HAB	2.46	0.46
15:1:97:PRO:C	15:1:102:LEU:CB	2.84	0.46
14:4:135:PHE:CD1	14:4:135:PHE:C	2.89	0.46
18:B:1240:CLA:H62	18:B:1240:CLA:H41	1.74	0.46
9:D:151:ILE:CG2	9:D:152:LYS:N	2.79	0.46
6:G:100:HIS:O	6:G:101:PHE:CD2	2.69	0.46
13:2:203:PRO:HD2	27:2:2501:LUT:C3	2.44	0.46
18:1:1005:CLA:CMD	18:1:1012:CLA:C1D	2.85	0.46
15:1:183:LYS:HZ2	18:1:1002:CLA:CGD	2.26	0.46
18:4:4017:CLA:HBA2	18:4:4017:CLA:H3A	1.66	0.46
18:4:4005:CLA:HMB1	27:4:4502:LUT:H403	1.97	0.46
6:G:149:LYS:O	6:G:149:LYS:HG3	2.14	0.46
9:D:166:TYR:OH	9:D:169:PRO:HD2	2.16	0.46
2:B:224:PRO:HG2	2:B:233:TYR:CZ	2.51	0.46
9:D:177:LYS:O	9:D:182:ARG:NH1	2.47	0.46
13:2:111:ARG:HA	13:2:114:MET:HE2	1.97	0.46
18:2:2004:CLA:HHD	18:2:2009:CLA:HBB2	1.98	0.46
27:2:2502:LUT:C36	27:2:2502:LUT:H28	2.42	0.46
18:1:1002:CLA:HMD2	18:1:1007:CLA:C1D	2.45	0.46
28:1:1009:CHL:HBA1	28:1:1009:CHL:H3A	1.67	0.46
15:1:97:PRO:HB2	15:1:102:LEU:CG	2.45	0.46
18:A:1151:CLA:HBC2	18:A:1151:CLA:HMC1	1.97	0.46
22:B:6005:BCR:H15C	22:B:6005:BCR:H351	1.74	0.46
7:L:145:LEU:HB3	7:L:186:THR:CG2	2.45	0.46
7:L:85:ASN:HA	7:L:90:ARG:NH2	2.30	0.46
16:3:94:GLU:CD	16:3:96:ARG:H	2.01	0.46
14:4:132:GLU:O	14:4:134:TYR:CD1	2.69	0.46
9:D:81:SER:HB3	9:D:129:LEU:O	2.16	0.46
18:B:1214:CLA:H3A	18:B:1214:CLA:HBA2	1.58	0.46
13:2:126:LEU:CB	13:2:134:THR:HA	2.45	0.46
18:2:2001:CLA:H41	18:2:2001:CLA:H62	1.63	0.46
13:2:127:THR:CG2	13:2:247:ILE:HD13	2.39	0.46
15:1:104:ASN:OD1	15:1:208:THR:HG23	2.15	0.46
18:4:4006:CLA:C3B	27:4:4503:LUT:C17	2.93	0.46
18:G:1003:CLA:H52	23:G:2021:LMG:H332	1.98	0.46
1:A:272:LEU:HD11	12:K:134:VAL:HG13	1.97	0.46
13:2:91:GLY:O	13:2:94:SER:HB2	2.16	0.46
5:F:146:PRO:O	5:F:147:HIS:HD2	1.99	0.46
15:1:173:ASP:HB3	15:1:176:LYS:HB3	1.97	0.46
13:2:126:LEU:HD12	13:2:126:LEU:C	2.36	0.46
16:3:225:LEU:CB	16:3:226:LYS:NZ	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:154:ILE:CG2	18:4:4008:CLA:HED1	2.46	0.46
15:1:97:PRO:HB2	15:1:102:LEU:CD2	2.43	0.46
18:4:4006:CLA:C2B	27:4:4503:LUT:C17	2.93	0.46
18:A:1151:CLA:C2C	18:A:1120:CLA:HMB3	2.46	0.46
13:2:59:VAL:O	13:2:59:VAL:HG12	2.16	0.46
13:2:188:LEU:CD2	13:2:197:GLY:C	2.84	0.46
16:3:225:LEU:C	16:3:225:LEU:HD13	2.36	0.46
18:3:3005:CLA:HMD2	18:3:3012:CLA:C4C	2.45	0.46
18:1:1002:CLA:CMC	18:1:1002:CLA:HBC2	2.45	0.46
15:1:200:VAL:CG1	18:1:1003:CLA:HAC2	2.44	0.46
15:1:183:LYS:HD3	18:1:1002:CLA:CGA	2.45	0.46
14:4:204:GLU:HG3	18:4:4001:CLA:NB	2.31	0.46
17:A:1011:CL0:H7	18:B:1021:CLA:HBB1	1.97	0.46
18:A:1013:CLA:HMA1	18:A:1013:CLA:H51	1.97	0.46
18:A:1104:CLA:H192	18:A:1104:CLA:H162	1.72	0.46
18:A:1122:CLA:H111	18:A:1122:CLA:H72	1.70	0.46
18:A:1132:CLA:H141	18:A:1132:CLA:H161	1.61	0.46
2:B:231:ASN:HA	18:B:1213:CLA:HAA2	1.98	0.46
7:L:96:LEU:CD2	7:L:96:LEU:C	2.85	0.46
18:G:1001:CLA:C4D	18:G:1001:CLA:CED	2.94	0.46
16:3:67:TYR:CZ	16:3:84:SER:C	2.89	0.46
7:L:203:LEU:HD12	7:L:203:LEU:N	2.30	0.46
10:E:76:ILE:O	10:E:77:LEU:HD12	2.16	0.46
1:A:197:GLN:O	1:A:199:VAL:N	2.49	0.46
16:3:135:ALA:HB1	16:3:137:PHE:CE2	2.52	0.45
27:4:4503:LUT:C36	28:1:1009:CHL:H8	2.36	0.45
15:1:108:ALA:O	15:1:111:TRP:CZ3	2.69	0.45
21:1:1801:LHG:C6	21:1:1801:LHG:HC81	2.39	0.45
15:1:183:LYS:HE3	18:1:1002:CLA:O1A	2.16	0.45
14:4:152:VAL:HG11	28:4:4011:CHL:C1B	2.45	0.45
14:4:204:GLU:HG3	18:4:4001:CLA:C4B	2.46	0.45
18:A:1140:CLA:HBA2	18:A:1140:CLA:H3A	1.69	0.45
2:B:142:LEU:HD21	22:B:6006:BCR:H24C	1.97	0.45
12:K:71:VAL:CG1	12:K:129:GLY:HA2	2.42	0.45
13:2:60:ALA:HB2	13:2:78:ASP:OD1	2.16	0.45
16:3:72:LEU:HA	16:3:72:LEU:HD23	1.73	0.45
13:2:131:ILE:HG21	13:2:133:LEU:HG	1.98	0.45
18:2:2016:CLA:CED	18:2:2016:CLA:CAD	2.94	0.45
16:3:226:LYS:H	16:3:226:LYS:CE	2.29	0.45
18:3:3013:CLA:H3A	18:3:3013:CLA:HBA1	1.54	0.45
18:1:1006:CLA:O1A	18:1:1013:CLA:HMD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:230:VAL:CG1	18:1:1014:CLA:C4B	2.94	0.45
15:1:232:ILE:CD1	18:1:1014:CLA:HMD2	2.45	0.45
23:G:2021:LMG:O5	15:1:131:LEU:HD11	2.15	0.45
18:A:1119:CLA:H111	18:A:1119:CLA:H143	1.67	0.45
18:A:1132:CLA:H193	18:A:1132:CLA:H162	1.70	0.45
18:B:1229:CLA:H121	22:F:6016:BCR:H271	1.98	0.45
2:B:9:SER:O	2:B:12:ILE:HG22	2.16	0.45
4:J:28:GLU:OE1	18:J:1302:CLA:ND	2.49	0.45
15:1:148:GLN:NE2	15:1:148:GLN:HA	2.31	0.45
2:B:560:ASP:OD1	8:C:66:ARG:NH1	2.47	0.45
14:4:54:GLY:O	14:4:74:ASN:HA	2.16	0.45
13:2:186:ASN:CG	18:2:2016:CLA:CMA	2.84	0.45
16:3:110:MET:HE2	27:3:3501:LUT:H201	1.98	0.45
16:3:190:LEU:HA	16:3:207:PHE:CE2	2.51	0.45
16:3:205:GLY:HA2	16:3:206:PRO:HD3	1.66	0.45
16:3:262:ASP:CB	16:3:265:ASN:HD22	2.29	0.45
15:1:104:ASN:CG	15:1:208:THR:CG2	2.84	0.45
15:1:127:PRO:O	15:1:128:TRP:CD1	2.70	0.45
15:1:63:PRO:HD2	27:1:1502:LUT:C3	2.47	0.45
15:1:212:GLU:O	15:1:215:ALA:HB3	2.16	0.45
15:1:225:ASN:N	15:1:225:ASN:ND2	2.60	0.45
14:4:154:ILE:O	28:1:1009:CHL:HED1	2.15	0.45
1:A:397:THR:HG23	1:A:613:ILE:HG21	1.97	0.45
18:B:1240:CLA:CED	18:B:1220:CLA:HHB	2.46	0.45
18:3:3008:CLA:CHD	18:3:3008:CLA:CBC	2.85	0.45
18:1:1002:CLA:CMD	18:1:1007:CLA:C4D	2.95	0.45
15:1:218:LEU:HD21	18:1:1008:CLA:HMC3	1.98	0.45
18:1:1011:CLA:CBA	18:1:1011:CLA:HBD	2.46	0.45
15:1:146:GLU:CG	15:1:149:ARG:NH1	2.73	0.45
15:1:158:LYS:C	15:1:159:LYS:CD	2.85	0.45
22:A:6017:BCR:H23C	22:A:6017:BCR:H392	1.99	0.45
16:3:121:TYR:C	16:3:121:TYR:CD1	2.89	0.45
1:A:570:PRO:HD2	9:D:136:GLU:OE1	2.15	0.45
1:A:503:THR:O	1:A:505:PRO:HD3	2.16	0.45
18:A:1110:CLA:H52	16:3:81:LEU:CD1	2.47	0.45
1:A:205:HIS:CE1	18:A:1118:CLA:HMD2	2.51	0.45
9:D:211:LEU:H	9:D:211:LEU:CD1	2.28	0.45
2:B:265:THR:HG22	2:B:360:PHE:CE1	2.52	0.45
2:B:551:LYS:C	2:B:553:PHE:H	2.20	0.45
13:2:164:GLU:O	13:2:168:TRP:HB2	2.16	0.45
16:3:157:LEU:O	16:3:161:GLU:N	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1240:CLA:HBA1	21:B:5004:LHG:HC42	1.98	0.45
2:B:282:PHE:CE2	22:G:2011:BCR:H281	2.51	0.45
7:L:166:LEU:CD2	7:L:166:LEU:C	2.85	0.45
10:E:111:ASN:ND2	10:E:113:ALA:N	2.60	0.45
18:A:1108:CLA:HED2	16:3:93:ILE:HB	1.98	0.45
22:F:6014:BCR:C8	22:F:6014:BCR:H331	2.46	0.45
14:4:74:ASN:N	14:4:74:ASN:HD22	2.14	0.45
5:F:111:ALA:O	5:F:113:SER:N	2.50	0.45
16:3:149:ASN:O	16:3:150:TYR:CD1	2.70	0.45
1:A:225:VAL:HG22	1:A:245:PRO:HB3	1.97	0.45
13:2:140:ALA:O	13:2:143:GLN:HG3	2.17	0.45
13:2:231:ALA:HA	18:2:2003:CLA:HBB1	1.99	0.45
16:3:225:LEU:CD1	16:3:225:LEU:C	2.84	0.45
16:3:263:PRO:CD	16:3:264:VAL:H	2.30	0.45
18:1:1001:CLA:C4A	18:1:1001:CLA:CGA	2.95	0.45
15:1:127:PRO:C	15:1:128:TRP:CG	2.87	0.45
18:4:4007:CLA:H92	18:4:4007:CLA:H52	1.99	0.45
1:A:62:HIS:HB2	18:A:1128:CLA:CGA	2.46	0.45
22:A:6007:BCR:H351	22:A:6007:BCR:H15C	1.65	0.45
23:B:5005:LMG:H212	22:F:6016:BCR:H362	1.98	0.45
22:B:6004:BCR:H383	6:G:126:ALA:HB1	1.98	0.45
3:I:24:LEU:O	3:I:28:VAL:HG23	2.16	0.45
6:G:76:ARG:HE	6:G:116:LYS:NZ	2.14	0.45
4:J:32:LEU:HB3	4:J:33:PHE:CD1	2.52	0.45
13:2:76:TRP:CD1	13:2:93:GLY:O	2.69	0.45
13:2:129:LEU:CD2	13:2:131:ILE:HG13	2.47	0.45
18:2:2002:CLA:HMC2	27:2:2501:LUT:C31	2.46	0.45
16:3:137:PHE:CD1	16:3:137:PHE:C	2.90	0.45
16:3:202:TYR:CD1	18:3:3001:CLA:O1D	2.70	0.45
18:3:3003:CLA:H62	18:3:3003:CLA:H2	1.79	0.45
18:3:3018:CLA:HBA1	18:3:3018:CLA:C4A	2.45	0.45
14:4:215:PHE:CE1	27:4:4502:LUT:H12	2.51	0.45
29:4:4505:ZEX:H191	29:4:4505:ZEX:H11	1.79	0.45
18:B:1207:CLA:H91	18:B:1207:CLA:H112	1.61	0.45
18:A:1237:CLA:HMC3	18:B:1238:CLA:ND	2.32	0.45
18:A:1130:CLA:C2	18:L:1502:CLA:H93	2.47	0.45
18:G:1001:CLA:C4	22:G:2011:BCR:C34	2.92	0.45
4:J:32:LEU:HD21	18:J:1302:CLA:C2	2.46	0.45
16:3:253:TYR:CD1	16:3:253:TYR:O	2.70	0.45
7:L:121:ARG:HG3	7:L:127:GLY:CA	2.39	0.45
1:A:222:GLN:NE2	1:A:300:ALA:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:548:PRO:HD2	8:C:62:PHE:CZ	2.52	0.45
2:B:473:GLY:O	2:B:474:PHE:HB2	2.17	0.45
7:L:148:TYR:CE1	7:L:152:SER:OG	2.70	0.45
13:2:122:ILE:HD12	13:2:122:ILE:N	2.31	0.45
16:3:130:GLN:C	16:3:132:THR:H	2.18	0.45
16:3:183:GLY:CA	16:3:194:PHE:C	2.85	0.45
16:3:186:TYR:CD1	16:3:186:TYR:N	2.85	0.45
16:3:62:LYS:HZ3	16:3:76:TYR:HD2	1.63	0.45
15:1:130:THR:HG22	15:1:131:LEU:H	1.80	0.45
14:4:99:GLY:O	14:4:103:MET:HG2	2.17	0.45
18:F:1302:CLA:H3A	18:F:1302:CLA:HBA1	1.74	0.45
3:I:9:VAL:HB	3:I:10:PRO:CD	2.47	0.45
7:L:145:LEU:CD1	22:L:6019:BCR:H392	2.25	0.45
22:K:2011:BCR:H24C	22:K:2011:BCR:H371	1.73	0.45
4:J:2:ARG:CD	4:J:4:LEU:HB2	2.42	0.45
6:G:114:VAL:CG1	18:G:1002:CLA:CBA	2.95	0.45
4:J:31:ARG:HH22	18:J:1302:CLA:H3A	1.81	0.45
4:J:9:SER:HA	4:J:13:VAL:HG21	1.99	0.45
14:4:132:GLU:O	14:4:134:TYR:CE1	2.70	0.45
5:F:167:PHE:HB2	22:F:6014:BCR:C40	2.47	0.45
2:B:374:HIS:O	2:B:378:ILE:HG12	2.17	0.45
1:A:304:LEU:HA	1:A:304:LEU:HD23	1.83	0.45
15:1:51:LEU:HD12	15:1:60:GLY:HA2	1.99	0.45
13:2:220:LYS:CA	18:2:2007:CLA:CED	2.90	0.45
18:3:3001:CLA:CBB	27:3:3501:LUT:H34	2.44	0.45
28:3:3011:CHL:HBC2	28:3:3011:CHL:HH2	1.99	0.45
18:4:4008:CLA:H3A	18:4:4008:CLA:HBA2	1.59	0.45
15:1:220:ASP:OD2	15:1:223:HIS:CD2	2.70	0.45
18:B:1205:CLA:C1A	18:B:1205:CLA:CGA	2.94	0.45
18:B:1207:CLA:H111	18:B:1207:CLA:H142	1.68	0.45
2:B:301:ILE:HG21	18:B:1221:CLA:HAC1	1.97	0.45
18:B:1223:CLA:H143	22:B:6009:BCR:C19	2.46	0.45
22:F:6016:BCR:C23	22:F:6016:BCR:C38	2.91	0.45
7:L:98:ARG:NH2	7:L:175:GLN:OE1	2.50	0.45
12:K:136:VAL:O	12:K:140:LEU:HD13	2.17	0.45
12:K:70:MET:CE	12:K:71:VAL:CA	2.85	0.45
16:3:94:GLU:OE2	16:3:95:PRO:N	2.50	0.45
14:4:167:ASN:OD1	14:4:168:GLN:N	2.49	0.45
7:L:204:LEU:CD1	7:L:204:LEU:C	2.85	0.45
14:4:60:LEU:CG	14:4:61:ALA:N	2.79	0.45
2:B:172:GLU:HB3	2:B:291:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:LEU:HD13	26:B:8002:LMU:H5B	1.99	0.45
7:L:55:GLN:O	7:L:56:VAL:HB	2.16	0.45
16:3:229:LYS:HD2	16:3:229:LYS:HA	1.67	0.45
8:C:5:VAL:HG22	8:C:67:VAL:HG22	1.98	0.45
13:2:177:VAL:C	13:2:179:THR:N	2.70	0.45
13:2:185:ASN:OD1	13:2:186:ASN:N	2.50	0.45
13:2:120:ILE:CG2	27:2:2501:LUT:C37	2.86	0.45
15:1:126:VAL:HG23	15:1:127:PRO:N	2.31	0.45
15:1:217:HIS:O	15:1:221:PRO:HA	2.17	0.45
2:B:585:ASN:HB2	18:B:1012:CLA:HBC2	1.98	0.45
2:B:358:TYR:CE2	18:B:1225:CLA:HED2	2.52	0.45
18:B:1235:CLA:H203	18:B:1235:CLA:H161	1.87	0.45
22:B:6009:BCR:H351	22:B:6009:BCR:H15C	1.71	0.45
5:F:157:TRP:CH2	18:F:1302:CLA:O1A	2.70	0.45
23:F:5002:LMG:H172	23:F:5002:LMG:H141	1.68	0.45
10:E:66:ILE:CG2	10:E:93:VAL:HG11	2.45	0.45
14:4:199:GLU:O	14:4:202:GLU:HB2	2.16	0.45
1:A:346:LEU:HG	1:A:429:ASN:HD21	1.81	0.45
1:A:229:ILE:HD11	1:A:245:PRO:HG3	1.99	0.45
7:L:164:LEU:N	7:L:164:LEU:HD23	2.31	0.45
13:2:194:GLY:O	13:2:195:TYR:CD1	2.70	0.44
16:3:100:TYR:CE1	16:3:104:ILE:HG13	2.52	0.44
15:1:105:TRP:H	15:1:105:TRP:HD1	1.62	0.44
18:4:4001:CLA:CGA	18:4:4001:CLA:C3A	2.95	0.44
14:4:98:ASN:ND2	18:4:4012:CLA:OBD	2.50	0.44
18:A:1131:CLA:C3B	18:A:1132:CLA:HMB2	2.47	0.44
18:B:1202:CLA:HBA2	18:B:1210:CLA:CED	2.47	0.44
2:B:22:TRP:CZ2	18:B:1238:CLA:HMB1	2.53	0.44
2:B:645:VAL:HG21	18:B:1205:CLA:HAC1	1.99	0.44
2:B:6:PRO:HG3	2:B:24:GLY:CA	2.47	0.44
18:G:1003:CLA:HBA2	18:G:1003:CLA:H3A	1.57	0.44
18:A:1237:CLA:H143	22:I:6020:BCR:H363	1.99	0.44
14:4:169:ASP:HB3	18:4:4016:CLA:C1D	2.47	0.44
1:A:453:LEU:HD21	18:A:1136:CLA:CAB	2.46	0.44
16:3:242:PHE:O	16:3:246:LEU:HB2	2.17	0.44
11:H:107:GLY:CA	11:H:110:THR:HG22	2.47	0.44
2:B:603:ARG:HH22	2:B:627:ASN:ND2	2.14	0.44
14:4:239:ASP:OD1	14:4:242:HIS:CD2	2.70	0.44
2:B:93:ASP:O	2:B:96:PHE:HB2	2.17	0.44
18:2:2004:CLA:H61	18:2:2004:CLA:H41	1.67	0.44
28:2:2010:CHL:HBB1	28:2:2013:CHL:CBB	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:3003:CLA:HAB	27:3:3501:LUT:C17	2.47	0.44
18:3:3012:CLA:CBB	18:3:3012:CLA:HMB1	2.12	0.44
27:3:3502:LUT:C28	27:3:3502:LUT:C37	2.85	0.44
14:4:135:PHE:O	14:4:135:PHE:CG	2.71	0.44
27:4:4502:LUT:H401	27:4:4502:LUT:H35	1.77	0.44
28:4:4013:CHL:HHB	27:4:4503:LUT:H191	1.98	0.44
1:A:382:TYR:CE2	18:A:1127:CLA:HED2	2.52	0.44
18:A:1237:CLA:H62	18:A:1237:CLA:H92	1.86	0.44
12:K:78:LEU:HD23	12:K:78:LEU:HA	1.75	0.44
4:J:2:ARG:O	4:J:2:ARG:HG2	2.16	0.44
18:B:1214:CLA:H92	18:B:1214:CLA:H61	1.74	0.44
1:A:721:GLN:NE2	10:E:109:LYS:HB2	2.32	0.44
1:A:614:PHE:HB3	1:A:652:TRP:HZ3	1.82	0.44
9:D:113:PHE:CD1	9:D:113:PHE:N	2.85	0.44
13:2:129:LEU:HD23	13:2:129:LEU:O	2.17	0.44
13:2:219:THR:CG2	18:2:2007:CLA:CED	2.86	0.44
13:2:238:GLN:NE2	18:2:2003:CLA:C1A	2.81	0.44
16:3:267:ASN:C	18:3:3003:CLA:HED2	2.37	0.44
18:3:3006:CLA:HMB1	18:3:3013:CLA:HBB1	1.99	0.44
18:3:3006:CLA:C4	18:3:3018:CLA:C1	2.94	0.44
14:4:219:ILE:CG2	14:4:220:ILE:N	2.81	0.44
18:1:1001:CLA:C1D	27:1:1501:LUT:H383	2.47	0.44
14:4:76:PHE:HB3	18:4:4004:CLA:CAD	2.48	0.44
18:B:1207:CLA:H92	18:B:1207:CLA:H61	1.65	0.44
12:K:128:VAL:CG2	22:K:2011:BCR:H311	2.47	0.44
6:G:132:HIS:CG	22:G:2011:BCR:H19C	2.53	0.44
18:G:1002:CLA:HBA2	18:G:1002:CLA:O2D	2.18	0.44
6:G:114:VAL:HG11	18:G:1002:CLA:HBA1	1.99	0.44
16:3:120:GLU:OE2	16:3:253:TYR:HB3	2.16	0.44
13:2:250:LEU:CD2	13:2:250:LEU:C	2.85	0.44
7:L:204:LEU:O	7:L:207:LEU:HD23	2.17	0.44
13:2:79:GLY:N	13:2:84:ASP:OD2	2.50	0.44
13:2:256:ASP:OD2	13:2:259:HIS:CD2	2.70	0.44
18:B:1215:CLA:H111	18:B:1215:CLA:H143	1.72	0.44
13:2:95:ASP:OD1	13:2:98:SER:HB2	2.17	0.44
13:2:162:TRP:CD1	13:2:162:TRP:O	2.70	0.44
18:2:2005:CLA:HMD2	18:2:2012:CLA:ND	2.33	0.44
15:1:120:THR:CG2	15:1:125:PRO:HA	2.48	0.44
18:A:1132:CLA:H111	18:A:1132:CLA:H143	1.65	0.44
18:B:1207:CLA:HAC2	27:I:6018:LUT:H181	1.99	0.44
18:B:1235:CLA:H162	18:B:1235:CLA:H141	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1107:CLA:HMA1	4:J:27:ILE:HD13	2.00	0.44
12:K:124:ALA:HA	12:K:127:THR:OG1	2.17	0.44
12:K:126:GLY:O	12:K:130:HIS:CD2	2.70	0.44
6:G:95:GLN:C	6:G:97:GLY:H	2.20	0.44
15:1:42:MET:O	15:1:42:MET:HE2	2.17	0.44
9:D:207:GLN:O	9:D:211:LEU:HD13	2.17	0.44
6:G:100:HIS:O	6:G:101:PHE:CG	2.70	0.44
6:G:72:LEU:HD23	6:G:127:TRP:HB2	1.99	0.44
6:G:125:LEU:HA	6:G:125:LEU:HD23	1.77	0.44
13:2:133:LEU:CD1	13:2:133:LEU:C	2.85	0.44
13:2:146:PHE:CD1	13:2:147:THR:N	2.85	0.44
13:2:188:LEU:O	13:2:189:THR:HG23	2.18	0.44
13:2:220:LYS:HD3	18:2:2002:CLA:HAA2	1.99	0.44
16:3:135:ALA:CB	16:3:137:PHE:CE2	3.00	0.44
16:3:236:LEU:HD11	18:3:3003:CLA:C15	2.48	0.44
18:3:3005:CLA:OBD	18:3:3012:CLA:HBA2	2.18	0.44
15:1:85:ARG:HH21	18:1:1001:CLA:C1D	2.29	0.44
14:4:153:GLU:HG3	14:4:156:ARG:HH11	1.82	0.44
22:A:6007:BCR:C11	18:A:1119:CLA:H112	2.47	0.44
21:A:5003:LHG:H371	18:A:1137:CLA:C4D	2.48	0.44
18:B:1221:CLA:H2	18:B:1210:CLA:H92	1.99	0.44
7:L:102:VAL:CG1	7:L:106:HIS:ND1	2.81	0.44
13:2:239:HIS:CE1	13:2:244:THR:O	2.70	0.44
22:A:6003:BCR:H351	22:A:6003:BCR:H15C	1.72	0.44
11:H:55:PHE:CD2	11:H:55:PHE:O	2.70	0.44
27:2:2502:LUT:H31	27:2:2502:LUT:H391	1.88	0.44
15:1:180:TYR:CD2	18:1:1001:CLA:O1A	2.71	0.44
23:F:5002:LMG:H292	18:1:1014:CLA:ND	2.32	0.44
15:1:116:GLY:O	15:1:118:GLN:HA	2.18	0.44
15:1:98:GLU:N	15:1:102:LEU:CB	2.81	0.44
18:B:1236:CLA:H52	18:B:1227:CLA:H191	1.99	0.44
7:L:174:ASP:CG	7:L:175:GLN:HG2	2.38	0.44
9:D:192:ILE:CG2	9:D:193:GLY:N	2.73	0.44
18:A:1110:CLA:H8	18:A:1110:CLA:HBB1	1.99	0.44
5:F:167:PHE:HB2	22:F:6014:BCR:H401	1.99	0.44
13:2:105:ALA:O	13:2:109:HIS:HD2	2.00	0.44
16:3:174:GLN:HB2	16:3:182:MET:CG	2.48	0.44
18:3:3012:CLA:HBC2	18:3:3013:CLA:HMB1	1.99	0.44
15:1:79:SER:CB	18:1:1012:CLA:HED2	2.47	0.44
18:B:1207:CLA:H51	18:B:1207:CLA:H11	1.77	0.44
18:B:1225:CLA:H202	18:B:1225:CLA:H161	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:5002:PQN:H292	20:B:5002:PQN:H261	1.71	0.44
7:L:91:THR:CG2	7:L:175:GLN:HE21	2.30	0.44
14:4:168:GLN:NE2	14:4:171:ILE:O	2.34	0.44
6:G:116:LYS:HZ1	18:G:1002:CLA:C4B	2.30	0.44
16:3:117:ILE:HG23	16:3:253:TYR:HB2	1.99	0.44
2:B:166:SER:OG	6:G:95:GLN:NE2	2.51	0.44
1:A:269:PHE:HA	1:A:274:TRP:NE1	2.27	0.44
13:2:199:LEU:C	13:2:199:LEU:CD2	2.85	0.44
18:A:1112:CLA:H142	18:A:1112:CLA:H112	1.78	0.44
16:3:205:GLY:O	16:3:209:ASN:HB3	2.17	0.44
16:3:241:TYR:CE1	27:3:3501:LUT:C16	2.85	0.44
16:3:268:VAL:HG22	18:3:3003:CLA:C3D	2.48	0.44
16:3:171:ARG:HB3	28:3:3011:CHL:CMC	2.48	0.44
18:3:3006:CLA:C2D	18:3:3018:CLA:CAB	2.95	0.44
27:I:6018:LUT:H381	27:I:6018:LUT:C28	2.45	0.44
7:L:132:LEU:C	7:L:132:LEU:HD12	2.35	0.44
12:K:70:MET:CE	12:K:71:VAL:CG2	2.85	0.44
14:4:113:GLU:CD	14:4:230:PHE:CB	2.86	0.44
1:A:492:ILE:HD11	18:A:1135:CLA:H11	1.99	0.44
1:A:375:HIS:ND1	18:A:1116:CLA:OBD	2.50	0.44
18:2:2006:CLA:CMA	28:2:2013:CHL:HAC2	2.46	0.44
18:2:2016:CLA:CGD	18:2:2016:CLA:CGA	2.96	0.44
13:2:223:LYS:HZ3	21:2:2801:LHG:P	2.23	0.44
16:3:78:PHE:O	16:3:78:PHE:CD1	2.70	0.44
15:1:106:VAL:HG21	15:1:208:THR:CG2	2.40	0.44
18:1:1004:CLA:H52	27:1:1502:LUT:H8	2.00	0.44
1:A:374:GLN:HG3	18:A:1124:CLA:HED2	2.00	0.44
22:A:6007:BCR:H371	22:A:6007:BCR:H24C	1.59	0.44
2:B:370:ALA:HB1	18:B:1224:CLA:HMA1	2.00	0.44
18:B:1229:CLA:H62	18:B:1229:CLA:H2	1.67	0.44
1:A:85:GLN:HG2	18:A:1103:CLA:HMA1	2.00	0.44
9:D:95:ALA:HA	9:D:99:GLU:O	2.16	0.44
15:1:193:LEU:C	15:1:193:LEU:CD2	2.85	0.44
16:3:202:TYR:HB3	18:3:3001:CLA:CGD	2.47	0.43
15:1:205:TYR:C	15:1:207:GLY:N	2.71	0.43
18:A:1013:CLA:H71	18:A:1140:CLA:HMC3	2.00	0.43
6:G:126:ALA:O	6:G:130:ILE:HG13	2.17	0.43
27:I:6018:LUT:H31	27:I:6018:LUT:H391	1.89	0.43
7:L:122:ASN:N	7:L:122:ASN:HD22	2.16	0.43
14:4:221:GLN:HE21	14:4:221:GLN:HB2	1.60	0.43
8:C:14:CYS:O	8:C:15:THR:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:183:GLY:HA2	16:3:191:GLU:O	2.18	0.43
16:3:225:LEU:CA	16:3:226:LYS:HZ2	2.31	0.43
16:3:62:LYS:NZ	16:3:76:TYR:HD2	2.16	0.43
21:1:1801:LHG:H382	21:1:1801:LHG:H223	1.88	0.43
27:4:4503:LUT:H191	27:4:4503:LUT:H11	1.80	0.43
18:B:1226:CLA:H161	18:B:1226:CLA:H141	1.70	0.43
14:4:118:ILE:CG2	14:4:120:ILE:H	2.30	0.43
1:A:615:HIS:CD2	18:A:1135:CLA:HMC2	2.53	0.43
13:2:209:ALA:HB3	13:2:214:LEU:CD2	2.48	0.43
1:A:295:TRP:HB3	1:A:297:THR:HG22	2.00	0.43
1:A:240:LYS:HB2	1:A:240:LYS:HE3	1.83	0.43
18:1:1004:CLA:H2	27:1:1502:LUT:C18	2.47	0.43
15:1:222:TRP:CD1	18:1:1008:CLA:HMA1	2.54	0.43
27:1:1502:LUT:H11	27:1:1502:LUT:H191	1.83	0.43
27:4:4503:LUT:H391	27:4:4503:LUT:H31	1.79	0.43
18:B:1204:CLA:C4D	18:B:1204:CLA:H12	2.48	0.43
18:B:1208:CLA:H3A	18:B:1208:CLA:HBA2	1.35	0.43
3:I:4:LEU:HD12	3:I:5:PRO:N	2.34	0.43
6:G:65:SER:HA	6:G:68:THR:CG2	2.48	0.43
5:F:143:ASP:OD1	5:F:144:GLY:N	2.51	0.43
13:2:253:HIS:CG	18:2:2003:CLA:HAA2	2.54	0.43
18:2:2003:CLA:HMA1	18:2:2008:CLA:CBC	2.42	0.43
18:2:2005:CLA:H61	18:2:2005:CLA:H93	1.79	0.43
16:3:100:TYR:CE1	16:3:104:ILE:CG1	3.01	0.43
16:3:184:LYS:CE	16:3:185:GLN:HE21	2.32	0.43
14:4:103:MET:CB	18:4:4001:CLA:HMC3	2.47	0.43
14:4:135:PHE:O	14:4:135:PHE:CD1	2.70	0.43
17:A:1011:CL0:H10	17:A:1011:CL0:H72	1.55	0.43
18:A:1127:CLA:H62	18:A:1127:CLA:H102	1.81	0.43
18:A:1128:CLA:H122	18:A:1128:CLA:H162	1.70	0.43
1:A:55:TRP:HE3	21:A:7001:LHG:H111	1.84	0.43
18:B:1218:CLA:H52	18:B:1218:CLA:H8	1.80	0.43
18:B:1232:CLA:H11	18:B:1232:CLA:H52	1.62	0.43
15:1:148:GLN:HE21	15:1:148:GLN:HA	1.83	0.43
1:A:158:ILE:HD11	18:A:1112:CLA:HMA2	1.99	0.43
10:E:79:GLN:HG3	10:E:84:TYR:OH	2.17	0.43
2:B:244:PHE:N	2:B:264:GLN:OE1	2.32	0.43
2:B:195:VAL:HA	2:B:199:ILE:HD12	2.00	0.43
6:G:67:SER:HB2	6:G:135:ALA:HB2	2.00	0.43
13:2:217:LEU:HD12	13:2:217:LEU:HA	1.77	0.43
18:3:3006:CLA:CHC	22:3:3503:BCR:HC41	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:4008:CLA:CHC	18:4:4008:CLA:HBB1	2.43	0.43
14:4:144:ILE:CD1	18:1:1008:CLA:HAA2	2.48	0.43
15:1:230:VAL:HG13	18:1:1014:CLA:NB	2.33	0.43
15:1:41:TRP:CD1	15:1:59:PHE:O	2.70	0.43
18:A:1109:CLA:H102	18:A:1101:CLA:HBB2	1.99	0.43
18:B:1220:CLA:H141	22:B:6009:BCR:HC32	1.99	0.43
22:G:2011:BCR:H321	22:G:2011:BCR:C8	2.48	0.43
16:3:257:LEU:HA	16:3:260:VAL:HB	1.99	0.43
14:4:243:ASN:C	14:4:244:THR:HG23	2.39	0.43
13:2:129:LEU:CD2	13:2:131:ILE:HG12	2.49	0.43
15:1:85:ARG:NH2	18:1:1001:CLA:C4D	2.72	0.43
15:1:58:ASP:CA	18:1:1004:CLA:CED	2.92	0.43
27:1:1501:LUT:H15	27:1:1501:LUT:H201	1.76	0.43
14:4:136:ALA:HA	15:1:223:HIS:NE2	2.33	0.43
14:4:105:GLY:CA	18:4:4006:CLA:CBB	2.95	0.43
14:4:154:ILE:HD12	14:4:157:TRP:HE3	1.83	0.43
18:4:4006:CLA:C2B	27:4:4503:LUT:H171	2.48	0.43
18:A:1237:CLA:HAA2	18:A:1130:CLA:HMB1	2.00	0.43
18:B:1224:CLA:O1D	18:B:1225:CLA:HMA1	2.19	0.43
7:L:85:ASN:CB	18:L:1501:CLA:HMC1	2.48	0.43
12:K:70:MET:CE	12:K:71:VAL:N	2.77	0.43
3:I:25:PHE:CE1	7:L:147:ILE:HG22	2.54	0.43
6:G:148:PRO:O	6:G:148:PRO:HD2	2.18	0.43
7:L:57:VAL:HG23	7:L:57:VAL:O	2.18	0.43
5:F:117:LEU:HA	5:F:117:LEU:HD23	1.77	0.43
15:1:168:LEU:HA	15:1:168:LEU:HD13	1.79	0.43
2:B:406:ASN:O	2:B:410:ARG:HG2	2.18	0.43
1:A:417:PHE:CD1	1:A:421:ASP:HB2	2.54	0.43
13:2:160:ILE:O	13:2:163:ALA:HB3	2.18	0.43
13:2:188:LEU:HD23	13:2:197:GLY:C	2.38	0.43
18:4:4005:CLA:HMD2	18:4:4012:CLA:ND	2.33	0.43
18:4:4005:CLA:O1A	18:4:4005:CLA:H2A	2.17	0.43
14:4:141:LEU:HD22	28:4:4013:CHL:C2D	2.49	0.43
28:4:4013:CHL:OMC	28:4:4013:CHL:HAC1	2.19	0.43
27:4:4503:LUT:H15	27:4:4503:LUT:H201	1.80	0.43
18:A:1122:CLA:H162	18:A:1122:CLA:H143	1.86	0.43
18:A:1140:CLA:H62	18:A:1140:CLA:H41	1.63	0.43
18:B:1211:CLA:HMC1	18:B:1212:CLA:HAB	2.00	0.43
18:B:1222:CLA:H61	18:B:1222:CLA:H41	1.67	0.43
18:B:1222:CLA:H62	18:B:1222:CLA:H92	1.75	0.43
18:B:1231:CLA:H112	18:B:1231:CLA:H142	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:6016:BCR:H24C	22:F:6016:BCR:H371	1.79	0.43
7:L:181:GLY:O	7:L:184:LYS:HB2	2.18	0.43
6:G:68:THR:HG23	6:G:69:GLY:N	2.34	0.43
6:G:116:LYS:HA	18:G:1002:CLA:C2D	2.49	0.43
5:F:221:LEU:HB2	5:F:222:LEU:HD23	1.99	0.43
1:A:445:HIS:O	1:A:449:VAL:HG23	2.19	0.43
1:A:103:PHE:HB3	1:A:122:VAL:HG23	2.00	0.43
13:2:181:PRO:CD	18:2:2016:CLA:CBB	2.95	0.43
18:3:3006:CLA:H43	18:3:3018:CLA:C1	2.48	0.43
27:3:3502:LUT:H31	27:3:3502:LUT:H391	1.88	0.43
15:1:85:ARG:HB3	18:1:1011:CLA:HED2	1.98	0.43
15:1:230:VAL:CG1	18:1:1014:CLA:NB	2.82	0.43
15:1:108:ALA:O	15:1:111:TRP:CE3	2.72	0.43
15:1:217:HIS:CE1	15:1:221:PRO:HB2	2.54	0.43
15:1:81:LEU:O	15:1:85:ARG:HG2	2.18	0.43
18:4:4007:CLA:HAA1	18:4:4007:CLA:HED2	2.00	0.43
22:A:6011:BCR:H15C	22:A:6011:BCR:H351	1.80	0.43
18:B:1205:CLA:H143	18:B:1205:CLA:H161	1.80	0.43
11:H:80:PRO:O	11:H:82:GLN:N	2.47	0.43
14:4:171:ILE:HD13	18:4:4016:CLA:CMA	2.49	0.43
7:L:169:ARG:C	7:L:171:LYS:N	2.72	0.43
15:1:224:ASN:N	15:1:224:ASN:OD1	2.51	0.43
16:3:185:GLN:HB2	16:3:186:TYR:HD1	1.77	0.43
28:1:1010:CHL:CMC	28:1:1010:CHL:CBC	2.86	0.43
15:1:85:ARG:NH1	15:1:85:ARG:HG3	2.34	0.43
28:4:4010:CHL:HAB	28:4:4010:CHL:HMB1	1.89	0.43
18:A:1120:CLA:H62	18:A:1120:CLA:H41	1.52	0.43
1:A:434:ARG:HA	1:A:437:ARG:HB2	2.01	0.43
18:B:1227:CLA:H102	18:B:1227:CLA:H62	1.74	0.43
18:B:1239:CLA:H62	18:B:1023:CLA:H201	2.00	0.43
2:B:95:HIS:NE2	18:B:1206:CLA:HMB3	2.33	0.43
12:K:78:LEU:C	12:K:80:ALA:N	2.72	0.43
6:G:116:LYS:HG2	6:G:117:SER:N	2.34	0.43
15:1:64:LEU:O	15:1:65:ARG:HB2	2.19	0.43
5:F:213:TRP:CG	5:F:214:PRO:HD3	2.54	0.43
16:3:148:TYR:O	16:3:150:TYR:CD1	2.72	0.43
2:B:17:THR:HA	2:B:696:LYS:HB2	2.01	0.43
13:2:104:GLN:NE2	13:2:193:VAL:CB	2.81	0.43
18:2:2006:CLA:O1A	28:2:2013:CHL:HMD2	2.19	0.43
18:1:1003:CLA:H2	18:1:1008:CLA:CMD	2.48	0.43
27:4:4503:LUT:C36	28:1:1009:CHL:C9	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:103:MET:HE3	14:4:207:ASN:CB	2.48	0.43
14:4:103:MET:HE3	14:4:207:ASN:HB3	1.96	0.43
18:4:4005:CLA:C2D	18:4:4012:CLA:C1D	2.97	0.43
18:B:1231:CLA:HAB	18:B:1223:CLA:HED1	2.01	0.43
23:F:5002:LMG:O9	18:1:1014:CLA:HED3	2.19	0.43
5:F:103:GLU:O	5:F:106:LEU:HB3	2.19	0.43
18:A:1110:CLA:C1	16:3:81:LEU:HD13	2.49	0.43
1:A:342:GLY:HA3	1:A:431:LEU:HG	2.00	0.43
12:K:119:LEU:HD12	12:K:119:LEU:HA	1.80	0.43
1:A:154:ARG:NH2	1:A:233:LEU:HB3	2.34	0.43
13:2:262:ILE:HD11	18:2:2003:CLA:C4	2.41	0.42
16:3:138:GLN:CB	16:3:145:ALA:CB	2.82	0.42
27:3:3501:LUT:C17	27:3:3501:LUT:H8	2.46	0.42
27:3:3502:LUT:H201	27:3:3502:LUT:H15	1.92	0.42
15:1:63:PRO:HD2	27:1:1502:LUT:O3	2.19	0.42
15:1:78:GLU:O	15:1:82:ILE:HG12	2.19	0.42
18:4:4001:CLA:HHD	28:4:4011:CHL:O1A	2.18	0.42
18:B:1203:CLA:OBD	18:B:1201:CLA:HMC3	2.19	0.42
18:B:1224:CLA:HBA2	18:B:1224:CLA:H3A	1.75	0.42
2:B:464:GLN:NE2	18:B:1234:CLA:HMD1	2.34	0.42
20:B:5002:PQN:H243	20:B:5002:PQN:H262	1.72	0.42
2:B:22:TRP:HZ3	20:B:5002:PQN:H302	1.84	0.42
6:G:141:THR:OG1	23:G:2021:LMG:HC91	2.18	0.42
3:I:7:LEU:HG	11:H:115:SER:HB2	2.00	0.42
22:L:6020:BCR:H24C	22:L:6020:BCR:H371	1.79	0.42
10:E:66:ILE:CG2	10:E:95:GLN:NE2	2.72	0.42
13:2:137:TRP:HH2	13:2:236:TRP:CA	2.24	0.42
6:G:121:LEU:CD2	6:G:121:LEU:C	2.84	0.42
13:2:254:LEU:HD23	13:2:254:LEU:H	1.83	0.42
4:J:16:THR:HG21	22:J:6013:BCR:H403	1.97	0.42
18:A:1112:CLA:C2	18:A:1114:CLA:HMB2	2.49	0.42
9:D:163:GLU:CD	9:D:164:VAL:N	2.72	0.42
13:2:123:PRO:CA	13:2:126:LEU:HG	2.49	0.42
13:2:238:GLN:HE21	18:2:2003:CLA:CHA	2.31	0.42
16:3:128:ILE:HG22	16:3:132:THR:HA	2.01	0.42
18:3:3002:CLA:HMD1	18:3:3007:CLA:HBA2	1.99	0.42
14:4:57:LEU:HD12	14:4:57:LEU:HA	1.72	0.42
18:1:1001:CLA:HHC	27:1:1501:LUT:C32	2.38	0.42
14:4:136:ALA:HB1	14:4:140:THR:CG2	2.46	0.42
18:4:4017:CLA:HED1	21:1:1801:LHG:C15	2.37	0.42
1:A:455:PHE:HB3	18:A:1132:CLA:HBB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1208:CLA:H41	18:B:1208:CLA:H62	1.56	0.42
18:B:1227:CLA:H121	18:B:1227:CLA:H162	1.78	0.42
4:J:11:ALA:HB1	4:J:12:PRO:HD2	2.01	0.42
18:A:1126:CLA:H192	22:J:6012:BCR:H14C	2.01	0.42
7:L:130:GLY:C	7:L:132:LEU:N	2.72	0.42
7:L:176:LEU:CD1	7:L:177:GLN:HG2	2.49	0.42
18:A:1121:CLA:H61	18:A:1121:CLA:H41	1.59	0.42
12:K:124:ALA:CB	22:K:2011:BCR:C33	2.92	0.42
6:G:116:LYS:CG	18:G:1002:CLA:ND	2.76	0.42
2:B:366:THR:HG1	2:B:733:PHE:HE1	1.67	0.42
11:H:56:ASP:HB2	11:H:59:ASP:OD1	2.18	0.42
1:A:205:HIS:HB3	18:A:1111:CLA:HBB1	2.01	0.42
8:C:30:PRO:HD3	9:D:179:ASN:O	2.18	0.42
22:F:6014:BCR:C23	22:F:6014:BCR:H403	2.48	0.42
1:A:302:HIS:HB2	18:A:1116:CLA:C1B	2.49	0.42
2:B:302:LYS:O	2:B:306:GLU:HG2	2.19	0.42
2:B:658:ALA:O	2:B:661:PHE:HB2	2.19	0.42
1:A:580:PRO:HB3	1:A:727:ILE:HB	2.01	0.42
13:2:118:ALA:HB2	18:2:2006:CLA:HMC3	2.01	0.42
16:3:240:GLY:HA2	18:3:3003:CLA:C3C	2.49	0.42
15:1:183:LYS:HZ3	18:1:1002:CLA:HBD	1.82	0.42
14:4:153:GLU:CG	14:4:156:ARG:NH1	2.82	0.42
18:4:4007:CLA:H112	18:4:4007:CLA:H91	1.74	0.42
18:4:4004:CLA:CBB	27:4:4502:LUT:C32	2.97	0.42
29:4:4505:ZEX:H15	29:4:4505:ZEX:H201	1.81	0.42
29:4:4505:ZEX:H362	29:4:4505:ZEX:C24	2.49	0.42
18:A:1013:CLA:HED2	2:B:532:LEU:HD21	2.01	0.42
18:B:1204:CLA:H42	3:I:8:PHE:HE2	1.84	0.42
18:B:1239:CLA:HED1	18:B:1226:CLA:H102	2.01	0.42
2:B:594:TRP:HB2	18:B:1234:CLA:HMC1	2.02	0.42
2:B:590:VAL:HG22	18:B:1234:CLA:HAB	2.01	0.42
7:L:94:ASN:O	7:L:98:ARG:HG3	2.19	0.42
12:K:71:VAL:HG12	12:K:129:GLY:C	2.40	0.42
8:C:9:ASP:OD1	9:D:191:SER:N	2.52	0.42
6:G:76:ARG:CD	6:G:116:LYS:NZ	2.82	0.42
16:3:81:LEU:HD23	16:3:81:LEU:HA	1.75	0.42
13:2:188:LEU:C	13:2:188:LEU:CD2	2.84	0.42
16:3:218:LYS:O	16:3:221:LYS:HG3	2.19	0.42
16:3:268:VAL:HG22	18:3:3003:CLA:CAD	2.49	0.42
16:3:169:GLU:HB3	18:3:3012:CLA:C1B	2.50	0.42
15:1:130:THR:CG2	15:1:132:PRO:CD	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LEU:HD11	22:A:6011:BCR:HC8	2.02	0.42
18:B:1220:CLA:H51	18:B:1220:CLA:H11	1.86	0.42
5:F:157:TRP:CZ2	18:F:1302:CLA:O1A	2.72	0.42
18:G:1003:CLA:C3	23:G:2021:LMG:H332	2.49	0.42
7:L:174:ASP:O	7:L:175:GLN:HB2	2.19	0.42
22:L:6019:BCR:C39	22:L:6019:BCR:C27	2.90	0.42
4:J:2:ARG:C	4:J:4:LEU:N	2.71	0.42
9:D:192:ILE:HB	9:D:194:LYS:HG3	2.02	0.42
16:3:120:GLU:CD	16:3:253:TYR:CB	2.81	0.42
13:2:222:ILE:H	13:2:222:ILE:CD1	2.32	0.42
2:B:221:GLY:O	26:B:8002:LMU:H6D	2.19	0.42
2:B:199:ILE:HB	2:B:200:PRO:HD3	2.00	0.42
10:E:75:LYS:HB2	10:E:128:VAL:HG21	2.02	0.42
1:A:398:HIS:O	1:A:402:ILE:HG12	2.19	0.42
15:1:58:ASP:HB2	18:1:1004:CLA:CED	2.48	0.42
18:1:1003:CLA:H12	18:1:1008:CLA:C2D	2.49	0.42
15:1:131:LEU:CD2	15:1:131:LEU:N	2.72	0.42
27:1:1502:LUT:H35	27:1:1502:LUT:H401	1.80	0.42
27:4:4502:LUT:H3	27:4:4502:LUT:H162	1.84	0.42
10:E:105:VAL:HG12	10:E:106:ARG:N	2.35	0.42
7:L:53:THR:O	7:L:53:THR:HG22	2.19	0.42
13:2:228:ALA:O	13:2:231:ALA:HB3	2.20	0.42
18:2:2001:CLA:H12	27:2:2501:LUT:H173	1.98	0.42
14:4:103:MET:HB2	18:4:4001:CLA:HMC3	2.01	0.42
14:4:108:GLY:HA2	18:4:4006:CLA:C2C	2.50	0.42
18:A:1102:CLA:H3A	18:A:1102:CLA:HBA1	1.66	0.42
18:A:1106:CLA:H61	18:A:1106:CLA:H93	1.76	0.42
1:A:364:MET:HE3	18:A:1119:CLA:H93	2.02	0.42
18:B:1202:CLA:H142	18:B:1202:CLA:H112	1.80	0.42
18:B:1202:CLA:HBD	18:B:1202:CLA:H122	2.02	0.42
18:B:1208:CLA:C4D	26:B:8001:LMU:H32	2.50	0.42
18:B:1216:CLA:H91	18:B:1216:CLA:H111	1.64	0.42
7:L:96:LEU:HB2	7:L:184:LYS:HB3	2.01	0.42
8:C:8:TYR:C	8:C:10:THR:N	2.72	0.42
5:F:85:CYS:SG	5:F:138:LEU:O	2.78	0.42
22:A:6002:BCR:C33	18:A:1112:CLA:HHB	2.48	0.42
1:A:340:GLY:HA2	7:L:55:GLN:OE1	2.20	0.42
14:4:222:HIS:HD1	14:4:222:HIS:C	2.23	0.42
2:B:136:TYR:O	2:B:140:ILE:HG12	2.19	0.42
18:2:2008:CLA:O2A	16:3:160:LEU:HD13	2.20	0.42
16:3:111:LEU:HD21	18:3:3006:CLA:CBB	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:121:TYR:CE1	18:1:1006:CLA:H2	2.53	0.42
15:1:66:LEU:HD12	27:1:1502:LUT:H41	2.02	0.42
21:A:7001:LHG:H202	18:A:1128:CLA:H13	2.02	0.42
1:A:440:ASP:HB2	9:D:88:THR:CG2	2.43	0.42
18:B:1207:CLA:C3B	3:I:14:LEU:HD21	2.50	0.42
8:C:8:TYR:HB3	9:D:191:SER:CA	2.47	0.42
9:D:77:PRO:CD	9:D:77:PRO:O	2.68	0.42
13:2:211:PRO:O	13:2:212:GLN:HB2	2.19	0.42
18:A:1135:CLA:O1A	18:A:1136:CLA:HBD	2.20	0.42
18:A:1112:CLA:H91	18:A:1112:CLA:H112	1.82	0.42
1:A:205:HIS:CG	18:A:1111:CLA:HMC2	2.54	0.42
1:A:232:PHE:HD1	1:A:237:VAL:HG11	1.85	0.42
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.00	0.42
13:2:133:LEU:C	13:2:135:PRO:HD2	2.39	0.42
13:2:186:ASN:ND2	18:2:2016:CLA:H2A	2.35	0.42
13:2:233:MET:CA	13:2:233:MET:HE3	2.50	0.42
27:3:3501:LUT:H401	27:3:3501:LUT:H35	1.80	0.42
15:1:119:ALA:O	15:1:120:THR:HG23	2.19	0.42
15:1:229:ASN:O	15:1:229:ASN:ND2	2.53	0.42
18:4:4002:CLA:C1D	18:4:4007:CLA:H71	2.50	0.42
18:4:4006:CLA:NB	27:4:4503:LUT:C17	2.80	0.42
1:A:34:TRP:HE1	18:A:1109:CLA:CHB	2.33	0.42
18:B:1207:CLA:H41	7:L:133:ALA:HB2	2.01	0.42
8:C:10:THR:CG2	8:C:64:SER:CB	2.97	0.42
14:4:223:ASN:OD1	14:4:223:ASN:N	2.53	0.42
18:A:1112:CLA:H162	18:A:1112:CLA:H141	1.70	0.42
1:A:191:PRO:HB2	1:A:196:PHE:CE2	2.54	0.42
5:F:173:TRP:CD1	5:F:210:GLY:HA3	2.55	0.42
16:3:102:GLU:OE2	16:3:232:ARG:HD3	2.20	0.42
16:3:102:GLU:CD	16:3:232:ARG:HH21	2.23	0.42
15:1:205:TYR:CE2	18:1:1003:CLA:O1D	2.70	0.42
18:1:1011:CLA:C3	27:1:1501:LUT:C23	2.86	0.42
15:1:200:VAL:HG21	18:1:1003:CLA:HAC1	2.02	0.42
14:4:156:ARG:O	14:4:160:ILE:HG13	2.20	0.42
18:A:1106:CLA:H3A	18:A:1106:CLA:HBA2	1.48	0.42
18:A:1109:CLA:HBB1	18:A:1109:CLA:HHC	2.01	0.42
3:I:7:LEU:HA	3:I:7:LEU:HD13	1.65	0.42
18:A:1130:CLA:H11	7:L:83:LEU:HD11	2.01	0.42
12:K:79:PHE:CD2	12:K:121:ASP:OD2	2.73	0.42
16:3:162:MET:HE2	16:3:162:MET:HA	1.98	0.42
18:A:1110:CLA:HBC2	18:A:1111:CLA:HAB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1215:CLA:H3A	18:B:1215:CLA:HBA2	1.76	0.42
15:1:51:LEU:CD1	15:1:60:GLY:HA2	2.50	0.42
6:G:83:GLN:O	6:G:87:VAL:HG23	2.20	0.42
13:2:207:GLY:CA	18:2:2001:CLA:HAA2	2.49	0.42
13:2:197:GLY:N	18:2:2001:CLA:HED2	2.35	0.42
16:3:206:PRO:HD2	16:3:207:PHE:CA	2.49	0.42
16:3:222:GLU:O	16:3:222:GLU:HG2	2.20	0.42
16:3:231:GLY:O	16:3:235:MET:CG	2.68	0.42
16:3:110:MET:HB3	18:3:3001:CLA:HMC3	2.02	0.42
15:1:83:HIS:ND1	18:1:1012:CLA:HMD1	2.34	0.42
15:1:158:LYS:C	15:1:160:TYR:H	2.22	0.42
15:1:166:ASP:O	15:1:169:GLY:N	2.52	0.42
14:4:95:GLU:HG3	18:4:4004:CLA:C1B	2.50	0.42
17:A:1011:CL0:H53	17:A:1011:CL0:H61	1.83	0.42
18:A:1106:CLA:H42	18:A:1126:CLA:HMD2	2.02	0.42
1:A:437:ARG:HG2	9:D:87:SER:HB2	2.02	0.42
18:B:1226:CLA:H143	18:B:1226:CLA:H111	1.85	0.42
2:B:6:PRO:HD2	2:B:12:ILE:HG23	2.01	0.42
1:A:315:HIS:NE2	22:K:2011:BCR:H352	2.34	0.42
6:G:64:ILE:HD12	18:G:1001:CLA:C2D	2.50	0.42
14:4:167:ASN:CG	14:4:168:GLN:N	2.72	0.42
10:E:92:THR:OG1	10:E:93:VAL:N	2.53	0.42
4:J:28:GLU:HG3	18:J:1302:CLA:C1D	2.49	0.42
16:3:122:LEU:C	16:3:124:LYS:N	2.73	0.42
16:3:119:PRO:HB3	16:3:133:ALA:HB2	1.95	0.42
13:2:254:LEU:N	13:2:254:LEU:CD2	2.73	0.42
13:2:64:ARG:HE	13:2:79:GLY:HA3	1.85	0.42
2:B:129:LEU:HD13	2:B:135:LEU:HD23	2.01	0.42
1:A:112:ASP:OD2	1:A:115:HIS:HB3	2.19	0.42
9:D:190:ARG:HG3	9:D:190:ARG:H	1.62	0.42
16:3:142:ILE:HA	16:3:147:THR:HG23	2.02	0.41
16:3:151:TRP:CE3	16:3:152:ALA:HB2	2.55	0.41
16:3:205:GLY:O	16:3:209:ASN:CB	2.68	0.41
18:1:1005:CLA:H43	18:1:1005:CLA:HED1	2.02	0.41
15:1:130:THR:CG2	15:1:131:LEU:H	2.32	0.41
15:1:112:ALA:O	15:1:131:LEU:HD11	2.20	0.41
15:1:229:ASN:C	15:1:229:ASN:ND2	2.72	0.41
14:4:105:GLY:C	14:4:109:MET:HE2	2.40	0.41
14:4:136:ALA:HB2	15:1:222:TRP:HB3	2.01	0.41
14:4:73:ASP:HA	18:4:4004:CLA:O1D	2.20	0.41
1:A:207:LEU:HD11	18:A:1119:CLA:C3B	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:6011:BCR:H402	18:B:1229:CLA:HMB3	2.02	0.41
2:B:115:ILE:O	18:B:1205:CLA:HMD3	2.21	0.41
1:A:470:LEU:HG	18:B:1206:CLA:HMC3	2.02	0.41
1:A:266:ALA:O	1:A:269:PHE:HB3	2.19	0.41
2:B:487:ASN:HA	2:B:490:ARG:HB2	2.01	0.41
16:3:188:LEU:HA	16:3:188:LEU:HD22	1.88	0.41
1:A:650:ASN:HB2	2:B:651:LEU:HD11	2.02	0.41
16:3:110:MET:CE	16:3:230:ASN:C	2.89	0.41
16:3:258:ASP:C	16:3:266:ASN:ND2	2.73	0.41
14:4:241:TRP:CE2	18:4:4008:CLA:HMA1	2.54	0.41
15:1:170:TYR:CE2	27:1:1501:LUT:C37	3.03	0.41
15:1:200:VAL:HG21	18:1:1003:CLA:CAC	2.50	0.41
13:2:182:ILE:HD12	18:4:4007:CLA:HAB	1.97	0.41
27:4:4501:LUT:H201	27:4:4501:LUT:H15	1.88	0.41
18:4:4004:CLA:HHC	27:4:4502:LUT:H32	2.02	0.41
1:A:694:PHE:HB2	18:A:1013:CLA:HBC2	2.02	0.41
18:B:1201:CLA:HBA2	18:B:1201:CLA:H3A	1.38	0.41
2:B:411:MET:HE3	18:B:1227:CLA:HMD3	2.01	0.41
22:J:6012:BCR:H371	22:J:6012:BCR:H24C	1.75	0.41
8:C:60:THR:HG1	8:C:64:SER:HG	1.55	0.41
14:4:113:GLU:OE2	14:4:230:PHE:HB3	2.20	0.41
2:B:73:ASN:HD22	2:B:74:PHE:N	2.07	0.41
1:A:163:GLN:CD	18:A:1112:CLA:HED1	2.40	0.41
8:C:14:CYS:O	8:C:15:THR:CB	2.69	0.41
16:3:93:ILE:HG23	16:3:93:ILE:O	2.21	0.41
6:G:100:HIS:O	6:G:101:PHE:CB	2.67	0.41
2:B:519:VAL:HG11	2:B:593:TYR:HB2	2.03	0.41
1:A:29:THR:HG23	1:A:187:HIS:HD2	1.84	0.41
2:B:569:ASP:HA	2:B:574:ASP:OD2	2.20	0.41
13:2:115:LEU:HD21	18:2:2001:CLA:HBC3	2.02	0.41
16:3:116:ALA:HA	16:3:136:TRP:HB3	2.03	0.41
16:3:267:ASN:O	18:3:3003:CLA:HED2	2.21	0.41
18:1:1004:CLA:HAA1	18:1:1004:CLA:HBD	2.01	0.41
15:1:158:LYS:C	15:1:160:TYR:N	2.73	0.41
15:1:167:PRO:C	15:1:169:GLY:N	2.72	0.41
18:4:4017:CLA:HMC2	29:4:4505:ZEX:C39	2.38	0.41
27:4:4502:LUT:H15	27:4:4502:LUT:H201	1.84	0.41
1:A:687:ALA:C	18:A:1013:CLA:HAB	2.41	0.41
1:A:395:LEU:HD11	18:A:1127:CLA:HED3	2.02	0.41
18:B:1213:CLA:H61	18:B:1213:CLA:H41	1.95	0.41
2:B:697:PRO:HB3	18:B:1238:CLA:C2C	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:65:SER:HA	18:G:1001:CLA:O2A	2.20	0.41
6:G:149:LYS:C	6:G:149:LYS:CE	2.85	0.41
5:F:188:GLU:HG3	5:F:189:LYS:HG3	2.03	0.41
2:B:80:ASP:HB2	2:B:84:VAL:HG23	2.01	0.41
15:1:197:GLY:O	15:1:201:GLN:HB2	2.20	0.41
1:A:701:GLN:O	1:A:705:GLU:HG3	2.20	0.41
18:2:2007:CLA:HBC2	18:2:2007:CLA:CMC	2.42	0.41
27:2:2501:LUT:H201	27:2:2501:LUT:H15	1.74	0.41
16:3:129:PRO:O	16:3:132:THR:CB	2.69	0.41
15:1:104:ASN:HB2	15:1:107:LYS:HB2	2.01	0.41
15:1:165:PHE:O	27:1:1501:LUT:O23	2.21	0.41
15:1:211:LEU:HD12	15:1:212:GLU:N	2.30	0.41
14:4:135:PHE:O	14:4:136:ALA:CB	2.68	0.41
18:4:4012:CLA:HBB	18:4:4017:CLA:HBC2	2.01	0.41
18:A:1126:CLA:H143	18:A:1126:CLA:H162	1.68	0.41
18:B:1222:CLA:H3A	18:B:1222:CLA:HBA2	1.61	0.41
22:B:6004:BCR:H24C	22:B:6004:BCR:H371	1.82	0.41
2:B:5:LEU:HA	2:B:6:PRO:HA	1.80	0.41
3:I:4:LEU:HD12	3:I:6:SER:N	2.26	0.41
6:G:116:LYS:HB2	18:G:1002:CLA:CHA	2.50	0.41
16:3:121:TYR:HA	16:3:253:TYR:HD2	1.84	0.41
15:1:153:LYS:HD3	15:1:153:LYS:N	2.31	0.41
22:A:6002:BCR:H342	18:A:1112:CLA:CHB	2.51	0.41
1:A:201:SER:O	1:A:205:HIS:HD2	2.03	0.41
1:A:209:GLY:HA3	18:A:1111:CLA:CBB	2.50	0.41
13:2:221:GLU:HB3	13:2:222:ILE:HD12	2.02	0.41
16:3:93:ILE:HA	16:3:93:ILE:HD12	1.85	0.41
13:2:157:LEU:HA	13:2:157:LEU:HD23	1.84	0.41
13:2:125:PHE:O	13:2:129:LEU:N	2.53	0.41
13:2:135:PRO:HG2	18:2:2006:CLA:HED3	2.01	0.41
28:2:2010:CHL:HAB	28:2:2010:CHL:HMB1	1.95	0.41
16:3:161:GLU:OE2	18:3:3010:CLA:HAB	2.20	0.41
16:3:102:GLU:CD	16:3:232:ARG:NH2	2.72	0.41
16:3:258:ASP:CB	16:3:266:ASN:ND2	2.73	0.41
18:1:1004:CLA:HHD	28:1:1009:CHL:HBB2	2.02	0.41
15:1:79:SER:OG	18:1:1012:CLA:OBD	2.33	0.41
15:1:226:ILE:O	15:1:229:ASN:HB3	2.20	0.41
15:1:58:ASP:OD1	18:1:1004:CLA:HED2	2.19	0.41
15:1:85:ARG:CG	15:1:85:ARG:NH1	2.72	0.41
14:4:111:LEU:HD12	18:4:4006:CLA:HBC1	2.02	0.41
13:2:182:ILE:HD13	18:4:4007:CLA:HAB	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7001:LHG:H161	18:A:1101:CLA:HMB2	2.02	0.41
18:B:1240:CLA:HMC3	18:1:1005:CLA:H11	2.02	0.41
23:J:5001:LMG:H453	23:J:5001:LMG:H422	1.81	0.41
9:D:107:SER:OG	9:D:109:LYS:O	2.36	0.41
13:2:242:THR:O	13:2:242:THR:CG2	2.68	0.41
11:H:125:ILE:O	11:H:127:LYS:N	2.54	0.41
13:2:167:ARG:O	13:2:171:ILE:HG12	2.21	0.41
13:2:186:ASN:CG	18:2:2016:CLA:C2A	2.89	0.41
13:2:188:LEU:HD21	13:2:197:GLY:O	2.20	0.41
16:3:209:ASN:OD1	27:3:3501:LUT:C24	2.69	0.41
16:3:223:LEU:HA	16:3:226:LYS:HG3	1.99	0.41
16:3:227:GLU:N	18:3:3001:CLA:HMB3	2.35	0.41
18:3:3005:CLA:O1D	18:3:3012:CLA:H2	2.21	0.41
16:3:80:PRO:HD2	27:3:3502:LUT:H24	2.02	0.41
15:1:85:ARG:HE	18:1:1001:CLA:CHD	2.33	0.41
18:1:1005:CLA:H3A	18:1:1005:CLA:HBA1	1.76	0.41
18:4:4005:CLA:ND	18:4:4012:CLA:H112	2.36	0.41
14:4:98:ASN:CG	18:4:4012:CLA:HMD1	2.41	0.41
18:4:4001:CLA:H71	27:4:4501:LUT:C30	2.51	0.41
1:A:127:VAL:HG22	18:B:1230:CLA:OBD	2.21	0.41
18:B:1211:CLA:CBB	18:B:1225:CLA:H162	2.51	0.41
18:B:1221:CLA:CBA	18:B:1202:CLA:H8	2.51	0.41
18:B:1235:CLA:H111	18:B:1235:CLA:H91	1.88	0.41
18:A:1237:CLA:H62	18:B:1238:CLA:H43	2.01	0.41
7:L:176:LEU:CD1	7:L:177:GLN:N	2.71	0.41
9:D:204:THR:C	9:D:206:LYS:N	2.72	0.41
2:B:507:SER:HA	2:B:510:LEU:HD21	2.02	0.41
2:B:158:GLN:HA	2:B:159:PRO:HD3	1.92	0.41
16:3:212:GLY:O	16:3:215:LYS:CB	2.68	0.41
14:4:70:LEU:HA	14:4:70:LEU:HD23	1.85	0.41
13:2:195:TYR:C	18:2:2001:CLA:HED3	2.41	0.41
13:2:219:THR:HG22	18:2:2007:CLA:HED1	1.99	0.41
18:3:3003:CLA:O2A	18:3:3003:CLA:CHA	2.69	0.41
18:1:1011:CLA:CMB	18:1:1011:CLA:HBB1	2.45	0.41
15:1:118:GLN:O	15:1:119:ALA:CB	2.69	0.41
14:4:111:LEU:HD12	18:4:4006:CLA:CBC	2.49	0.41
18:A:1117:CLA:H3A	18:A:1117:CLA:HBA2	1.65	0.41
2:B:12:ILE:HD11	2:B:23:PHE:CB	2.47	0.41
18:F:1302:CLA:HMB2	22:F:6016:BCR:C7	2.50	0.41
7:L:175:GLN:HB3	7:L:176:LEU:H	1.70	0.41
7:L:91:THR:CA	7:L:98:ARG:HH21	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:114:VAL:HG12	6:G:115:SER:N	2.36	0.41
7:L:120:LEU:O	7:L:124:GLU:CB	2.69	0.41
7:L:121:ARG:HG2	7:L:127:GLY:CA	2.48	0.41
7:L:121:ARG:HB3	7:L:122:ASN:H	1.66	0.41
13:2:254:LEU:O	13:2:257:PRO:HD3	2.21	0.41
18:A:1116:CLA:NB	18:A:1116:CLA:H43	2.36	0.41
13:2:131:ILE:CD1	13:2:133:LEU:CD2	2.85	0.41
27:2:2502:LUT:C36	27:2:2502:LUT:C28	2.94	0.41
16:3:222:GLU:O	16:3:226:LYS:HD2	2.21	0.41
18:3:3007:CLA:HBC2	18:3:3007:CLA:CMC	2.49	0.41
16:3:141:VAL:HG23	18:3:3010:CLA:CAD	2.51	0.41
28:3:3011:CHL:HMB3	22:3:3503:BCR:C16	2.51	0.41
18:1:1002:CLA:HHC	18:1:1002:CLA:CBB	2.50	0.41
18:1:1004:CLA:H91	18:1:1004:CLA:H112	1.77	0.41
23:G:2021:LMG:C6	15:1:115:PRO:HA	2.44	0.41
14:4:212:MET:HB2	18:4:4004:CLA:CMC	2.49	0.41
18:A:1124:CLA:CHB	18:A:1137:CLA:HAA2	2.51	0.41
1:A:334:HIS:O	21:A:5003:LHG:O1	2.38	0.41
18:B:1204:CLA:H11	18:B:1204:CLA:H51	1.80	0.41
18:A:1107:CLA:HAB	18:B:1230:CLA:HMD2	2.02	0.41
6:G:116:LYS:NZ	18:G:1002:CLA:NB	2.69	0.41
9:D:77:PRO:O	9:D:77:PRO:HD2	2.20	0.41
16:3:117:ILE:O	16:3:117:ILE:HG22	2.20	0.41
16:3:250:VAL:CG1	16:3:254:GLN:HG2	2.50	0.41
5:F:156:HIS:HB3	5:F:159:GLU:OE1	2.21	0.41
18:A:1112:CLA:HBA1	18:A:1112:CLA:H3A	1.77	0.41
16:3:246:LEU:CD2	16:3:246:LEU:C	2.85	0.41
10:E:103:VAL:O	10:E:105:VAL:HG23	2.21	0.41
10:E:97:PRO:C	10:E:99:THR:H	2.24	0.41
5:F:101:LYS:HE2	5:F:101:LYS:HB3	1.88	0.41
5:F:152:GLY:HA2	5:F:161:ILE:HD11	2.02	0.41
13:2:153:PHE:CD1	28:2:2010:CHL:HAC2	2.55	0.41
16:3:134:LEU:HB2	16:3:138:GLN:CG	2.49	0.41
16:3:228:VAL:O	16:3:232:ARG:HG2	2.20	0.41
18:3:3010:CLA:H61	18:3:3010:CLA:H41	1.74	0.41
18:3:3012:CLA:C1	18:3:3017:CLA:HBB2	2.50	0.41
18:3:3017:CLA:HHC	18:3:3017:CLA:CBB	2.50	0.41
18:1:1012:CLA:H3A	18:1:1012:CLA:HBA2	1.76	0.41
15:1:146:GLU:HG2	15:1:149:ARG:HD3	2.02	0.41
15:1:158:LYS:O	15:1:159:LYS:CG	2.69	0.41
15:1:215:ALA:O	15:1:218:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:126:TRP:O	27:4:4502:LUT:O3	2.36	0.41
14:4:209:ARG:NH1	18:4:4004:CLA:C2D	2.83	0.41
18:A:1106:CLA:H162	18:A:1106:CLA:H193	1.77	0.41
18:B:1221:CLA:H112	18:B:1221:CLA:H142	1.69	0.41
2:B:189:ALA:O	18:B:1211:CLA:HMC3	2.21	0.41
18:1:1005:CLA:H12	18:1:1005:CLA:CED	2.43	0.41
1:A:206:HIS:ND1	18:A:1123:CLA:OBD	2.49	0.41
18:A:1137:CLA:H41	18:A:1137:CLA:H61	1.83	0.41
18:B:1209:CLA:O1D	18:B:1210:CLA:HMC1	2.20	0.41
18:B:1218:CLA:H202	18:B:1218:CLA:H161	1.75	0.41
18:B:1221:CLA:H61	18:B:1221:CLA:H41	1.77	0.41
18:B:1223:CLA:H62	18:B:1223:CLA:H92	1.86	0.41
7:L:182:TRP:O	7:L:186:THR:HG23	2.21	0.41
7:L:104:LEU:O	22:L:6020:BCR:H14C	2.20	0.41
22:K:2011:BCR:H15C	22:K:2011:BCR:H351	1.82	0.41
8:C:9:ASP:OD1	9:D:191:SER:CB	2.69	0.41
5:F:85:CYS:SG	5:F:139:LEU:O	2.78	0.41
1:A:542:HIS:HB2	18:A:1136:CLA:HED2	2.03	0.41
18:A:1112:CLA:H192	18:A:1112:CLA:H162	1.83	0.41
2:B:292:ARG:NH2	6:G:107:ARG:NH1	2.69	0.41
18:A:1111:CLA:H62	18:A:1111:CLA:H101	1.89	0.41
15:1:204:ALA:C	15:1:206:PRO:CD	2.87	0.41
1:A:283:PHE:CZ	18:A:1116:CLA:H42	2.56	0.41
18:A:1116:CLA:H112	18:A:1116:CLA:H91	1.66	0.41
2:B:268:LEU:HG	2:B:356:PRO:O	2.21	0.41
1:A:549:ILE:O	1:A:553:VAL:HG23	2.21	0.41
7:L:173:PRO:CD	7:L:173:PRO:O	2.69	0.41
16:3:83:LEU:HD23	16:3:83:LEU:HA	1.82	0.41
13:2:125:PHE:HB2	13:2:133:LEU:HD21	2.03	0.41
18:3:3004:CLA:H2	27:3:3502:LUT:C36	2.49	0.41
18:3:3006:CLA:CHA	18:3:3018:CLA:HMB3	2.51	0.41
16:3:161:GLU:OE2	18:3:3010:CLA:CAB	2.69	0.41
15:1:85:ARG:NH2	18:1:1001:CLA:C1D	2.83	0.41
15:1:170:TYR:CE2	27:1:1501:LUT:H372	2.52	0.41
18:4:4005:CLA:HMC2	27:4:4502:LUT:H12	2.01	0.41
18:B:1023:CLA:H143	18:B:1023:CLA:H111	1.82	0.41
18:B:1236:CLA:HED2	18:B:1235:CLA:CMA	2.51	0.41
2:B:526:GLY:HA2	2:B:582:TRP:CZ3	2.56	0.41
18:G:1001:CLA:HBC2	18:G:1001:CLA:HMC1	2.02	0.41
1:A:266:ALA:HB1	1:A:270:PHE:CD1	2.56	0.41
11:H:111:LEU:HA	11:H:111:LEU:HD12	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:25:VAL:O	8:C:43:PRO:HD2	2.22	0.41
10:E:78:ARG:O	10:E:79:GLN:CB	2.69	0.41
10:E:106:ARG:HA	10:E:116:SER:O	2.21	0.41
1:A:307:ALA:O	1:A:311:LEU:HG	2.21	0.41
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.83	0.41
18:2:2005:CLA:CB	18:2:2012:CLA:HBC2	2.51	0.40
18:3:3005:CLA:H61	18:3:3005:CLA:H41	1.80	0.40
18:3:3010:CLA:CB	18:3:3010:CLA:HAA1	2.50	0.40
16:3:161:GLU:OE2	18:3:3010:CLA:HBB2	2.22	0.40
16:3:168:ALA:HB1	28:3:3011:CHL:C1B	2.51	0.40
18:3:3012:CLA:CBA	18:3:3017:CLA:HBB2	2.51	0.40
18:1:1006:CLA:O1A	18:1:1013:CLA:C2D	2.70	0.40
15:1:205:TYR:O	15:1:207:GLY:N	2.54	0.40
15:1:94:ILE:O	15:1:102:LEU:CD2	2.69	0.40
14:4:212:MET:HB3	27:4:4502:LUT:C33	2.49	0.40
14:4:152:VAL:CG1	28:4:4011:CHL:NB	2.81	0.40
27:4:4501:LUT:C17	27:4:4501:LUT:H8	2.51	0.40
21:A:7001:LHG:H101	18:A:1128:CLA:H41	2.03	0.40
18:A:1139:CLA:H62	18:A:1139:CLA:H41	1.50	0.40
20:A:5001:PQN:H141	20:A:5001:PQN:H161	1.60	0.40
1:A:451:ILE:HA	18:B:1023:CLA:CGA	2.51	0.40
18:B:1213:CLA:H51	18:B:1213:CLA:H11	1.71	0.40
18:B:1231:CLA:HBA2	18:B:1232:CLA:HMB3	2.03	0.40
7:L:59:PRO:HD3	9:D:85:GLY:O	2.21	0.40
9:D:77:PRO:O	9:D:77:PRO:CG	2.69	0.40
16:3:248:THR:CG2	16:3:250:VAL:HG23	2.39	0.40
16:3:248:THR:CG2	16:3:255:ASN:ND2	2.73	0.40
7:L:203:LEU:CD1	7:L:203:LEU:N	2.84	0.40
13:2:250:LEU:O	13:2:254:LEU:HG	2.21	0.40
7:L:207:LEU:O	7:L:208:ASP:CB	2.69	0.40
13:2:204:LEU:HD12	13:2:206:TRP:CE2	2.56	0.40
5:F:160:PHE:C	5:F:163:PRO:HD2	2.41	0.40
2:B:477:LEU:C	2:B:479:SER:H	2.25	0.40
22:F:6014:BCR:H15C	22:F:6014:BCR:H351	1.87	0.40
1:A:529:LEU:HD12	1:A:529:LEU:HA	1.86	0.40
12:K:77:MET:SD	12:K:77:MET:O	2.79	0.40
13:2:149:THR:HG21	28:2:2010:CHL:CMD	2.52	0.40
18:2:2003:CLA:O2A	18:2:2003:CLA:C1A	2.70	0.40
21:2:2801:LHG:P	21:2:2801:LHG:O2	2.79	0.40
16:3:107:ARG:CZ	16:3:227:GLU:OE1	2.69	0.40
18:4:4009:CLA:HBA2	18:4:4009:CLA:H3A	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:80:GLU:CD	15:1:189:ARG:HH21	2.23	0.40
18:4:4004:CLA:CGA	18:4:4004:CLA:C3A	2.99	0.40
2:B:330:ILE:HG22	18:B:1202:CLA:HHD	2.02	0.40
18:B:1216:CLA:C1D	18:B:1220:CLA:H43	2.50	0.40
2:B:387:PHE:HZ	18:B:1222:CLA:HAB	1.87	0.40
18:L:1502:CLA:CHD	22:L:6019:BCR:H292	2.50	0.40
18:A:1121:CLA:HAA1	12:K:83:PHE:CE2	2.56	0.40
12:K:128:VAL:HG21	22:K:2011:BCR:C31	2.51	0.40
12:K:75:THR:O	12:K:78:LEU:HB2	2.21	0.40
8:C:60:THR:CB	8:C:64:SER:HG	2.34	0.40
18:A:1112:CLA:H2	18:A:1114:CLA:HMB2	2.02	0.40
9:D:174:TYR:HB3	9:D:176:GLU:OE2	2.22	0.40
14:4:52:LYS:O	14:4:53:LYS:CB	2.69	0.40
13:2:102:ASN:OD1	18:2:2004:CLA:C1	2.70	0.40
13:2:147:THR:O	13:2:148:ASP:CB	2.69	0.40
16:3:227:GLU:HB2	18:3:3001:CLA:C2B	2.52	0.40
16:3:266:ASN:O	16:3:267:ASN:CB	2.69	0.40
16:3:102:GLU:HB2	18:3:3004:CLA:C1B	2.51	0.40
16:3:114:VAL:HG12	18:3:3006:CLA:HAC1	2.02	0.40
18:4:4009:CLA:CBB	18:4:4009:CLA:HHC	2.20	0.40
15:1:183:LYS:CE	18:1:1002:CLA:O1A	2.70	0.40
14:4:154:ILE:O	28:1:1009:CHL:CED	2.69	0.40
18:1:1013:CLA:HBA1	18:1:1013:CLA:H3A	1.80	0.40
15:1:85:ARG:CZ	15:1:184:GLU:OE1	2.70	0.40
14:4:153:GLU:OE1	18:4:4012:CLA:C4B	2.70	0.40
18:4:4002:CLA:OBD	18:4:4007:CLA:CGA	2.70	0.40
18:B:1207:CLA:CAB	3:I:14:LEU:HD21	2.51	0.40
18:B:1210:CLA:H193	18:B:1210:CLA:H161	1.80	0.40
11:H:95:LYS:O	11:H:96:ARG:CB	2.69	0.40
5:F:221:LEU:CB	5:F:222:LEU:HD23	2.50	0.40
16:3:272:LEU:HA	16:3:272:LEU:HD23	1.96	0.40
1:A:278:ALA:HA	18:A:1115:CLA:HMA2	2.02	0.40
7:L:122:ASN:O	7:L:123:THR:OG1	2.35	0.40
1:A:343:HIS:CE1	1:A:431:LEU:HD11	2.55	0.40
18:B:1215:CLA:H61	18:B:1215:CLA:H41	1.66	0.40
14:4:222:HIS:C	14:4:222:HIS:ND1	2.72	0.40
13:2:223:LYS:HB3	18:2:2007:CLA:HMD3	2.03	0.40
16:3:227:GLU:OE2	18:3:3001:CLA:C4A	2.69	0.40
15:1:218:LEU:HA	15:1:218:LEU:HD23	1.82	0.40
15:1:230:VAL:HG13	18:1:1014:CLA:C2B	2.48	0.40
15:1:66:LEU:HG	15:1:66:LEU:H	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:4505:ZEX:H27	29:4:4505:ZEX:H391	1.75	0.40
22:B:6004:BCR:H402	18:B:1218:CLA:C1D	2.50	0.40
18:B:1239:CLA:H172	7:L:144:CYS:SG	2.62	0.40
7:L:145:LEU:HB3	7:L:186:THR:HG22	2.04	0.40
12:K:123:LEU:O	12:K:127:THR:HG23	2.21	0.40
18:A:1125:CLA:HBB1	18:A:1133:CLA:HAA2	2.04	0.40
7:L:128:GLN:CB	7:L:204:LEU:CG	2.97	0.40
15:1:86:TRP:O	15:1:89:LEU:N	2.54	0.40
15:1:40:ASP:OD1	15:1:40:ASP:N	2.54	0.40
1:A:537:ALA:O	1:A:541:VAL:HG23	2.21	0.40
18:2:2002:CLA:O2D	18:2:2002:CLA:CGA	2.69	0.40
28:2:2011:CHL:HAB	28:2:2011:CHL:HMB1	1.84	0.40
13:2:246:PRO:HG2	13:2:247:ILE:N	2.36	0.40
16:3:210:PRO:HD2	27:3:3501:LUT:O23	2.21	0.40
18:3:3008:CLA:C4A	18:3:3008:CLA:O1A	2.70	0.40
18:1:1011:CLA:C2	27:1:1501:LUT:H23	2.47	0.40
15:1:218:LEU:HD22	18:1:1008:CLA:CBB	2.51	0.40
13:2:182:ILE:CG2	13:2:183:PHE:CE1	3.05	0.40
27:4:4501:LUT:H31	27:4:4501:LUT:H391	1.81	0.40
27:4:4502:LUT:H191	27:4:4502:LUT:H11	1.98	0.40
18:B:1021:CLA:H202	18:B:1021:CLA:H161	1.76	0.40
18:B:1206:CLA:CMA	18:B:1207:CLA:HBB1	2.52	0.40
22:J:6012:BCR:H15C	22:J:6012:BCR:H351	1.70	0.40
7:L:122:ASN:O	7:L:123:THR:CB	2.69	0.40
18:A:1136:CLA:H61	18:A:1136:CLA:H92	1.89	0.40
1:A:488:PHE:HB3	18:A:1135:CLA:H2	2.04	0.40
7:L:162:PRO:O	7:L:162:PRO:CG	2.70	0.40
15:1:203:SER:O	15:1:204:ALA:CB	2.69	0.40
15:1:204:ALA:O	15:1:206:PRO:CD	2.70	0.40
10:E:84:TYR:C	10:E:84:TYR:CD1	2.95	0.40
2:B:558:PRO:HB3	2:B:702:ILE:HB	2.03	0.40
4:J:26:LEU:HA	4:J:26:LEU:HD23	1.86	0.40
11:H:117:THR:OG1	11:H:118:ALA:N	2.54	0.40

All (3) 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)
5:F:96:LYS:CD	7:L:170:LYS:NZ[3_555]	1.69	0.51
5:F:96:LYS:CE	7:L:170:LYS:NZ[3_555]	1.86	0.34
5:F:96:LYS:CG	7:L:170:LYS:NZ[3_555]	1.99	0.21

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	A	740/758 (98%)	691 (93%)	45 (6%)	4 (0%)	34	69
2	B	730/733 (100%)	695 (95%)	30 (4%)	5 (1%)	26	62
3	I	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	4	14
4	J	39/42 (93%)	34 (87%)	3 (8%)	2 (5%)	2	8
5	F	148/154 (96%)	138 (93%)	8 (5%)	2 (1%)	14	42
6	G	89/97 (92%)	76 (85%)	8 (9%)	5 (6%)	2	6
7	L	158/167 (95%)	133 (84%)	15 (10%)	10 (6%)	2	4
8	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
9	D	139/147 (95%)	116 (84%)	14 (10%)	9 (6%)	1	4
10	E	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	12	38
11	H	82/90 (91%)	65 (79%)	10 (12%)	7 (8%)	1	2
12	K	53/129 (41%)	49 (92%)	2 (4%)	2 (4%)	4	13
13	2	205/269 (76%)	184 (90%)	7 (3%)	14 (7%)	1	4
14	4	196/252 (78%)	174 (89%)	15 (8%)	7 (4%)	4	14
15	1	192/202 (95%)	168 (88%)	17 (9%)	7 (4%)	4	14
16	3	213/275 (78%)	189 (89%)	15 (7%)	9 (4%)	3	11
All	All	3153/3492 (90%)	2866 (91%)	202 (6%)	85 (3%)	6	21

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
3	I	6	SER
4	J	11	ALA
6	G	101	PHE
6	G	102	GLU
6	G	104	GLY

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Mol	Chain	Res	Type
7	L	67	GLY
7	L	125	ILE
7	L	152	SER
9	D	77	PRO
9	D	192	ILE
11	H	69	LEU
11	H	97	GLY
11	H	125	ILE
11	H	126	VAL
11	H	133	PRO
11	H	135	LEU
12	K	80	ALA
12	K	86	ALA
13	2	71	SER
13	2	131	ILE
13	2	176	CYS
13	2	178	ASN
13	2	188	LEU
13	2	193	VAL
13	2	212	GLN
14	4	154	ILE
15	1	43	PRO
15	1	155	PRO
16	3	129	PRO
16	3	206	PRO
16	3	250	VAL
16	3	267	ASN
2	B	74	PHE
5	F	112	ASP
7	L	208	ASP
9	D	205	GLY
10	E	102	PRO
13	2	148	ASP
14	4	179	ALA
15	1	219	ALA
16	3	144	PRO
1	A	198	ASP
1	A	581	CYS
2	B	559	CYS
6	G	107	ARG
6	G	148	PRO
7	L	61	ASN

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Mol	Chain	Res	Type
9	D	76	ASP
13	2	174	PRO
13	2	209	ALA
14	4	167	ASN
14	4	199	GLU
15	1	126	VAL
15	1	166	ASP
16	3	179	PRO
16	3	263	PRO
5	F	189	LYS
9	D	160	PRO
9	D	191	SER
9	D	206	LYS
13	2	185	ASN
14	4	170	PRO
14	4	178	PRO
16	3	188	LEU
7	L	158	PRO
7	L	176	LEU
9	D	159	PHE
13	2	165	GLY
16	3	120	GLU
7	L	172	GLN
14	4	127	TYR
15	1	205	TYR
7	L	162	PRO
13	2	203	PRO
2	B	257	ILE
2	B	639	VAL
7	L	56	VAL
15	1	196	VAL
2	B	492	ILE
4	J	10	VAL
13	2	173	ASN
1	A	26	PRO
9	D	172	GLY
11	H	132	PRO

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	A	603/619 (97%)	595 (99%)	8 (1%)	76	94
2	B	599/600 (100%)	587 (98%)	12 (2%)	63	90
3	I	25/26 (96%)	23 (92%)	2 (8%)	15	40
4	J	33/35 (94%)	29 (88%)	4 (12%)	6	18
5	F	123/127 (97%)	115 (94%)	8 (6%)	21	52
6	G	71/76 (93%)	65 (92%)	6 (8%)	13	36
7	L	124/133 (93%)	107 (86%)	17 (14%)	4	13
8	C	69/70 (99%)	65 (94%)	4 (6%)	25	57
9	D	120/125 (96%)	110 (92%)	10 (8%)	14	38
10	E	59/59 (100%)	57 (97%)	2 (3%)	44	78
11	H	69/74 (93%)	63 (91%)	6 (9%)	13	35
12	K	38/99 (38%)	32 (84%)	6 (16%)	3	9
13	2	166/216 (77%)	148 (89%)	18 (11%)	8	23
14	4	161/202 (80%)	145 (90%)	16 (10%)	10	28
15	1	158/167 (95%)	141 (89%)	17 (11%)	8	23
16	3	159/213 (75%)	135 (85%)	24 (15%)	3	10
All	All	2577/2841 (91%)	2417 (94%)	160 (6%)	23	54

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	A	187	HIS
1	A	204	ASN
1	A	207	LEU
1	A	339	THR
1	A	433	ASP
1	A	465	ASP
1	A	590	CYS
2	B	73	ASN
2	B	127	ILE
2	B	155	LEU
2	B	172	GLU

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Mol	Chain	Res	Type
2	B	176	ASN
2	B	220	GLN
2	B	226	LEU
2	B	444	LEU
2	B	552	ASP
2	B	568	CYS
2	B	583	MET
2	B	640	CYS
3	I	4	LEU
3	I	11	LEU
4	J	3	ASP
4	J	10	VAL
4	J	13	VAL
4	J	16	THR
5	F	82	LEU
5	F	106	LEU
5	F	108	ILE
5	F	113	SER
5	F	185	ILE
5	F	218	TYR
5	F	222	LEU
5	F	225	GLU
6	G	92	LEU
6	G	99	THR
6	G	111	TYR
6	G	123	ASP
6	G	141	THR
6	G	149	LYS
7	L	54	TYR
7	L	68	SER
7	L	121	ARG
7	L	123	THR
7	L	142	SER
7	L	146	THR
7	L	151	SER
7	L	162	PRO
7	L	163	SER
7	L	165	THR
7	L	169	ARG
7	L	172	GLN
7	L	174	ASP
7	L	176	LEU

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Mol	Chain	Res	Type
7	L	178	THR
7	L	180	ASP
7	L	204	LEU
8	C	14	CYS
8	C	26	LEU
8	C	38	GLN
8	C	48	CYS
9	D	77	PRO
9	D	79	THR
9	D	99	GLU
9	D	109	LYS
9	D	128	ASN
9	D	139	LEU
9	D	156	TYR
9	D	163	GLU
9	D	190	ARG
9	D	195	ASN
10	E	110	VAL
10	E	127	GLU
11	H	54	TYR
11	H	59	ASP
11	H	69	LEU
11	H	121	ASP
11	H	123	LEU
11	H	125	ILE
12	K	62	ILE
12	K	69	ILE
12	K	70	MET
12	K	79	PHE
12	K	88	SER
12	K	140	LEU
13	2	102	ASN
13	2	110	SER
13	2	133	LEU
13	2	134	THR
13	2	138	TYR
13	2	145	TYR
13	2	146	PHE
13	2	148	ASP
13	2	164	GLU
13	2	173	ASN
13	2	176	CYS

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Mol	Chain	Res	Type
13	2	178	ASN
13	2	188	LEU
13	2	189	THR
13	2	233	MET
13	2	238	GLN
13	2	250	LEU
13	2	254	LEU
14	4	74	ASN
14	4	103	MET
14	4	116	THR
14	4	135	PHE
14	4	140	THR
14	4	156	ARG
14	4	162	ASN
14	4	168	GLN
14	4	169	ASP
14	4	172	PHE
14	4	174	GLN
14	4	193	ASN
14	4	221	GLN
14	4	222	HIS
14	4	225	THR
14	4	234	LEU
15	1	40	ASP
15	1	43	PRO
15	1	85	ARG
15	1	88	MET
15	1	105	TRP
15	1	124	ASN
15	1	126	VAL
15	1	128	TRP
15	1	131	LEU
15	1	135	LEU
15	1	155	PRO
15	1	159	LYS
15	1	202	GLN
15	1	206	PRO
15	1	211	LEU
15	1	214	LEU
15	1	225	ASN
16	3	68	LEU
16	3	87	GLU

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Mol	Chain	Res	Type
16	3	93	ILE
16	3	100	TYR
16	3	131	GLU
16	3	132	THR
16	3	138	GLN
16	3	148	TYR
16	3	149	ASN
16	3	188	LEU
16	3	190	LEU
16	3	206	PRO
16	3	211	LEU
16	3	220	LEU
16	3	225	LEU
16	3	226	LYS
16	3	232	ARG
16	3	235	MET
16	3	236	LEU
16	3	238	ILE
16	3	244	GLN
16	3	250	VAL
16	3	253	TYR
16	3	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	204	ASN
1	A	205	HIS
1	A	222	GLN
1	A	224	HIS
1	A	234	ASN
1	A	303	HIS
1	A	325	HIS
1	A	485	GLN
1	A	615	HIS
1	A	629	ASN
1	A	631	GLN
2	B	14	GLN
2	B	44	GLN
2	B	73	ASN
2	B	95	HIS

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Mol	Chain	Res	Type
2	B	176	ASN
2	B	276	HIS
2	B	294	ASN
2	B	368	GLN
2	B	627	ASN
5	F	132	ASN
5	F	136	GLN
6	G	59	ASN
6	G	95	GLN
6	G	132	HIS
6	G	144	ASN
7	L	122	ASN
8	C	71	HIS
9	D	78	ASN
9	D	96	GLN
9	D	137	GLN
9	D	195	ASN
10	E	111	ASN
11	H	82	GLN
12	K	130	HIS
13	2	104	GLN
13	2	109	HIS
13	2	178	ASN
13	2	238	GLN
13	2	259	HIS
14	4	98	ASN
14	4	158	GLN
14	4	162	ASN
14	4	174	GLN
14	4	242	HIS
15	1	83	HIS
15	1	148	GLN
15	1	187	ASN
15	1	201	GLN
15	1	225	ASN
15	1	229	ASN
16	3	105	ASN
16	3	154	ASN
16	3	174	GLN
16	3	185	GLN
16	3	255	ASN
16	3	265	ASN

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Mol	Chain	Res	Type
16	3	266	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 209 ligands modelled in this entry, 1 is monoatomic - leaving 208 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$
18	CLA	1	1001	15	52,68,73	1.80	12 (23%)	55,107,113	2.25	12 (21%)
18	CLA	1	1002	-	38,54,73	2.21	13 (34%)	41,90,113	2.47	16 (39%)
18	CLA	1	1003	15	47,63,73	1.93	13 (27%)	49,101,113	2.45	19 (38%)
18	CLA	1	1004	15	57,73,73	1.74	13 (22%)	61,113,113	2.21	14 (22%)
18	CLA	1	1005	-	47,63,73	1.85	12 (25%)	49,101,113	2.42	15 (30%)
18	CLA	1	1006	-	42,58,73	2.00	14 (33%)	44,95,113	2.57	15 (34%)
18	CLA	1	1007	21	38,54,73	2.15	13 (34%)	41,90,113	2.52	13 (31%)
18	CLA	1	1008	-	38,54,73	2.17	12 (31%)	41,90,113	2.54	15 (36%)
28	CHL	1	1009	-	48,64,74	1.83	8 (16%)	46,102,114	1.36	5 (10%)
28	CHL	1	1010	15	39,55,74	1.93	7 (17%)	38,91,114	1.52	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	1	1011	-	42,58,73	2.02	13 (30%)	44,95,113	2.50	15 (34%)
18	CLA	1	1012	15	42,58,73	2.01	13 (30%)	44,95,113	2.45	14 (31%)
18	CLA	1	1013	-	38,54,73	2.18	13 (34%)	41,90,113	2.56	13 (31%)
18	CLA	1	1014	15	38,54,73	2.23	13 (34%)	41,90,113	2.49	12 (29%)
27	LUT	1	1501	-	42,43,43	2.58	5 (11%)	49,60,60	1.94	12 (24%)
27	LUT	1	1502	-	42,43,43	2.53	6 (14%)	49,60,60	2.12	16 (32%)
21	LHG	1	1801	18	48,48,48	0.89	2 (4%)	49,54,54	1.21	3 (6%)
18	CLA	2	2001	13	52,68,73	1.79	14 (26%)	55,107,113	2.40	20 (36%)
18	CLA	2	2002	-	38,54,73	2.12	13 (34%)	41,90,113	2.39	14 (34%)
18	CLA	2	2003	-	47,63,73	1.92	13 (27%)	49,101,113	2.41	15 (30%)
18	CLA	2	2004	13	57,73,73	1.78	12 (21%)	61,113,113	2.20	13 (21%)
18	CLA	2	2005	-	47,63,73	1.99	12 (25%)	49,101,113	2.21	12 (24%)
18	CLA	2	2006	-	47,63,73	1.98	12 (25%)	49,101,113	2.35	14 (28%)
18	CLA	2	2007	-	52,68,73	1.88	12 (23%)	55,107,113	2.19	13 (23%)
18	CLA	2	2008	-	42,58,73	1.99	12 (28%)	44,95,113	2.73	18 (40%)
18	CLA	2	2009	13	42,58,73	2.01	13 (30%)	44,95,113	2.46	14 (31%)
28	CHL	2	2010	-	39,55,74	2.24	10 (25%)	38,91,114	1.66	6 (15%)
28	CHL	2	2011	-	40,56,74	2.26	11 (27%)	39,92,114	1.65	4 (10%)
18	CLA	2	2012	13	47,63,73	1.82	13 (27%)	49,101,113	2.38	15 (30%)
28	CHL	2	2013	-	35,54,74	1.87	5 (14%)	34,90,114	1.60	4 (11%)
18	CLA	2	2016	13	42,58,73	2.12	12 (28%)	44,95,113	2.99	17 (38%)
18	CLA	2	2019	-	20,35,73	2.80	9 (45%)	25,60,113	3.01	12 (48%)
27	LUT	2	2501	-	42,43,43	2.45	5 (11%)	49,60,60	2.07	15 (30%)
27	LUT	2	2502	-	42,43,43	2.53	5 (11%)	49,60,60	1.98	13 (26%)
21	LHG	2	2801	-	23,23,48	1.29	2 (8%)	24,29,54	1.17	3 (12%)
23	LMG	2	2802	-	35,35,55	1.06	2 (5%)	43,43,63	1.38	7 (16%)
18	CLA	3	3001	16	42,58,73	2.05	13 (30%)	44,95,113	2.33	11 (25%)
18	CLA	3	3002	-	38,54,73	2.14	12 (31%)	41,90,113	2.68	18 (43%)
18	CLA	3	3003	16	52,68,73	1.79	13 (25%)	55,107,113	2.37	13 (23%)
18	CLA	3	3004	16	52,68,73	1.81	13 (25%)	55,107,113	2.35	13 (23%)
18	CLA	3	3005	-	47,63,73	1.85	12 (25%)	49,101,113	2.56	14 (28%)
18	CLA	3	3006	-	42,58,73	2.01	13 (30%)	44,95,113	2.69	16 (36%)
18	CLA	3	3007	-	42,58,73	2.06	13 (30%)	44,95,113	2.48	17 (38%)
18	CLA	3	3008	-	40,56,73	2.10	11 (27%)	42,92,113	2.93	18 (42%)
18	CLA	3	3010	-	52,68,73	1.79	13 (25%)	55,107,113	2.34	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CHL	3	3011	-	48,64,74	2.09	11 (22%)	46,102,114	1.48	4 (8%)
18	CLA	3	3012	16	42,58,73	2.03	13 (30%)	44,95,113	2.51	14 (31%)
18	CLA	3	3013	-	38,54,73	2.21	12 (31%)	41,90,113	2.26	11 (26%)
18	CLA	3	3017	-	38,54,73	2.17	13 (34%)	41,90,113	2.32	14 (34%)
18	CLA	3	3018	16	42,58,73	2.02	13 (30%)	44,95,113	2.55	17 (38%)
18	CLA	3	3019	-	20,35,73	3.01	11 (55%)	25,60,113	2.95	13 (52%)
27	LUT	3	3501	-	42,43,43	2.37	4 (9%)	49,60,60	2.20	16 (32%)
27	LUT	3	3502	-	42,43,43	2.44	4 (9%)	49,60,60	2.22	17 (34%)
22	BCR	3	3503	-	41,41,41	3.04	9 (21%)	56,56,56	6.32	32 (57%)
18	CLA	4	4001	14	52,68,73	1.77	13 (25%)	55,107,113	2.28	18 (32%)
18	CLA	4	4002	-	42,58,73	1.98	13 (30%)	44,95,113	2.64	16 (36%)
18	CLA	4	4003	14	57,73,73	1.75	13 (22%)	61,113,113	2.13	16 (26%)
18	CLA	4	4004	14	52,68,73	1.78	12 (23%)	55,107,113	2.28	13 (23%)
18	CLA	4	4005	14	52,68,73	1.73	12 (23%)	55,107,113	2.54	19 (34%)
18	CLA	4	4006	-	42,58,73	1.98	13 (30%)	44,95,113	2.41	17 (38%)
18	CLA	4	4007	-	52,68,73	1.78	13 (25%)	55,107,113	2.35	13 (23%)
18	CLA	4	4008	-	38,54,73	2.03	12 (31%)	41,90,113	2.76	15 (36%)
18	CLA	4	4009	14	42,58,73	1.93	13 (30%)	44,95,113	2.46	12 (27%)
28	CHL	4	4010	-	39,55,74	2.32	11 (28%)	38,91,114	1.84	8 (21%)
28	CHL	4	4011	-	43,59,74	2.11	11 (25%)	41,96,114	1.65	5 (12%)
18	CLA	4	4012	14	57,73,73	1.65	12 (21%)	61,113,113	2.14	14 (22%)
28	CHL	4	4013	-	39,55,74	2.27	10 (25%)	38,91,114	1.80	4 (10%)
18	CLA	4	4016	-	38,54,73	2.29	12 (31%)	41,90,113	2.37	16 (39%)
18	CLA	4	4017	-	57,73,73	1.70	12 (21%)	61,113,113	2.15	15 (24%)
27	LUT	4	4501	-	42,43,43	2.47	6 (14%)	49,60,60	2.13	14 (28%)
27	LUT	4	4502	-	42,43,43	2.41	5 (11%)	49,60,60	2.03	14 (28%)
27	LUT	4	4503	-	42,43,43	2.48	5 (11%)	49,60,60	2.27	11 (22%)
29	ZEX	4	4505	-	41,43,43	1.08	3 (7%)	51,60,60	2.04	17 (33%)
23	LMG	4	4801	-	35,35,55	1.01	2 (5%)	43,43,63	1.65	9 (20%)
17	CL0	A	1011	-	57,73,73	1.84	13 (22%)	61,113,113	2.16	12 (19%)
18	CLA	A	1013	-	57,73,73	1.87	12 (21%)	61,113,113	2.01	14 (22%)
18	CLA	A	1022	-	57,73,73	1.83	12 (21%)	61,113,113	2.19	14 (22%)
18	CLA	A	1101	-	57,73,73	1.86	12 (21%)	61,113,113	2.17	14 (22%)
18	CLA	A	1102	-	42,58,73	2.18	12 (28%)	44,95,113	2.40	14 (31%)
18	CLA	A	1103	-	57,73,73	1.84	12 (21%)	61,113,113	2.11	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1104	-	57,73,73	1.86	13 (22%)	61,113,113	2.06	12 (19%)
18	CLA	A	1105	-	43,59,73	2.15	13 (30%)	43,96,113	2.31	12 (27%)
18	CLA	A	1106	1	57,73,73	1.89	13 (22%)	61,113,113	2.21	14 (22%)
18	CLA	A	1107	1	57,73,73	1.87	12 (21%)	61,113,113	2.10	13 (21%)
18	CLA	A	1108	-	38,54,73	2.40	13 (34%)	41,90,113	2.40	13 (31%)
18	CLA	A	1109	-	57,73,73	1.85	12 (21%)	61,113,113	2.02	11 (18%)
18	CLA	A	1110	-	47,63,73	2.07	13 (27%)	49,101,113	2.24	13 (26%)
18	CLA	A	1111	-	52,68,73	1.93	12 (23%)	55,107,113	2.20	15 (27%)
18	CLA	A	1112	-	57,73,73	1.82	12 (21%)	61,113,113	2.20	13 (21%)
18	CLA	A	1113	-	38,54,73	2.35	12 (31%)	41,90,113	2.42	15 (36%)
18	CLA	A	1114	-	38,54,73	2.35	12 (31%)	41,90,113	2.48	11 (26%)
18	CLA	A	1115	-	38,54,73	2.37	13 (34%)	41,90,113	2.36	12 (29%)
18	CLA	A	1116	-	52,68,73	1.94	12 (23%)	55,107,113	2.24	14 (25%)
18	CLA	A	1117	-	57,73,73	1.86	12 (21%)	61,113,113	2.08	14 (22%)
18	CLA	A	1118	-	38,54,73	2.36	11 (28%)	41,90,113	2.53	13 (31%)
18	CLA	A	1119	-	57,73,73	1.83	12 (21%)	61,113,113	2.13	13 (21%)
18	CLA	A	1120	-	52,68,73	1.94	12 (23%)	55,107,113	2.18	14 (25%)
18	CLA	A	1121	-	47,63,73	2.05	13 (27%)	49,101,113	2.38	15 (30%)
18	CLA	A	1122	-	57,73,73	1.85	12 (21%)	61,113,113	2.10	13 (21%)
18	CLA	A	1123	-	57,73,73	1.88	13 (22%)	61,113,113	2.21	15 (24%)
18	CLA	A	1124	-	47,63,73	2.05	13 (27%)	49,101,113	2.39	14 (28%)
18	CLA	A	1125	-	52,68,73	1.90	12 (23%)	55,107,113	2.22	15 (27%)
18	CLA	A	1126	-	57,73,73	1.85	13 (22%)	61,113,113	2.14	17 (27%)
18	CLA	A	1127	-	57,73,73	1.87	12 (21%)	61,113,113	2.14	13 (21%)
18	CLA	A	1128	-	57,73,73	1.85	12 (21%)	61,113,113	2.26	14 (22%)
18	CLA	A	1129	-	42,58,73	2.16	12 (28%)	44,95,113	2.47	15 (34%)
18	CLA	A	1130	-	42,58,73	2.21	13 (30%)	44,95,113	2.43	13 (29%)
18	CLA	A	1131	-	57,73,73	1.86	12 (21%)	61,113,113	2.10	13 (21%)
18	CLA	A	1132	-	57,73,73	1.86	13 (22%)	61,113,113	2.22	13 (21%)
18	CLA	A	1133	-	47,63,73	2.04	13 (27%)	49,101,113	2.42	14 (28%)
18	CLA	A	1134	-	47,63,73	2.05	12 (25%)	49,101,113	2.36	14 (28%)
18	CLA	A	1135	-	43,59,73	2.13	12 (27%)	43,96,113	2.50	13 (30%)
18	CLA	A	1136	-	48,64,73	2.03	13 (27%)	49,102,113	2.33	14 (28%)
18	CLA	A	1137	-	47,63,73	2.06	13 (27%)	49,101,113	2.30	14 (28%)
18	CLA	A	1138	-	57,73,73	1.90	12 (21%)	61,113,113	1.99	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1139	-	57,73,73	1.86	13 (22%)	61,113,113	2.10	14 (22%)
18	CLA	A	1140	-	57,73,73	1.88	13 (22%)	61,113,113	2.01	14 (22%)
18	CLA	A	1151	21	42,58,73	2.22	13 (30%)	44,95,113	2.51	13 (29%)
18	CLA	A	1237	-	52,68,73	1.94	12 (23%)	55,107,113	2.22	15 (27%)
19	SF4	A	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
20	PQN	A	5001	-	34,34,34	1.42	2 (5%)	45,45,45	1.16	2 (4%)
21	LHG	A	5003	18	39,39,48	1.02	2 (5%)	40,45,54	1.21	4 (10%)
22	BCR	A	6002	-	41,41,41	2.82	7 (17%)	56,56,56	6.34	23 (41%)
22	BCR	A	6003	-	41,41,41	2.87	6 (14%)	56,56,56	6.37	20 (35%)
22	BCR	A	6007	-	41,41,41	2.84	7 (17%)	56,56,56	6.41	22 (39%)
22	BCR	A	6008	-	41,41,41	2.92	6 (14%)	56,56,56	6.46	26 (46%)
22	BCR	A	6011	-	41,41,41	2.97	6 (14%)	56,56,56	6.62	28 (50%)
22	BCR	A	6017	-	41,41,41	2.75	6 (14%)	56,56,56	7.01	28 (50%)
21	LHG	A	7001	-	48,48,48	0.94	2 (4%)	49,54,54	1.15	4 (8%)
18	CLA	B	1012	-	57,73,73	1.83	12 (21%)	61,113,113	2.25	17 (27%)
18	CLA	B	1021	-	57,73,73	1.87	11 (19%)	61,113,113	2.12	17 (27%)
18	CLA	B	1023	-	57,73,73	1.86	12 (21%)	61,113,113	2.08	17 (27%)
18	CLA	B	1201	-	42,58,73	2.17	13 (30%)	44,95,113	2.32	14 (31%)
18	CLA	B	1202	-	57,73,73	1.87	12 (21%)	61,113,113	2.11	14 (22%)
18	CLA	B	1203	2	57,73,73	1.82	12 (21%)	61,113,113	2.09	13 (21%)
18	CLA	B	1204	-	47,63,73	2.08	12 (25%)	49,101,113	2.22	12 (24%)
18	CLA	B	1205	-	57,73,73	1.84	12 (21%)	61,113,113	2.03	14 (22%)
18	CLA	B	1206	2	57,73,73	1.87	12 (21%)	61,113,113	2.21	15 (24%)
18	CLA	B	1207	-	57,73,73	1.86	13 (22%)	61,113,113	2.07	15 (24%)
18	CLA	B	1208	-	47,63,73	2.08	13 (27%)	49,101,113	2.31	13 (26%)
18	CLA	B	1209	-	38,54,73	2.40	12 (31%)	41,90,113	2.47	12 (29%)
18	CLA	B	1210	-	57,73,73	1.83	12 (21%)	61,113,113	2.07	13 (21%)
18	CLA	B	1211	-	57,73,73	1.85	12 (21%)	61,113,113	2.12	14 (22%)
18	CLA	B	1212	-	47,63,73	2.06	13 (27%)	49,101,113	2.36	14 (28%)
18	CLA	B	1213	-	52,68,73	1.96	11 (21%)	55,107,113	2.11	12 (21%)
18	CLA	B	1214	-	51,67,73	1.96	12 (23%)	53,105,113	2.27	15 (28%)
18	CLA	B	1215	-	52,68,73	1.97	13 (25%)	55,107,113	2.21	14 (25%)
18	CLA	B	1216	-	57,73,73	1.83	13 (22%)	61,113,113	2.16	13 (21%)
18	CLA	B	1217	-	38,54,73	2.36	13 (34%)	41,90,113	2.44	12 (29%)
18	CLA	B	1218	-	57,73,73	1.86	13 (22%)	61,113,113	2.23	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1219	-	52,68,73	1.96	13 (25%)	55,107,113	2.19	13 (23%)
18	CLA	B	1220	-	57,73,73	1.84	13 (22%)	61,113,113	2.03	16 (26%)
18	CLA	B	1221	-	57,73,73	1.85	12 (21%)	61,113,113	2.23	16 (26%)
18	CLA	B	1222	-	57,73,73	1.86	12 (21%)	61,113,113	2.12	15 (24%)
18	CLA	B	1223	-	57,73,73	1.81	11 (19%)	61,113,113	2.20	14 (22%)
18	CLA	B	1224	-	57,73,73	1.83	12 (21%)	61,113,113	2.20	16 (26%)
18	CLA	B	1225	-	57,73,73	1.88	12 (21%)	61,113,113	2.13	13 (21%)
18	CLA	B	1226	-	57,73,73	1.79	12 (21%)	61,113,113	2.20	14 (22%)
18	CLA	B	1227	-	57,73,73	1.85	13 (22%)	61,113,113	2.14	14 (22%)
18	CLA	B	1228	-	52,68,73	1.96	11 (21%)	55,107,113	2.10	14 (25%)
18	CLA	B	1229	-	57,73,73	1.87	12 (21%)	61,113,113	2.18	15 (24%)
18	CLA	B	1230	-	50,66,73	1.99	11 (22%)	52,104,113	2.46	15 (28%)
18	CLA	B	1231	-	52,68,73	1.97	13 (25%)	55,107,113	2.09	12 (21%)
18	CLA	B	1232	-	47,63,73	2.04	13 (27%)	49,101,113	2.23	12 (24%)
18	CLA	B	1234	-	52,68,73	1.98	13 (25%)	55,107,113	2.22	15 (27%)
18	CLA	B	1235	-	57,73,73	1.86	12 (21%)	61,113,113	2.15	14 (22%)
18	CLA	B	1236	-	47,63,73	2.05	12 (25%)	49,101,113	2.32	14 (28%)
18	CLA	B	1238	-	57,73,73	1.87	12 (21%)	61,113,113	2.13	12 (19%)
18	CLA	B	1239	-	57,73,73	1.86	13 (22%)	61,113,113	2.11	13 (21%)
18	CLA	B	1240	21	57,73,73	1.84	11 (19%)	61,113,113	2.14	15 (24%)
20	PQN	B	5002	-	34,34,34	1.49	2 (5%)	45,45,45	1.04	1 (2%)
21	LHG	B	5004	18	20,20,48	1.32	2 (10%)	21,26,54	1.56	3 (14%)
23	LMG	B	5005	-	38,38,55	1.05	2 (5%)	46,46,63	1.07	3 (6%)
22	BCR	B	6004	-	41,41,41	2.86	6 (14%)	56,56,56	6.58	29 (51%)
22	BCR	B	6005	-	41,41,41	2.79	6 (14%)	56,56,56	6.70	24 (42%)
22	BCR	B	6006	-	41,41,41	2.87	6 (14%)	56,56,56	6.74	27 (48%)
22	BCR	B	6009	-	41,41,41	2.89	6 (14%)	56,56,56	6.29	21 (37%)
22	BCR	B	6010	-	41,41,41	2.81	6 (14%)	56,56,56	6.45	23 (41%)
25	DGD	B	7101	-	62,62,67	0.89	1 (1%)	76,76,81	1.34	11 (14%)
26	LMU	B	8001	-	36,36,36	0.48	0	47,47,47	1.18	4 (8%)
26	LMU	B	8002	-	36,36,36	0.44	0	47,47,47	1.05	3 (6%)
19	SF4	C	3002	8	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	C	3003	8	0,12,12	0.00	-	0,24,24	0.00	-
18	CLA	F	1301	-	34,53,73	2.17	11 (32%)	37,89,113	2.35	9 (24%)
18	CLA	F	1302	5	42,58,73	2.10	12 (28%)	44,95,113	2.50	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMG	F	5001	-	23,23,55	1.22	2 (8%)	31,31,63	1.69	6 (19%)
23	LMG	F	5002	-	37,37,55	1.04	2 (5%)	45,45,63	1.27	5 (11%)
22	BCR	F	6014	-	41,41,41	3.12	7 (17%)	56,56,56	6.58	23 (41%)
22	BCR	F	6016	-	41,41,41	3.15	9 (21%)	56,56,56	6.59	25 (44%)
18	CLA	G	1001	-	47,63,73	1.89	13 (27%)	49,101,113	2.64	16 (32%)
18	CLA	G	1002	-	38,54,73	2.21	12 (31%)	41,90,113	2.66	13 (31%)
18	CLA	G	1003	-	52,68,73	1.82	12 (23%)	55,107,113	2.24	15 (27%)
22	BCR	G	2011	-	41,41,41	3.13	7 (17%)	56,56,56	6.64	29 (51%)
23	LMG	G	2021	-	41,41,55	0.93	2 (4%)	49,49,63	1.17	5 (10%)
18	CLA	H	1000	11	38,54,73	2.35	12 (31%)	41,90,113	2.46	13 (31%)
27	LUT	I	6018	-	42,43,43	2.50	4 (9%)	49,60,60	2.13	17 (34%)
22	BCR	I	6020	-	41,41,41	2.85	7 (17%)	56,56,56	6.55	21 (37%)
18	CLA	J	1302	4	42,58,73	2.17	13 (30%)	44,95,113	2.57	16 (36%)
23	LMG	J	5001	-	55,55,55	0.86	2 (3%)	63,63,63	1.43	6 (9%)
22	BCR	J	6012	-	41,41,41	2.99	8 (19%)	56,56,56	6.47	29 (51%)
22	BCR	J	6013	-	41,41,41	2.97	8 (19%)	56,56,56	6.46	29 (51%)
18	CLA	K	1001	-	38,54,73	2.22	13 (34%)	41,90,113	2.63	14 (34%)
22	BCR	K	2011	-	41,41,41	2.79	6 (14%)	56,56,56	6.64	29 (51%)
18	CLA	L	1501	7	42,58,73	2.00	13 (30%)	44,95,113	2.58	18 (40%)
18	CLA	L	1502	-	52,68,73	1.84	13 (25%)	55,107,113	2.26	14 (25%)
18	CLA	L	1503	-	42,58,73	2.04	13 (30%)	44,95,113	2.50	15 (34%)
22	BCR	L	6019	-	41,41,41	3.01	8 (19%)	56,56,56	6.44	24 (42%)
22	BCR	L	6020	-	41,41,41	2.91	7 (17%)	56,56,56	6.44	29 (51%)

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
18	CLA	1	1001	15	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	1	1002	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	1	1003	15	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	1	1004	15	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	1	1005	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	1	1006	-	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	1007	21	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	1	1008	-	3/3/16/25	0/15/113/135	0/0/9/9
28	CHL	1	1009	-	-	0/27/125/137	0/0/9/9
28	CHL	1	1010	15	-	0/17/115/137	0/0/9/9
18	CLA	1	1011	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	1	1012	15	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	1	1013	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	1	1014	15	3/3/16/25	0/15/113/135	0/0/9/9
27	LUT	1	1501	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	1	1502	-	1/1/12/27	0/29/67/67	0/2/2/2
21	LHG	1	1801	18	-	2/53/53/53	0/0/0/0
18	CLA	2	2001	13	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	2	2002	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	2	2003	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	2	2004	13	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	2	2005	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	2	2006	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	2	2007	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	2	2008	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	2	2009	13	3/3/17/25	0/19/117/135	0/0/9/9
28	CHL	2	2010	-	-	0/17/115/137	0/0/9/9
28	CHL	2	2011	-	-	0/18/116/137	0/0/9/9
18	CLA	2	2012	13	3/3/18/25	0/25/123/135	0/0/9/9
28	CHL	2	2013	-	-	0/13/113/137	0/0/9/9
18	CLA	2	2016	13	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	2	2019	-	3/3/8/25	0/0/75/135	0/0/9/9
27	LUT	2	2501	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	2	2502	-	1/1/12/27	0/29/67/67	0/2/2/2
21	LHG	2	2801	-	-	0/28/28/53	0/0/0/0
23	LMG	2	2802	-	-	0/30/50/70	0/1/1/1
18	CLA	3	3001	16	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3002	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	3	3003	16	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	3	3004	16	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	3	3005	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	3	3006	-	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	3007	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3008	-	3/3/16/25	0/17/115/135	0/0/9/9
18	CLA	3	3010	-	3/3/19/25	0/31/129/135	0/0/9/9
28	CHL	3	3011	-	-	0/27/125/137	0/0/9/9
18	CLA	3	3012	16	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3013	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	3	3017	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	3	3018	16	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3019	-	3/3/8/25	0/0/75/135	0/0/9/9
27	LUT	3	3501	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	3	3502	-	1/1/12/27	1/29/67/67	0/2/2/2
22	BCR	3	3503	-	-	0/29/63/63	0/2/2/2
18	CLA	4	4001	14	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	4	4002	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	4	4003	14	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	4	4004	14	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	4	4005	14	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	4	4006	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	4	4007	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	4	4008	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	4	4009	14	3/3/17/25	0/19/117/135	0/0/9/9
28	CHL	4	4010	-	-	0/17/115/137	0/0/9/9
28	CHL	4	4011	-	-	0/21/119/137	0/0/9/9
18	CLA	4	4012	14	3/3/20/25	0/37/135/135	0/0/9/9
28	CHL	4	4013	-	-	0/17/115/137	0/0/9/9
18	CLA	4	4016	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	4	4017	-	3/3/20/25	0/37/135/135	0/0/9/9
27	LUT	4	4501	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	4	4502	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	4	4503	-	1/1/12/27	0/29/67/67	0/2/2/2
29	ZEX	4	4505	-	-	0/29/67/67	0/2/2/2
23	LMG	4	4801	-	-	1/30/50/70	0/1/1/1
17	CL0	A	1011	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1013	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1022	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1101	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1102	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	A	1103	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1104	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1105	-	3/3/17/25	0/21/119/135	0/0/9/9
18	CLA	A	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1107	1	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1108	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1109	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1110	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1111	-	2/2/19/25	0/31/129/135	0/0/9/9
18	CLA	A	1112	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1113	-	2/2/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1114	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1115	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1116	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	A	1117	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1118	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1120	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	A	1121	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1122	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1125	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	A	1126	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1129	-	2/2/17/25	0/19/117/135	0/0/9/9
18	CLA	A	1130	-	2/2/17/25	0/19/117/135	0/0/9/9
18	CLA	A	1131	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1133	-	2/2/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1134	-	2/2/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1135	-	2/2/17/25	0/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1136	-	3/3/18/25	0/27/125/135	0/0/9/9
18	CLA	A	1137	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1138	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1139	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1151	21	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	A	1237	-	3/3/19/25	0/31/129/135	0/0/9/9
19	SF4	A	3001	1,2	-	0/0/48/48	0/6/5/5
20	PQN	A	5001	-	-	0/23/43/43	0/2/2/2
21	LHG	A	5003	18	-	0/44/44/53	0/0/0/0
22	BCR	A	6002	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6003	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6007	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6008	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6011	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6017	-	-	0/29/63/63	0/2/2/2
21	LHG	A	7001	-	-	0/53/53/53	0/0/0/0
18	CLA	B	1012	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1023	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1201	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	B	1202	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1203	2	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1204	-	2/2/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1205	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1206	2	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1207	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1208	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1209	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	B	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1211	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1212	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1213	-	2/2/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1214	-	3/3/18/25	0/30/128/135	0/0/9/9
18	CLA	B	1215	-	2/2/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1216	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1217	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	B	1218	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1219	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1220	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1221	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1222	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1223	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1224	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1227	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1228	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1229	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1230	-	3/3/18/25	0/29/127/135	0/0/9/9
18	CLA	B	1231	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1232	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1234	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1235	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1236	-	2/2/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1238	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1239	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1240	21	2/2/20/25	0/37/135/135	0/0/9/9
20	PQN	B	5002	-	-	0/23/43/43	0/2/2/2
21	LHG	B	5004	18	-	0/23/23/53	0/0/0/0
23	LMG	B	5005	-	-	0/33/53/70	0/1/1/1
22	BCR	B	6004	-	-	0/29/63/63	0/2/2/2
22	BCR	B	6005	-	-	0/29/63/63	0/2/2/2
22	BCR	B	6006	-	-	0/29/63/63	0/2/2/2
22	BCR	B	6009	-	-	0/29/63/63	0/2/2/2
22	BCR	B	6010	-	-	0/29/63/63	0/2/2/2
25	DGD	B	7101	-	-	0/50/90/95	0/2/2/2
26	LMU	B	8001	-	-	0/21/61/61	0/2/2/2
26	LMU	B	8002	-	-	0/21/61/61	0/2/2/2
19	SF4	C	3002	8	-	0/0/48/48	0/6/5/5
19	SF4	C	3003	8	-	0/0/48/48	0/6/5/5
18	CLA	F	1301	-	3/3/16/25	0/11/111/135	0/0/9/9
18	CLA	F	1302	5	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMG	F	5001	-	-	0/16/36/70	0/1/1/1
23	LMG	F	5002	-	-	0/32/52/70	0/1/1/1
22	BCR	F	6014	-	-	0/29/63/63	0/2/2/2
22	BCR	F	6016	-	-	0/29/63/63	0/2/2/2
18	CLA	G	1001	-	3/3/18/25	1/25/123/135	0/0/9/9
18	CLA	G	1002	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	G	1003	-	3/3/19/25	0/31/129/135	0/0/9/9
22	BCR	G	2011	-	-	0/29/63/63	0/2/2/2
23	LMG	G	2021	-	-	0/36/56/70	0/1/1/1
18	CLA	H	1000	11	3/3/16/25	0/15/113/135	0/0/9/9
27	LUT	I	6018	-	1/1/12/27	0/29/67/67	0/2/2/2
22	BCR	I	6020	-	-	0/29/63/63	0/2/2/2
18	CLA	J	1302	4	3/3/17/25	0/19/117/135	0/0/9/9
23	LMG	J	5001	-	-	0/50/70/70	0/1/1/1
22	BCR	J	6012	-	-	0/29/63/63	0/2/2/2
22	BCR	J	6013	-	-	0/29/63/63	0/2/2/2
18	CLA	K	1001	-	3/3/16/25	0/15/113/135	0/0/9/9
22	BCR	K	2011	-	-	0/29/63/63	0/2/2/2
18	CLA	L	1501	7	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	L	1502	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	L	1503	-	3/3/17/25	0/19/117/135	0/0/9/9
22	BCR	L	6019	-	-	0/29/63/63	0/2/2/2
22	BCR	L	6020	-	-	0/29/63/63	0/2/2/2

All (2131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	2011	BCR	C11-C10	-9.27	1.16	1.43
22	F	6016	BCR	C11-C10	-9.02	1.17	1.43
22	F	6014	BCR	C11-C10	-8.85	1.17	1.43
22	A	6011	BCR	C11-C10	-8.79	1.17	1.43
22	A	6008	BCR	C11-C10	-8.72	1.18	1.43
22	L	6019	BCR	C11-C10	-8.64	1.18	1.43
22	3	3503	BCR	C11-C10	-8.61	1.18	1.43
22	G	2011	BCR	C10-C9	-8.60	1.24	1.35
22	J	6012	BCR	C11-C10	-8.57	1.18	1.43
22	J	6013	BCR	C11-C10	-8.55	1.18	1.43
22	A	6003	BCR	C11-C10	-8.53	1.18	1.43
22	B	6009	BCR	C11-C10	-8.50	1.18	1.43
22	B	6006	BCR	C11-C10	-8.47	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	6020	BCR	C11-C10	-8.45	1.18	1.43
22	A	6007	BCR	C11-C10	-8.42	1.19	1.43
22	B	6004	BCR	C11-C10	-8.42	1.19	1.43
22	A	6002	BCR	C11-C10	-8.37	1.19	1.43
22	F	6014	BCR	C10-C9	-8.34	1.24	1.35
22	B	6005	BCR	C11-C10	-8.31	1.19	1.43
22	B	6010	BCR	C11-C10	-8.31	1.19	1.43
22	F	6016	BCR	C16-C17	-8.31	1.19	1.43
22	F	6016	BCR	C10-C9	-8.30	1.24	1.35
22	A	6017	BCR	C11-C10	-8.29	1.19	1.43
22	K	2011	BCR	C11-C10	-8.26	1.19	1.43
22	L	6020	BCR	C11-C10	-8.23	1.19	1.43
22	A	6011	BCR	C8-C9	-8.22	1.27	1.45
22	G	2011	BCR	C8-C9	-8.11	1.28	1.45
22	B	6006	BCR	C8-C9	-8.11	1.28	1.45
22	G	2011	BCR	C20-C21	-8.08	1.20	1.43
22	A	6003	BCR	C8-C9	-8.08	1.28	1.45
22	J	6012	BCR	C20-C21	-8.05	1.20	1.43
22	3	3503	BCR	C10-C9	-8.05	1.24	1.35
22	F	6014	BCR	C8-C9	-8.05	1.28	1.45
22	3	3503	BCR	C16-C17	-8.04	1.20	1.43
22	A	6008	BCR	C8-C9	-8.04	1.28	1.45
22	A	6011	BCR	C20-C21	-8.03	1.20	1.43
22	B	6004	BCR	C8-C9	-8.01	1.28	1.45
22	F	6016	BCR	C8-C9	-8.00	1.28	1.45
22	3	3503	BCR	C20-C21	-7.99	1.20	1.43
22	L	6019	BCR	C8-C9	-7.98	1.28	1.45
22	B	6009	BCR	C8-C9	-7.97	1.28	1.45
22	L	6019	BCR	C10-C9	-7.97	1.25	1.35
22	F	6014	BCR	C16-C17	-7.95	1.20	1.43
22	B	6010	BCR	C8-C9	-7.94	1.28	1.45
22	B	6010	BCR	C20-C21	-7.93	1.20	1.43
22	A	6011	BCR	C16-C17	-7.93	1.20	1.43
22	F	6016	BCR	C20-C21	-7.90	1.20	1.43
22	I	6020	BCR	C20-C21	-7.90	1.20	1.43
22	A	6008	BCR	C16-C17	-7.86	1.20	1.43
22	L	6020	BCR	C20-C21	-7.85	1.20	1.43
22	A	6007	BCR	C8-C9	-7.85	1.28	1.45
22	G	2011	BCR	C16-C17	-7.85	1.20	1.43
22	B	6006	BCR	C20-C21	-7.84	1.20	1.43
22	L	6019	BCR	C20-C21	-7.84	1.20	1.43
22	B	6004	BCR	C20-C21	-7.84	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	6020	BCR	C8-C9	-7.83	1.28	1.45
22	J	6012	BCR	C8-C9	-7.82	1.28	1.45
22	A	6008	BCR	C20-C21	-7.82	1.20	1.43
22	3	3503	BCR	C8-C9	-7.82	1.28	1.45
22	K	2011	BCR	C8-C9	-7.81	1.28	1.45
22	I	6020	BCR	C8-C9	-7.81	1.28	1.45
22	F	6014	BCR	C20-C21	-7.80	1.20	1.43
22	A	6002	BCR	C8-C9	-7.79	1.28	1.45
22	B	6005	BCR	C8-C9	-7.78	1.28	1.45
22	J	6013	BCR	C16-C17	-7.78	1.20	1.43
22	J	6013	BCR	C20-C21	-7.77	1.20	1.43
22	B	6009	BCR	C16-C17	-7.77	1.20	1.43
22	B	6009	BCR	C20-C21	-7.77	1.20	1.43
22	L	6020	BCR	C16-C17	-7.76	1.20	1.43
22	A	6003	BCR	C20-C21	-7.75	1.20	1.43
22	A	6007	BCR	C20-C21	-7.73	1.21	1.43
22	B	6004	BCR	C16-C17	-7.72	1.21	1.43
22	A	6002	BCR	C20-C21	-7.72	1.21	1.43
22	J	6013	BCR	C8-C9	-7.71	1.28	1.45
22	B	6006	BCR	C16-C17	-7.71	1.21	1.43
22	I	6020	BCR	C16-C17	-7.70	1.21	1.43
22	A	6011	BCR	C10-C9	-7.68	1.25	1.35
22	B	6005	BCR	C20-C21	-7.67	1.21	1.43
22	K	2011	BCR	C20-C21	-7.67	1.21	1.43
22	A	6017	BCR	C20-C21	-7.66	1.21	1.43
22	A	6003	BCR	C16-C17	-7.65	1.21	1.43
22	L	6019	BCR	C16-C17	-7.64	1.21	1.43
22	K	2011	BCR	C16-C17	-7.63	1.21	1.43
22	A	6007	BCR	C16-C17	-7.62	1.21	1.43
22	J	6012	BCR	C16-C17	-7.62	1.21	1.43
22	A	6017	BCR	C16-C17	-7.62	1.21	1.43
22	A	6002	BCR	C16-C17	-7.60	1.21	1.43
22	B	6005	BCR	C16-C17	-7.56	1.21	1.43
22	B	6010	BCR	C16-C17	-7.56	1.21	1.43
22	J	6013	BCR	C10-C9	-7.55	1.25	1.35
22	B	6009	BCR	C10-C9	-7.52	1.25	1.35
22	A	6017	BCR	C8-C9	-7.52	1.29	1.45
22	L	6020	BCR	C10-C9	-7.49	1.25	1.35
22	A	6008	BCR	C10-C9	-7.41	1.25	1.35
22	J	6012	BCR	C10-C9	-7.28	1.26	1.35
22	A	6003	BCR	C10-C9	-7.26	1.26	1.35
22	B	6006	BCR	C10-C9	-7.10	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	6007	BCR	C10-C9	-7.07	1.26	1.35
22	B	6004	BCR	C10-C9	-7.05	1.26	1.35
22	I	6020	BCR	C10-C9	-7.01	1.26	1.35
22	A	6002	BCR	C10-C9	-6.92	1.26	1.35
22	K	2011	BCR	C10-C9	-6.86	1.26	1.35
22	B	6005	BCR	C10-C9	-6.83	1.26	1.35
28	4	4010	CHL	C3D-C4D	-6.81	1.31	1.41
22	B	6010	BCR	C10-C9	-6.80	1.26	1.35
28	4	4011	CHL	C3D-C4D	-6.70	1.31	1.41
28	4	4013	CHL	C3D-C4D	-6.59	1.31	1.41
22	A	6017	BCR	C10-C9	-6.54	1.27	1.35
28	2	2010	CHL	C3D-C4D	-6.54	1.31	1.41
28	2	2011	CHL	C3D-C4D	-6.52	1.31	1.41
28	3	3011	CHL	C3D-C4D	-6.47	1.31	1.41
28	1	1009	CHL	C3D-C4D	-6.47	1.31	1.41
28	1	1010	CHL	C3D-C4D	-6.32	1.31	1.41
28	4	4011	CHL	C4D-CHA	-6.21	1.37	1.45
28	3	3011	CHL	C4D-CHA	-6.20	1.37	1.45
28	2	2010	CHL	C4D-CHA	-6.18	1.37	1.45
28	2	2011	CHL	C4D-CHA	-6.17	1.37	1.45
28	2	2013	CHL	C3D-C4D	-6.14	1.32	1.41
28	1	1009	CHL	C4D-CHA	-6.13	1.37	1.45
28	4	4010	CHL	C4D-CHA	-6.11	1.37	1.45
28	4	4013	CHL	C4D-CHA	-6.10	1.37	1.45
28	1	1010	CHL	C4D-CHA	-5.97	1.37	1.45
28	2	2010	CHL	C3B-C2B	-5.94	1.32	1.40
28	4	4013	CHL	C3B-C2B	-5.93	1.32	1.40
28	2	2013	CHL	C4D-CHA	-5.88	1.37	1.45
28	4	4010	CHL	C3B-C2B	-5.77	1.33	1.40
28	3	3011	CHL	C3B-C2B	-5.74	1.33	1.40
28	2	2011	CHL	C3B-C2B	-5.49	1.33	1.40
28	1	1009	CHL	C3B-C2B	-4.81	1.34	1.40
27	3	3502	LUT	C21-C26	-4.60	1.50	1.56
27	2	2502	LUT	C21-C26	-4.54	1.50	1.56
28	4	4011	CHL	C3B-C2B	-4.49	1.34	1.40
28	2	2011	CHL	C1A-CHA	-4.42	1.29	1.37
22	G	2011	BCR	C11-C12	-4.41	1.24	1.34
28	3	3011	CHL	C1A-CHA	-4.19	1.29	1.37
18	2	2004	CLA	C4C-NC	-4.18	1.31	1.37
27	4	4501	LUT	C21-C26	-4.12	1.51	1.56
28	4	4010	CHL	C3A-C2A	-4.08	1.42	1.54
22	F	6016	BCR	C11-C12	-4.07	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	4503	LUT	C21-C26	-4.04	1.51	1.56
22	F	6014	BCR	C11-C12	-3.93	1.25	1.34
22	A	6011	BCR	C11-C12	-3.90	1.25	1.34
27	1	1502	LUT	C26-C27	-3.89	1.47	1.50
22	J	6012	BCR	C11-C12	-3.87	1.25	1.34
27	1	1501	LUT	C26-C27	-3.86	1.47	1.50
18	2	2004	CLA	C1C-NC	-3.86	1.31	1.37
27	1	1502	LUT	C21-C26	-3.84	1.51	1.56
27	4	4502	LUT	C21-C26	-3.81	1.51	1.56
22	A	6008	BCR	C11-C12	-3.80	1.25	1.34
27	4	4503	LUT	C26-C27	-3.80	1.47	1.50
18	4	4004	CLA	C4C-NC	-3.79	1.32	1.37
22	L	6019	BCR	C11-C12	-3.77	1.25	1.34
28	2	2013	CHL	C3B-C2B	-3.74	1.35	1.40
27	3	3501	LUT	C21-C26	-3.69	1.51	1.56
18	2	2008	CLA	C4C-NC	-3.68	1.32	1.37
18	2	2012	CLA	C1C-NC	-3.66	1.32	1.37
22	J	6013	BCR	C11-C12	-3.64	1.26	1.34
18	G	1001	CLA	C1C-NC	-3.63	1.32	1.37
27	1	1501	LUT	C21-C26	-3.62	1.51	1.56
28	4	4011	CHL	C3A-C2A	-3.60	1.44	1.54
22	A	6003	BCR	C11-C12	-3.59	1.26	1.34
18	4	4007	CLA	C1C-NC	-3.56	1.32	1.37
22	3	3503	BCR	C11-C12	-3.55	1.26	1.34
18	4	4001	CLA	C4C-NC	-3.55	1.32	1.37
18	L	1501	CLA	C1C-NC	-3.54	1.32	1.37
22	A	6007	BCR	C11-C12	-3.53	1.26	1.34
18	4	4004	CLA	C1C-NC	-3.52	1.32	1.37
18	L	1501	CLA	C4C-NC	-3.51	1.32	1.37
22	B	6006	BCR	C11-C12	-3.51	1.26	1.34
18	4	4002	CLA	C1C-NC	-3.50	1.32	1.37
27	I	6018	LUT	C21-C26	-3.50	1.51	1.56
22	B	6009	BCR	C11-C12	-3.49	1.26	1.34
18	4	4009	CLA	C4C-NC	-3.49	1.32	1.37
18	4	4009	CLA	C1C-NC	-3.46	1.32	1.37
18	4	4006	CLA	C1C-NC	-3.46	1.32	1.37
22	I	6020	BCR	C11-C12	-3.45	1.26	1.34
18	2	2016	CLA	C4C-NC	-3.44	1.32	1.37
18	3	3001	CLA	C4C-NC	-3.44	1.32	1.37
28	4	4011	CHL	C1A-CHA	-3.44	1.31	1.37
18	4	4005	CLA	C1C-NC	-3.44	1.32	1.37
18	2	2001	CLA	C1C-NC	-3.43	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3012	CLA	C1C-NC	-3.42	1.32	1.37
22	B	6004	BCR	C11-C12	-3.41	1.26	1.34
18	2	2008	CLA	C1C-NC	-3.41	1.32	1.37
22	A	6002	BCR	C11-C12	-3.41	1.26	1.34
28	2	2010	CHL	C1A-CHA	-3.41	1.31	1.37
27	2	2502	LUT	C26-C27	-3.39	1.47	1.50
18	4	4012	CLA	C4C-NC	-3.39	1.32	1.37
22	B	6010	BCR	C11-C12	-3.39	1.26	1.34
18	4	4012	CLA	C1C-NC	-3.38	1.32	1.37
18	4	4005	CLA	C4C-NC	-3.38	1.32	1.37
18	G	1001	CLA	C4C-NC	-3.36	1.32	1.37
18	1	1001	CLA	C1C-NC	-3.36	1.32	1.37
18	1	1014	CLA	C4C-NC	-3.36	1.32	1.37
22	K	2011	BCR	C11-C12	-3.33	1.26	1.34
18	1	1012	CLA	C4C-NC	-3.32	1.32	1.37
22	B	6005	BCR	C11-C12	-3.31	1.26	1.34
18	3	3012	CLA	C4C-NC	-3.31	1.32	1.37
18	1	1005	CLA	C1C-NC	-3.30	1.32	1.37
28	3	3011	CHL	C3A-C2A	-3.28	1.44	1.54
22	L	6020	BCR	C11-C12	-3.27	1.26	1.34
22	A	6017	BCR	C11-C12	-3.26	1.26	1.34
27	2	2501	LUT	C21-C26	-3.25	1.52	1.56
18	1	1007	CLA	C1C-NC	-3.25	1.32	1.37
22	F	6014	BCR	C1-C6	-3.25	1.49	1.53
18	1	1014	CLA	C1C-NC	-3.24	1.32	1.37
18	2	2001	CLA	C4C-NC	-3.24	1.32	1.37
18	1	1004	CLA	C1C-NC	-3.22	1.32	1.37
18	4	4008	CLA	C1C-NC	-3.21	1.32	1.37
28	1	1010	CHL	C3B-C2B	-3.21	1.36	1.40
18	1	1007	CLA	C4C-NC	-3.21	1.33	1.37
18	4	4002	CLA	C4C-NC	-3.21	1.33	1.37
18	4	4007	CLA	C4C-NC	-3.19	1.33	1.37
27	I	6018	LUT	C26-C27	-3.19	1.47	1.50
18	4	4017	CLA	C1C-NC	-3.18	1.32	1.37
18	4	4006	CLA	C4C-NC	-3.16	1.33	1.37
18	3	3006	CLA	C1C-NC	-3.15	1.32	1.37
18	3	3004	CLA	C1C-NC	-3.15	1.32	1.37
18	3	3017	CLA	C1C-NC	-3.13	1.32	1.37
18	1	1012	CLA	C1C-NC	-3.13	1.32	1.37
29	4	4505	ZEX	C1-C6	-3.13	1.49	1.53
22	J	6013	BCR	C30-C25	-3.13	1.49	1.53
18	3	3001	CLA	C1C-NC	-3.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	4	4013	CHL	C1A-CHA	-3.10	1.31	1.37
18	2	2012	CLA	C4C-NC	-3.08	1.33	1.37
18	1	1005	CLA	C4C-NC	-3.08	1.33	1.37
18	3	3010	CLA	C1C-NC	-3.08	1.33	1.37
18	3	3019	CLA	CAD-CBD	-3.07	1.50	1.54
18	3	3010	CLA	C4C-NC	-3.05	1.33	1.37
18	1	1002	CLA	C1C-NC	-3.04	1.33	1.37
18	1	1003	CLA	C1C-NC	-3.04	1.33	1.37
18	2	2016	CLA	C1C-NC	-3.04	1.33	1.37
18	3	3005	CLA	C1C-NC	-3.04	1.33	1.37
18	3	3003	CLA	C1C-NC	-3.03	1.33	1.37
18	3	3007	CLA	C1C-NC	-3.02	1.33	1.37
18	2	2009	CLA	C4C-NC	-3.02	1.33	1.37
18	3	3005	CLA	C4C-NC	-3.01	1.33	1.37
18	2	2009	CLA	C1C-NC	-3.00	1.33	1.37
18	3	3018	CLA	C1C-NC	-2.99	1.33	1.37
18	K	1001	CLA	C1C-NC	-2.99	1.33	1.37
18	3	3018	CLA	C4C-NC	-2.98	1.33	1.37
18	1	1002	CLA	C4C-NC	-2.98	1.33	1.37
18	3	3013	CLA	C1C-NC	-2.97	1.33	1.37
18	2	2002	CLA	C1C-NC	-2.97	1.33	1.37
18	3	3017	CLA	C4C-NC	-2.97	1.33	1.37
18	4	4001	CLA	C1C-NC	-2.97	1.33	1.37
18	L	1502	CLA	C4C-NC	-2.95	1.33	1.37
28	4	4010	CHL	C3D-C2D	-2.95	1.33	1.40
18	3	3004	CLA	C4C-NC	-2.95	1.33	1.37
18	1	1001	CLA	C4C-NC	-2.93	1.33	1.37
18	1	1011	CLA	C4C-NC	-2.93	1.33	1.37
18	K	1001	CLA	C4C-NC	-2.92	1.33	1.37
18	2	2019	CLA	C4C-NC	-2.92	1.33	1.37
28	4	4013	CHL	C1C-NC	-2.91	1.33	1.37
18	2	2002	CLA	C4C-NC	-2.86	1.33	1.37
18	1	1006	CLA	C1C-NC	-2.86	1.33	1.37
18	1	1011	CLA	C1C-NC	-2.85	1.33	1.37
18	1	1003	CLA	C4C-NC	-2.84	1.33	1.37
28	2	2011	CHL	C3A-C2A	-2.84	1.46	1.54
18	L	1503	CLA	C1C-NC	-2.82	1.33	1.37
18	2	2003	CLA	C4C-NC	-2.82	1.33	1.37
18	3	3002	CLA	C1C-NC	-2.81	1.33	1.37
18	L	1502	CLA	C1C-NC	-2.81	1.33	1.37
18	G	1003	CLA	C1C-NC	-2.79	1.33	1.37
18	4	4016	CLA	C1C-NC	-2.79	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1006	CLA	C4C-NC	-2.78	1.33	1.37
18	4	4017	CLA	C4C-NC	-2.77	1.33	1.37
18	1	1004	CLA	C4C-NC	-2.77	1.33	1.37
18	2	2019	CLA	CAD-CBD	-2.76	1.50	1.54
18	L	1503	CLA	C4C-NC	-2.76	1.33	1.37
18	2	2019	CLA	C1C-NC	-2.76	1.33	1.37
28	4	4010	CHL	C1A-CHA	-2.75	1.32	1.37
28	2	2010	CHL	C3A-C2A	-2.75	1.46	1.54
18	3	3013	CLA	C4C-NC	-2.73	1.33	1.37
18	3	3008	CLA	C4C-NC	-2.72	1.33	1.37
18	2	2005	CLA	C1C-NC	-2.69	1.33	1.37
18	3	3007	CLA	C4C-NC	-2.69	1.33	1.37
28	2	2011	CHL	C1B-NB	-2.67	1.31	1.37
18	4	4008	CLA	C4C-NC	-2.66	1.33	1.37
22	J	6012	BCR	C30-C25	-2.65	1.50	1.53
28	2	2011	CHL	C3D-C2D	-2.64	1.34	1.40
18	F	1302	CLA	C1C-NC	-2.64	1.33	1.37
18	1	1013	CLA	C1C-NC	-2.63	1.33	1.37
18	3	3003	CLA	C4C-NC	-2.61	1.33	1.37
18	F	1301	CLA	C1C-NC	-2.60	1.33	1.37
18	3	3005	CLA	C1D-ND	-2.58	1.31	1.37
18	2	2008	CLA	C1D-ND	-2.57	1.31	1.37
27	2	2501	LUT	C26-C27	-2.57	1.48	1.50
27	4	4502	LUT	C26-C27	-2.55	1.48	1.50
18	1	1005	CLA	C1D-ND	-2.55	1.31	1.37
29	4	4505	ZEX	C21-C26	-2.54	1.50	1.53
18	B	1210	CLA	C1C-NC	-2.52	1.33	1.37
18	4	4003	CLA	C1C-NC	-2.52	1.33	1.37
18	2	2012	CLA	C1D-ND	-2.52	1.31	1.37
18	2	2003	CLA	C1C-NC	-2.52	1.33	1.37
18	2	2006	CLA	C1C-NC	-2.51	1.33	1.37
28	3	3011	CHL	C1C-NC	-2.51	1.34	1.37
28	2	2010	CHL	C1C-NC	-2.51	1.34	1.37
18	4	4003	CLA	C4C-NC	-2.51	1.34	1.37
18	G	1003	CLA	C4C-NC	-2.50	1.34	1.37
18	G	1002	CLA	C1C-NC	-2.50	1.33	1.37
18	B	1211	CLA	C1C-NC	-2.49	1.33	1.37
22	G	2011	BCR	C1-C6	-2.49	1.50	1.53
28	3	3011	CHL	C3D-C2D	-2.48	1.34	1.40
28	4	4013	CHL	C3A-C2A	-2.48	1.47	1.54
18	1	1014	CLA	C1D-ND	-2.46	1.32	1.37
18	1	1012	CLA	C1D-ND	-2.46	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	4	4013	CHL	C1B-NB	-2.45	1.32	1.37
18	1	1008	CLA	C1C-NC	-2.45	1.34	1.37
18	4	4006	CLA	C1D-ND	-2.44	1.32	1.37
18	G	1002	CLA	C4C-NC	-2.44	1.34	1.37
18	2	2007	CLA	C1C-NC	-2.44	1.34	1.37
28	3	3011	CHL	C1B-NB	-2.43	1.32	1.37
18	A	1137	CLA	C1C-NC	-2.43	1.34	1.37
27	3	3502	LUT	C26-C27	-2.43	1.48	1.50
22	F	6016	BCR	C1-C6	-2.43	1.50	1.53
18	2	2001	CLA	C2A-C1A	-2.43	1.46	1.52
22	L	6019	BCR	C1-C6	-2.42	1.50	1.53
27	3	3502	LUT	C1-C6	-2.42	1.50	1.53
28	4	4013	CHL	CHB-C4A	-2.41	1.34	1.41
18	3	3010	CLA	C1D-ND	-2.41	1.32	1.37
27	1	1501	LUT	C1-C6	-2.40	1.50	1.53
22	3	3503	BCR	C1-C6	-2.40	1.50	1.53
18	K	1001	CLA	C1D-ND	-2.40	1.32	1.37
18	2	2004	CLA	C1D-ND	-2.39	1.32	1.37
18	4	4002	CLA	C1D-ND	-2.39	1.32	1.37
18	3	3006	CLA	C4C-NC	-2.39	1.34	1.37
28	2	2011	CHL	CHB-C4A	-2.38	1.34	1.41
18	B	1223	CLA	C1C-NC	-2.38	1.34	1.37
18	1	1013	CLA	C4C-NC	-2.38	1.34	1.37
22	J	6013	BCR	C1-C6	-2.37	1.50	1.53
27	1	1502	LUT	C10-C9	-2.36	1.32	1.35
18	3	3002	CLA	C4C-NC	-2.36	1.34	1.37
18	A	1125	CLA	C1C-NC	-2.36	1.34	1.37
27	4	4503	LUT	C1-C6	-2.35	1.50	1.53
18	F	1301	CLA	C4C-NC	-2.34	1.34	1.37
18	A	1151	CLA	C1C-NC	-2.34	1.34	1.37
18	A	1111	CLA	C1C-NC	-2.34	1.34	1.37
18	1	1008	CLA	C4C-NC	-2.34	1.34	1.37
18	2	2005	CLA	C4C-NC	-2.34	1.34	1.37
18	B	1220	CLA	C1C-NC	-2.34	1.34	1.37
28	4	4011	CHL	CHB-C4A	-2.33	1.34	1.41
28	3	3011	CHL	CHB-C4A	-2.33	1.34	1.41
18	B	1229	CLA	C1C-NC	-2.33	1.34	1.37
18	B	1207	CLA	C1C-NC	-2.32	1.34	1.37
18	A	1132	CLA	C1C-NC	-2.32	1.34	1.37
18	A	1133	CLA	C1C-NC	-2.31	1.34	1.37
18	B	1205	CLA	C1C-NC	-2.31	1.34	1.37
18	1	1007	CLA	C1D-ND	-2.31	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1204	CLA	C1C-NC	-2.31	1.34	1.37
18	2	2016	CLA	C1D-ND	-2.30	1.32	1.37
18	A	1101	CLA	C1C-NC	-2.30	1.34	1.37
18	4	4005	CLA	C1D-ND	-2.30	1.32	1.37
28	1	1009	CHL	C1A-CHA	-2.30	1.33	1.37
18	L	1501	CLA	C1D-ND	-2.30	1.32	1.37
27	1	1502	LUT	C1-C6	-2.29	1.50	1.53
18	A	1110	CLA	C1C-NC	-2.29	1.34	1.37
18	A	1237	CLA	C1C-NC	-2.29	1.34	1.37
18	G	1001	CLA	C1D-ND	-2.29	1.32	1.37
18	3	3008	CLA	C1C-NC	-2.28	1.34	1.37
18	3	3012	CLA	C1D-ND	-2.28	1.32	1.37
28	1	1010	CHL	C3D-C2D	-2.27	1.35	1.40
18	3	3001	CLA	C1D-ND	-2.27	1.32	1.37
18	A	1114	CLA	C1C-NC	-2.27	1.34	1.37
28	4	4010	CHL	C1B-NB	-2.27	1.32	1.37
27	3	3501	LUT	C26-C27	-2.26	1.48	1.50
18	4	4012	CLA	C1D-ND	-2.26	1.32	1.37
18	A	1119	CLA	C1C-NC	-2.26	1.34	1.37
18	B	1236	CLA	C1C-NC	-2.26	1.34	1.37
18	B	1213	CLA	C1C-NC	-2.26	1.34	1.37
18	4	4004	CLA	C1D-ND	-2.26	1.32	1.37
22	3	3503	BCR	C17-C18	-2.26	1.32	1.35
18	A	1121	CLA	C1C-NC	-2.26	1.34	1.37
23	F	5001	LMG	O7-C8	-2.26	1.40	1.46
18	B	1217	CLA	C1C-NC	-2.26	1.34	1.37
18	B	1023	CLA	C1C-NC	-2.26	1.34	1.37
18	1	1001	CLA	C1D-ND	-2.26	1.32	1.37
18	H	1000	CLA	C1C-NC	-2.25	1.34	1.37
18	4	4009	CLA	C1D-ND	-2.25	1.32	1.37
22	F	6016	BCR	C30-C25	-2.25	1.50	1.53
22	3	3503	BCR	C30-C25	-2.25	1.50	1.53
18	A	1113	CLA	C1C-NC	-2.25	1.34	1.37
18	A	1105	CLA	C1C-NC	-2.25	1.34	1.37
18	B	1228	CLA	C1C-NC	-2.25	1.34	1.37
18	B	1232	CLA	C1C-NC	-2.25	1.34	1.37
18	A	1128	CLA	C1C-NC	-2.24	1.34	1.37
18	A	1109	CLA	C1C-NC	-2.24	1.34	1.37
27	4	4502	LUT	C22-C21	-2.24	1.52	1.54
18	A	1120	CLA	C1C-NC	-2.24	1.34	1.37
18	B	1209	CLA	C1C-NC	-2.24	1.34	1.37
18	A	1106	CLA	C1C-NC	-2.24	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	7101	DGD	O2G-C2G	-2.24	1.40	1.46
18	A	1112	CLA	C1C-NC	-2.24	1.34	1.37
18	2	2001	CLA	C1D-ND	-2.23	1.32	1.37
18	B	1202	CLA	C1C-NC	-2.23	1.34	1.37
18	B	1214	CLA	C1C-NC	-2.23	1.34	1.37
18	A	1103	CLA	C1C-NC	-2.23	1.34	1.37
28	4	4011	CHL	C1C-NC	-2.23	1.34	1.37
18	A	1138	CLA	C1C-NC	-2.23	1.34	1.37
18	B	1238	CLA	C1C-NC	-2.23	1.34	1.37
17	A	1011	CL0	C1C-NC	-2.22	1.34	1.37
28	4	4011	CHL	C3D-C2D	-2.22	1.35	1.40
18	B	1239	CLA	C1C-NC	-2.22	1.34	1.37
18	2	2006	CLA	C4C-NC	-2.22	1.34	1.37
18	A	1108	CLA	C1C-NC	-2.22	1.34	1.37
18	3	3004	CLA	C1D-ND	-2.22	1.32	1.37
28	1	1009	CHL	CHB-C4A	-2.22	1.34	1.41
18	A	1140	CLA	C1C-NC	-2.21	1.34	1.37
28	4	4010	CHL	CHB-C4A	-2.21	1.34	1.41
18	B	1230	CLA	C1C-NC	-2.21	1.34	1.37
18	3	3003	CLA	C1D-ND	-2.21	1.32	1.37
18	B	1203	CLA	C1C-NC	-2.21	1.34	1.37
18	B	1222	CLA	C1C-NC	-2.21	1.34	1.37
18	B	1212	CLA	C1C-NC	-2.21	1.34	1.37
22	I	6020	BCR	C30-C25	-2.20	1.50	1.53
28	4	4010	CHL	C1C-NC	-2.20	1.34	1.37
18	B	1240	CLA	C1C-NC	-2.20	1.34	1.37
27	4	4501	LUT	C1-C6	-2.19	1.50	1.53
18	4	4016	CLA	C4C-NC	-2.19	1.34	1.37
18	A	1118	CLA	C1C-NC	-2.19	1.34	1.37
18	A	1126	CLA	C1C-NC	-2.19	1.34	1.37
18	2	2003	CLA	C1D-ND	-2.19	1.32	1.37
28	2	2010	CHL	C1B-NB	-2.19	1.32	1.37
18	A	1013	CLA	C1C-NC	-2.19	1.34	1.37
18	A	1130	CLA	C1C-NC	-2.18	1.34	1.37
18	F	1302	CLA	C4C-NC	-2.18	1.34	1.37
18	A	1116	CLA	C1C-NC	-2.18	1.34	1.37
18	A	1136	CLA	C1C-NC	-2.18	1.34	1.37
18	B	1226	CLA	C1C-NC	-2.18	1.34	1.37
18	3	3018	CLA	C1D-ND	-2.18	1.32	1.37
18	4	4008	CLA	C1D-ND	-2.18	1.32	1.37
18	A	1123	CLA	C1C-NC	-2.17	1.34	1.37
18	A	1102	CLA	C1C-NC	-2.17	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1003	CLA	C1D-ND	-2.17	1.32	1.37
18	B	1012	CLA	C1C-NC	-2.17	1.34	1.37
18	A	1139	CLA	C1C-NC	-2.17	1.34	1.37
18	A	1127	CLA	C1C-NC	-2.17	1.34	1.37
18	A	1117	CLA	C1C-NC	-2.16	1.34	1.37
28	2	2010	CHL	CHB-C4A	-2.16	1.34	1.41
18	B	1235	CLA	C1C-NC	-2.16	1.34	1.37
28	1	1010	CHL	CHB-C4A	-2.16	1.34	1.41
18	B	1219	CLA	C1C-NC	-2.16	1.34	1.37
18	B	1208	CLA	C1C-NC	-2.16	1.34	1.37
18	1	1006	CLA	C1D-ND	-2.15	1.32	1.37
18	B	1216	CLA	C1C-NC	-2.15	1.34	1.37
18	A	1122	CLA	C1C-NC	-2.15	1.34	1.37
18	4	4001	CLA	C1D-ND	-2.14	1.32	1.37
18	A	1135	CLA	C1C-NC	-2.14	1.34	1.37
18	A	1134	CLA	C1C-NC	-2.14	1.34	1.37
28	4	4011	CHL	C1B-NB	-2.14	1.32	1.37
18	3	3017	CLA	C1D-ND	-2.14	1.32	1.37
18	J	1302	CLA	C1C-NC	-2.13	1.34	1.37
18	A	1104	CLA	C1C-NC	-2.13	1.34	1.37
18	1	1002	CLA	C1D-ND	-2.13	1.32	1.37
18	2	2007	CLA	C4C-NC	-2.13	1.34	1.37
18	2	2002	CLA	C1D-ND	-2.13	1.32	1.37
27	1	1502	LUT	C22-C21	-2.13	1.52	1.54
18	B	1201	CLA	C1C-NC	-2.12	1.34	1.37
18	B	1218	CLA	C1C-NC	-2.12	1.34	1.37
18	B	1206	CLA	C1C-NC	-2.12	1.34	1.37
18	B	1215	CLA	C1C-NC	-2.12	1.34	1.37
27	2	2502	LUT	C1-C6	-2.12	1.50	1.53
18	A	1124	CLA	C1C-NC	-2.11	1.34	1.37
18	4	4007	CLA	C1D-ND	-2.11	1.32	1.37
18	B	1227	CLA	C1C-NC	-2.11	1.34	1.37
28	2	2011	CHL	C1C-NC	-2.11	1.34	1.37
18	B	1021	CLA	C1C-NC	-2.10	1.34	1.37
29	4	4505	ZEX	C30-C29	-2.10	1.33	1.35
18	A	1131	CLA	C1C-NC	-2.10	1.34	1.37
18	A	1115	CLA	C1C-NC	-2.09	1.34	1.37
27	4	4501	LUT	C10-C9	-2.08	1.33	1.35
28	1	1009	CHL	C1C-NC	-2.08	1.34	1.37
28	2	2013	CHL	CHB-C4A	-2.08	1.35	1.41
18	A	1129	CLA	C1C-NC	-2.08	1.34	1.37
18	1	1011	CLA	C1D-ND	-2.08	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	6007	BCR	C30-C25	-2.07	1.51	1.53
18	B	1225	CLA	C1C-NC	-2.07	1.34	1.37
18	B	1224	CLA	C1C-NC	-2.07	1.34	1.37
27	4	4502	LUT	C1-C6	-2.06	1.51	1.53
22	F	6016	BCR	C14-C13	-2.06	1.33	1.35
27	4	4501	LUT	C26-C27	-2.06	1.48	1.50
18	3	3019	CLA	C1C-NC	-2.06	1.34	1.37
18	L	1502	CLA	C1D-ND	-2.06	1.32	1.37
18	B	1231	CLA	C1C-NC	-2.06	1.34	1.37
22	L	6020	BCR	C1-C6	-2.05	1.51	1.53
18	1	1004	CLA	C1D-ND	-2.05	1.32	1.37
18	3	3007	CLA	C1D-ND	-2.05	1.32	1.37
18	B	1234	CLA	C1C-NC	-2.05	1.34	1.37
22	L	6019	BCR	C30-C25	-2.05	1.51	1.53
22	J	6012	BCR	C14-C13	-2.04	1.33	1.35
18	3	3006	CLA	C1D-ND	-2.04	1.33	1.37
27	2	2501	LUT	C1-C6	-2.04	1.51	1.53
22	A	6002	BCR	C30-C25	-2.03	1.51	1.53
18	L	1503	CLA	C1D-ND	-2.03	1.33	1.37
18	2	2009	CLA	C1D-ND	-2.03	1.33	1.37
18	B	1221	CLA	C1C-NC	-2.03	1.34	1.37
18	4	4003	CLA	C1D-ND	-2.02	1.33	1.37
18	2	2016	CLA	C1A-CHA	2.00	1.51	1.43
18	A	1140	CLA	C4C-C3C	2.00	1.48	1.45
18	A	1133	CLA	C1C-C2C	2.00	1.48	1.44
18	B	1217	CLA	C1C-C2C	2.00	1.48	1.44
18	B	1211	CLA	C4C-C3C	2.00	1.48	1.45
18	1	1006	CLA	C4C-C3C	2.00	1.48	1.45
18	A	1136	CLA	C1C-C2C	2.01	1.48	1.44
18	J	1302	CLA	C1C-C2C	2.01	1.48	1.44
18	B	1225	CLA	C1C-C2C	2.01	1.48	1.44
18	A	1110	CLA	C1C-C2C	2.01	1.48	1.44
18	A	1137	CLA	C4C-C3C	2.01	1.48	1.45
18	A	1115	CLA	C1C-C2C	2.02	1.48	1.44
18	A	1121	CLA	C1C-C2C	2.02	1.48	1.44
18	B	1212	CLA	C1C-C2C	2.03	1.48	1.44
18	B	1220	CLA	C1C-C2C	2.03	1.48	1.44
18	A	1140	CLA	C1C-C2C	2.03	1.48	1.44
18	A	1106	CLA	C4C-C3C	2.03	1.48	1.45
18	A	1124	CLA	C1C-C2C	2.03	1.48	1.44
18	A	1132	CLA	C1C-C2C	2.03	1.48	1.44
18	B	1212	CLA	C4C-C3C	2.04	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1011	CL0	C4C-C3C	2.04	1.48	1.45
18	B	1012	CLA	C1C-C2C	2.04	1.48	1.44
18	A	1108	CLA	C1C-C2C	2.04	1.48	1.44
18	A	1130	CLA	C4C-C3C	2.04	1.48	1.45
18	A	1106	CLA	C1C-C2C	2.04	1.48	1.44
18	B	1227	CLA	C4C-C3C	2.05	1.48	1.45
18	A	1126	CLA	C1C-C2C	2.05	1.48	1.44
18	A	1123	CLA	C1C-C2C	2.05	1.48	1.44
18	A	1022	CLA	C1C-C2C	2.05	1.48	1.44
18	B	1215	CLA	C4C-C3C	2.05	1.48	1.45
18	A	1120	CLA	C1C-C2C	2.06	1.48	1.44
18	B	1234	CLA	C1C-C2C	2.06	1.48	1.44
18	B	1208	CLA	C4C-C3C	2.06	1.48	1.45
18	3	3010	CLA	C4B-CHC	2.06	1.45	1.40
18	B	1216	CLA	C4C-C3C	2.06	1.48	1.45
18	A	1105	CLA	C1C-C2C	2.07	1.48	1.44
18	B	1218	CLA	C1C-C2C	2.07	1.48	1.44
18	B	1239	CLA	C1C-C2C	2.07	1.48	1.44
18	A	1103	CLA	C4C-C3C	2.07	1.48	1.45
18	A	1128	CLA	C4C-C3C	2.07	1.48	1.45
18	B	1219	CLA	C1C-C2C	2.07	1.48	1.44
18	A	1237	CLA	C4C-C3C	2.07	1.48	1.45
18	B	1238	CLA	C1C-C2C	2.08	1.48	1.44
18	B	1218	CLA	C4C-C3C	2.08	1.48	1.45
18	B	1216	CLA	C1C-C2C	2.08	1.48	1.44
18	A	1130	CLA	C1C-C2C	2.09	1.48	1.44
18	B	1217	CLA	C4C-C3C	2.09	1.48	1.45
18	B	1215	CLA	C1C-C2C	2.09	1.48	1.44
18	A	1132	CLA	C4C-C3C	2.09	1.48	1.45
18	4	4002	CLA	OBD-CAD	2.09	1.25	1.22
18	3	3003	CLA	C4C-C3C	2.09	1.48	1.45
18	A	1125	CLA	C1C-C2C	2.09	1.48	1.44
18	B	1236	CLA	C1C-C2C	2.09	1.48	1.44
18	B	1239	CLA	C4C-C3C	2.09	1.48	1.45
18	A	1151	CLA	C1C-C2C	2.09	1.48	1.44
18	A	1137	CLA	C1C-C2C	2.10	1.48	1.44
18	A	1129	CLA	C4C-C3C	2.10	1.48	1.45
18	B	1207	CLA	C4C-C3C	2.10	1.48	1.45
18	B	1221	CLA	C4C-C3C	2.10	1.48	1.45
18	A	1131	CLA	C1C-C2C	2.10	1.48	1.44
18	A	1111	CLA	C4C-C3C	2.10	1.48	1.45
18	2	2019	CLA	C3C-C4C	2.11	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1203	CLA	C1C-C2C	2.11	1.48	1.44
18	A	1117	CLA	C4C-C3C	2.11	1.48	1.45
18	A	1116	CLA	C4C-C3C	2.11	1.48	1.45
18	A	1107	CLA	C1C-C2C	2.11	1.48	1.44
18	A	1121	CLA	C4C-C3C	2.11	1.48	1.45
18	1	1013	CLA	C4C-C3C	2.12	1.48	1.45
18	B	1229	CLA	C1C-C2C	2.12	1.48	1.44
18	B	1206	CLA	C4C-C3C	2.12	1.48	1.45
18	A	1104	CLA	C4C-C3C	2.12	1.48	1.45
18	A	1139	CLA	C1C-C2C	2.12	1.48	1.44
18	2	2008	CLA	C3D-C2D	2.12	1.44	1.40
18	B	1220	CLA	C4C-C3C	2.12	1.48	1.45
18	B	1227	CLA	C1C-C2C	2.12	1.48	1.44
18	A	1102	CLA	C1C-C2C	2.12	1.48	1.44
18	A	1107	CLA	C4C-C3C	2.12	1.48	1.45
18	B	1207	CLA	C1C-C2C	2.13	1.48	1.44
27	4	4501	LUT	C23-C24	2.13	1.52	1.50
18	B	1219	CLA	C4C-C3C	2.13	1.48	1.45
18	B	1201	CLA	C1C-C2C	2.13	1.48	1.44
18	B	1201	CLA	C4C-C3C	2.13	1.48	1.45
27	2	2502	LUT	C23-C24	2.14	1.52	1.50
18	B	1235	CLA	C1C-C2C	2.14	1.48	1.44
18	B	1231	CLA	C4C-C3C	2.14	1.48	1.45
18	B	1231	CLA	C1C-C2C	2.15	1.48	1.44
18	A	1109	CLA	C4C-C3C	2.15	1.48	1.45
18	A	1110	CLA	C4C-C3C	2.15	1.48	1.45
18	4	4005	CLA	C4B-CHC	2.15	1.45	1.40
18	A	1127	CLA	C4C-C3C	2.15	1.48	1.45
18	A	1139	CLA	C4C-C3C	2.16	1.48	1.45
18	A	1124	CLA	C4C-C3C	2.16	1.48	1.45
18	4	4002	CLA	CHD-C4C	2.16	1.46	1.41
18	B	1214	CLA	C4C-C3C	2.16	1.48	1.45
18	B	1208	CLA	C1C-C2C	2.16	1.48	1.44
18	A	1013	CLA	C1C-C2C	2.16	1.48	1.44
18	B	1202	CLA	C4C-C3C	2.17	1.49	1.45
18	B	1205	CLA	C4C-C3C	2.17	1.49	1.45
18	3	3017	CLA	C1B-CHB	2.18	1.46	1.40
18	4	4006	CLA	CHD-C4C	2.18	1.46	1.41
18	B	1226	CLA	C4C-C3C	2.18	1.49	1.45
18	A	1108	CLA	C4C-C3C	2.18	1.49	1.45
18	A	1105	CLA	C4C-C3C	2.18	1.49	1.45
18	B	1232	CLA	C4C-C3C	2.18	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1232	CLA	C1C-C2C	2.18	1.48	1.44
18	A	1119	CLA	C4C-C3C	2.19	1.49	1.45
18	4	4007	CLA	CHD-C4C	2.19	1.46	1.41
18	B	1222	CLA	C1C-C2C	2.19	1.48	1.44
18	2	2003	CLA	CHD-C4C	2.20	1.46	1.41
18	A	1138	CLA	C4C-C3C	2.20	1.49	1.45
18	A	1133	CLA	C4C-C3C	2.20	1.49	1.45
18	A	1136	CLA	C4C-C3C	2.20	1.49	1.45
18	1	1002	CLA	CHD-C4C	2.21	1.46	1.41
27	2	2501	LUT	C23-C24	2.22	1.52	1.50
18	4	4007	CLA	C3D-C2D	2.22	1.44	1.40
18	A	1123	CLA	C4C-C3C	2.22	1.49	1.45
18	4	4008	CLA	C4B-CHC	2.22	1.46	1.40
18	A	1122	CLA	C4C-C3C	2.22	1.49	1.45
18	H	1000	CLA	C4C-C3C	2.22	1.49	1.45
18	A	1112	CLA	C4C-C3C	2.22	1.49	1.45
18	A	1134	CLA	C4C-C3C	2.22	1.49	1.45
18	J	1302	CLA	C4C-C3C	2.23	1.49	1.45
18	1	1014	CLA	CHD-C4C	2.23	1.46	1.41
18	B	1204	CLA	C4C-C3C	2.23	1.49	1.45
18	B	1234	CLA	C4C-C3C	2.23	1.49	1.45
18	3	3001	CLA	C3D-C2D	2.24	1.45	1.40
18	2	2001	CLA	C4B-CHC	2.24	1.46	1.40
18	A	1135	CLA	C4C-C3C	2.25	1.49	1.45
18	3	3019	CLA	C4B-CHC	2.25	1.48	1.43
18	4	4008	CLA	C3D-C2D	2.25	1.45	1.40
18	4	4007	CLA	C4B-CHC	2.25	1.46	1.40
18	A	1022	CLA	C4C-C3C	2.26	1.49	1.45
18	1	1007	CLA	C3D-C2D	2.26	1.45	1.40
18	4	4009	CLA	CHD-C4C	2.27	1.46	1.41
18	1	1007	CLA	CHD-C4C	2.27	1.46	1.41
18	A	1101	CLA	C4C-C3C	2.27	1.49	1.45
17	A	1011	CL0	C1C-C2C	2.27	1.49	1.44
18	B	1209	CLA	C4C-C3C	2.28	1.49	1.45
18	B	1210	CLA	C4C-C3C	2.28	1.49	1.45
18	3	3012	CLA	CHD-C4C	2.28	1.46	1.41
18	1	1006	CLA	C3D-C2D	2.29	1.45	1.40
18	A	1115	CLA	C4C-C3C	2.29	1.49	1.45
18	4	4002	CLA	C4B-CHC	2.29	1.46	1.40
18	A	1104	CLA	C1C-C2C	2.29	1.49	1.44
18	3	3008	CLA	C4B-CHC	2.31	1.46	1.40
18	4	4001	CLA	CHD-C4C	2.31	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1114	CLA	C4C-C3C	2.32	1.49	1.45
18	A	1113	CLA	C4C-C3C	2.32	1.49	1.45
18	3	3005	CLA	C3D-C2D	2.32	1.45	1.40
18	3	3010	CLA	CHD-C4C	2.32	1.46	1.41
18	2	2002	CLA	C3D-C2D	2.32	1.45	1.40
18	1	1005	CLA	C3D-C2D	2.34	1.45	1.40
18	4	4004	CLA	C1B-CHB	2.34	1.46	1.40
18	4	4006	CLA	C4B-CHC	2.35	1.46	1.40
18	2	2002	CLA	CHD-C4C	2.35	1.46	1.41
18	G	1001	CLA	C4B-CHC	2.36	1.46	1.40
18	2	2012	CLA	C4B-CHC	2.36	1.46	1.40
18	A	1151	CLA	C4C-C3C	2.36	1.49	1.45
18	2	2016	CLA	C4B-CHC	2.37	1.46	1.40
18	1	1004	CLA	CHD-C4C	2.37	1.46	1.41
18	4	4001	CLA	C3D-C2D	2.38	1.45	1.40
18	B	1023	CLA	C4C-C3C	2.38	1.49	1.45
18	3	3006	CLA	C3D-C2D	2.38	1.45	1.40
18	3	3018	CLA	C3D-C2D	2.38	1.45	1.40
18	A	1126	CLA	C4C-C3C	2.39	1.49	1.45
18	B	1224	CLA	C4C-C3C	2.39	1.49	1.45
18	4	4009	CLA	C3D-C2D	2.39	1.45	1.40
18	3	3002	CLA	C3D-C2D	2.39	1.45	1.40
21	B	5004	LHG	O8-C23	2.40	1.45	1.33
18	K	1001	CLA	C3D-C2D	2.41	1.45	1.40
18	G	1001	CLA	CHD-C4C	2.42	1.46	1.41
18	3	3019	CLA	C1B-CHB	2.42	1.48	1.43
18	4	4017	CLA	CHD-C4C	2.43	1.46	1.41
18	3	3008	CLA	C3D-C2D	2.44	1.45	1.40
18	1	1008	CLA	CHD-C4C	2.44	1.46	1.41
18	4	4004	CLA	C3D-C2D	2.44	1.45	1.40
18	2	2012	CLA	CHD-C4C	2.44	1.46	1.41
18	L	1502	CLA	CHD-C4C	2.45	1.46	1.41
18	1	1014	CLA	C4B-CHC	2.45	1.46	1.40
27	4	4503	LUT	C23-C24	2.45	1.52	1.50
18	L	1501	CLA	C3D-C2D	2.45	1.45	1.40
18	3	3003	CLA	CHD-C4C	2.46	1.47	1.41
18	1	1013	CLA	C3D-C2D	2.48	1.45	1.40
18	1	1007	CLA	C4B-CHC	2.49	1.46	1.40
18	3	3010	CLA	C1B-CHB	2.49	1.46	1.40
18	2	2001	CLA	CHD-C4C	2.50	1.47	1.41
18	3	3013	CLA	C1B-CHB	2.50	1.46	1.40
18	2	2001	CLA	C1B-CHB	2.50	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1012	CLA	CHD-C4C	2.50	1.47	1.41
18	3	3001	CLA	C1B-CHB	2.50	1.46	1.40
18	1	1005	CLA	C4B-CHC	2.51	1.46	1.40
18	3	3019	CLA	C2C-C1C	2.51	1.48	1.42
18	3	3004	CLA	CHD-C4C	2.52	1.47	1.41
18	2	2012	CLA	C1B-CHB	2.52	1.46	1.40
18	1	1001	CLA	C1B-CHB	2.53	1.46	1.40
18	4	4002	CLA	C3D-C2D	2.54	1.45	1.40
18	4	4001	CLA	C1B-CHB	2.54	1.47	1.40
18	1	1003	CLA	C4B-CHC	2.54	1.47	1.40
18	4	4009	CLA	C1B-CHB	2.54	1.47	1.40
18	3	3018	CLA	C1B-CHB	2.55	1.47	1.40
18	L	1502	CLA	C3D-C2D	2.56	1.45	1.40
18	3	3019	CLA	C3C-C4C	2.56	1.48	1.42
18	2	2002	CLA	C4B-CHC	2.56	1.47	1.40
18	1	1002	CLA	C4B-CHC	2.56	1.47	1.40
18	4	4012	CLA	CHD-C4C	2.56	1.47	1.41
18	1	1013	CLA	C4B-CHC	2.57	1.47	1.40
18	4	4006	CLA	C1B-CHB	2.57	1.47	1.40
18	K	1001	CLA	CHD-C4C	2.57	1.47	1.41
18	1	1008	CLA	C4B-CHC	2.57	1.47	1.40
18	K	1001	CLA	C4B-CHC	2.57	1.47	1.40
18	2	2008	CLA	C4B-CHC	2.58	1.47	1.40
27	I	6018	LUT	C23-C24	2.59	1.52	1.50
18	3	3010	CLA	C3D-C2D	2.60	1.45	1.40
18	1	1011	CLA	CHD-C4C	2.61	1.47	1.41
18	4	4003	CLA	CHD-C4C	2.61	1.47	1.41
18	2	2003	CLA	C3D-C2D	2.61	1.45	1.40
18	G	1003	CLA	C3D-C2D	2.61	1.45	1.40
18	4	4001	CLA	C4B-CHC	2.62	1.47	1.40
18	L	1503	CLA	CHD-C4C	2.62	1.47	1.41
18	3	3012	CLA	C3D-C2D	2.62	1.45	1.40
18	2	2004	CLA	CHD-C4C	2.62	1.47	1.41
18	3	3006	CLA	C4B-CHC	2.62	1.47	1.40
18	3	3004	CLA	C4B-CHC	2.63	1.47	1.40
18	3	3007	CLA	CHD-C4C	2.63	1.47	1.41
18	1	1008	CLA	C3D-C2D	2.63	1.45	1.40
18	3	3018	CLA	CHD-C4C	2.64	1.47	1.41
18	L	1501	CLA	C1B-CHB	2.64	1.47	1.40
18	1	1011	CLA	C1B-CHB	2.64	1.47	1.40
18	3	3001	CLA	CHD-C4C	2.65	1.47	1.41
18	4	4017	CLA	C1B-CHB	2.65	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1014	CLA	C1B-CHB	2.66	1.47	1.40
18	1	1001	CLA	C4B-CHC	2.66	1.47	1.40
18	F	1301	CLA	CHD-C4C	2.66	1.47	1.41
18	2	2003	CLA	C4B-CHC	2.67	1.47	1.40
18	3	3007	CLA	C1B-CHB	2.68	1.47	1.40
18	3	3012	CLA	C1B-CHB	2.68	1.47	1.40
18	3	3012	CLA	C4B-CHC	2.68	1.47	1.40
18	4	4016	CLA	C3D-C2D	2.68	1.45	1.40
18	3	3006	CLA	CHD-C4C	2.68	1.47	1.41
18	3	3003	CLA	C3D-C2D	2.68	1.45	1.40
18	1	1004	CLA	C4B-CHC	2.69	1.47	1.40
18	2	2009	CLA	C3D-C2D	2.69	1.45	1.40
18	B	1211	CLA	C1B-CHB	2.69	1.47	1.40
18	1	1012	CLA	C4B-CHC	2.69	1.47	1.40
18	3	3017	CLA	C3D-C2D	2.69	1.46	1.40
18	4	4009	CLA	C4B-CHC	2.69	1.47	1.40
18	3	3017	CLA	CHD-C4C	2.70	1.47	1.41
18	G	1002	CLA	CHD-C4C	2.70	1.47	1.41
18	1	1007	CLA	C1B-CHB	2.71	1.47	1.40
18	K	1001	CLA	C1B-CHB	2.71	1.47	1.40
18	3	3018	CLA	C4B-CHC	2.71	1.47	1.40
18	1	1004	CLA	C3D-C2D	2.71	1.46	1.40
18	3	3002	CLA	C4B-CHC	2.72	1.47	1.40
18	2	2004	CLA	C3D-C2D	2.72	1.46	1.40
18	4	4012	CLA	C1B-CHB	2.72	1.47	1.40
18	A	1125	CLA	CHD-C4C	2.73	1.47	1.41
18	1	1006	CLA	C1B-CHB	2.73	1.47	1.40
18	1	1014	CLA	C3D-C2D	2.73	1.46	1.40
18	B	1230	CLA	CHD-C4C	2.73	1.47	1.41
18	G	1001	CLA	C3D-C2D	2.73	1.46	1.40
18	B	1216	CLA	C1B-CHB	2.73	1.47	1.40
18	4	4016	CLA	CHD-C4C	2.74	1.47	1.41
18	2	2007	CLA	CHD-C4C	2.74	1.47	1.41
18	A	1111	CLA	C1B-CHB	2.74	1.47	1.40
18	A	1112	CLA	C1B-CHB	2.74	1.47	1.40
18	2	2009	CLA	CHD-C4C	2.74	1.47	1.41
18	G	1002	CLA	C4B-CHC	2.75	1.47	1.40
18	4	4012	CLA	C3D-C2D	2.75	1.46	1.40
18	A	1013	CLA	C1B-CHB	2.75	1.47	1.40
18	1	1012	CLA	C1B-CHB	2.76	1.47	1.40
18	L	1501	CLA	CHD-C4C	2.76	1.47	1.41
18	4	4016	CLA	C4B-CHC	2.76	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1003	CLA	C1B-CHB	2.76	1.47	1.40
18	B	1226	CLA	C4B-CHC	2.76	1.47	1.40
18	B	1224	CLA	C1B-CHB	2.76	1.47	1.40
18	3	3004	CLA	C3B-C2B	2.78	1.43	1.40
18	1	1011	CLA	C3D-C2D	2.78	1.46	1.40
18	2	2008	CLA	C1B-CHB	2.78	1.47	1.40
18	4	4003	CLA	C4B-CHC	2.78	1.47	1.40
18	G	1003	CLA	C1B-CHB	2.78	1.47	1.40
18	2	2009	CLA	C4B-CHC	2.78	1.47	1.40
18	B	1222	CLA	CHD-C4C	2.79	1.47	1.41
18	3	3002	CLA	CHD-C4C	2.79	1.47	1.41
18	3	3004	CLA	C1B-CHB	2.79	1.47	1.40
18	A	1104	CLA	CHD-C4C	2.79	1.47	1.41
18	4	4008	CLA	C1B-CHB	2.80	1.47	1.40
18	2	2009	CLA	C1B-CHB	2.80	1.47	1.40
18	A	1102	CLA	CHD-C4C	2.80	1.47	1.41
18	G	1003	CLA	CHD-C4C	2.80	1.47	1.41
18	A	1132	CLA	C1B-CHB	2.81	1.47	1.40
18	B	1210	CLA	C1B-CHB	2.81	1.47	1.40
18	2	2005	CLA	CHD-C4C	2.81	1.47	1.41
18	B	1223	CLA	CHD-C4C	2.81	1.47	1.41
18	4	4004	CLA	C4B-CHC	2.82	1.47	1.40
17	A	1011	CL0	C1B-CHB	2.82	1.47	1.40
18	3	3001	CLA	C4B-CHC	2.82	1.47	1.40
18	B	1229	CLA	CHD-C4C	2.82	1.47	1.41
18	3	3004	CLA	C3D-C2D	2.82	1.46	1.40
18	A	1126	CLA	C1B-CHB	2.83	1.47	1.40
18	B	1012	CLA	CHD-C4C	2.84	1.47	1.41
18	A	1128	CLA	C4B-CHC	2.84	1.47	1.40
18	3	3002	CLA	OBD-CAD	2.84	1.26	1.22
18	F	1302	CLA	CHD-C4C	2.84	1.47	1.41
18	B	1207	CLA	CHD-C4C	2.84	1.47	1.41
18	A	1109	CLA	C1B-CHB	2.84	1.47	1.40
18	B	1206	CLA	C4B-CHC	2.84	1.47	1.40
18	A	1101	CLA	C1B-CHB	2.84	1.47	1.40
18	3	3007	CLA	C4B-CHC	2.84	1.47	1.40
18	2	2001	CLA	C3D-C2D	2.85	1.46	1.40
18	3	3013	CLA	CHD-C4C	2.85	1.47	1.41
18	3	3005	CLA	C1B-CHB	2.85	1.47	1.40
18	2	2006	CLA	CHD-C4C	2.85	1.47	1.41
18	3	3017	CLA	C4B-CHC	2.85	1.47	1.40
18	B	1023	CLA	C1B-CHB	2.85	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1011	CLA	C4B-CHC	2.86	1.47	1.40
18	4	4017	CLA	C4B-CHC	2.86	1.47	1.40
18	B	1203	CLA	CHD-C4C	2.86	1.47	1.41
18	B	1212	CLA	CHD-C4C	2.86	1.47	1.41
18	B	1021	CLA	CHD-C4C	2.86	1.47	1.41
18	G	1002	CLA	C3D-C2D	2.86	1.46	1.40
18	1	1006	CLA	C4B-CHC	2.86	1.47	1.40
18	G	1002	CLA	C1B-CHB	2.87	1.47	1.40
18	L	1503	CLA	C1B-CHB	2.87	1.47	1.40
18	1	1005	CLA	C1B-CHB	2.87	1.47	1.40
18	4	4005	CLA	OBD-CAD	2.87	1.26	1.22
18	A	1110	CLA	C1B-CHB	2.87	1.47	1.40
18	B	1228	CLA	C1B-CHB	2.87	1.47	1.40
18	B	1227	CLA	C1B-CHB	2.87	1.47	1.40
18	4	4003	CLA	C3D-C2D	2.87	1.46	1.40
18	A	1137	CLA	CHD-C4C	2.88	1.48	1.41
18	3	3005	CLA	C4B-CHC	2.88	1.47	1.40
17	A	1011	CL0	CHD-C4C	2.88	1.48	1.41
18	B	1231	CLA	C1B-CHB	2.88	1.47	1.40
18	B	1232	CLA	C1B-CHB	2.88	1.47	1.40
18	B	1221	CLA	C1B-CHB	2.89	1.47	1.40
18	A	1022	CLA	C1B-CHB	2.89	1.47	1.40
18	1	1012	CLA	C3D-C2D	2.89	1.46	1.40
18	A	1119	CLA	C1B-CHB	2.89	1.47	1.40
18	2	2012	CLA	C3D-C2D	2.90	1.46	1.40
18	B	1222	CLA	C1B-CHB	2.90	1.47	1.40
18	B	1221	CLA	CHD-C4C	2.90	1.48	1.41
18	2	2002	CLA	C1B-CHB	2.90	1.47	1.40
18	A	1106	CLA	C1B-CHB	2.90	1.47	1.40
18	A	1108	CLA	C1B-CHB	2.91	1.47	1.40
18	B	1235	CLA	CHD-C4C	2.91	1.48	1.41
18	B	1224	CLA	C4B-CHC	2.91	1.47	1.40
18	A	1129	CLA	CHD-C4C	2.91	1.48	1.41
18	B	1223	CLA	C1B-CHB	2.91	1.48	1.40
18	A	1118	CLA	CHD-C4C	2.91	1.48	1.41
18	4	4006	CLA	C3D-C2D	2.91	1.46	1.40
18	A	1121	CLA	C1B-CHB	2.92	1.48	1.40
18	1	1006	CLA	CHD-C4C	2.92	1.48	1.41
18	2	2007	CLA	C4B-CHC	2.92	1.48	1.40
18	B	1225	CLA	CHD-C4C	2.92	1.48	1.41
18	4	4005	CLA	C3D-C2D	2.92	1.46	1.40
18	B	1220	CLA	C1B-CHB	2.92	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1138	CLA	C1B-CHB	2.92	1.48	1.40
18	A	1104	CLA	C1B-CHB	2.92	1.48	1.40
18	3	3019	CLA	CHD-C4C	2.92	1.48	1.41
18	A	1123	CLA	C1B-CHB	2.92	1.48	1.40
18	G	1003	CLA	C4B-CHC	2.92	1.48	1.40
18	2	2006	CLA	C4B-CHC	2.92	1.48	1.40
18	B	1209	CLA	C1B-CHB	2.93	1.48	1.40
18	1	1003	CLA	CHD-C4C	2.93	1.48	1.41
18	2	2005	CLA	C4B-CHC	2.93	1.48	1.40
18	B	1012	CLA	C1B-CHB	2.93	1.48	1.40
18	B	1226	CLA	C1B-CHB	2.93	1.48	1.40
18	B	1236	CLA	CHD-C4C	2.93	1.48	1.41
18	A	1123	CLA	CHD-C4C	2.94	1.48	1.41
18	A	1120	CLA	CHD-C4C	2.94	1.48	1.41
18	A	1124	CLA	C1B-CHB	2.94	1.48	1.40
18	A	1111	CLA	C4B-CHC	2.94	1.48	1.40
18	H	1000	CLA	C4B-CHC	2.94	1.48	1.40
18	B	1214	CLA	C1B-CHB	2.94	1.48	1.40
18	A	1131	CLA	CHD-C4C	2.94	1.48	1.41
18	B	1213	CLA	CHD-C4C	2.94	1.48	1.41
18	A	1102	CLA	C1B-CHB	2.94	1.48	1.40
18	G	1001	CLA	C1B-CHB	2.94	1.48	1.40
18	B	1021	CLA	C1B-CHB	2.94	1.48	1.40
18	A	1128	CLA	CHD-C4C	2.94	1.48	1.41
18	4	4017	CLA	C3D-C2D	2.94	1.46	1.40
18	L	1502	CLA	C1B-CHB	2.94	1.48	1.40
18	A	1133	CLA	C4B-CHC	2.94	1.48	1.40
18	B	1206	CLA	CHD-C4C	2.95	1.48	1.41
18	A	1128	CLA	C1B-CHB	2.95	1.48	1.40
18	A	1117	CLA	C1B-CHB	2.95	1.48	1.40
18	2	2012	CLA	C3B-C2B	2.95	1.44	1.40
18	A	1111	CLA	CHD-C4C	2.95	1.48	1.41
18	A	1103	CLA	CHD-C4C	2.95	1.48	1.41
18	B	1240	CLA	C1B-CHB	2.95	1.48	1.40
18	B	1234	CLA	CHD-C4C	2.96	1.48	1.41
18	B	1215	CLA	C1B-CHB	2.96	1.48	1.40
18	B	1239	CLA	CHD-C4C	2.96	1.48	1.41
18	B	1202	CLA	C1B-CHB	2.96	1.48	1.40
18	F	1301	CLA	C4B-CHC	2.96	1.48	1.40
18	3	3013	CLA	C4B-CHC	2.96	1.48	1.40
18	B	1204	CLA	C1B-CHB	2.96	1.48	1.40
18	L	1501	CLA	C4B-CHC	2.96	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	1302	CLA	C4B-CHC	2.96	1.48	1.40
18	B	1238	CLA	C1B-CHB	2.96	1.48	1.40
18	B	1238	CLA	CHD-C4C	2.96	1.48	1.41
18	A	1139	CLA	C1B-CHB	2.96	1.48	1.40
18	B	1207	CLA	C1B-CHB	2.97	1.48	1.40
18	A	1113	CLA	C1B-CHB	2.97	1.48	1.40
18	A	1133	CLA	CHD-C4C	2.97	1.48	1.41
18	A	1133	CLA	C1B-CHB	2.97	1.48	1.40
18	A	1136	CLA	C1B-CHB	2.97	1.48	1.40
18	3	3002	CLA	C1B-CHB	2.97	1.48	1.40
27	3	3501	LUT	C23-C24	2.97	1.52	1.50
18	B	1219	CLA	CHD-C4C	2.97	1.48	1.41
18	1	1004	CLA	C1B-CHB	2.98	1.48	1.40
18	3	3013	CLA	C3D-C2D	2.98	1.46	1.40
18	H	1000	CLA	C1B-CHB	2.98	1.48	1.40
18	A	1140	CLA	CHD-C4C	2.98	1.48	1.41
18	A	1105	CLA	C1B-CHB	2.98	1.48	1.40
18	A	1119	CLA	CHD-C4C	2.98	1.48	1.41
18	B	1201	CLA	CHD-C4C	2.98	1.48	1.41
18	L	1503	CLA	C3D-C2D	2.98	1.46	1.40
18	A	1136	CLA	CHD-C4C	2.98	1.48	1.41
18	A	1115	CLA	C1B-CHB	2.98	1.48	1.40
18	A	1106	CLA	C4B-CHC	2.98	1.48	1.40
18	A	1110	CLA	CHD-C4C	2.98	1.48	1.41
18	A	1116	CLA	C1B-CHB	2.98	1.48	1.40
18	3	3017	CLA	OBD-CAD	2.99	1.26	1.22
18	A	1125	CLA	C1B-CHB	2.99	1.48	1.40
18	A	1127	CLA	CHD-C4C	2.99	1.48	1.41
18	F	1302	CLA	C1B-CHB	2.99	1.48	1.40
18	B	1232	CLA	CHD-C4C	2.99	1.48	1.41
18	A	1151	CLA	CHD-C4C	2.99	1.48	1.41
18	B	1219	CLA	C1B-CHB	2.99	1.48	1.40
18	A	1101	CLA	C4B-CHC	2.99	1.48	1.40
18	A	1122	CLA	C1B-CHB	2.99	1.48	1.40
18	F	1301	CLA	C3D-C2D	2.99	1.46	1.40
18	B	1217	CLA	CHD-C4C	2.99	1.48	1.41
18	A	1237	CLA	C4B-CHC	2.99	1.48	1.40
18	J	1302	CLA	C1B-CHB	2.99	1.48	1.40
18	2	2019	CLA	CHD-C4C	2.99	1.48	1.41
18	B	1224	CLA	CHD-C4C	3.00	1.48	1.41
18	B	1202	CLA	C4B-CHC	3.00	1.48	1.40
18	B	1201	CLA	C1B-CHB	3.00	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4003	CLA	C1B-CHB	3.00	1.48	1.40
18	B	1203	CLA	C1B-CHB	3.00	1.48	1.40
18	4	4005	CLA	C1B-CHB	3.00	1.48	1.40
18	B	1227	CLA	CHD-C4C	3.00	1.48	1.41
18	2	2004	CLA	C4B-CHC	3.00	1.48	1.40
18	A	1135	CLA	C4B-CHC	3.00	1.48	1.40
18	A	1135	CLA	CHD-C4C	3.00	1.48	1.41
18	A	1135	CLA	C1B-CHB	3.00	1.48	1.40
18	B	1210	CLA	CHD-C4C	3.01	1.48	1.41
18	A	1113	CLA	CHD-C4C	3.01	1.48	1.41
18	B	1211	CLA	CHD-C4C	3.01	1.48	1.41
18	3	3006	CLA	C1B-CHB	3.01	1.48	1.40
18	A	1127	CLA	C4B-CHC	3.01	1.48	1.40
18	A	1101	CLA	CHD-C4C	3.01	1.48	1.41
18	B	1205	CLA	CHD-C4C	3.01	1.48	1.41
18	A	1121	CLA	CHD-C4C	3.01	1.48	1.41
18	A	1127	CLA	C1B-CHB	3.01	1.48	1.40
18	A	1119	CLA	C4B-CHC	3.01	1.48	1.40
18	A	1125	CLA	C3D-C2D	3.01	1.46	1.40
18	A	1132	CLA	CHD-C4C	3.02	1.48	1.41
18	A	1117	CLA	C4B-CHC	3.02	1.48	1.40
18	B	1213	CLA	C1B-CHB	3.02	1.48	1.40
18	B	1205	CLA	C1B-CHB	3.02	1.48	1.40
18	B	1212	CLA	C1B-CHB	3.02	1.48	1.40
18	4	4008	CLA	OBD-CAD	3.02	1.26	1.22
18	A	1105	CLA	CHD-C4C	3.02	1.48	1.41
18	4	4016	CLA	C1B-CHB	3.02	1.48	1.40
18	A	1237	CLA	C3D-C2D	3.02	1.46	1.40
18	A	1114	CLA	CHD-C4C	3.02	1.48	1.41
18	3	3007	CLA	C3D-C2D	3.02	1.46	1.40
18	B	1218	CLA	C1B-CHB	3.02	1.48	1.40
18	B	1208	CLA	C1B-CHB	3.02	1.48	1.40
18	B	1215	CLA	CHD-C4C	3.02	1.48	1.41
18	A	1129	CLA	C1B-CHB	3.02	1.48	1.40
18	A	1151	CLA	C1B-CHB	3.03	1.48	1.40
18	A	1120	CLA	C1B-CHB	3.03	1.48	1.40
18	B	1239	CLA	C1B-CHB	3.03	1.48	1.40
18	A	1130	CLA	CHD-C4C	3.03	1.48	1.41
18	B	1235	CLA	C1B-CHB	3.03	1.48	1.40
18	A	1122	CLA	CHD-C4C	3.03	1.48	1.41
18	1	1003	CLA	C3D-C2D	3.03	1.46	1.40
18	L	1503	CLA	C4B-CHC	3.03	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	C1B-CHB	3.03	1.48	1.40
18	A	1237	CLA	CHD-C4C	3.03	1.48	1.41
18	B	1229	CLA	C1B-CHB	3.03	1.48	1.40
18	1	1002	CLA	C3D-C2D	3.03	1.46	1.40
18	A	1108	CLA	CHD-C4C	3.04	1.48	1.41
18	4	4007	CLA	C1B-CHB	3.04	1.48	1.40
18	A	1106	CLA	CHD-C4C	3.04	1.48	1.41
18	B	1023	CLA	CHD-C4C	3.04	1.48	1.41
18	A	1103	CLA	C4B-CHC	3.04	1.48	1.40
18	B	1210	CLA	C4B-CHC	3.04	1.48	1.40
18	B	1214	CLA	C4B-CHC	3.04	1.48	1.40
18	B	1212	CLA	C4B-CHC	3.04	1.48	1.40
18	A	1123	CLA	C4B-CHC	3.04	1.48	1.40
18	A	1013	CLA	CHD-C4C	3.05	1.48	1.41
18	B	1215	CLA	C4B-CHC	3.05	1.48	1.40
18	J	1302	CLA	CHD-C4C	3.05	1.48	1.41
18	B	1021	CLA	C4B-CHC	3.05	1.48	1.40
18	B	1220	CLA	CHD-C4C	3.05	1.48	1.41
18	A	1107	CLA	CHD-C4C	3.05	1.48	1.41
18	A	1107	CLA	C1B-CHB	3.05	1.48	1.40
18	A	1125	CLA	C4B-CHC	3.05	1.48	1.40
18	A	1122	CLA	C4B-CHC	3.05	1.48	1.40
18	A	1237	CLA	C1B-CHB	3.05	1.48	1.40
18	A	1134	CLA	C1B-CHB	3.05	1.48	1.40
18	A	1114	CLA	C1B-CHB	3.05	1.48	1.40
18	1	1002	CLA	C1B-CHB	3.05	1.48	1.40
23	4	4801	LMG	O8-C28	3.05	1.42	1.33
18	B	1209	CLA	CHD-C4C	3.05	1.48	1.41
18	L	1502	CLA	C4B-CHC	3.06	1.48	1.40
18	A	1109	CLA	CHD-C4C	3.06	1.48	1.41
18	B	1220	CLA	C4B-CHC	3.06	1.48	1.40
18	B	1228	CLA	CHD-C4C	3.06	1.48	1.41
18	A	1139	CLA	CHD-C4C	3.06	1.48	1.41
18	B	1208	CLA	CHD-C4C	3.06	1.48	1.41
18	J	1302	CLA	C4B-CHC	3.06	1.48	1.40
18	B	1218	CLA	CHD-C4C	3.06	1.48	1.41
18	B	1203	CLA	C4B-CHC	3.06	1.48	1.40
18	B	1209	CLA	C4B-CHC	3.06	1.48	1.40
18	B	1240	CLA	CHD-C4C	3.06	1.48	1.41
18	A	1151	CLA	C4B-CHC	3.07	1.48	1.40
18	A	1118	CLA	C1B-CHB	3.07	1.48	1.40
18	B	1234	CLA	C1B-CHB	3.07	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1223	CLA	C4B-CHC	3.07	1.48	1.40
18	A	1114	CLA	C4B-CHC	3.07	1.48	1.40
18	B	1214	CLA	CHD-C4C	3.07	1.48	1.41
18	B	1203	CLA	C3D-C2D	3.07	1.46	1.40
18	B	1202	CLA	CHD-C4C	3.07	1.48	1.41
18	B	1230	CLA	C1B-CHB	3.07	1.48	1.40
18	B	1219	CLA	C4B-CHC	3.07	1.48	1.40
18	A	1130	CLA	C1B-CHB	3.07	1.48	1.40
18	A	1126	CLA	CHD-C4C	3.07	1.48	1.41
18	A	1112	CLA	CHD-C4C	3.08	1.48	1.41
18	B	1228	CLA	C4B-CHC	3.08	1.48	1.40
18	B	1216	CLA	CHD-C4C	3.08	1.48	1.41
18	B	1217	CLA	C4B-CHC	3.08	1.48	1.40
18	A	1116	CLA	CHD-C4C	3.08	1.48	1.41
18	H	1000	CLA	CHD-C4C	3.09	1.48	1.41
18	3	3005	CLA	OBD-CAD	3.09	1.27	1.22
18	A	1131	CLA	C1B-CHB	3.09	1.48	1.40
18	B	1204	CLA	CHD-C4C	3.09	1.48	1.41
18	A	1103	CLA	C1B-CHB	3.09	1.48	1.40
18	1	1008	CLA	C1B-CHB	3.09	1.48	1.40
18	2	2005	CLA	C3D-C2D	3.09	1.46	1.40
18	A	1124	CLA	CHD-C4C	3.09	1.48	1.41
18	2	2007	CLA	C3D-C2D	3.10	1.46	1.40
18	B	1225	CLA	C4B-CHC	3.10	1.48	1.40
18	A	1118	CLA	C4B-CHC	3.10	1.48	1.40
18	A	1117	CLA	CHD-C4C	3.10	1.48	1.41
18	B	1222	CLA	C4B-CHC	3.10	1.48	1.40
18	A	1022	CLA	CHD-C4C	3.10	1.48	1.41
18	1	1013	CLA	CHD-C4C	3.10	1.48	1.41
18	A	1102	CLA	C4B-CHC	3.10	1.48	1.40
18	1	1001	CLA	C3D-C2D	3.10	1.46	1.40
18	A	1140	CLA	C1B-CHB	3.10	1.48	1.40
18	B	1213	CLA	C4B-CHC	3.10	1.48	1.40
18	B	1205	CLA	C4B-CHC	3.10	1.48	1.40
18	A	1137	CLA	C1B-CHB	3.10	1.48	1.40
18	B	1223	CLA	C3D-C2D	3.11	1.46	1.40
18	A	1113	CLA	C4B-CHC	3.11	1.48	1.40
18	B	1207	CLA	C4B-CHC	3.11	1.48	1.40
18	B	1216	CLA	C4B-CHC	3.11	1.48	1.40
18	A	1120	CLA	C3D-C2D	3.11	1.46	1.40
18	F	1302	CLA	C3D-C2D	3.11	1.46	1.40
18	B	1236	CLA	C1B-CHB	3.11	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2005	CLA	C1B-CHB	3.11	1.48	1.40
18	2	2007	CLA	C1B-CHB	3.11	1.48	1.40
18	A	1138	CLA	CHD-C4C	3.11	1.48	1.41
18	A	1130	CLA	C4B-CHC	3.11	1.48	1.40
18	A	1129	CLA	C4B-CHC	3.11	1.48	1.40
18	B	1225	CLA	C1B-CHB	3.11	1.48	1.40
18	B	1204	CLA	C4B-CHC	3.11	1.48	1.40
18	B	1201	CLA	C4B-CHC	3.11	1.48	1.40
18	B	1023	CLA	C4B-CHC	3.11	1.48	1.40
18	A	1112	CLA	C4B-CHC	3.12	1.48	1.40
18	A	1115	CLA	C4B-CHC	3.12	1.48	1.40
18	A	1134	CLA	CHD-C4C	3.12	1.48	1.41
18	A	1136	CLA	C4B-CHC	3.12	1.48	1.40
18	2	2006	CLA	C1B-CHB	3.13	1.48	1.40
18	B	1240	CLA	C4B-CHC	3.13	1.48	1.40
18	A	1121	CLA	C4B-CHC	3.14	1.48	1.40
18	2	2006	CLA	C3D-C2D	3.14	1.46	1.40
18	A	1139	CLA	C4B-CHC	3.14	1.48	1.40
18	B	1221	CLA	C4B-CHC	3.14	1.48	1.40
18	A	1131	CLA	C4B-CHC	3.14	1.48	1.40
18	B	1226	CLA	CHD-C4C	3.14	1.48	1.41
18	A	1126	CLA	C4B-CHC	3.14	1.48	1.40
18	A	1116	CLA	C4B-CHC	3.14	1.48	1.40
18	4	4008	CLA	C3C-C2C	3.14	1.43	1.36
18	B	1238	CLA	C3D-C2D	3.14	1.46	1.40
18	A	1115	CLA	CHD-C4C	3.14	1.48	1.41
18	A	1134	CLA	C4B-CHC	3.15	1.48	1.40
18	B	1207	CLA	C3D-C2D	3.15	1.47	1.40
18	A	1107	CLA	C4B-CHC	3.15	1.48	1.40
18	A	1129	CLA	C3D-C2D	3.15	1.47	1.40
18	B	1231	CLA	CHD-C4C	3.15	1.48	1.41
18	A	1022	CLA	C4B-CHC	3.16	1.48	1.40
18	2	2016	CLA	C1B-CHB	3.16	1.48	1.40
18	4	4012	CLA	OBD-CAD	3.16	1.27	1.22
18	B	1229	CLA	C4B-CHC	3.16	1.48	1.40
18	B	1218	CLA	C4B-CHC	3.16	1.48	1.40
18	B	1230	CLA	C4B-CHC	3.16	1.48	1.40
17	A	1011	CL0	C4B-CHC	3.17	1.48	1.40
18	B	1012	CLA	C4B-CHC	3.17	1.48	1.40
18	3	3003	CLA	OBD-CAD	3.17	1.27	1.22
18	A	1107	CLA	C3D-C2D	3.17	1.47	1.40
18	B	1206	CLA	C1B-CHB	3.17	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1120	CLA	C4B-CHC	3.17	1.48	1.40
18	B	1239	CLA	C4B-CHC	3.17	1.48	1.40
18	A	1140	CLA	C4B-CHC	3.17	1.48	1.40
18	4	4009	CLA	OBD-CAD	3.17	1.27	1.22
18	A	1138	CLA	C4B-CHC	3.17	1.48	1.40
18	B	1227	CLA	C4B-CHC	3.18	1.48	1.40
18	B	1240	CLA	C3D-C2D	3.18	1.47	1.40
18	B	1238	CLA	C4B-CHC	3.18	1.48	1.40
18	B	1235	CLA	C4B-CHC	3.19	1.48	1.40
18	A	1108	CLA	C4B-CHC	3.19	1.48	1.40
18	A	1118	CLA	C3D-C2D	3.19	1.47	1.40
18	A	1124	CLA	C4B-CHC	3.19	1.48	1.40
18	A	1103	CLA	C3D-C2D	3.20	1.47	1.40
18	A	1130	CLA	C3D-C2D	3.20	1.47	1.40
18	B	1201	CLA	C3D-C2D	3.20	1.47	1.40
18	2	2001	CLA	OBD-CAD	3.20	1.27	1.22
18	A	1110	CLA	C4B-CHC	3.20	1.48	1.40
18	B	1236	CLA	C4B-CHC	3.20	1.48	1.40
18	B	1227	CLA	C3D-C2D	3.21	1.47	1.40
18	B	1217	CLA	C3D-C2D	3.21	1.47	1.40
18	F	1301	CLA	C1B-CHB	3.21	1.48	1.40
18	A	1135	CLA	C3D-C2D	3.21	1.47	1.40
18	A	1013	CLA	C4B-CHC	3.21	1.48	1.40
18	A	1137	CLA	C4B-CHC	3.21	1.48	1.40
18	A	1109	CLA	C4B-CHC	3.21	1.48	1.40
18	A	1105	CLA	C4B-CHC	3.21	1.48	1.40
18	B	1234	CLA	C3D-C2D	3.22	1.47	1.40
18	B	1232	CLA	C4B-CHC	3.22	1.48	1.40
18	A	1101	CLA	C3D-C2D	3.22	1.47	1.40
18	B	1214	CLA	C3D-C2D	3.22	1.47	1.40
18	A	1136	CLA	C3D-C2D	3.22	1.47	1.40
18	B	1208	CLA	C4B-CHC	3.23	1.48	1.40
18	A	1114	CLA	C3D-C2D	3.23	1.47	1.40
18	A	1104	CLA	C4B-CHC	3.24	1.48	1.40
18	2	2003	CLA	C1B-CHB	3.24	1.48	1.40
18	B	1205	CLA	C3D-C2D	3.24	1.47	1.40
18	A	1121	CLA	C3D-C2D	3.24	1.47	1.40
18	A	1132	CLA	C4B-CHC	3.24	1.48	1.40
18	B	1226	CLA	C3D-C2D	3.24	1.47	1.40
18	B	1231	CLA	C3D-C2D	3.24	1.47	1.40
18	B	1213	CLA	C3D-C2D	3.25	1.47	1.40
18	A	1119	CLA	C3D-C2D	3.25	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1137	CLA	C3D-C2D	3.25	1.47	1.40
18	B	1239	CLA	C3D-C2D	3.25	1.47	1.40
18	A	1109	CLA	C3D-C2D	3.25	1.47	1.40
18	4	4002	CLA	C1B-CHB	3.26	1.48	1.40
18	A	1113	CLA	C3D-C2D	3.26	1.47	1.40
18	B	1234	CLA	C4B-CHC	3.26	1.48	1.40
18	B	1211	CLA	C3D-C2D	3.26	1.47	1.40
18	B	1211	CLA	C4B-CHC	3.26	1.48	1.40
18	3	3008	CLA	C1B-CHB	3.26	1.48	1.40
18	A	1108	CLA	C3D-C2D	3.26	1.47	1.40
18	4	4001	CLA	OBD-CAD	3.26	1.27	1.22
18	1	1013	CLA	C1B-CHB	3.27	1.48	1.40
18	2	2004	CLA	C3B-C2B	3.27	1.44	1.40
18	A	1104	CLA	C3D-C2D	3.27	1.47	1.40
18	J	1302	CLA	C3D-C2D	3.27	1.47	1.40
18	A	1123	CLA	C3D-C2D	3.28	1.47	1.40
18	1	1005	CLA	OBD-CAD	3.28	1.27	1.22
18	A	1105	CLA	C3D-C2D	3.28	1.47	1.40
18	B	1221	CLA	C3D-C2D	3.28	1.47	1.40
18	B	1230	CLA	C3D-C2D	3.29	1.47	1.40
18	B	1212	CLA	C3D-C2D	3.29	1.47	1.40
18	B	1218	CLA	C3D-C2D	3.29	1.47	1.40
18	3	3003	CLA	C1B-CHB	3.29	1.49	1.40
18	B	1208	CLA	C3D-C2D	3.29	1.47	1.40
18	B	1210	CLA	C3D-C2D	3.29	1.47	1.40
18	A	1117	CLA	C3D-C2D	3.30	1.47	1.40
18	A	1122	CLA	C3D-C2D	3.30	1.47	1.40
18	A	1134	CLA	C3D-C2D	3.30	1.47	1.40
18	B	1236	CLA	C3D-C2D	3.30	1.47	1.40
18	B	1229	CLA	C3D-C2D	3.30	1.47	1.40
18	A	1124	CLA	C3D-C2D	3.31	1.47	1.40
18	A	1131	CLA	C3D-C2D	3.31	1.47	1.40
18	A	1111	CLA	C3D-C2D	3.31	1.47	1.40
18	H	1000	CLA	C3D-C2D	3.31	1.47	1.40
18	A	1151	CLA	C3D-C2D	3.31	1.47	1.40
18	B	1225	CLA	C3D-C2D	3.31	1.47	1.40
18	3	3006	CLA	OBD-CAD	3.31	1.27	1.22
18	A	1110	CLA	C3D-C2D	3.31	1.47	1.40
18	B	1219	CLA	C3D-C2D	3.31	1.47	1.40
18	A	1139	CLA	C3D-C2D	3.31	1.47	1.40
18	B	1232	CLA	C3D-C2D	3.31	1.47	1.40
18	G	1001	CLA	C3C-C2C	3.32	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1106	CLA	C3D-C2D	3.33	1.47	1.40
18	A	1112	CLA	C3D-C2D	3.33	1.47	1.40
18	B	1204	CLA	C3D-C2D	3.33	1.47	1.40
18	B	1235	CLA	C3D-C2D	3.34	1.47	1.40
18	A	1115	CLA	C3D-C2D	3.34	1.47	1.40
18	B	1222	CLA	C3D-C2D	3.34	1.47	1.40
18	3	3003	CLA	CHC-C1C	3.35	1.45	1.35
18	B	1220	CLA	C3D-C2D	3.35	1.47	1.40
18	2	2012	CLA	OBD-CAD	3.35	1.27	1.22
18	B	1228	CLA	C3D-C2D	3.35	1.47	1.40
18	B	1209	CLA	C3D-C2D	3.35	1.47	1.40
18	A	1116	CLA	C3D-C2D	3.36	1.47	1.40
18	B	1224	CLA	C3D-C2D	3.36	1.47	1.40
18	4	4004	CLA	C3B-C2B	3.36	1.44	1.40
18	2	2002	CLA	OBD-CAD	3.36	1.27	1.22
18	B	1021	CLA	C3D-C2D	3.36	1.47	1.40
18	A	1126	CLA	C3D-C2D	3.36	1.47	1.40
18	A	1140	CLA	C3D-C2D	3.37	1.47	1.40
18	A	1127	CLA	C3D-C2D	3.37	1.47	1.40
18	A	1013	CLA	C3D-C2D	3.38	1.47	1.40
18	B	1216	CLA	C3D-C2D	3.38	1.47	1.40
18	B	1231	CLA	C4B-CHC	3.38	1.49	1.40
18	B	1215	CLA	C3D-C2D	3.39	1.47	1.40
18	B	1206	CLA	C3D-C2D	3.39	1.47	1.40
18	2	2004	CLA	OBD-CAD	3.40	1.27	1.22
18	B	1202	CLA	C3D-C2D	3.40	1.47	1.40
18	2	2002	CLA	C3C-C2C	3.41	1.44	1.36
23	J	5001	LMG	O8-C28	3.41	1.43	1.33
18	4	4006	CLA	OBD-CAD	3.41	1.27	1.22
18	A	1138	CLA	C3D-C2D	3.41	1.47	1.40
17	A	1011	CL0	C3D-C2D	3.42	1.47	1.40
18	2	2016	CLA	C3C-C2C	3.43	1.44	1.36
18	B	1023	CLA	C3D-C2D	3.43	1.47	1.40
23	4	4801	LMG	O7-C10	3.43	1.44	1.34
18	A	1022	CLA	C3D-C2D	3.43	1.47	1.40
18	4	4012	CLA	C3B-C2B	3.45	1.44	1.40
18	4	4012	CLA	C3C-C2C	3.45	1.44	1.36
18	4	4005	CLA	C3B-C2B	3.46	1.44	1.40
18	1	1007	CLA	C3C-C2C	3.46	1.44	1.36
18	A	1102	CLA	C3D-C2D	3.46	1.47	1.40
18	2	2008	CLA	OBD-CAD	3.46	1.27	1.22
18	A	1132	CLA	C3D-C2D	3.47	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	1001	CLA	OBD-CAD	3.48	1.27	1.22
18	3	3010	CLA	OBD-CAD	3.48	1.27	1.22
18	1	1006	CLA	OBD-CAD	3.50	1.27	1.22
18	1	1008	CLA	OBD-CAD	3.52	1.27	1.22
18	A	1133	CLA	C3D-C2D	3.52	1.47	1.40
18	L	1501	CLA	OBD-CAD	3.53	1.27	1.22
18	4	4002	CLA	C3C-C2C	3.53	1.44	1.36
18	2	2003	CLA	C3C-C2C	3.54	1.44	1.36
18	1	1001	CLA	OBD-CAD	3.54	1.27	1.22
18	A	1128	CLA	C3D-C2D	3.55	1.47	1.40
18	4	4009	CLA	C3C-C2C	3.55	1.44	1.36
18	L	1501	CLA	C3C-C2C	3.57	1.44	1.36
18	4	4005	CLA	C3C-C2C	3.57	1.44	1.36
18	3	3012	CLA	C3B-C2B	3.58	1.44	1.40
18	1	1002	CLA	C3C-C2C	3.58	1.44	1.36
18	L	1501	CLA	C3B-C2B	3.59	1.44	1.40
18	B	1012	CLA	C3D-C2D	3.60	1.47	1.40
23	G	2021	LMG	O8-C28	3.61	1.44	1.33
18	1	1001	CLA	C3C-C2C	3.61	1.44	1.36
23	F	5002	LMG	O7-C10	3.61	1.44	1.34
18	4	4002	CLA	CHC-C1C	3.62	1.46	1.35
18	3	3013	CLA	C3B-C2B	3.62	1.44	1.40
18	4	4001	CLA	C3B-C2B	3.62	1.45	1.40
18	1	1007	CLA	C3B-C2B	3.63	1.45	1.40
18	1	1014	CLA	C3C-C2C	3.63	1.44	1.36
18	2	2008	CLA	C3C-C2C	3.65	1.44	1.36
18	4	4007	CLA	C3C-C2C	3.65	1.44	1.36
28	1	1009	CHL	O2D-CGD	3.65	1.42	1.33
18	2	2009	CLA	OBD-CAD	3.65	1.27	1.22
23	G	2021	LMG	O7-C10	3.65	1.45	1.34
18	3	3005	CLA	C3C-C2C	3.66	1.44	1.36
18	4	4007	CLA	CHC-C1C	3.66	1.46	1.35
23	J	5001	LMG	O7-C10	3.68	1.45	1.34
18	4	4004	CLA	OBD-CAD	3.69	1.27	1.22
18	1	1011	CLA	OBD-CAD	3.69	1.27	1.22
18	1	1006	CLA	C3C-C2C	3.69	1.44	1.36
18	1	1014	CLA	OBD-CAD	3.69	1.27	1.22
18	2	2001	CLA	C3C-C2C	3.69	1.44	1.36
18	2	2012	CLA	O2D-CGD	3.70	1.42	1.33
18	4	4009	CLA	C3B-C2B	3.70	1.45	1.40
18	2	2001	CLA	CHC-C1C	3.71	1.46	1.35
18	4	4012	CLA	CHC-C1C	3.71	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	4	4013	CHL	O2D-CGD	3.71	1.42	1.33
18	4	4006	CLA	C3C-C2C	3.72	1.44	1.36
18	L	1503	CLA	C3C-C2C	3.72	1.44	1.36
18	3	3017	CLA	C3B-C2B	3.73	1.45	1.40
18	L	1503	CLA	OBD-CAD	3.73	1.28	1.22
28	2	2010	CHL	O2D-CGD	3.73	1.42	1.33
18	1	1013	CLA	OBD-CAD	3.74	1.28	1.22
18	1	1007	CLA	OBD-CAD	3.74	1.28	1.22
18	3	3017	CLA	C3C-C2C	3.74	1.44	1.36
28	4	4011	CHL	O2D-CGD	3.75	1.42	1.33
18	1	1008	CLA	C3C-C2C	3.75	1.44	1.36
18	3	3005	CLA	C3B-C2B	3.76	1.45	1.40
18	4	4007	CLA	C3B-C2B	3.77	1.45	1.40
18	4	4008	CLA	CHC-C1C	3.77	1.46	1.35
18	G	1003	CLA	OBD-CAD	3.77	1.28	1.22
18	G	1001	CLA	CHC-C1C	3.77	1.46	1.35
21	2	2801	LHG	O7-C7	3.78	1.45	1.34
18	2	2016	CLA	C3B-C2B	3.78	1.45	1.40
18	1	1005	CLA	C3C-C2C	3.79	1.44	1.36
28	1	1010	CHL	O2A-CGA	3.79	1.45	1.32
28	2	2011	CHL	O2D-CGD	3.79	1.43	1.33
18	1	1012	CLA	C3C-C2C	3.79	1.45	1.36
18	2	2012	CLA	C3C-C2C	3.80	1.45	1.36
18	L	1502	CLA	OBD-CAD	3.80	1.28	1.22
18	1	1005	CLA	C3B-C2B	3.80	1.45	1.40
28	4	4013	CHL	O2A-CGA	3.81	1.45	1.32
18	4	4009	CLA	O2D-CGD	3.83	1.43	1.33
18	4	4017	CLA	OBD-CAD	3.83	1.28	1.22
23	2	2802	LMG	O7-C10	3.83	1.45	1.34
21	1	1801	LHG	O7-C7	3.83	1.45	1.34
18	3	3013	CLA	OBD-CAD	3.83	1.28	1.22
18	1	1013	CLA	C3C-C2C	3.84	1.45	1.36
18	4	4005	CLA	CHC-C1C	3.84	1.46	1.35
18	B	1203	CLA	OBD-CAD	3.84	1.28	1.22
18	2	2004	CLA	C3C-C2C	3.85	1.45	1.36
18	A	1125	CLA	OBD-CAD	3.85	1.28	1.22
18	1	1005	CLA	O2D-CGD	3.85	1.43	1.33
18	2	2001	CLA	O2D-CGD	3.85	1.43	1.33
18	G	1002	CLA	OBD-CAD	3.85	1.28	1.22
18	3	3008	CLA	CHC-C1C	3.86	1.46	1.35
28	2	2011	CHL	O2A-CGA	3.86	1.44	1.33
18	3	3001	CLA	O2D-CGD	3.86	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1013	CLA	C3B-C2B	3.86	1.45	1.40
28	3	3011	CHL	O2D-CGD	3.87	1.43	1.33
21	1	1801	LHG	O8-C23	3.87	1.44	1.33
18	4	4012	CLA	O2D-CGD	3.89	1.43	1.33
18	4	4007	CLA	O2D-CGD	3.89	1.43	1.33
18	2	2008	CLA	O2D-CGD	3.89	1.43	1.33
18	3	3010	CLA	C3B-C2B	3.89	1.45	1.40
18	2	2003	CLA	OBD-CAD	3.90	1.28	1.22
18	3	3002	CLA	C3C-C2C	3.90	1.45	1.36
18	1	1004	CLA	OBD-CAD	3.90	1.28	1.22
18	2	2012	CLA	CHC-C1C	3.90	1.46	1.35
18	G	1002	CLA	C3C-C2C	3.90	1.45	1.36
18	K	1001	CLA	C3B-C2B	3.90	1.45	1.40
23	F	5002	LMG	O8-C28	3.90	1.44	1.33
18	F	1301	CLA	OBD-CAD	3.91	1.28	1.22
28	4	4011	CHL	O2A-CGA	3.91	1.45	1.33
18	1	1011	CLA	C3C-C2C	3.91	1.45	1.36
28	1	1009	CHL	O2A-CGA	3.91	1.45	1.33
18	4	4006	CLA	CHC-C1C	3.91	1.46	1.35
18	3	3001	CLA	C3C-C2C	3.92	1.45	1.36
18	3	3008	CLA	OBD-CAD	3.92	1.28	1.22
23	2	2802	LMG	O8-C28	3.92	1.45	1.33
18	4	4007	CLA	OBD-CAD	3.92	1.28	1.22
18	1	1001	CLA	C3B-C2B	3.93	1.45	1.40
18	4	4001	CLA	C3C-C2C	3.93	1.45	1.36
18	G	1001	CLA	C3B-C2B	3.93	1.45	1.40
18	4	4017	CLA	C3C-C2C	3.93	1.45	1.36
18	1	1003	CLA	OBD-CAD	3.93	1.28	1.22
18	4	4008	CLA	O2D-CGD	3.93	1.43	1.33
18	2	2016	CLA	CHC-C1C	3.94	1.46	1.35
28	4	4010	CHL	O2D-CGD	3.94	1.43	1.33
23	F	5001	LMG	O7-C10	3.95	1.44	1.35
18	2	2001	CLA	C3B-C2B	3.95	1.45	1.40
23	B	5005	LMG	O7-C10	3.95	1.45	1.34
18	4	4016	CLA	OBD-CAD	3.95	1.28	1.22
18	2	2002	CLA	C3B-C2B	3.96	1.45	1.40
18	3	3012	CLA	OBD-CAD	3.96	1.28	1.22
18	L	1502	CLA	C3C-C2C	3.96	1.45	1.36
18	K	1001	CLA	OBD-CAD	3.96	1.28	1.22
27	1	1501	LUT	C23-C24	3.96	1.53	1.50
21	A	5003	LHG	O7-C7	3.97	1.46	1.34
18	2	2002	CLA	O2D-CGD	3.97	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2003	CLA	O2D-CGD	3.97	1.43	1.33
18	G	1002	CLA	C3B-C2B	3.97	1.45	1.40
18	3	3012	CLA	C3C-C2C	3.97	1.45	1.36
21	A	7001	LHG	O7-C7	3.97	1.46	1.34
18	4	4004	CLA	C3C-C2C	3.97	1.45	1.36
18	K	1001	CLA	CHC-C1C	3.97	1.47	1.35
18	B	1223	CLA	OBD-CAD	3.97	1.28	1.22
18	4	4003	CLA	OBD-CAD	3.98	1.28	1.22
28	2	2013	CHL	O2D-CGD	3.98	1.43	1.33
18	1	1002	CLA	O2D-CGD	3.98	1.43	1.33
18	4	4003	CLA	C3C-C2C	3.98	1.45	1.36
18	2	2019	CLA	C3B-C4B	3.99	1.47	1.40
18	3	3007	CLA	C3C-C2C	3.99	1.45	1.36
28	2	2010	CHL	O2A-CGA	3.99	1.46	1.32
18	3	3006	CLA	C3C-C2C	3.99	1.45	1.36
18	3	3010	CLA	CHC-C1C	3.99	1.47	1.35
18	1	1012	CLA	OBD-CAD	3.99	1.28	1.22
18	4	4004	CLA	O2D-CGD	4.00	1.43	1.33
18	3	3004	CLA	OBD-CAD	4.01	1.28	1.22
18	3	3006	CLA	CHC-C1C	4.02	1.47	1.35
18	1	1013	CLA	CHC-C1C	4.02	1.47	1.35
18	3	3018	CLA	C3C-C2C	4.02	1.45	1.36
18	2	2007	CLA	OBD-CAD	4.02	1.28	1.22
18	1	1012	CLA	C3B-C2B	4.03	1.45	1.40
18	4	4008	CLA	C3B-C2B	4.03	1.45	1.40
18	4	4017	CLA	O2D-CGD	4.04	1.43	1.33
18	A	1119	CLA	OBD-CAD	4.04	1.28	1.22
18	1	1002	CLA	CHC-C1C	4.04	1.47	1.35
28	1	1010	CHL	O2D-CGD	4.04	1.43	1.33
28	4	4010	CHL	O2A-CGA	4.05	1.46	1.32
18	3	3002	CLA	C3B-C2B	4.05	1.45	1.40
18	1	1003	CLA	CHC-C1C	4.05	1.47	1.35
18	2	2008	CLA	CHC-C1C	4.05	1.47	1.35
18	3	3007	CLA	OBD-CAD	4.06	1.28	1.22
18	A	1120	CLA	OBD-CAD	4.06	1.28	1.22
18	2	2009	CLA	C3B-C2B	4.06	1.45	1.40
18	3	3018	CLA	C3B-C2B	4.06	1.45	1.40
18	4	4004	CLA	O2A-C1	4.06	1.58	1.46
18	3	3002	CLA	CHC-C1C	4.07	1.47	1.35
18	2	2003	CLA	CHC-C1C	4.07	1.47	1.35
18	1	1012	CLA	CHC-C1C	4.07	1.47	1.35
18	2	2006	CLA	OBD-CAD	4.07	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4001	CLA	CHC-C1C	4.08	1.47	1.35
18	3	3018	CLA	CHC-C1C	4.08	1.47	1.35
18	4	4017	CLA	C3B-C2B	4.08	1.45	1.40
18	1	1012	CLA	O2A-C1	4.08	1.58	1.46
18	1	1011	CLA	O2D-CGD	4.08	1.43	1.33
18	1	1004	CLA	CHC-C1C	4.09	1.47	1.35
18	1	1004	CLA	C3C-C2C	4.09	1.45	1.36
21	2	2801	LHG	O8-C23	4.09	1.45	1.33
18	1	1002	CLA	OBD-CAD	4.10	1.28	1.22
18	2	2002	CLA	CHC-C1C	4.11	1.47	1.35
18	2	2005	CLA	OBD-CAD	4.11	1.28	1.22
18	4	4009	CLA	CHC-C1C	4.11	1.47	1.35
18	1	1002	CLA	C3B-C2B	4.12	1.45	1.40
18	1	1007	CLA	CHC-C1C	4.12	1.47	1.35
18	4	4006	CLA	O2A-C1	4.12	1.58	1.46
18	2	2012	CLA	O2A-C1	4.12	1.58	1.46
18	1	1014	CLA	CHC-C1C	4.13	1.47	1.35
18	1	1006	CLA	C3B-C2B	4.13	1.45	1.40
18	1	1008	CLA	CHC-C1C	4.13	1.47	1.35
18	1	1003	CLA	C3C-C2C	4.13	1.45	1.36
18	1	1006	CLA	CHC-C1C	4.14	1.47	1.35
18	1	1011	CLA	O2A-C1	4.14	1.58	1.46
18	K	1001	CLA	C3C-C2C	4.14	1.45	1.36
18	G	1003	CLA	O2D-CGD	4.14	1.43	1.33
18	A	1133	CLA	OBD-CAD	4.15	1.28	1.22
28	3	3011	CHL	O2A-CGA	4.15	1.45	1.33
18	4	4005	CLA	O2D-CGD	4.15	1.43	1.33
18	F	1302	CLA	OBD-CAD	4.15	1.28	1.22
18	3	3010	CLA	C3C-C2C	4.15	1.45	1.36
18	3	3004	CLA	CHC-C1C	4.16	1.47	1.35
18	F	1301	CLA	C3C-C2C	4.16	1.45	1.36
18	3	3003	CLA	C3C-C2C	4.16	1.45	1.36
18	2	2004	CLA	O2D-CGD	4.16	1.43	1.33
18	4	4016	CLA	C3C-C2C	4.16	1.45	1.36
21	A	5003	LHG	O8-C23	4.17	1.45	1.33
18	B	1226	CLA	CHC-C1C	4.17	1.47	1.35
18	1	1012	CLA	O2D-CGD	4.17	1.43	1.33
18	G	1003	CLA	C3B-C2B	4.17	1.45	1.40
18	3	3004	CLA	C3C-C2C	4.18	1.45	1.36
18	L	1501	CLA	O2D-CGD	4.18	1.44	1.33
18	3	3002	CLA	O2D-CGD	4.18	1.44	1.33
18	G	1003	CLA	C3C-C2C	4.18	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3001	CLA	C3B-C2B	4.19	1.45	1.40
18	B	1226	CLA	OBD-CAD	4.19	1.28	1.22
18	B	1211	CLA	OBD-CAD	4.19	1.28	1.22
18	3	3013	CLA	O2D-CGD	4.19	1.44	1.33
18	B	1206	CLA	CHC-C1C	4.19	1.47	1.35
18	3	3006	CLA	O2A-C1	4.19	1.59	1.46
18	3	3012	CLA	CHC-C1C	4.19	1.47	1.35
18	L	1501	CLA	CHC-C1C	4.20	1.47	1.35
18	1	1001	CLA	CHC-C1C	4.20	1.47	1.35
23	B	5005	LMG	O8-C28	4.21	1.45	1.33
18	B	1235	CLA	OBD-CAD	4.22	1.28	1.22
18	1	1005	CLA	CHC-C1C	4.22	1.47	1.35
18	3	3001	CLA	OBD-CAD	4.22	1.28	1.22
18	4	4017	CLA	CHC-C1C	4.22	1.47	1.35
18	3	3005	CLA	CHC-C1C	4.23	1.47	1.35
18	3	3007	CLA	C3B-C2B	4.23	1.45	1.40
18	3	3013	CLA	CHC-C1C	4.23	1.47	1.35
18	1	1007	CLA	O2D-CGD	4.23	1.44	1.33
18	2	2007	CLA	C3C-C2C	4.23	1.45	1.36
18	2	2005	CLA	C3C-C2C	4.23	1.45	1.36
18	L	1503	CLA	O2D-CGD	4.23	1.44	1.33
18	B	1220	CLA	OBD-CAD	4.24	1.28	1.22
18	1	1008	CLA	O2D-CGD	4.24	1.44	1.33
18	1	1003	CLA	O2A-C1	4.24	1.59	1.46
18	1	1004	CLA	O2D-CGD	4.24	1.44	1.33
18	2	2008	CLA	O2A-C1	4.24	1.59	1.46
18	G	1002	CLA	CHC-C1C	4.24	1.47	1.35
18	A	1130	CLA	OBD-CAD	4.24	1.28	1.22
18	3	3005	CLA	O2D-CGD	4.24	1.44	1.33
18	2	2009	CLA	CHC-C1C	4.25	1.47	1.35
18	3	3007	CLA	CHC-C1C	4.26	1.47	1.35
18	B	1205	CLA	OBD-CAD	4.26	1.28	1.22
18	A	1135	CLA	OBD-CAD	4.26	1.28	1.22
18	A	1114	CLA	CHC-C1C	4.27	1.47	1.35
18	A	1109	CLA	OBD-CAD	4.27	1.28	1.22
18	3	3013	CLA	C3C-C2C	4.27	1.46	1.36
18	B	1224	CLA	OBD-CAD	4.27	1.28	1.22
18	3	3004	CLA	O2D-CGD	4.27	1.44	1.33
18	2	2009	CLA	C3C-C2C	4.28	1.46	1.36
18	A	1128	CLA	OBD-CAD	4.28	1.28	1.22
18	3	3017	CLA	CHC-C1C	4.28	1.48	1.35
18	2	2009	CLA	O2D-CGD	4.28	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1126	CLA	OBD-CAD	4.28	1.28	1.22
18	3	3018	CLA	O2A-C1	4.29	1.59	1.46
18	3	3008	CLA	C3C-C2C	4.29	1.46	1.36
18	B	1238	CLA	OBD-CAD	4.29	1.28	1.22
18	A	1128	CLA	CHC-C1C	4.29	1.48	1.35
18	A	1103	CLA	C3C-C2C	4.29	1.46	1.36
18	B	1201	CLA	OBD-CAD	4.29	1.28	1.22
18	3	3001	CLA	CHC-C1C	4.29	1.48	1.35
18	A	1131	CLA	OBD-CAD	4.29	1.28	1.22
18	B	1236	CLA	OBD-CAD	4.30	1.28	1.22
18	A	1114	CLA	OBD-CAD	4.30	1.28	1.22
18	1	1011	CLA	C3B-C2B	4.30	1.45	1.40
18	2	2006	CLA	C3C-C2C	4.30	1.46	1.36
18	F	1302	CLA	C3C-C2C	4.30	1.46	1.36
18	4	4016	CLA	CHC-C1C	4.31	1.48	1.35
18	A	1022	CLA	C3B-C2B	4.31	1.45	1.40
18	A	1103	CLA	OBD-CAD	4.31	1.28	1.22
18	A	1137	CLA	OBD-CAD	4.31	1.28	1.22
18	1	1014	CLA	O2D-CGD	4.31	1.44	1.33
18	B	1230	CLA	C3C-C2C	4.31	1.46	1.36
18	A	1140	CLA	OBD-CAD	4.31	1.28	1.22
18	A	1133	CLA	CHC-C1C	4.32	1.48	1.35
18	2	2006	CLA	CHC-C1C	4.32	1.48	1.35
18	3	3012	CLA	O2D-CGD	4.32	1.44	1.33
21	A	7001	LHG	O8-C23	4.32	1.46	1.33
18	A	1139	CLA	OBD-CAD	4.32	1.28	1.22
18	B	1239	CLA	OBD-CAD	4.32	1.28	1.22
18	B	1202	CLA	CHC-C1C	4.33	1.48	1.35
18	A	1127	CLA	CHC-C1C	4.33	1.48	1.35
18	B	1210	CLA	CHC-C1C	4.33	1.48	1.35
18	2	2007	CLA	CHC-C1C	4.33	1.48	1.35
18	1	1003	CLA	C3B-C2B	4.33	1.45	1.40
18	4	4006	CLA	O2D-CGD	4.34	1.44	1.33
18	H	1000	CLA	CHC-C1C	4.34	1.48	1.35
18	A	1110	CLA	OBD-CAD	4.34	1.28	1.22
18	B	1213	CLA	OBD-CAD	4.34	1.28	1.22
18	B	1012	CLA	OBD-CAD	4.34	1.28	1.22
18	B	1228	CLA	OBD-CAD	4.34	1.28	1.22
18	G	1003	CLA	CHC-C1C	4.34	1.48	1.35
18	4	4003	CLA	O2A-C1	4.35	1.59	1.46
18	4	4003	CLA	CHC-C1C	4.35	1.48	1.35
18	4	4006	CLA	C3B-C2B	4.35	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1118	CLA	CHC-C1C	4.35	1.48	1.35
18	1	1004	CLA	C3B-C2B	4.35	1.45	1.40
18	4	4017	CLA	O2A-C1	4.35	1.59	1.46
18	A	1108	CLA	OBD-CAD	4.35	1.28	1.22
18	A	1135	CLA	CHC-C1C	4.35	1.48	1.35
18	A	1111	CLA	OBD-CAD	4.35	1.28	1.22
18	1	1014	CLA	C3B-C2B	4.36	1.45	1.40
18	B	1226	CLA	C3C-C2C	4.36	1.46	1.36
18	B	1021	CLA	C3C-C2C	4.36	1.46	1.36
18	B	1207	CLA	OBD-CAD	4.36	1.28	1.22
18	B	1224	CLA	CHC-C1C	4.36	1.48	1.35
18	B	1214	CLA	OBD-CAD	4.36	1.28	1.22
18	L	1503	CLA	C3B-C2B	4.36	1.45	1.40
18	B	1207	CLA	C3C-C2C	4.36	1.46	1.36
18	2	2003	CLA	O2A-C1	4.36	1.59	1.46
18	A	1117	CLA	OBD-CAD	4.36	1.28	1.22
18	B	1222	CLA	OBD-CAD	4.36	1.28	1.22
18	B	1021	CLA	CHC-C1C	4.37	1.48	1.35
18	B	1216	CLA	OBD-CAD	4.37	1.28	1.22
18	F	1302	CLA	CHC-C1C	4.37	1.48	1.35
18	A	1115	CLA	OBD-CAD	4.37	1.28	1.22
18	B	1209	CLA	CHC-C1C	4.37	1.48	1.35
18	J	1302	CLA	CHC-C1C	4.37	1.48	1.35
18	2	2005	CLA	CHC-C1C	4.37	1.48	1.35
18	A	1022	CLA	OBD-CAD	4.37	1.28	1.22
18	A	1112	CLA	OBD-CAD	4.37	1.28	1.22
18	A	1119	CLA	CHC-C1C	4.38	1.48	1.35
18	B	1201	CLA	C3C-C2C	4.38	1.46	1.36
18	L	1502	CLA	O2D-CGD	4.38	1.44	1.33
18	B	1232	CLA	OBD-CAD	4.38	1.28	1.22
18	B	1023	CLA	OBD-CAD	4.38	1.28	1.22
18	A	1134	CLA	CHC-C1C	4.38	1.48	1.35
18	H	1000	CLA	OBD-CAD	4.38	1.28	1.22
18	A	1129	CLA	OBD-CAD	4.38	1.28	1.22
18	B	1239	CLA	CHC-C1C	4.38	1.48	1.35
18	A	1113	CLA	OBD-CAD	4.38	1.28	1.22
18	A	1123	CLA	CHC-C1C	4.38	1.48	1.35
18	A	1111	CLA	C3C-C2C	4.38	1.46	1.36
18	1	1013	CLA	O2D-CGD	4.38	1.44	1.33
18	B	1213	CLA	C3C-C2C	4.39	1.46	1.36
18	A	1013	CLA	OBD-CAD	4.39	1.28	1.22
18	A	1116	CLA	CHC-C1C	4.39	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1006	CLA	O2D-CGD	4.39	1.44	1.33
18	A	1105	CLA	OBD-CAD	4.39	1.28	1.22
18	A	1107	CLA	OBD-CAD	4.39	1.29	1.22
18	B	1209	CLA	OBD-CAD	4.39	1.29	1.22
18	B	1234	CLA	OBD-CAD	4.39	1.29	1.22
18	B	1210	CLA	C3C-C2C	4.40	1.46	1.36
18	B	1218	CLA	OBD-CAD	4.40	1.29	1.22
18	4	4004	CLA	CHC-C1C	4.40	1.48	1.35
18	A	1132	CLA	OBD-CAD	4.40	1.29	1.22
18	B	1223	CLA	CHC-C1C	4.40	1.48	1.35
18	A	1122	CLA	OBD-CAD	4.40	1.29	1.22
18	3	3010	CLA	O2D-CGD	4.40	1.44	1.33
18	A	1237	CLA	CHC-C1C	4.40	1.48	1.35
18	B	1217	CLA	CHC-C1C	4.40	1.48	1.35
18	A	1137	CLA	CHC-C1C	4.40	1.48	1.35
18	F	1301	CLA	CHC-C1C	4.40	1.48	1.35
17	A	1011	CL0	OBD-CAD	4.40	1.29	1.22
18	3	3005	CLA	O2A-C1	4.41	1.59	1.46
18	B	1217	CLA	OBD-CAD	4.41	1.29	1.22
18	A	1151	CLA	OBD-CAD	4.41	1.29	1.22
18	3	3007	CLA	O2D-CGD	4.41	1.44	1.33
18	A	1124	CLA	OBD-CAD	4.41	1.29	1.22
18	B	1214	CLA	C3C-C2C	4.41	1.46	1.36
18	A	1136	CLA	OBD-CAD	4.41	1.29	1.22
18	B	1219	CLA	CHC-C1C	4.41	1.48	1.35
18	A	1121	CLA	CHC-C1C	4.41	1.48	1.35
18	B	1206	CLA	OBD-CAD	4.41	1.29	1.22
18	A	1111	CLA	CHC-C1C	4.41	1.48	1.35
18	B	1206	CLA	C3C-C2C	4.41	1.46	1.36
18	A	1122	CLA	CHC-C1C	4.41	1.48	1.35
18	A	1121	CLA	OBD-CAD	4.41	1.29	1.22
18	B	1204	CLA	OBD-CAD	4.42	1.29	1.22
18	B	1227	CLA	OBD-CAD	4.42	1.29	1.22
18	A	1138	CLA	OBD-CAD	4.42	1.29	1.22
18	A	1113	CLA	CHC-C1C	4.42	1.48	1.35
18	A	1117	CLA	CHC-C1C	4.42	1.48	1.35
18	A	1106	CLA	CHC-C1C	4.42	1.48	1.35
18	L	1503	CLA	CHC-C1C	4.42	1.48	1.35
18	A	1116	CLA	OBD-CAD	4.42	1.29	1.22
18	A	1109	CLA	CHC-C1C	4.42	1.48	1.35
18	B	1205	CLA	CHC-C1C	4.43	1.48	1.35
18	3	3003	CLA	C3B-C2B	4.43	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1127	CLA	OBD-CAD	4.43	1.29	1.22
18	B	1229	CLA	OBD-CAD	4.43	1.29	1.22
18	G	1001	CLA	O2D-CGD	4.43	1.44	1.33
18	B	1214	CLA	CHC-C1C	4.43	1.48	1.35
18	3	3018	CLA	OBD-CAD	4.43	1.29	1.22
17	A	1011	CL0	C3B-C2B	4.43	1.46	1.40
18	B	1219	CLA	OBD-CAD	4.43	1.29	1.22
18	B	1212	CLA	CHC-C1C	4.43	1.48	1.35
18	J	1302	CLA	OBD-CAD	4.43	1.29	1.22
18	A	1101	CLA	CHC-C1C	4.43	1.48	1.35
18	1	1004	CLA	O2A-C1	4.43	1.59	1.46
18	1	1001	CLA	O2D-CGD	4.44	1.44	1.33
18	3	3006	CLA	O2D-CGD	4.44	1.44	1.33
18	B	1212	CLA	OBD-CAD	4.44	1.29	1.22
18	A	1118	CLA	OBD-CAD	4.44	1.29	1.22
18	A	1104	CLA	OBD-CAD	4.44	1.29	1.22
18	A	1102	CLA	OBD-CAD	4.44	1.29	1.22
18	B	1207	CLA	CHC-C1C	4.44	1.48	1.35
18	2	2008	CLA	C3B-C2B	4.44	1.46	1.40
18	1	1006	CLA	O2A-C1	4.44	1.59	1.46
18	A	1125	CLA	C3C-C2C	4.44	1.46	1.36
18	A	1105	CLA	CHC-C1C	4.44	1.48	1.35
18	A	1112	CLA	O2D-CGD	4.44	1.44	1.33
18	B	1240	CLA	OBD-CAD	4.45	1.29	1.22
18	A	1101	CLA	OBD-CAD	4.45	1.29	1.22
18	A	1134	CLA	OBD-CAD	4.45	1.29	1.22
18	A	1120	CLA	CHC-C1C	4.45	1.48	1.35
18	B	1223	CLA	C3C-C2C	4.45	1.46	1.36
18	A	1103	CLA	CHC-C1C	4.45	1.48	1.35
18	B	1216	CLA	C3C-C2C	4.45	1.46	1.36
18	L	1502	CLA	CHC-C1C	4.45	1.48	1.35
18	A	1139	CLA	CHC-C1C	4.45	1.48	1.35
18	A	1237	CLA	C3C-C2C	4.45	1.46	1.36
18	A	1115	CLA	CHC-C1C	4.46	1.48	1.35
18	2	2009	CLA	O2A-C1	4.46	1.59	1.46
18	A	1134	CLA	C3C-C2C	4.46	1.46	1.36
17	A	1011	CL0	CHC-C1C	4.46	1.48	1.35
18	A	1140	CLA	C3C-C2C	4.46	1.46	1.36
18	A	1126	CLA	CHC-C1C	4.46	1.48	1.35
18	B	1222	CLA	O2A-C1	4.46	1.59	1.46
18	B	1208	CLA	OBD-CAD	4.46	1.29	1.22
18	B	1221	CLA	C3C-C2C	4.46	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1130	CLA	CHC-C1C	4.46	1.48	1.35
18	B	1218	CLA	CHC-C1C	4.46	1.48	1.35
18	A	1123	CLA	OBD-CAD	4.47	1.29	1.22
18	B	1210	CLA	OBD-CAD	4.47	1.29	1.22
18	F	1301	CLA	C3B-C2B	4.47	1.46	1.40
18	A	1151	CLA	CHC-C1C	4.47	1.48	1.35
18	B	1220	CLA	CHC-C1C	4.47	1.48	1.35
18	A	1139	CLA	C3C-C2C	4.47	1.46	1.36
18	B	1225	CLA	OBD-CAD	4.47	1.29	1.22
18	B	1204	CLA	CHC-C1C	4.47	1.48	1.35
18	B	1226	CLA	O2D-CGD	4.47	1.44	1.33
18	A	1125	CLA	CHC-C1C	4.47	1.48	1.35
18	A	1129	CLA	CHC-C1C	4.47	1.48	1.35
18	B	1228	CLA	CHC-C1C	4.47	1.48	1.35
18	B	1225	CLA	CHC-C1C	4.48	1.48	1.35
18	4	4009	CLA	O2A-C1	4.48	1.59	1.46
18	A	1117	CLA	C3C-C2C	4.48	1.46	1.36
18	B	1023	CLA	CHC-C1C	4.48	1.48	1.35
18	B	1203	CLA	C3C-C2C	4.48	1.46	1.36
18	B	1221	CLA	OBD-CAD	4.48	1.29	1.22
18	B	1203	CLA	CHC-C1C	4.48	1.48	1.35
18	A	1136	CLA	CHC-C1C	4.48	1.48	1.35
18	A	1114	CLA	C3C-C2C	4.48	1.46	1.36
18	A	1101	CLA	C3C-C2C	4.48	1.46	1.36
18	B	1240	CLA	C3C-C2C	4.48	1.46	1.36
18	B	1222	CLA	CHC-C1C	4.48	1.48	1.35
18	4	4002	CLA	O2D-CGD	4.48	1.44	1.33
18	B	1232	CLA	CHC-C1C	4.48	1.48	1.35
18	3	3003	CLA	O2A-C1	4.49	1.60	1.46
18	B	1215	CLA	C3C-C2C	4.49	1.46	1.36
18	B	1012	CLA	C3C-C2C	4.49	1.46	1.36
18	A	1112	CLA	CHC-C1C	4.49	1.48	1.35
18	1	1011	CLA	CHC-C1C	4.49	1.48	1.35
18	A	1131	CLA	CHC-C1C	4.49	1.48	1.35
18	B	1240	CLA	CHC-C1C	4.49	1.48	1.35
18	B	1215	CLA	OBD-CAD	4.49	1.29	1.22
18	B	1236	CLA	CHC-C1C	4.49	1.48	1.35
18	A	1127	CLA	C3C-C2C	4.50	1.46	1.36
18	A	1237	CLA	OBD-CAD	4.50	1.29	1.22
18	4	4001	CLA	O2D-CGD	4.50	1.44	1.33
18	A	1132	CLA	CHC-C1C	4.50	1.48	1.35
18	A	1102	CLA	CHC-C1C	4.50	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1123	CLA	C3C-C2C	4.50	1.46	1.36
18	B	1012	CLA	CHC-C1C	4.50	1.48	1.35
18	B	1213	CLA	CHC-C1C	4.50	1.48	1.35
18	A	1113	CLA	C3C-C2C	4.50	1.46	1.36
18	B	1227	CLA	C3C-C2C	4.50	1.46	1.36
18	B	1205	CLA	O2D-CGD	4.50	1.44	1.33
18	B	1215	CLA	CHC-C1C	4.50	1.48	1.35
18	A	1116	CLA	O2A-C1	4.50	1.60	1.46
18	A	1133	CLA	C3C-C2C	4.50	1.46	1.36
18	B	1234	CLA	O2A-C1	4.50	1.60	1.46
18	A	1022	CLA	CHC-C1C	4.50	1.48	1.35
18	B	1216	CLA	CHC-C1C	4.51	1.48	1.35
18	A	1102	CLA	C3C-C2C	4.51	1.46	1.36
18	A	1013	CLA	O2A-C1	4.51	1.60	1.46
18	A	1140	CLA	CHC-C1C	4.51	1.48	1.35
18	B	1201	CLA	CHC-C1C	4.51	1.48	1.35
18	A	1110	CLA	CHC-C1C	4.51	1.48	1.35
18	B	1023	CLA	C3C-C2C	4.51	1.46	1.36
18	B	1227	CLA	CHC-C1C	4.51	1.48	1.35
18	A	1126	CLA	O2A-C1	4.51	1.60	1.46
18	B	1238	CLA	CHC-C1C	4.52	1.48	1.35
18	1	1005	CLA	O2A-C1	4.52	1.60	1.46
18	A	1137	CLA	C3C-C2C	4.52	1.46	1.36
18	B	1202	CLA	C3C-C2C	4.52	1.46	1.36
18	A	1013	CLA	C3C-C2C	4.52	1.46	1.36
18	B	1220	CLA	C3C-C2C	4.52	1.46	1.36
18	L	1502	CLA	O2A-C1	4.52	1.60	1.46
18	B	1229	CLA	C3C-C2C	4.52	1.46	1.36
18	B	1236	CLA	C3C-C2C	4.52	1.46	1.36
18	B	1230	CLA	OBD-CAD	4.53	1.29	1.22
18	B	1021	CLA	OBD-CAD	4.53	1.29	1.22
18	B	1222	CLA	C3C-C2C	4.53	1.46	1.36
18	A	1106	CLA	OBD-CAD	4.53	1.29	1.22
18	B	1217	CLA	C3C-C2C	4.53	1.46	1.36
18	B	1202	CLA	OBD-CAD	4.53	1.29	1.22
18	A	1138	CLA	CHC-C1C	4.53	1.48	1.35
18	B	1205	CLA	C3C-C2C	4.53	1.46	1.36
18	J	1302	CLA	C3C-C2C	4.54	1.46	1.36
18	A	1122	CLA	C3C-C2C	4.54	1.46	1.36
18	2	2004	CLA	CHC-C1C	4.54	1.48	1.35
18	B	1216	CLA	O2A-C1	4.54	1.60	1.46
18	B	1209	CLA	C3C-C2C	4.54	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1229	CLA	CHC-C1C	4.54	1.48	1.35
18	A	1105	CLA	C3C-C2C	4.54	1.46	1.36
18	4	4003	CLA	C3B-C2B	4.54	1.46	1.40
18	A	1112	CLA	C3C-C2C	4.54	1.46	1.36
18	A	1104	CLA	O2D-CGD	4.54	1.44	1.33
18	A	1129	CLA	C3C-C2C	4.54	1.46	1.36
18	A	1109	CLA	C3C-C2C	4.54	1.46	1.36
18	H	1000	CLA	C3C-C2C	4.54	1.46	1.36
18	A	1107	CLA	CHC-C1C	4.54	1.48	1.35
18	B	1221	CLA	CHC-C1C	4.54	1.48	1.35
18	B	1240	CLA	O2A-C1	4.54	1.60	1.46
18	A	1116	CLA	C3C-C2C	4.54	1.46	1.36
18	B	1211	CLA	C3C-C2C	4.54	1.46	1.36
18	L	1502	CLA	C3B-C2B	4.55	1.46	1.40
18	A	1120	CLA	C3C-C2C	4.55	1.46	1.36
18	A	1106	CLA	C3C-C2C	4.55	1.46	1.36
18	A	1118	CLA	C3C-C2C	4.55	1.46	1.36
18	B	1238	CLA	C3C-C2C	4.55	1.46	1.36
18	A	1124	CLA	CHC-C1C	4.55	1.48	1.35
18	B	1218	CLA	C3C-C2C	4.55	1.46	1.36
18	B	1239	CLA	C3C-C2C	4.56	1.46	1.36
18	G	1001	CLA	O2A-C1	4.56	1.60	1.46
18	B	1231	CLA	O2A-C1	4.56	1.60	1.46
18	B	1012	CLA	O2A-C1	4.56	1.60	1.46
18	B	1230	CLA	CHC-C1C	4.56	1.48	1.35
18	A	1121	CLA	C3C-C2C	4.56	1.46	1.36
18	A	1108	CLA	CHC-C1C	4.57	1.48	1.35
18	2	2007	CLA	O2D-CGD	4.57	1.45	1.33
18	B	1225	CLA	C3C-C2C	4.57	1.46	1.36
18	A	1119	CLA	C3C-C2C	4.57	1.46	1.36
18	A	1103	CLA	O2A-C1	4.57	1.60	1.46
18	A	1136	CLA	C3C-C2C	4.57	1.46	1.36
18	B	1235	CLA	CHC-C1C	4.57	1.48	1.35
18	A	1126	CLA	C3C-C2C	4.57	1.46	1.36
18	3	3017	CLA	O2D-CGD	4.57	1.45	1.33
18	4	4003	CLA	O2D-CGD	4.57	1.45	1.33
18	2	2006	CLA	O2A-C1	4.57	1.60	1.46
18	A	1022	CLA	C3C-C2C	4.58	1.46	1.36
18	A	1132	CLA	C3C-C2C	4.58	1.46	1.36
18	A	1104	CLA	C3C-C2C	4.58	1.46	1.36
18	B	1208	CLA	CHC-C1C	4.58	1.48	1.35
18	F	1302	CLA	C3B-C2B	4.58	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1107	CLA	C3C-C2C	4.58	1.46	1.36
18	B	1222	CLA	O2D-CGD	4.58	1.45	1.33
18	4	4005	CLA	O2A-C1	4.58	1.60	1.46
18	B	1212	CLA	C3C-C2C	4.58	1.46	1.36
18	3	3008	CLA	O2D-CGD	4.59	1.45	1.33
18	B	1208	CLA	C3C-C2C	4.59	1.46	1.36
18	A	1115	CLA	C3C-C2C	4.59	1.46	1.36
18	2	2007	CLA	O2A-C1	4.59	1.60	1.46
18	B	1231	CLA	C3C-C2C	4.59	1.46	1.36
18	B	1232	CLA	C3C-C2C	4.59	1.46	1.36
17	A	1011	CL0	C3C-C2C	4.59	1.46	1.36
18	3	3018	CLA	O2D-CGD	4.59	1.45	1.33
18	2	2005	CLA	O2D-CGD	4.60	1.45	1.33
18	B	1230	CLA	O2A-C1	4.60	1.60	1.46
18	2	2005	CLA	O2A-C1	4.60	1.60	1.46
18	A	1124	CLA	C3C-C2C	4.60	1.46	1.36
18	A	1127	CLA	O2A-C1	4.60	1.60	1.46
18	B	1202	CLA	O2A-C1	4.60	1.60	1.46
18	B	1235	CLA	O2A-C1	4.60	1.60	1.46
18	A	1138	CLA	C3C-C2C	4.60	1.46	1.36
18	B	1219	CLA	C3C-C2C	4.60	1.46	1.36
18	A	1131	CLA	C3C-C2C	4.61	1.46	1.36
18	B	1232	CLA	O2A-C1	4.61	1.60	1.46
18	1	1003	CLA	O2D-CGD	4.61	1.45	1.33
18	2	2006	CLA	O2D-CGD	4.61	1.45	1.33
18	A	1110	CLA	C3C-C2C	4.61	1.46	1.36
18	F	1302	CLA	O2D-CGD	4.61	1.45	1.33
18	A	1108	CLA	C3C-C2C	4.61	1.46	1.36
18	A	1135	CLA	C3C-C2C	4.61	1.46	1.36
18	B	1235	CLA	C3C-C2C	4.61	1.46	1.36
18	B	1210	CLA	O2D-CGD	4.61	1.45	1.33
18	B	1231	CLA	OBD-CAD	4.62	1.29	1.22
18	A	1112	CLA	O2A-C1	4.62	1.60	1.46
18	G	1002	CLA	O2D-CGD	4.62	1.45	1.33
18	F	1302	CLA	O2A-C1	4.62	1.60	1.46
18	L	1503	CLA	O2A-C1	4.62	1.60	1.46
18	B	1224	CLA	C3C-C2C	4.62	1.46	1.36
18	A	1128	CLA	C3C-C2C	4.62	1.46	1.36
18	4	4012	CLA	O2A-C1	4.62	1.60	1.46
18	A	1013	CLA	CHC-C1C	4.62	1.49	1.35
18	4	4002	CLA	O2A-C1	4.63	1.60	1.46
18	B	1218	CLA	O2A-C1	4.63	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1119	CLA	O2A-C1	4.63	1.60	1.46
18	B	1216	CLA	C3B-C2B	4.63	1.46	1.40
18	B	1204	CLA	C3C-C2C	4.63	1.46	1.36
18	A	1112	CLA	C3B-C2B	4.63	1.46	1.40
18	L	1501	CLA	O2A-C1	4.63	1.60	1.46
18	4	4001	CLA	O2A-C1	4.63	1.60	1.46
18	B	1234	CLA	CHC-C1C	4.63	1.49	1.35
18	3	3010	CLA	O2A-C1	4.64	1.60	1.46
18	B	1226	CLA	C3B-C2B	4.64	1.46	1.40
18	A	1104	CLA	O2A-C1	4.64	1.60	1.46
18	B	1227	CLA	O2A-C1	4.64	1.60	1.46
18	B	1023	CLA	O2A-C1	4.64	1.60	1.46
18	3	3012	CLA	O2A-C1	4.64	1.60	1.46
18	A	1106	CLA	O2A-C1	4.64	1.60	1.46
18	A	1122	CLA	O2A-C1	4.64	1.60	1.46
18	B	1012	CLA	C3B-C2B	4.64	1.46	1.40
18	A	1133	CLA	O2A-C1	4.65	1.60	1.46
18	B	1203	CLA	O2A-C1	4.65	1.60	1.46
18	A	1130	CLA	C3C-C2C	4.65	1.46	1.36
18	B	1226	CLA	O2A-C1	4.65	1.60	1.46
18	A	1139	CLA	O2A-C1	4.65	1.60	1.46
18	A	1237	CLA	O2A-C1	4.65	1.60	1.46
18	B	1210	CLA	O2A-C1	4.65	1.60	1.46
18	A	1121	CLA	O2A-C1	4.65	1.60	1.46
18	A	1022	CLA	O2A-C1	4.65	1.60	1.46
18	B	1223	CLA	O2A-C1	4.65	1.60	1.46
18	A	1123	CLA	O2A-C1	4.66	1.60	1.46
17	A	1011	CL0	O2A-C1	4.66	1.60	1.46
18	4	4002	CLA	C3B-C2B	4.66	1.46	1.40
18	A	1132	CLA	O2D-CGD	4.66	1.45	1.33
18	2	2004	CLA	O2A-C1	4.66	1.60	1.46
18	B	1211	CLA	CHC-C1C	4.66	1.49	1.35
18	B	1213	CLA	O2A-C1	4.66	1.60	1.46
18	3	3019	CLA	C3B-C4B	4.67	1.48	1.40
18	A	1136	CLA	O2A-C1	4.67	1.60	1.46
18	3	3003	CLA	O2D-CGD	4.67	1.45	1.33
18	A	1117	CLA	O2A-C1	4.67	1.60	1.46
18	B	1229	CLA	O2A-C1	4.67	1.60	1.46
18	A	1135	CLA	O2A-C1	4.67	1.60	1.46
18	2	2005	CLA	C3B-C2B	4.67	1.46	1.40
18	A	1134	CLA	O2A-C1	4.68	1.60	1.46
18	B	1021	CLA	O2A-C1	4.68	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1104	CLA	CHC-C1C	4.68	1.49	1.35
18	B	1224	CLA	O2A-C1	4.68	1.60	1.46
18	2	2001	CLA	O2A-C1	4.68	1.60	1.46
18	A	1124	CLA	O2A-C1	4.68	1.60	1.46
18	F	1301	CLA	O2D-CGD	4.68	1.45	1.33
18	B	1234	CLA	C3C-C2C	4.69	1.46	1.36
18	B	1219	CLA	O2A-C1	4.69	1.60	1.46
18	A	1151	CLA	O2A-C1	4.69	1.60	1.46
18	B	1228	CLA	O2A-C1	4.70	1.60	1.46
18	A	1131	CLA	O2A-C1	4.70	1.60	1.46
18	B	1218	CLA	O2D-CGD	4.71	1.45	1.33
18	A	1125	CLA	O2A-C1	4.71	1.60	1.46
18	A	1109	CLA	O2A-C1	4.71	1.60	1.46
18	2	2006	CLA	C3B-C2B	4.71	1.46	1.40
18	A	1102	CLA	O2D-CGD	4.71	1.45	1.33
18	A	1138	CLA	O2A-C1	4.71	1.60	1.46
18	B	1228	CLA	C3C-C2C	4.71	1.47	1.36
18	B	1220	CLA	O2A-C1	4.71	1.60	1.46
18	A	1136	CLA	O2D-CGD	4.72	1.45	1.33
18	G	1003	CLA	O2A-C1	4.72	1.60	1.46
18	B	1214	CLA	O2A-C1	4.72	1.60	1.46
18	B	1231	CLA	CHC-C1C	4.72	1.49	1.35
18	1	1008	CLA	C3B-C2B	4.72	1.46	1.40
18	A	1101	CLA	O2A-C1	4.73	1.60	1.46
18	A	1107	CLA	O2D-CGD	4.73	1.45	1.33
18	A	1129	CLA	O2A-C1	4.73	1.60	1.46
18	B	1212	CLA	O2A-C1	4.73	1.60	1.46
18	B	1229	CLA	O2D-CGD	4.73	1.45	1.33
21	B	5004	LHG	O7-C7	4.73	1.45	1.35
18	A	1105	CLA	O2A-C1	4.74	1.60	1.46
18	A	1120	CLA	O2A-C1	4.74	1.60	1.46
18	A	1139	CLA	O2D-CGD	4.74	1.45	1.33
18	A	1129	CLA	O2D-CGD	4.74	1.45	1.33
18	A	1102	CLA	O2A-C1	4.74	1.60	1.46
18	B	1206	CLA	O2A-C1	4.75	1.60	1.46
18	A	1125	CLA	O2D-CGD	4.75	1.45	1.33
18	A	1128	CLA	O2A-C1	4.75	1.60	1.46
18	B	1207	CLA	O2A-C1	4.75	1.60	1.46
18	B	1201	CLA	O2D-CGD	4.75	1.45	1.33
18	B	1240	CLA	O2D-CGD	4.75	1.45	1.33
18	B	1211	CLA	O2A-C1	4.75	1.60	1.46
18	B	1208	CLA	O2A-C1	4.75	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1124	CLA	O2D-CGD	4.75	1.45	1.33
18	A	1130	CLA	O2A-C1	4.76	1.60	1.46
18	3	3001	CLA	O2A-C1	4.76	1.60	1.46
18	B	1239	CLA	O2A-C1	4.76	1.60	1.46
18	A	1137	CLA	O2A-C1	4.76	1.60	1.46
18	H	1000	CLA	C3B-C2B	4.76	1.46	1.40
18	B	1211	CLA	O2D-CGD	4.76	1.45	1.33
18	A	1132	CLA	O2A-C1	4.76	1.60	1.46
18	B	1205	CLA	O2A-C1	4.76	1.60	1.46
18	B	1232	CLA	C3B-C2B	4.77	1.46	1.40
18	1	1001	CLA	O2A-C1	4.77	1.60	1.46
18	B	1221	CLA	O2D-CGD	4.77	1.45	1.33
18	K	1001	CLA	O2D-CGD	4.77	1.45	1.33
18	3	3004	CLA	O2A-C1	4.77	1.60	1.46
18	J	1302	CLA	O2A-C1	4.77	1.60	1.46
18	B	1223	CLA	O2D-CGD	4.77	1.45	1.33
18	B	1220	CLA	C3B-C2B	4.78	1.46	1.40
18	B	1210	CLA	C3B-C2B	4.78	1.46	1.40
18	B	1220	CLA	O2D-CGD	4.78	1.45	1.33
18	B	1201	CLA	O2A-C1	4.78	1.60	1.46
18	A	1137	CLA	O2D-CGD	4.78	1.45	1.33
18	B	1224	CLA	C3B-C2B	4.78	1.46	1.40
18	A	1126	CLA	O2D-CGD	4.79	1.45	1.33
18	3	3008	CLA	O2A-C1	4.79	1.60	1.46
18	B	1203	CLA	O2D-CGD	4.79	1.45	1.33
18	B	1212	CLA	O2D-CGD	4.79	1.45	1.33
18	B	1215	CLA	O2A-C1	4.80	1.60	1.46
18	B	1235	CLA	O2D-CGD	4.80	1.45	1.33
18	B	1236	CLA	O2A-C1	4.80	1.60	1.46
18	A	1135	CLA	O2D-CGD	4.80	1.45	1.33
18	A	1110	CLA	O2D-CGD	4.80	1.45	1.33
18	B	1205	CLA	C3B-C2B	4.81	1.46	1.40
18	A	1122	CLA	O2D-CGD	4.82	1.45	1.33
18	A	1140	CLA	O2A-C1	4.82	1.61	1.46
18	B	1202	CLA	O2D-CGD	4.82	1.45	1.33
18	B	1225	CLA	O2A-C1	4.82	1.61	1.46
18	A	1117	CLA	O2D-CGD	4.82	1.45	1.33
18	2	2007	CLA	C3B-C2B	4.82	1.46	1.40
18	A	1101	CLA	O2D-CGD	4.82	1.45	1.33
18	B	1238	CLA	O2A-C1	4.82	1.61	1.46
18	B	1204	CLA	O2A-C1	4.82	1.61	1.46
18	A	1134	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1011	CL0	O2D-CGD	4.83	1.45	1.33
18	B	1012	CLA	O2D-CGD	4.83	1.45	1.33
18	B	1231	CLA	O2D-CGD	4.83	1.45	1.33
18	A	1111	CLA	O2A-C1	4.83	1.61	1.46
18	3	3007	CLA	O2A-C1	4.83	1.61	1.46
18	A	1109	CLA	O2D-CGD	4.83	1.45	1.33
18	A	1131	CLA	O2D-CGD	4.83	1.45	1.33
18	A	1128	CLA	C3B-C2B	4.83	1.46	1.40
18	B	1215	CLA	O2D-CGD	4.83	1.45	1.33
18	B	1239	CLA	O2D-CGD	4.84	1.45	1.33
18	4	4016	CLA	O2D-CGD	4.84	1.45	1.33
18	B	1232	CLA	O2D-CGD	4.84	1.45	1.33
18	B	1211	CLA	C3B-C2B	4.84	1.46	1.40
18	A	1116	CLA	O2D-CGD	4.84	1.45	1.33
18	2	2019	CLA	C2B-C1B	4.84	1.48	1.40
18	J	1302	CLA	O2D-CGD	4.84	1.45	1.33
18	A	1110	CLA	O2A-C1	4.85	1.61	1.46
18	A	1237	CLA	O2D-CGD	4.85	1.45	1.33
18	B	1221	CLA	C3B-C2B	4.85	1.46	1.40
18	B	1221	CLA	O2A-C1	4.85	1.61	1.46
18	B	1236	CLA	O2D-CGD	4.85	1.45	1.33
18	A	1119	CLA	C3B-C2B	4.85	1.46	1.40
18	B	1224	CLA	O2D-CGD	4.86	1.45	1.33
18	A	1013	CLA	O2D-CGD	4.86	1.45	1.33
18	A	1118	CLA	O2D-CGD	4.86	1.45	1.33
18	B	1208	CLA	O2D-CGD	4.86	1.45	1.33
18	B	1023	CLA	C3B-C2B	4.86	1.46	1.40
18	B	1217	CLA	O2D-CGD	4.87	1.45	1.33
18	A	1123	CLA	O2D-CGD	4.87	1.45	1.33
18	2	2016	CLA	O2A-C1	4.87	1.61	1.46
18	B	1223	CLA	C3B-C2B	4.87	1.46	1.40
18	B	1227	CLA	O2D-CGD	4.87	1.45	1.33
18	A	1128	CLA	O2D-CGD	4.87	1.45	1.33
18	B	1228	CLA	O2D-CGD	4.88	1.45	1.33
18	B	1214	CLA	O2D-CGD	4.88	1.45	1.33
18	B	1207	CLA	O2D-CGD	4.89	1.45	1.33
18	B	1234	CLA	O2D-CGD	4.89	1.45	1.33
18	A	1133	CLA	C3B-C2B	4.89	1.46	1.40
18	2	2019	CLA	C3C-C2C	4.89	1.46	1.35
18	A	1115	CLA	O2D-CGD	4.89	1.45	1.33
18	B	1213	CLA	O2D-CGD	4.89	1.45	1.33
18	B	1209	CLA	O2D-CGD	4.89	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1114	CLA	O2D-CGD	4.90	1.45	1.33
18	A	1124	CLA	C3B-C2B	4.90	1.46	1.40
18	B	1206	CLA	O2D-CGD	4.90	1.45	1.33
18	B	1023	CLA	O2D-CGD	4.90	1.45	1.33
18	A	1111	CLA	O2D-CGD	4.90	1.45	1.33
18	A	1127	CLA	O2D-CGD	4.90	1.45	1.33
18	A	1140	CLA	O2D-CGD	4.90	1.45	1.33
18	A	1121	CLA	O2D-CGD	4.90	1.45	1.33
18	A	1105	CLA	O2D-CGD	4.91	1.45	1.33
18	B	1216	CLA	O2D-CGD	4.91	1.45	1.33
18	B	1021	CLA	O2D-CGD	4.91	1.45	1.33
18	A	1132	CLA	C3B-C2B	4.91	1.46	1.40
18	A	1103	CLA	O2D-CGD	4.91	1.45	1.33
18	A	1119	CLA	O2D-CGD	4.92	1.45	1.33
18	A	1108	CLA	O2D-CGD	4.92	1.45	1.33
18	A	1126	CLA	C3B-C2B	4.92	1.46	1.40
18	A	1105	CLA	C3B-C2B	4.92	1.46	1.40
18	B	1225	CLA	C3B-C2B	4.92	1.46	1.40
18	B	1230	CLA	O2D-CGD	4.92	1.45	1.33
18	A	1130	CLA	O2D-CGD	4.92	1.45	1.33
18	A	1111	CLA	C3B-C2B	4.92	1.46	1.40
18	A	1122	CLA	C3B-C2B	4.92	1.46	1.40
18	B	1238	CLA	O2D-CGD	4.93	1.45	1.33
18	A	1114	CLA	C3B-C2B	4.93	1.46	1.40
18	A	1151	CLA	O2D-CGD	4.93	1.45	1.33
18	B	1204	CLA	O2D-CGD	4.93	1.45	1.33
18	B	1225	CLA	O2D-CGD	4.93	1.45	1.33
18	A	1237	CLA	C3B-C2B	4.94	1.46	1.40
18	B	1239	CLA	C3B-C2B	4.94	1.46	1.40
18	4	4007	CLA	O2A-C1	4.94	1.61	1.46
18	B	1219	CLA	O2D-CGD	4.94	1.45	1.33
18	A	1113	CLA	O2D-CGD	4.95	1.46	1.33
18	B	1227	CLA	C3B-C2B	4.95	1.46	1.40
18	B	1214	CLA	C3B-C2B	4.95	1.46	1.40
18	A	1113	CLA	C3B-C2B	4.96	1.46	1.40
18	A	1107	CLA	O2A-C1	4.96	1.61	1.46
18	A	1120	CLA	O2D-CGD	4.96	1.46	1.33
18	A	1022	CLA	O2D-CGD	4.97	1.46	1.33
18	A	1107	CLA	C3B-C2B	4.97	1.46	1.40
18	2	2003	CLA	C3B-C2B	4.97	1.46	1.40
18	A	1106	CLA	O2D-CGD	4.97	1.46	1.33
18	B	1240	CLA	C3B-C2B	4.98	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1133	CLA	O2D-CGD	4.99	1.46	1.33
18	H	1000	CLA	O2D-CGD	5.00	1.46	1.33
18	A	1109	CLA	C3B-C2B	5.00	1.46	1.40
18	A	1129	CLA	C3B-C2B	5.01	1.46	1.40
18	B	1231	CLA	C3B-C2B	5.01	1.46	1.40
18	B	1219	CLA	C3B-C2B	5.01	1.46	1.40
18	A	1103	CLA	C3B-C2B	5.01	1.46	1.40
18	A	1138	CLA	O2D-CGD	5.02	1.46	1.33
18	A	1151	CLA	C3C-C2C	5.02	1.47	1.36
18	A	1121	CLA	C3B-C2B	5.02	1.46	1.40
18	B	1204	CLA	C3B-C2B	5.03	1.46	1.40
18	B	1203	CLA	C3B-C2B	5.03	1.46	1.40
18	4	4016	CLA	C3B-C2B	5.03	1.46	1.40
18	A	1115	CLA	C3B-C2B	5.04	1.46	1.40
18	3	3019	CLA	C3C-C2C	5.04	1.46	1.35
18	B	1235	CLA	C3B-C2B	5.04	1.46	1.40
18	A	1104	CLA	C3B-C2B	5.05	1.46	1.40
18	A	1013	CLA	C3B-C2B	5.05	1.46	1.40
18	A	1101	CLA	C3B-C2B	5.05	1.46	1.40
18	J	1302	CLA	C3B-C2B	5.06	1.46	1.40
18	A	1131	CLA	C3B-C2B	5.06	1.46	1.40
18	A	1116	CLA	C3B-C2B	5.06	1.46	1.40
18	B	1236	CLA	C3B-C2B	5.06	1.46	1.40
18	A	1120	CLA	C3B-C2B	5.06	1.46	1.40
18	B	1208	CLA	C3B-C2B	5.08	1.46	1.40
18	3	3006	CLA	C3B-C2B	5.09	1.46	1.40
18	A	1140	CLA	C3B-C2B	5.09	1.46	1.40
18	A	1125	CLA	C3B-C2B	5.09	1.46	1.40
18	A	1139	CLA	C3B-C2B	5.09	1.46	1.40
18	A	1110	CLA	C3B-C2B	5.09	1.46	1.40
18	A	1136	CLA	C3B-C2B	5.11	1.46	1.40
18	A	1134	CLA	C3B-C2B	5.11	1.46	1.40
18	B	1238	CLA	C3B-C2B	5.11	1.46	1.40
18	2	2016	CLA	OBD-CAD	5.13	1.30	1.22
18	B	1217	CLA	C3B-C2B	5.13	1.46	1.40
18	B	1228	CLA	C3B-C2B	5.13	1.46	1.40
18	A	1118	CLA	C3B-C2B	5.14	1.46	1.40
18	B	1212	CLA	C3B-C2B	5.15	1.46	1.40
18	B	1218	CLA	C3B-C2B	5.17	1.46	1.40
18	A	1135	CLA	C3B-C2B	5.18	1.46	1.40
18	A	1117	CLA	C3B-C2B	5.19	1.46	1.40
18	A	1151	CLA	C3B-C2B	5.20	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	5001	PQN	C10-C5	5.21	1.48	1.40
18	A	1137	CLA	C3B-C2B	5.22	1.47	1.40
18	B	1229	CLA	C3B-C2B	5.23	1.47	1.40
18	B	1206	CLA	C3B-C2B	5.23	1.47	1.40
18	B	1201	CLA	C3B-C2B	5.24	1.47	1.40
18	B	1202	CLA	C3B-C2B	5.24	1.47	1.40
18	B	1207	CLA	C3B-C2B	5.24	1.47	1.40
18	B	1215	CLA	C3B-C2B	5.24	1.47	1.40
18	B	1230	CLA	C3B-C2B	5.27	1.47	1.40
18	A	1127	CLA	C3B-C2B	5.31	1.47	1.40
18	A	1138	CLA	C3B-C2B	5.32	1.47	1.40
18	A	1108	CLA	C3B-C2B	5.35	1.47	1.40
18	B	1021	CLA	C3B-C2B	5.35	1.47	1.40
18	3	3008	CLA	C3B-C2B	5.37	1.47	1.40
18	B	1234	CLA	C3B-C2B	5.39	1.47	1.40
18	A	1102	CLA	C3B-C2B	5.44	1.47	1.40
18	B	1222	CLA	C3B-C2B	5.49	1.47	1.40
18	2	2016	CLA	O2D-CGD	5.49	1.47	1.33
18	B	1213	CLA	C3B-C2B	5.50	1.47	1.40
18	A	1106	CLA	C3B-C2B	5.51	1.47	1.40
18	3	3019	CLA	C2B-C1B	5.56	1.49	1.40
18	A	1123	CLA	C3B-C2B	5.56	1.47	1.40
18	A	1130	CLA	C3B-C2B	5.63	1.47	1.40
18	B	1209	CLA	C3B-C2B	5.66	1.47	1.40
20	B	5002	PQN	C10-C5	5.69	1.49	1.40
18	4	4008	CLA	O2A-C1	5.90	1.59	1.45
18	2	2019	CLA	CHC-C1C	5.99	1.47	1.38
18	3	3002	CLA	O2A-C1	6.00	1.60	1.45
18	1	1002	CLA	O2A-C1	6.03	1.60	1.45
18	1	1008	CLA	O2A-C1	6.03	1.60	1.45
20	A	5001	PQN	C3-C2	6.04	1.49	1.35
18	1	1007	CLA	O2A-C1	6.11	1.60	1.45
18	1	1013	CLA	O2A-C1	6.11	1.60	1.45
18	B	1217	CLA	O2A-C1	6.11	1.60	1.45
18	3	3017	CLA	O2A-C1	6.13	1.60	1.45
18	K	1001	CLA	O2A-C1	6.13	1.60	1.45
18	A	1108	CLA	O2A-C1	6.15	1.60	1.45
18	2	2002	CLA	O2A-C1	6.16	1.60	1.45
20	B	5002	PQN	C3-C2	6.16	1.49	1.35
18	H	1000	CLA	O2A-C1	6.17	1.60	1.45
18	A	1115	CLA	O2A-C1	6.17	1.60	1.45
18	3	3013	CLA	O2A-C1	6.17	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4016	CLA	O2A-C1	6.18	1.60	1.45
18	A	1113	CLA	O2A-C1	6.18	1.60	1.45
18	B	1209	CLA	O2A-C1	6.19	1.60	1.45
18	A	1118	CLA	O2A-C1	6.21	1.60	1.45
18	A	1114	CLA	O2A-C1	6.21	1.60	1.45
18	G	1002	CLA	O2A-C1	6.21	1.60	1.45
18	1	1014	CLA	O2A-C1	6.33	1.60	1.45
18	3	3019	CLA	CHC-C1C	6.72	1.48	1.38
27	3	3501	LUT	C24-C25	13.57	1.50	1.33
27	4	4502	LUT	C24-C25	13.61	1.50	1.33
27	3	3502	LUT	C24-C25	13.62	1.50	1.33
27	4	4501	LUT	C24-C25	13.82	1.50	1.33
27	4	4503	LUT	C24-C25	13.82	1.50	1.33
27	1	1502	LUT	C24-C25	13.84	1.51	1.33
27	1	1501	LUT	C24-C25	14.25	1.51	1.33
27	2	2501	LUT	C24-C25	14.32	1.51	1.33
27	I	6018	LUT	C24-C25	14.39	1.51	1.33
27	2	2502	LUT	C24-C25	14.40	1.51	1.33

All (2912) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	4013	CHL	C3C-C4C-NC	-8.29	105.27	110.05
22	A	6017	BCR	C15-C14-C13	-7.65	116.11	127.22
28	2	2011	CHL	C3C-C4C-NC	-7.47	105.74	110.05
28	4	4011	CHL	C3C-C4C-NC	-7.44	105.76	110.05
18	2	2019	CLA	C3B-C2B-C1B	-7.35	99.86	106.29
18	3	3019	CLA	C3B-C2B-C1B	-7.35	99.86	106.29
28	4	4010	CHL	C3C-C4C-NC	-7.05	105.99	110.05
28	3	3011	CHL	C3C-C4C-NC	-7.05	105.99	110.05
27	4	4503	LUT	C7-C8-C9	-6.89	115.80	126.21
27	3	3502	LUT	C7-C8-C9	-6.80	115.93	126.21
28	2	2010	CHL	C3C-C4C-NC	-6.75	106.16	110.05
28	1	1009	CHL	C3C-C4C-NC	-6.48	106.31	110.05
18	3	3008	CLA	C1C-C2C-C3C	-6.21	100.04	106.93
22	A	6007	BCR	C24-C23-C22	-6.19	116.86	126.21
18	4	4001	CLA	C1C-C2C-C3C	-6.16	100.10	106.93
18	3	3006	CLA	OBD-CAD-C3D	-6.06	117.38	128.09
22	A	6008	BCR	C15-C14-C13	-6.04	118.44	127.22
22	J	6012	BCR	C24-C23-C22	-6.00	117.15	126.21
28	2	2013	CHL	C3C-C4C-NC	-5.97	106.61	110.05
22	J	6013	BCR	C24-C23-C22	-5.86	117.35	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4007	CLA	O2A-CGA-O1A	-5.84	108.20	123.51
28	1	1010	CHL	C3C-C4C-NC	-5.81	106.70	110.05
18	2	2001	CLA	C1C-C2C-C3C	-5.72	100.58	106.93
18	K	1001	CLA	C1C-C2C-C3C	-5.67	100.64	106.93
18	2	2019	CLA	C3C-C2C-C1C	-5.65	99.90	107.18
18	2	2009	CLA	C1C-C2C-C3C	-5.62	100.70	106.93
18	3	3010	CLA	C1C-C2C-C3C	-5.62	100.70	106.93
18	3	3001	CLA	C1C-C2C-C3C	-5.61	100.71	106.93
18	2	2016	CLA	C1C-C2C-C3C	-5.60	100.72	106.93
18	1	1003	CLA	O2A-CGA-O1A	-5.58	108.87	123.51
22	3	3503	BCR	C33-C5-C6	-5.57	118.69	124.62
22	L	6020	BCR	C24-C23-C22	-5.57	117.80	126.21
18	3	3003	CLA	C1C-C2C-C3C	-5.56	100.77	106.93
18	4	4002	CLA	C1C-C2C-C3C	-5.56	100.77	106.93
18	1	1004	CLA	O2A-CGA-O1A	-5.55	108.95	123.51
27	1	1502	LUT	C7-C8-C9	-5.51	117.88	126.21
18	2	2001	CLA	O2A-CGA-O1A	-5.46	109.20	123.51
22	B	6009	BCR	C24-C23-C22	-5.43	118.00	126.21
18	1	1013	CLA	C1C-C2C-C3C	-5.43	100.91	106.93
27	3	3501	LUT	C22-C23-C24	-5.41	104.89	111.19
18	2	2008	CLA	C1C-C2C-C3C	-5.40	100.94	106.93
18	B	1205	CLA	O2A-CGA-O1A	-5.39	109.38	123.51
18	3	3004	CLA	C1C-C2C-C3C	-5.37	100.97	106.93
18	B	1226	CLA	O2A-CGA-O1A	-5.37	109.44	123.51
18	G	1001	CLA	O2A-CGA-O1A	-5.35	109.48	123.51
18	3	3005	CLA	C1C-C2C-C3C	-5.35	101.00	106.93
29	4	4505	ZEX	C7-C8-C9	-5.35	118.13	126.21
18	4	4007	CLA	C1C-C2C-C3C	-5.35	101.00	106.93
18	B	1235	CLA	O2A-CGA-O1A	-5.33	109.53	123.51
27	3	3502	LUT	C18-C5-C6	-5.33	118.94	124.62
18	2	2008	CLA	O2A-CGA-O1A	-5.32	109.55	123.51
18	B	1206	CLA	C1C-C2C-C3C	-5.32	101.03	106.93
18	A	1118	CLA	C1C-C2C-C3C	-5.30	101.05	106.93
18	B	1226	CLA	C1C-C2C-C3C	-5.29	101.06	106.93
18	B	1229	CLA	O2A-CGA-O1A	-5.29	109.65	123.51
18	4	4004	CLA	C1C-C2C-C3C	-5.28	101.07	106.93
18	4	4017	CLA	O2A-CGA-O1A	-5.28	109.67	123.51
18	L	1502	CLA	O2A-CGA-O1A	-5.28	109.68	123.51
22	B	6004	BCR	C24-C23-C22	-5.25	118.28	126.21
18	4	4012	CLA	C1C-C2C-C3C	-5.25	101.11	106.93
18	A	1101	CLA	O2A-CGA-O1A	-5.24	109.77	123.51
18	1	1012	CLA	C1C-C2C-C3C	-5.23	101.13	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1139	CLA	C1C-C2C-C3C	-5.22	101.15	106.93
18	L	1503	CLA	O2A-CGA-O1A	-5.21	109.84	123.51
18	4	4005	CLA	C1C-C2C-C3C	-5.21	101.15	106.93
18	1	1003	CLA	C1C-C2C-C3C	-5.19	101.17	106.93
27	4	4503	LUT	C1-C6-C5	-5.19	115.56	122.50
18	1	1005	CLA	O2A-CGA-O1A	-5.18	109.92	123.51
18	2	2004	CLA	O2A-CGA-O1A	-5.18	109.94	123.51
18	3	3018	CLA	C1C-C2C-C3C	-5.17	101.20	106.93
17	A	1011	CL0	O2A-CGA-O1A	-5.17	109.97	123.51
18	4	4009	CLA	C1C-C2C-C3C	-5.17	101.20	106.93
18	J	1302	CLA	O2A-CGA-O1A	-5.17	109.97	123.51
27	2	2502	LUT	C22-C23-C24	-5.16	105.17	111.19
18	A	1128	CLA	O2A-CGA-O1A	-5.16	109.98	123.51
18	3	3006	CLA	O2A-CGA-O1A	-5.14	110.04	123.51
18	B	1217	CLA	C1C-C2C-C3C	-5.13	101.24	106.93
18	3	3012	CLA	C3B-CAB-CBB	-5.13	116.09	126.40
18	B	1239	CLA	C1C-C2C-C3C	-5.12	101.26	106.93
18	B	1224	CLA	O2A-CGA-O1A	-5.12	110.10	123.51
18	2	2012	CLA	C3B-CAB-CBB	-5.11	116.11	126.40
18	1	1006	CLA	C1C-C2C-C3C	-5.11	101.26	106.93
18	B	1218	CLA	C1C-C2C-C3C	-5.11	101.27	106.93
18	4	4008	CLA	C1C-C2C-C3C	-5.10	101.27	106.93
18	H	1000	CLA	C1C-C2C-C3C	-5.10	101.28	106.93
18	1	1008	CLA	C1C-C2C-C3C	-5.10	101.28	106.93
17	A	1011	CL0	C1C-C2C-C3C	-5.09	101.28	106.93
18	G	1001	CLA	C1C-C2C-C3C	-5.09	101.29	106.93
22	A	6008	BCR	C24-C23-C22	-5.08	118.54	126.21
18	3	3012	CLA	C1C-C2C-C3C	-5.07	101.30	106.93
22	A	6011	BCR	C3-C4-C5	-5.07	105.47	113.87
18	G	1003	CLA	C1C-C2C-C3C	-5.06	101.32	106.93
18	2	2005	CLA	C1C-C2C-C3C	-5.06	101.32	106.93
22	K	2011	BCR	C24-C23-C22	-5.05	118.57	126.21
18	A	1116	CLA	O2A-CGA-O1A	-5.05	110.27	123.51
18	B	1218	CLA	O2A-CGA-O1A	-5.04	110.29	123.51
18	A	1151	CLA	C1C-C2C-C3C	-5.04	101.34	106.93
22	F	6014	BCR	C24-C23-C22	-5.04	118.59	126.21
18	A	1123	CLA	C1C-C2C-C3C	-5.04	101.34	106.93
18	A	1135	CLA	C1C-C2C-C3C	-5.04	101.34	106.93
18	A	1114	CLA	C1C-C2C-C3C	-5.04	101.34	106.93
18	A	1116	CLA	C1C-C2C-C3C	-5.04	101.34	106.93
27	3	3501	LUT	C18-C5-C6	-5.04	119.25	124.62
18	4	4001	CLA	O2A-CGA-O1A	-5.04	110.31	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	3503	BCR	C34-C9-C10	-5.04	115.56	122.89
18	4	4005	CLA	O2A-CGA-O1A	-5.03	110.31	123.51
18	A	1106	CLA	C1C-C2C-C3C	-5.03	101.35	106.93
18	A	1124	CLA	O2A-CGA-O1A	-5.03	110.32	123.51
18	A	1132	CLA	C1C-C2C-C3C	-5.03	101.35	106.93
18	4	4004	CLA	O2A-CGA-O1A	-5.03	110.34	123.51
18	A	1130	CLA	C1C-C2C-C3C	-5.02	101.36	106.93
18	B	1224	CLA	C1C-C2C-C3C	-5.02	101.36	106.93
18	A	1134	CLA	C1C-C2C-C3C	-5.02	101.36	106.93
18	A	1133	CLA	C1C-C2C-C3C	-5.01	101.37	106.93
18	A	1119	CLA	C1C-C2C-C3C	-5.01	101.37	106.93
18	A	1101	CLA	C1C-C2C-C3C	-5.01	101.37	106.93
18	3	3012	CLA	O2A-CGA-O1A	-5.01	110.37	123.51
18	G	1002	CLA	C1C-C2C-C3C	-5.01	101.38	106.93
18	A	1122	CLA	O2A-CGA-O1A	-5.01	110.38	123.51
18	1	1004	CLA	C1C-C2C-C3C	-5.00	101.38	106.93
18	B	1214	CLA	C1C-C2C-C3C	-5.00	101.38	106.93
18	J	1302	CLA	C1C-C2C-C3C	-5.00	101.38	106.93
18	B	1209	CLA	C1C-C2C-C3C	-5.00	101.38	106.93
18	B	1215	CLA	C1C-C2C-C3C	-5.00	101.39	106.93
18	A	1121	CLA	C1C-C2C-C3C	-4.99	101.39	106.93
18	A	1109	CLA	C1C-C2C-C3C	-4.99	101.40	106.93
18	B	1021	CLA	C1C-C2C-C3C	-4.99	101.40	106.93
18	B	1203	CLA	C1C-C2C-C3C	-4.99	101.40	106.93
18	A	1136	CLA	O2A-CGA-O1A	-4.99	110.44	123.51
18	B	1225	CLA	C1C-C2C-C3C	-4.98	101.41	106.93
18	2	2006	CLA	O2A-CGA-O1A	-4.98	110.46	123.51
18	3	3002	CLA	C1C-C2C-C3C	-4.98	101.41	106.93
18	B	1230	CLA	O2A-CGA-O1A	-4.98	110.47	123.51
18	A	1121	CLA	O2A-CGA-O1A	-4.97	110.47	123.51
18	A	1124	CLA	C1C-C2C-C3C	-4.97	101.41	106.93
18	3	3019	CLA	C3C-C2C-C1C	-4.97	100.78	107.18
18	1	1001	CLA	O2A-CGA-O1A	-4.97	110.48	123.51
18	A	1115	CLA	C1C-C2C-C3C	-4.97	101.42	106.93
18	4	4009	CLA	O2A-CGA-O1A	-4.97	110.49	123.51
18	A	1134	CLA	O2A-CGA-O1A	-4.96	110.50	123.51
18	A	1137	CLA	C1C-C2C-C3C	-4.96	101.42	106.93
18	2	2004	CLA	C1C-C2C-C3C	-4.96	101.43	106.93
18	1	1007	CLA	C1C-C2C-C3C	-4.96	101.43	106.93
18	2	2007	CLA	C1C-C2C-C3C	-4.95	101.44	106.93
18	4	4002	CLA	O2A-CGA-O1A	-4.95	110.52	123.51
18	2	2006	CLA	C1C-C2C-C3C	-4.95	101.44	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1232	CLA	O2A-CGA-O1A	-4.95	110.53	123.51
18	A	1131	CLA	O2A-CGA-O1A	-4.95	110.54	123.51
18	B	1236	CLA	O2A-CGA-O1A	-4.95	110.54	123.51
18	B	1210	CLA	O2A-CGA-O1A	-4.94	110.55	123.51
18	1	1011	CLA	C1C-C2C-C3C	-4.94	101.45	106.93
18	A	1107	CLA	C1C-C2C-C3C	-4.94	101.45	106.93
22	L	6019	BCR	C24-C23-C22	-4.94	118.74	126.21
18	A	1133	CLA	O2A-CGA-O1A	-4.94	110.56	123.51
18	B	1202	CLA	C1C-C2C-C3C	-4.94	101.45	106.93
18	A	1127	CLA	O2A-CGA-O1A	-4.94	110.57	123.51
18	A	1128	CLA	C1C-C2C-C3C	-4.94	101.46	106.93
18	B	1219	CLA	C1C-C2C-C3C	-4.94	101.46	106.93
22	B	6010	BCR	C38-C26-C25	-4.93	119.37	124.62
18	B	1214	CLA	O2A-CGA-O1A	-4.93	110.59	123.51
18	3	3007	CLA	C1C-C2C-C3C	-4.93	101.47	106.93
18	A	1120	CLA	C1C-C2C-C3C	-4.93	101.47	106.93
18	F	1302	CLA	C1C-C2C-C3C	-4.92	101.47	106.93
18	B	1222	CLA	C1C-C2C-C3C	-4.92	101.47	106.93
18	B	1227	CLA	C1C-C2C-C3C	-4.92	101.47	106.93
18	B	1208	CLA	C1C-C2C-C3C	-4.92	101.48	106.93
22	B	6010	BCR	C33-C5-C6	-4.91	119.39	124.62
27	4	4501	LUT	C22-C23-C24	-4.91	105.47	111.19
18	1	1002	CLA	C1C-C2C-C3C	-4.91	101.48	106.93
18	A	1117	CLA	C1C-C2C-C3C	-4.90	101.49	106.93
18	A	1127	CLA	C1C-C2C-C3C	-4.90	101.49	106.93
18	B	1235	CLA	C1C-C2C-C3C	-4.90	101.49	106.93
18	4	4006	CLA	C1C-C2C-C3C	-4.90	101.49	106.93
18	B	1240	CLA	C1C-C2C-C3C	-4.90	101.50	106.93
18	A	1109	CLA	O2A-CGA-O1A	-4.90	110.68	123.51
18	B	1012	CLA	O2A-CGA-O1A	-4.90	110.68	123.51
18	B	1238	CLA	C1C-C2C-C3C	-4.89	101.50	106.93
18	L	1503	CLA	C1C-C2C-C3C	-4.89	101.50	106.93
18	B	1206	CLA	O2A-CGA-O1A	-4.89	110.69	123.51
18	4	4003	CLA	C1C-C2C-C3C	-4.89	101.51	106.93
22	A	6002	BCR	C24-C23-C22	-4.89	118.82	126.21
18	A	1237	CLA	C1C-C2C-C3C	-4.89	101.51	106.93
18	A	1105	CLA	C1C-C2C-C3C	-4.88	101.52	106.93
22	B	6006	BCR	C33-C5-C6	-4.88	119.42	124.62
18	A	1119	CLA	O2A-CGA-O1A	-4.88	110.72	123.51
18	G	1002	CLA	C3B-CAB-CBB	-4.88	116.59	126.40
18	B	1212	CLA	C1C-C2C-C3C	-4.87	101.53	106.93
18	B	1238	CLA	O2A-CGA-O1A	-4.87	110.73	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1104	CLA	C1C-C2C-C3C	-4.87	101.53	106.93
18	A	1108	CLA	C1C-C2C-C3C	-4.87	101.53	106.93
18	3	3004	CLA	O2A-CGA-O1A	-4.87	110.74	123.51
18	1	1006	CLA	O2A-CGA-O1A	-4.87	110.75	123.51
18	B	1232	CLA	C1C-C2C-C3C	-4.87	101.53	106.93
18	F	1301	CLA	C1C-C2C-C3C	-4.86	101.54	106.93
18	4	4003	CLA	O2A-CGA-O1A	-4.86	110.76	123.51
18	F	1302	CLA	O2A-CGA-O1A	-4.86	110.77	123.51
18	L	1502	CLA	C1C-C2C-C3C	-4.85	101.55	106.93
18	A	1131	CLA	C1C-C2C-C3C	-4.85	101.55	106.93
18	A	1132	CLA	O2A-CGA-O1A	-4.85	110.79	123.51
18	A	1112	CLA	C1C-C2C-C3C	-4.85	101.55	106.93
18	2	2009	CLA	O2A-CGA-O1A	-4.85	110.80	123.51
18	A	1151	CLA	O2A-CGA-O1A	-4.85	110.80	123.51
18	2	2002	CLA	C1C-C2C-C3C	-4.85	101.55	106.93
18	A	1123	CLA	O2A-CGA-O1A	-4.85	110.80	123.51
18	A	1106	CLA	O2A-CGA-O1A	-4.84	110.81	123.51
18	3	3004	CLA	C3B-CAB-CBB	-4.84	116.66	126.40
18	B	1204	CLA	C1C-C2C-C3C	-4.84	101.56	106.93
18	B	1236	CLA	C1C-C2C-C3C	-4.84	101.56	106.93
18	A	1122	CLA	C1C-C2C-C3C	-4.84	101.56	106.93
18	A	1237	CLA	O2A-CGA-O1A	-4.82	110.87	123.51
18	A	1102	CLA	C1C-C2C-C3C	-4.82	101.58	106.93
18	B	1211	CLA	O2A-CGA-O1A	-4.82	110.88	123.51
18	A	1130	CLA	O2A-CGA-O1A	-4.81	110.89	123.51
18	B	1221	CLA	C1C-C2C-C3C	-4.81	101.59	106.93
18	B	1223	CLA	O2A-CGA-O1A	-4.81	110.91	123.51
18	A	1103	CLA	C1C-C2C-C3C	-4.81	101.60	106.93
18	B	1216	CLA	C1C-C2C-C3C	-4.80	101.61	106.93
18	A	1135	CLA	O2A-CGA-O1A	-4.80	110.93	123.51
22	J	6012	BCR	C4-C5-C6	-4.79	117.46	122.73
18	A	1138	CLA	C1C-C2C-C3C	-4.79	101.61	106.93
18	A	1136	CLA	C1C-C2C-C3C	-4.79	101.62	106.93
27	4	4503	LUT	C35-C34-C33	-4.78	120.27	127.22
18	K	1001	CLA	C3B-CAB-CBB	-4.78	116.78	126.40
18	B	1208	CLA	O2A-CGA-O1A	-4.78	110.98	123.51
18	B	1220	CLA	C1C-C2C-C3C	-4.78	101.63	106.93
18	B	1023	CLA	O2A-CGA-O1A	-4.78	110.99	123.51
18	B	1228	CLA	C1C-C2C-C3C	-4.78	101.63	106.93
18	B	1222	CLA	O2A-CGA-O1A	-4.78	110.99	123.51
22	A	6007	BCR	C38-C26-C25	-4.77	119.53	124.62
18	2	2007	CLA	O2A-CGA-O1A	-4.77	111.01	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6003	BCR	C38-C26-C25	-4.76	119.55	124.62
22	B	6004	BCR	C33-C5-C6	-4.76	119.55	124.62
18	3	3013	CLA	C1C-C2C-C3C	-4.76	101.65	106.93
18	A	1126	CLA	C1C-C2C-C3C	-4.76	101.66	106.93
18	B	1213	CLA	O2A-CGA-O1A	-4.76	111.05	123.51
18	2	2012	CLA	O2A-CGA-O1A	-4.75	111.05	123.51
18	4	4017	CLA	C1C-C2C-C3C	-4.75	101.66	106.93
18	2	2003	CLA	C1C-C2C-C3C	-4.75	101.66	106.93
18	A	1129	CLA	C1C-C2C-C3C	-4.74	101.67	106.93
18	1	1012	CLA	C3B-CAB-CBB	-4.74	116.87	126.40
22	A	6003	BCR	C33-C5-C6	-4.73	119.58	124.62
18	B	1234	CLA	O2A-CGA-O1A	-4.73	111.11	123.51
18	3	3006	CLA	C1C-C2C-C3C	-4.73	101.69	106.93
18	A	1022	CLA	C1C-C2C-C3C	-4.72	101.70	106.93
18	A	1013	CLA	C1C-C2C-C3C	-4.72	101.70	106.93
18	4	4016	CLA	C1C-C2C-C3C	-4.72	101.70	106.93
18	B	1205	CLA	C1C-C2C-C3C	-4.72	101.70	106.93
18	3	3005	CLA	O2A-CGA-O1A	-4.72	111.15	123.51
18	4	4005	CLA	C3B-CAB-CBB	-4.72	116.91	126.40
18	B	1201	CLA	C1C-C2C-C3C	-4.72	101.70	106.93
18	A	1107	CLA	O2A-CGA-O1A	-4.72	111.15	123.51
18	3	3008	CLA	O2A-CGA-O1A	-4.72	111.15	123.51
18	A	1110	CLA	O2A-CGA-O1A	-4.71	111.16	123.51
22	A	6002	BCR	C7-C8-C9	-4.71	119.09	126.21
18	A	1129	CLA	O2A-CGA-O1A	-4.70	111.18	123.51
18	3	3017	CLA	C1C-C2C-C3C	-4.70	101.72	106.93
18	3	3018	CLA	O2A-CGA-O1A	-4.70	111.19	123.51
18	A	1112	CLA	O2A-CGA-O1A	-4.70	111.19	123.51
18	A	1111	CLA	C1C-C2C-C3C	-4.70	101.72	106.93
18	B	1207	CLA	C1C-C2C-C3C	-4.69	101.73	106.93
18	L	1501	CLA	C1C-C2C-C3C	-4.69	101.73	106.93
18	A	1111	CLA	O2A-CGA-O1A	-4.69	111.22	123.51
18	A	1120	CLA	O2A-CGA-O1A	-4.68	111.23	123.51
18	A	1138	CLA	O2A-CGA-O1A	-4.68	111.25	123.51
18	B	1012	CLA	C1C-C2C-C3C	-4.67	101.75	106.93
22	G	2011	BCR	C37-C22-C21	-4.67	116.09	122.89
18	B	1203	CLA	O2A-CGA-O1A	-4.67	111.28	123.51
18	A	1110	CLA	C1C-C2C-C3C	-4.66	101.76	106.93
22	J	6013	BCR	C34-C9-C10	-4.66	116.11	122.89
18	B	1231	CLA	C1C-C2C-C3C	-4.65	101.77	106.93
18	B	1219	CLA	O2A-CGA-O1A	-4.65	111.33	123.51
18	B	1225	CLA	O2A-CGA-O1A	-4.65	111.33	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	4501	LUT	C18-C5-C6	-4.64	119.68	124.62
18	B	1223	CLA	C1C-C2C-C3C	-4.64	101.78	106.93
18	2	2003	CLA	O2A-CGA-O1A	-4.64	111.35	123.51
18	B	1021	CLA	O2A-CGA-O1A	-4.63	111.36	123.51
18	B	1216	CLA	O2A-CGA-O1A	-4.63	111.37	123.51
18	A	1113	CLA	C1C-C2C-C3C	-4.63	101.80	106.93
18	B	1234	CLA	C1C-C2C-C3C	-4.63	101.80	106.93
18	A	1102	CLA	O2A-CGA-O1A	-4.62	111.39	123.51
18	A	1013	CLA	O2A-CGA-O1A	-4.62	111.39	123.51
22	B	6009	BCR	C33-C5-C6	-4.62	119.70	124.62
18	3	3010	CLA	O2A-CGA-O1A	-4.62	111.39	123.51
18	B	1212	CLA	O2A-CGA-O1A	-4.62	111.40	123.51
18	A	1125	CLA	C1C-C2C-C3C	-4.62	101.81	106.93
18	B	1229	CLA	C1C-C2C-C3C	-4.62	101.81	106.93
22	B	6006	BCR	C7-C8-C9	-4.61	119.24	126.21
18	B	1228	CLA	O2A-CGA-O1A	-4.61	111.42	123.51
18	B	1220	CLA	O2A-CGA-O1A	-4.60	111.44	123.51
27	2	2501	LUT	C15-C14-C13	-4.60	120.54	127.22
18	1	1005	CLA	C1C-C2C-C3C	-4.58	101.85	106.93
18	A	1132	CLA	C3B-CAB-CBB	-4.58	117.19	126.40
18	A	1140	CLA	C1C-C2C-C3C	-4.58	101.86	106.93
18	A	1022	CLA	O2A-CGA-O1A	-4.58	111.52	123.51
27	I	6018	LUT	C22-C23-C24	-4.57	105.87	111.19
18	B	1202	CLA	O2A-CGA-O1A	-4.56	111.55	123.51
18	1	1014	CLA	C1C-C2C-C3C	-4.56	101.87	106.93
22	3	3503	BCR	C24-C23-C22	-4.56	119.32	126.21
18	3	3005	CLA	C3B-CAB-CBB	-4.56	117.23	126.40
18	1	1001	CLA	C1C-C2C-C3C	-4.54	101.90	106.93
18	B	1213	CLA	C1C-C2C-C3C	-4.54	101.90	106.93
22	A	6008	BCR	C7-C8-C9	-4.53	119.36	126.21
18	B	1201	CLA	O2A-CGA-O1A	-4.53	111.63	123.51
22	G	2011	BCR	C34-C9-C10	-4.53	116.30	122.89
22	A	6007	BCR	C33-C5-C6	-4.53	119.80	124.62
18	A	1125	CLA	O2A-CGA-O1A	-4.52	111.66	123.51
18	A	1104	CLA	O2A-CGA-O1A	-4.52	111.67	123.51
22	A	6008	BCR	C38-C26-C25	-4.50	119.83	124.62
18	4	4012	CLA	C3B-CAB-CBB	-4.48	117.40	126.40
18	B	1210	CLA	C1C-C2C-C3C	-4.47	101.98	106.93
22	A	6003	BCR	C7-C8-C9	-4.46	119.47	126.21
18	2	2004	CLA	O1D-CGD-CBD	-4.45	117.71	124.64
27	2	2501	LUT	C22-C23-C24	-4.45	106.01	111.19
18	1	1011	CLA	O2A-CGA-O1A	-4.45	111.84	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6017	BCR	C7-C8-C9	-4.45	119.49	126.21
18	B	1239	CLA	O2A-CGA-O1A	-4.44	111.87	123.51
18	B	1204	CLA	O2A-CGA-O1A	-4.43	111.89	123.51
18	A	1126	CLA	O2A-CGA-O1A	-4.43	111.89	123.51
18	1	1014	CLA	C3B-CAB-CBB	-4.43	117.48	126.40
22	A	6002	BCR	C38-C26-C25	-4.43	119.90	124.62
18	3	3017	CLA	O2A-CGA-O1A	-4.42	109.92	123.05
18	3	3001	CLA	C3B-CAB-CBB	-4.42	117.51	126.40
18	4	4002	CLA	C3B-CAB-CBB	-4.41	117.54	126.40
18	A	1137	CLA	O2A-CGA-O1A	-4.40	111.98	123.51
18	G	1003	CLA	O2A-CGA-O1A	-4.40	111.98	123.51
18	A	1139	CLA	O2A-CGA-O1A	-4.40	111.98	123.51
18	2	2002	CLA	C3B-CAB-CBB	-4.40	117.56	126.40
22	A	6017	BCR	C38-C26-C25	-4.39	119.94	124.62
22	B	6005	BCR	C38-C26-C25	-4.39	119.94	124.62
18	B	1230	CLA	C1C-C2C-C3C	-4.39	102.06	106.93
22	A	6011	BCR	C7-C8-C9	-4.39	119.58	126.21
18	2	2012	CLA	C1C-C2C-C3C	-4.39	102.06	106.93
18	4	4006	CLA	O2A-CGA-O1A	-4.39	112.01	123.51
22	L	6020	BCR	C34-C9-C10	-4.39	116.51	122.89
22	A	6007	BCR	C7-C8-C9	-4.38	119.58	126.21
18	B	1215	CLA	O2A-CGA-O1A	-4.38	112.02	123.51
29	4	4505	ZEX	C27-C28-C29	-4.38	119.59	126.21
22	G	2011	BCR	C33-C5-C6	-4.38	119.96	124.62
18	2	2005	CLA	O2A-CGA-O1A	-4.37	112.05	123.51
29	4	4505	ZEX	C18-C5-C6	-4.37	119.97	124.62
27	1	1502	LUT	C22-C23-C24	-4.36	106.11	111.19
18	3	3007	CLA	O2A-CGA-O1A	-4.35	112.10	123.51
18	3	3002	CLA	C3B-CAB-CBB	-4.35	117.65	126.40
22	A	6011	BCR	C28-C27-C26	-4.35	106.66	113.87
18	A	1105	CLA	O2A-CGA-O1A	-4.35	112.12	123.51
18	1	1008	CLA	O2A-CGA-O1A	-4.35	110.14	123.05
18	B	1227	CLA	O2A-CGA-O1A	-4.34	112.14	123.51
18	L	1501	CLA	O2A-CGA-O1A	-4.33	112.16	123.51
27	3	3501	LUT	C11-C10-C9	-4.32	120.93	127.22
18	B	1240	CLA	O2A-CGA-O1A	-4.32	112.17	123.51
22	J	6013	BCR	C1-C6-C5	-4.31	116.73	122.50
18	1	1005	CLA	C3B-CAB-CBB	-4.30	117.74	126.40
27	I	6018	LUT	C15-C35-C34	-4.30	113.96	123.23
18	B	1207	CLA	O2A-CGA-O1A	-4.28	112.28	123.51
18	A	1103	CLA	O2A-CGA-O1A	-4.28	112.28	123.51
18	3	3001	CLA	O2A-CGA-O1A	-4.28	112.30	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	1501	LUT	C22-C23-C24	-4.27	106.21	111.19
27	4	4503	LUT	C31-C30-C29	-4.27	121.01	127.22
18	B	1012	CLA	OBD-CAD-CBD	-4.26	119.50	125.94
22	J	6013	BCR	C37-C22-C21	-4.26	116.69	122.89
18	B	1231	CLA	O2A-CGA-O1A	-4.26	112.34	123.51
18	3	3004	CLA	OBD-CAD-CBD	-4.25	119.52	125.94
18	G	1001	CLA	CAA-C2A-C3A	-4.25	101.25	112.79
18	A	1140	CLA	O2A-CGA-O1A	-4.21	112.48	123.51
18	A	1117	CLA	O2A-CGA-O1A	-4.20	112.50	123.51
22	A	6008	BCR	C33-C5-C6	-4.18	120.17	124.62
22	3	3503	BCR	C7-C8-C9	-4.18	119.90	126.21
18	4	4004	CLA	C3B-CAB-CBB	-4.17	118.02	126.40
18	4	4012	CLA	O2A-CGA-O1A	-4.16	112.59	123.51
18	A	1118	CLA	O2A-CGA-O1A	-4.16	110.69	123.05
18	L	1501	CLA	C3B-CAB-CBB	-4.16	118.03	126.40
18	4	4016	CLA	O2A-CGA-O1A	-4.16	110.70	123.05
22	A	6002	BCR	C36-C18-C17	-4.16	116.84	122.89
27	2	2501	LUT	C18-C5-C6	-4.15	120.19	124.62
22	3	3503	BCR	C36-C18-C17	-4.15	116.85	122.89
18	B	1211	CLA	C1C-C2C-C3C	-4.15	102.33	106.93
18	H	1000	CLA	O2A-CGA-O1A	-4.14	110.75	123.05
18	2	2008	CLA	OBD-CAD-C3D	-4.14	120.78	128.09
18	A	1108	CLA	O2A-CGA-O1A	-4.13	110.78	123.05
18	B	1023	CLA	C1C-C2C-C3C	-4.12	102.36	106.93
22	L	6019	BCR	C34-C9-C10	-4.12	116.90	122.89
18	2	2016	CLA	O1D-CGD-CBD	-4.12	118.23	124.64
22	B	6004	BCR	C7-C8-C9	-4.11	119.99	126.21
22	J	6013	BCR	C4-C5-C6	-4.11	118.21	122.73
22	J	6013	BCR	C36-C18-C17	-4.11	116.91	122.89
22	J	6013	BCR	C7-C8-C9	-4.10	120.01	126.21
18	3	3006	CLA	C1-C2-C3	-4.10	119.66	126.64
18	1	1007	CLA	C3B-CAB-CBB	-4.09	118.17	126.40
22	L	6020	BCR	C37-C22-C21	-4.09	116.94	122.89
18	B	1217	CLA	O2A-CGA-O1A	-4.09	110.91	123.05
22	B	6009	BCR	C38-C26-C25	-4.09	120.27	124.62
22	A	6017	BCR	C36-C18-C17	-4.08	116.96	122.89
27	4	4503	LUT	C15-C14-C13	-4.07	121.30	127.22
22	B	6010	BCR	C7-C8-C9	-4.06	120.07	126.21
18	2	2004	CLA	C3B-CAB-CBB	-4.06	118.23	126.40
18	1	1001	CLA	C6-C5-C3	-4.05	105.49	112.76
22	F	6016	BCR	C24-C23-C22	-4.05	120.09	126.21
18	1	1001	CLA	CAA-C2A-C3A	-4.05	101.80	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4002	CLA	OBD-CAD-C3D	-4.04	120.94	128.09
18	A	1115	CLA	O2A-CGA-O1A	-4.04	111.06	123.05
18	1	1001	CLA	C3B-CAB-CBB	-4.03	118.29	126.40
22	L	6019	BCR	C36-C18-C17	-4.02	117.04	122.89
22	L	6019	BCR	C33-C5-C6	-4.02	120.34	124.62
18	A	1113	CLA	O2A-CGA-O1A	-4.01	111.15	123.05
27	2	2502	LUT	C15-C14-C13	-4.00	121.40	127.22
27	4	4503	LUT	C11-C10-C9	-3.98	121.43	127.22
18	L	1502	CLA	C3B-CAB-CBB	-3.98	118.39	126.40
22	B	6009	BCR	C3-C4-C5	-3.98	107.27	113.87
18	3	3013	CLA	O2A-CGA-O1A	-3.97	111.27	123.05
18	A	1126	CLA	C3B-CAB-CBB	-3.96	118.43	126.40
18	A	1114	CLA	O2A-CGA-O1A	-3.96	111.29	123.05
22	F	6016	BCR	C34-C9-C10	-3.95	117.14	122.89
18	3	3006	CLA	C3B-CAB-CBB	-3.95	118.45	126.40
18	4	4008	CLA	O2A-CGA-O1A	-3.95	111.33	123.05
18	3	3008	CLA	OBD-CAD-C3D	-3.95	121.11	128.09
18	2	2008	CLA	C3B-CAB-CBB	-3.95	118.46	126.40
18	J	1302	CLA	C1-C2-C3	-3.95	119.92	126.64
22	3	3503	BCR	C37-C22-C21	-3.94	117.15	122.89
18	2	2008	CLA	C1-C2-C3	-3.94	119.92	126.64
18	B	1209	CLA	O2A-CGA-O1A	-3.94	111.34	123.05
18	3	3007	CLA	C1-C2-C3	-3.93	119.94	126.64
18	L	1503	CLA	C3B-CAB-CBB	-3.93	118.49	126.40
22	A	6003	BCR	C24-C23-C22	-3.93	120.27	126.21
18	2	2009	CLA	C3B-CAB-CBB	-3.93	118.50	126.40
18	L	1501	CLA	O1D-CGD-CBD	-3.92	118.53	124.64
22	I	6020	BCR	C33-C5-C6	-3.92	120.45	124.62
18	1	1008	CLA	C3B-CAB-CBB	-3.91	118.53	126.40
18	3	3018	CLA	CAA-C2A-C3A	-3.91	102.17	112.79
18	1	1012	CLA	C1-C2-C3	-3.91	119.97	126.64
27	1	1502	LUT	C15-C14-C13	-3.91	121.53	127.22
18	K	1001	CLA	O2A-CGA-O1A	-3.91	111.44	123.05
18	B	1221	CLA	O2A-CGA-O1A	-3.90	113.29	123.51
22	J	6013	BCR	C39-C30-C25	-3.89	104.39	110.33
18	4	4003	CLA	C3B-CAB-CBB	-3.88	118.59	126.40
18	1	1011	CLA	C3B-CAB-CBB	-3.88	118.59	126.40
22	A	6017	BCR	C3-C4-C5	-3.88	107.44	113.87
22	K	2011	BCR	C3-C4-C5	-3.87	107.45	113.87
18	2	2002	CLA	O2A-CGA-O1A	-3.87	111.56	123.05
18	3	3007	CLA	C3B-CAB-CBB	-3.86	118.64	126.40
27	2	2502	LUT	C18-C5-C6	-3.86	120.51	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	1003	CLA	C3B-CAB-CBB	-3.86	118.64	126.40
27	4	4502	LUT	C31-C30-C29	-3.86	121.61	127.22
22	F	6014	BCR	C31-C1-C6	-3.86	104.44	110.33
22	G	2011	BCR	C36-C18-C17	-3.85	117.28	122.89
22	A	6007	BCR	C15-C14-C13	-3.85	121.62	127.22
22	A	6017	BCR	C33-C5-C6	-3.85	120.52	124.62
18	G	1002	CLA	O2A-CGA-O1A	-3.85	111.63	123.05
18	G	1002	CLA	O1D-CGD-CBD	-3.84	118.66	124.64
22	A	6017	BCR	C34-C9-C10	-3.84	117.30	122.89
22	I	6020	BCR	C38-C26-C25	-3.84	120.53	124.62
18	2	2016	CLA	O2A-CGA-O1A	-3.84	113.46	123.51
18	1	1011	CLA	C1-C2-C3	-3.83	120.11	126.64
18	B	1230	CLA	O1D-CGD-CBD	-3.83	118.69	124.64
18	A	1022	CLA	OBD-CAD-C3D	-3.82	121.33	128.09
18	1	1007	CLA	O2A-CGA-O1A	-3.80	111.76	123.05
18	G	1001	CLA	C3B-CAB-CBB	-3.80	118.76	126.40
18	B	1236	CLA	C3B-CAB-CBB	-3.80	118.77	126.40
18	4	4006	CLA	C1-C2-C3	-3.79	120.17	126.64
27	2	2501	LUT	C7-C8-C9	-3.79	120.48	126.21
22	L	6019	BCR	C39-C30-C25	-3.79	104.54	110.33
22	B	6004	BCR	C28-C27-C26	-3.78	107.59	113.87
22	J	6012	BCR	C7-C8-C9	-3.78	120.49	126.21
27	1	1501	LUT	C31-C30-C29	-3.78	121.73	127.22
18	K	1001	CLA	OBD-CAD-C3D	-3.78	121.41	128.09
27	2	2502	LUT	C31-C30-C29	-3.78	121.73	127.22
22	J	6012	BCR	C34-C9-C10	-3.78	117.40	122.89
18	B	1220	CLA	C3B-CAB-CBB	-3.78	118.80	126.40
22	L	6020	BCR	C33-C5-C6	-3.77	120.60	124.62
18	1	1014	CLA	O1D-CGD-CBD	-3.76	118.78	124.64
22	B	6005	BCR	C36-C18-C17	-3.75	117.43	122.89
27	3	3501	LUT	C35-C34-C33	-3.75	121.76	127.22
22	B	6006	BCR	C3-C4-C5	-3.75	107.65	113.87
18	L	1503	CLA	C1-C2-C3	-3.73	120.28	126.64
22	B	6005	BCR	C7-C8-C9	-3.73	120.57	126.21
22	B	6009	BCR	C7-C8-C9	-3.73	120.57	126.21
18	4	4007	CLA	C3B-CAB-CBB	-3.72	118.92	126.40
27	I	6018	LUT	C18-C5-C6	-3.70	120.68	124.62
22	K	2011	BCR	C36-C18-C17	-3.69	117.52	122.89
18	2	2009	CLA	C1-C2-C3	-3.69	120.34	126.64
18	F	1302	CLA	C1-C2-C3	-3.69	120.35	126.64
26	B	8001	LMU	C1B-O1B-C4'	-3.69	108.19	118.00
18	1	1013	CLA	O2A-CGA-O1A	-3.69	112.09	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	6019	BCR	C30-C25-C26	-3.69	117.57	122.50
18	3	3006	CLA	OBD-CAD-CBD	-3.68	120.38	125.94
18	1	1014	CLA	O2A-CGA-O1A	-3.68	112.11	123.05
22	B	6004	BCR	C3-C4-C5	-3.68	107.77	113.87
18	A	1119	CLA	C3B-CAB-CBB	-3.68	119.00	126.40
22	A	6017	BCR	C28-C27-C26	-3.67	107.78	113.87
18	B	1224	CLA	C3B-CAB-CBB	-3.67	119.02	126.40
18	3	3002	CLA	OBD-CAD-C3D	-3.67	121.61	128.09
18	1	1003	CLA	C3B-CAB-CBB	-3.66	119.03	126.40
22	K	2011	BCR	C7-C8-C9	-3.66	120.68	126.21
22	B	6004	BCR	C36-C18-C17	-3.65	117.58	122.89
18	1	1002	CLA	OBD-CAD-CBD	-3.65	120.43	125.94
22	A	6008	BCR	C3-C4-C5	-3.65	107.82	113.87
22	A	6017	BCR	C35-C13-C14	-3.64	117.59	122.89
18	A	1124	CLA	C3B-CAB-CBB	-3.64	119.08	126.40
18	2	2016	CLA	C1-C2-C3	-3.64	120.43	126.64
27	1	1501	LUT	C18-C5-C6	-3.63	120.75	124.62
27	3	3502	LUT	C22-C23-C24	-3.63	106.96	111.19
27	I	6018	LUT	C10-C11-C12	-3.62	111.92	123.11
27	1	1501	LUT	C15-C14-C13	-3.62	121.96	127.22
18	1	1012	CLA	CAA-CBA-CGA	-3.61	102.84	113.28
18	2	2003	CLA	C3B-CAB-CBB	-3.61	119.14	126.40
18	4	4009	CLA	C3B-CAB-CBB	-3.61	119.14	126.40
18	K	1001	CLA	OBD-CAD-CBD	-3.61	120.49	125.94
18	2	2001	CLA	C3B-CAB-CBB	-3.59	119.17	126.40
18	3	3002	CLA	O2A-CGA-O1A	-3.58	112.42	123.05
28	4	4010	CHL	CGD-CBD-CAD	-3.58	98.58	110.70
18	4	4016	CLA	C3B-CAB-CBB	-3.58	119.20	126.40
22	F	6014	BCR	C33-C5-C6	-3.57	120.81	124.62
22	L	6020	BCR	C36-C18-C17	-3.57	117.69	122.89
18	B	1023	CLA	C3B-CAB-CBB	-3.57	119.21	126.40
22	B	6006	BCR	C29-C30-C25	-3.57	105.16	110.48
18	2	2019	CLA	C3A-C4A-CHB	-3.57	120.39	123.97
18	4	4005	CLA	OBD-CAD-C3D	-3.56	121.80	128.09
28	4	4011	CHL	C1D-CHD-C4C	-3.55	122.28	129.34
18	L	1501	CLA	C1-C2-C3	-3.55	120.60	126.64
18	1	1002	CLA	C3B-CAB-CBB	-3.54	119.28	126.40
18	B	1012	CLA	C3B-CAB-CBB	-3.54	119.28	126.40
18	1	1011	CLA	CAA-CBA-CGA	-3.54	103.05	113.28
18	A	1022	CLA	C3B-CAB-CBB	-3.54	119.29	126.40
22	3	3503	BCR	C15-C14-C13	-3.53	122.09	127.22
23	F	5001	LMG	C8-O7-C10	-3.53	111.29	117.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1116	CLA	C4-C3-C2	-3.52	116.76	123.58
22	F	6014	BCR	C37-C22-C21	-3.52	117.77	122.89
22	J	6012	BCR	C37-C22-C21	-3.51	117.78	122.89
18	3	3003	CLA	O2A-CGA-O1A	-3.51	114.31	123.51
18	3	3010	CLA	C3B-CAB-CBB	-3.51	119.34	126.40
22	B	6010	BCR	C1-C6-C5	-3.50	117.81	122.50
22	B	6006	BCR	C34-C9-C10	-3.50	117.80	122.89
27	4	4501	LUT	C15-C14-C13	-3.50	122.14	127.22
18	F	1302	CLA	C3B-CAB-CBB	-3.49	119.38	126.40
22	L	6020	BCR	C7-C8-C9	-3.49	120.94	126.21
27	4	4503	LUT	C17-C1-C6	-3.48	105.01	110.33
18	F	1301	CLA	C3B-CAB-CBB	-3.48	119.41	126.40
18	2	2007	CLA	C3B-CAB-CBB	-3.48	119.41	126.40
22	J	6013	BCR	C28-C27-C26	-3.48	108.11	113.87
18	1	1006	CLA	C3B-CAB-CBB	-3.47	119.42	126.40
22	A	6011	BCR	C33-C5-C6	-3.47	120.93	124.62
27	4	4502	LUT	C22-C23-C24	-3.46	107.16	111.19
18	A	1129	CLA	C1-C2-C3	-3.46	120.74	126.64
22	J	6013	BCR	C33-C5-C6	-3.46	120.94	124.62
27	4	4502	LUT	C35-C34-C33	-3.46	122.20	127.22
18	4	4001	CLA	CAA-C2A-C3A	-3.45	103.42	112.79
27	4	4501	LUT	C10-C11-C12	-3.45	112.46	123.11
27	4	4502	LUT	C18-C5-C6	-3.44	120.96	124.62
21	B	5004	LHG	C5-O7-C7	-3.43	111.48	117.93
18	3	3001	CLA	CAA-C2A-C3A	-3.42	103.49	112.79
18	B	1216	CLA	C3B-CAB-CBB	-3.42	119.53	126.40
18	2	2006	CLA	C3B-CAB-CBB	-3.41	119.53	126.40
18	B	1012	CLA	OBD-CAD-C3D	-3.41	122.06	128.09
22	3	3503	BCR	C38-C26-C25	-3.41	120.99	124.62
27	4	4503	LUT	C18-C5-C6	-3.40	121.00	124.62
18	1	1005	CLA	OBD-CAD-C3D	-3.40	122.08	128.09
18	A	1151	CLA	C1-C2-C3	-3.40	120.84	126.64
22	A	6003	BCR	C36-C18-C17	-3.40	117.95	122.89
18	3	3018	CLA	C3B-CAB-CBB	-3.40	119.57	126.40
22	A	6002	BCR	C33-C5-C6	-3.39	121.01	124.62
28	4	4013	CHL	C1D-CHD-C4C	-3.39	122.60	129.34
18	G	1001	CLA	O1D-CGD-CBD	-3.39	119.37	124.64
22	L	6020	BCR	C15-C14-C13	-3.38	122.30	127.22
22	J	6012	BCR	C38-C26-C25	-3.38	121.02	124.62
28	3	3011	CHL	C1D-CHD-C4C	-3.38	122.63	129.34
22	B	6004	BCR	C15-C14-C13	-3.37	122.32	127.22
28	2	2013	CHL	C1D-CHD-C4C	-3.37	122.65	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3004	CLA	OBD-CAD-C3D	-3.37	122.14	128.09
18	1	1011	CLA	O1D-CGD-CBD	-3.36	119.42	124.64
22	K	2011	BCR	C33-C5-C6	-3.35	121.05	124.62
22	L	6019	BCR	C37-C22-C21	-3.35	118.02	122.89
18	B	1227	CLA	C3B-CAB-CBB	-3.35	119.66	126.40
18	A	1131	CLA	C3B-CAB-CBB	-3.34	119.67	126.40
22	F	6014	BCR	C34-C9-C10	-3.34	118.03	122.89
18	1	1012	CLA	O2A-CGA-O1A	-3.34	114.76	123.51
18	H	1000	CLA	C3B-CAB-CBB	-3.33	119.70	126.40
22	J	6013	BCR	C38-C26-C25	-3.33	121.08	124.62
27	3	3501	LUT	C15-C14-C13	-3.32	122.40	127.22
18	4	4008	CLA	O2D-CGD-O1D	-3.32	116.79	123.77
18	B	1205	CLA	C3B-CAB-CBB	-3.31	119.73	126.40
22	I	6020	BCR	C7-C8-C9	-3.31	121.20	126.21
18	A	1122	CLA	C4-C3-C2	-3.31	117.17	123.58
22	B	6004	BCR	C37-C22-C21	-3.31	118.07	122.89
18	B	1219	CLA	C3B-CAB-CBB	-3.31	119.74	126.40
28	2	2010	CHL	C3B-C4B-NB	-3.31	104.70	110.94
18	1	1002	CLA	O2A-CGA-O1A	-3.31	113.23	123.05
28	4	4010	CHL	C3B-C4B-NB	-3.30	104.71	110.94
18	3	3012	CLA	OBD-CAD-C3D	-3.30	122.26	128.09
22	J	6013	BCR	C3-C4-C5	-3.30	108.40	113.87
18	A	1022	CLA	OBD-CAD-CBD	-3.30	120.97	125.94
27	2	2501	LUT	C15-C35-C34	-3.30	116.13	123.23
18	B	1212	CLA	C3B-CAB-CBB	-3.29	119.78	126.40
22	G	2011	BCR	C4-C5-C6	-3.29	119.12	122.73
18	4	4005	CLA	C4-C3-C2	-3.29	117.22	123.58
28	2	2011	CHL	C1D-CHD-C4C	-3.29	122.81	129.34
22	J	6012	BCR	C1-C6-C5	-3.28	118.11	122.50
22	G	2011	BCR	C24-C23-C22	-3.28	121.25	126.21
22	B	6006	BCR	C30-C25-C26	-3.27	118.12	122.50
22	F	6016	BCR	C36-C18-C17	-3.27	118.13	122.89
27	3	3502	LUT	C1-C6-C5	-3.27	118.13	122.50
18	A	1237	CLA	C3B-CAB-CBB	-3.27	119.83	126.40
22	A	6007	BCR	C36-C18-C17	-3.26	118.14	122.89
27	4	4502	LUT	C15-C14-C13	-3.26	122.48	127.22
18	3	3008	CLA	C3B-CAB-CBB	-3.26	119.85	126.40
18	A	1112	CLA	C3B-CAB-CBB	-3.25	119.86	126.40
18	B	1221	CLA	O1D-CGD-CBD	-3.25	119.58	124.64
25	B	7101	DGD	O3G-C3G-C2G	-3.24	103.27	110.99
28	1	1010	CHL	C3B-C4B-NB	-3.24	104.82	110.94
22	K	2011	BCR	C38-C26-C25	-3.23	121.18	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	1502	LUT	C11-C10-C9	-3.23	122.53	127.22
18	B	1234	CLA	C3B-CAB-CBB	-3.23	119.90	126.40
29	4	4505	ZEX	C15-C14-C13	-3.23	122.53	127.22
18	A	1115	CLA	C3B-CAB-CBB	-3.23	119.91	126.40
18	B	1203	CLA	C3B-CAB-CBB	-3.23	119.91	126.40
18	B	1201	CLA	C1-C2-C3	-3.22	121.15	126.64
27	I	6018	LUT	C31-C30-C29	-3.22	122.54	127.22
22	L	6020	BCR	C27-C26-C25	-3.22	119.19	122.73
18	B	1230	CLA	C3B-CAB-CBB	-3.22	119.93	126.40
22	A	6002	BCR	C37-C22-C21	-3.22	118.21	122.89
22	A	6017	BCR	C37-C22-C21	-3.21	118.22	122.89
22	B	6009	BCR	C36-C18-C17	-3.21	118.22	122.89
27	4	4501	LUT	C31-C30-C29	-3.21	122.56	127.22
22	A	6008	BCR	C36-C18-C17	-3.21	118.22	122.89
22	A	6011	BCR	C34-C9-C10	-3.21	118.23	122.89
22	L	6020	BCR	C38-C26-C25	-3.20	121.21	124.62
27	1	1502	LUT	C18-C5-C6	-3.20	121.22	124.62
22	B	6004	BCR	C30-C25-C26	-3.20	118.22	122.50
18	A	1128	CLA	O1D-CGD-CBD	-3.20	119.67	124.64
22	B	6004	BCR	C27-C26-C25	-3.19	119.22	122.73
22	F	6014	BCR	C36-C18-C17	-3.19	118.25	122.89
25	B	7101	DGD	O5D-C6D-C5D	-3.19	103.47	109.14
18	B	1201	CLA	C3B-CAB-CBB	-3.19	119.99	126.40
18	B	1211	CLA	O1D-CGD-CBD	-3.19	119.68	124.64
18	1	1006	CLA	C1-C2-C3	-3.18	121.22	126.64
18	A	1013	CLA	C3B-CAB-CBB	-3.18	120.01	126.40
18	1	1002	CLA	CBA-CAA-C2A	-3.18	105.77	113.96
27	4	4501	LUT	C2-C3-C4	-3.17	105.39	110.29
29	4	4505	ZEX	C38-C24-C25	-3.17	105.83	110.84
27	1	1501	LUT	C31-C32-C33	-3.17	117.05	126.34
22	K	2011	BCR	C37-C22-C21	-3.17	118.28	122.89
22	A	6011	BCR	C12-C13-C14	-3.17	113.85	118.95
22	J	6012	BCR	C36-C18-C17	-3.17	118.28	122.89
22	A	6002	BCR	C3-C4-C5	-3.16	108.63	113.87
18	B	1204	CLA	C3B-CAB-CBB	-3.16	120.04	126.40
18	1	1004	CLA	C3B-CAB-CBB	-3.16	120.04	126.40
18	4	4005	CLA	O1D-CGD-CBD	-3.16	119.72	124.64
28	1	1010	CHL	C1D-CHD-C4C	-3.16	123.07	129.34
18	4	4008	CLA	C3B-CAB-CBB	-3.15	120.06	126.40
23	4	4801	LMG	C8-O7-C10	-3.15	110.13	117.91
26	B	8002	LMU	C1B-O1B-C4'	-3.14	109.64	118.00
21	1	1801	LHG	C6-C5-C4	-3.14	104.77	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	2502	LUT	C35-C34-C33	-3.14	122.66	127.22
18	3	3001	CLA	CMD-C2D-C3D	-3.12	118.98	125.09
18	2	2008	CLA	O1D-CGD-CBD	-3.12	119.78	124.64
18	4	4004	CLA	O1D-CGD-CBD	-3.12	119.79	124.64
22	I	6020	BCR	C24-C23-C22	-3.11	121.52	126.21
25	B	7101	DGD	O6D-C1D-O3G	-3.10	102.55	109.99
22	F	6016	BCR	C38-C26-C25	-3.10	121.32	124.62
18	1	1007	CLA	O1D-CGD-CBD	-3.10	119.82	124.64
22	F	6014	BCR	C7-C8-C9	-3.09	121.53	126.21
18	2	2016	CLA	CAA-C2A-C3A	-3.09	104.39	112.79
18	B	1211	CLA	O2D-CGD-O1D	-3.09	117.27	123.77
18	A	1118	CLA	O1D-CGD-CBD	-3.09	119.83	124.64
18	3	3003	CLA	OBD-CAD-C3D	-3.08	122.64	128.09
18	A	1133	CLA	C3B-CAB-CBB	-3.08	120.20	126.40
18	A	1237	CLA	C4-C3-C2	-3.08	117.62	123.58
18	A	1106	CLA	O1D-CGD-CBD	-3.08	119.84	124.64
27	4	4501	LUT	C8-C7-C6	-3.08	118.30	127.24
22	B	6009	BCR	C37-C22-C21	-3.07	118.42	122.89
18	1	1006	CLA	CAA-C2A-C3A	-3.07	104.44	112.79
18	L	1502	CLA	CAA-C2A-C3A	-3.07	104.46	112.79
18	3	3008	CLA	OBD-CAD-CBD	-3.07	121.31	125.94
18	4	4007	CLA	O1D-CGD-CBD	-3.06	119.87	124.64
22	F	6016	BCR	C23-C24-C25	-3.06	118.35	127.24
18	B	1214	CLA	C3B-CAB-CBB	-3.06	120.25	126.40
18	A	1101	CLA	O2D-CGD-O1D	-3.06	117.33	123.77
18	4	4009	CLA	C1-C2-C3	-3.06	121.43	126.64
27	I	6018	LUT	C7-C8-C9	-3.06	121.59	126.21
18	1	1004	CLA	O1D-CGD-CBD	-3.05	119.89	124.64
22	3	3503	BCR	C3-C4-C5	-3.05	108.81	113.87
18	3	3013	CLA	OBD-CAD-C3D	-3.05	122.71	128.09
18	4	4002	CLA	C1-C2-C3	-3.05	121.45	126.64
27	3	3501	LUT	C17-C1-C6	-3.05	105.68	110.33
18	G	1003	CLA	OBD-CAD-C3D	-3.04	122.72	128.09
28	3	3011	CHL	C3B-C4B-NB	-3.03	105.22	110.94
22	B	6005	BCR	C1-C6-C5	-3.03	118.44	122.50
18	A	1151	CLA	C3B-CAB-CBB	-3.03	120.31	126.40
18	A	1107	CLA	C3B-CAB-CBB	-3.03	120.31	126.40
18	4	4006	CLA	CAA-C2A-C3A	-3.02	104.58	112.79
18	4	4008	CLA	OBD-CAD-C3D	-3.02	122.75	128.09
23	J	5001	LMG	O8-C28-O10	-3.02	115.60	123.51
27	3	3501	LUT	C8-C7-C6	-3.01	118.49	127.24
18	B	1227	CLA	O1D-CGD-CBD	-3.01	119.95	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6007	BCR	C37-C22-C21	-3.01	118.51	122.89
22	I	6020	BCR	C3-C4-C5	-3.01	108.88	113.87
29	4	4505	ZEX	C17-C1-C6	-3.01	105.73	110.33
18	B	1221	CLA	O2D-CGD-O1D	-3.01	117.43	123.77
18	1	1013	CLA	C3B-CAB-CBB	-3.01	120.35	126.40
18	3	3012	CLA	C1-C2-C3	-3.00	121.52	126.64
29	4	4505	ZEX	C31-C30-C29	-3.00	122.86	127.22
18	B	1238	CLA	C3B-CAB-CBB	-2.99	120.38	126.40
18	A	1111	CLA	O1D-CGD-CBD	-2.98	120.00	124.64
18	B	1218	CLA	O1D-CGD-CBD	-2.98	120.00	124.64
18	2	2019	CLA	C2A-C3A-C4A	-2.98	100.86	103.96
18	J	1302	CLA	C3B-CAB-CBB	-2.98	120.40	126.40
18	3	3003	CLA	C3B-CAB-CBB	-2.98	120.41	126.40
18	B	1229	CLA	O1D-CGD-CBD	-2.98	120.01	124.64
18	2	2016	CLA	C3B-CAB-CBB	-2.97	120.42	126.40
22	F	6016	BCR	C33-C5-C6	-2.97	121.46	124.62
18	A	1129	CLA	C3B-CAB-CBB	-2.97	120.43	126.40
18	B	1240	CLA	C4-C3-C2	-2.97	117.84	123.58
27	1	1502	LUT	C10-C11-C12	-2.96	113.96	123.11
22	J	6012	BCR	C31-C1-C6	-2.96	105.81	110.33
18	3	3018	CLA	C1-C2-C3	-2.96	121.59	126.64
22	B	6010	BCR	C36-C18-C17	-2.96	118.58	122.89
22	3	3503	BCR	C31-C1-C6	-2.96	105.82	110.33
18	2	2012	CLA	O1D-CGD-CBD	-2.95	120.04	124.64
18	B	1223	CLA	C3B-CAB-CBB	-2.95	120.46	126.40
27	1	1502	LUT	C35-C34-C33	-2.95	122.93	127.22
22	B	6006	BCR	C38-C26-C25	-2.95	121.48	124.62
29	4	4505	ZEX	C11-C10-C9	-2.94	122.94	127.22
22	B	6005	BCR	C33-C5-C6	-2.94	121.48	124.62
18	A	1104	CLA	CAA-C2A-C3A	-2.94	104.82	112.79
23	J	5001	LMG	C12-C11-C10	-2.93	102.13	113.57
27	4	4503	LUT	C22-C23-C24	-2.93	107.78	111.19
22	K	2011	BCR	C34-C9-C10	-2.93	118.63	122.89
18	4	4005	CLA	C6-C5-C3	-2.92	107.52	112.76
18	B	1221	CLA	C6-C5-C3	-2.92	107.52	112.76
18	B	1208	CLA	O1D-CGD-CBD	-2.92	120.10	124.64
18	A	1102	CLA	C1-C2-C3	-2.92	121.67	126.64
23	2	2802	LMG	C9-C8-C7	-2.92	105.29	112.08
18	4	4017	CLA	C3B-CAB-CBB	-2.92	120.53	126.40
22	G	2011	BCR	C27-C26-C25	-2.92	119.53	122.73
27	3	3502	LUT	C35-C34-C33	-2.91	122.99	127.22
18	3	3012	CLA	CAA-C2A-C3A	-2.91	104.88	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1113	CLA	C3B-CAB-CBB	-2.91	120.54	126.40
18	A	1123	CLA	O1D-CGD-CBD	-2.91	120.12	124.64
22	L	6020	BCR	C39-C30-C25	-2.90	105.90	110.33
28	1	1009	CHL	C3B-C4B-NB	-2.90	105.47	110.94
18	A	1128	CLA	C3B-CAB-CBB	-2.89	120.58	126.40
18	A	1108	CLA	C3B-CAB-CBB	-2.89	120.58	126.40
22	I	6020	BCR	C36-C18-C17	-2.89	118.68	122.89
18	L	1502	CLA	O2D-CGD-O1D	-2.89	117.69	123.77
28	2	2011	CHL	C3B-C4B-NB	-2.88	105.50	110.94
18	2	2016	CLA	O2D-CGD-O1D	-2.88	117.71	123.77
18	2	2007	CLA	O1D-CGD-CBD	-2.88	120.16	124.64
20	A	5001	PQN	C11-C12-C13	-2.88	121.81	126.70
27	2	2501	LUT	C38-C25-C24	-2.87	117.49	123.75
22	A	6011	BCR	C27-C26-C25	-2.87	119.58	122.73
18	A	1114	CLA	O1D-CGD-CBD	-2.87	120.18	124.64
18	B	1221	CLA	C3B-CAB-CBB	-2.86	120.64	126.40
18	A	1118	CLA	C3B-CAB-CBB	-2.86	120.64	126.40
23	J	5001	LMG	O6-C5-C4	-2.86	104.21	109.67
18	B	1230	CLA	O2D-CGD-O1D	-2.86	117.75	123.77
18	J	1302	CLA	CBA-CAA-C2A	-2.86	106.59	113.96
18	A	1112	CLA	O2D-CGD-O1D	-2.86	117.76	123.77
28	4	4013	CHL	C3B-C4B-NB	-2.86	105.55	110.94
18	4	4017	CLA	O2D-CGD-O1D	-2.85	117.77	123.77
18	2	2005	CLA	C3B-CAB-CBB	-2.85	120.66	126.40
18	B	1229	CLA	C3B-CAB-CBB	-2.85	120.67	126.40
18	3	3008	CLA	CHC-C1C-C2C	-2.85	118.42	126.31
18	2	2006	CLA	CAA-C2A-C3A	-2.84	105.07	112.79
18	A	1128	CLA	O2D-CGD-O1D	-2.84	117.78	123.77
22	B	6009	BCR	C34-C9-C10	-2.84	118.75	122.89
18	A	1121	CLA	O1D-CGD-CBD	-2.84	120.22	124.64
18	B	1224	CLA	O1D-CGD-CBD	-2.84	120.22	124.64
18	B	1228	CLA	C3B-CAB-CBB	-2.84	120.70	126.40
27	3	3502	LUT	C11-C10-C9	-2.83	123.11	127.22
18	B	1238	CLA	O1D-CGD-CBD	-2.83	120.24	124.64
27	I	6018	LUT	C8-C7-C6	-2.83	119.04	127.24
18	2	2012	CLA	CAA-C2A-C3A	-2.82	105.12	112.79
18	B	1225	CLA	C3B-CAB-CBB	-2.82	120.72	126.40
18	3	3002	CLA	O1D-CGD-CBD	-2.82	120.25	124.64
18	B	1216	CLA	CAA-C2A-C3A	-2.82	105.13	112.79
18	A	1132	CLA	O2D-CGD-O1D	-2.82	117.83	123.77
18	B	1234	CLA	O1D-CGD-CBD	-2.82	120.25	124.64
18	B	1222	CLA	CAA-C2A-C3A	-2.81	105.16	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1003	CLA	C6-C5-C3	-2.81	107.72	112.76
22	L	6020	BCR	C31-C1-C6	-2.81	106.04	110.33
29	4	4505	ZEX	C19-C9-C10	-2.81	118.81	122.89
18	A	1132	CLA	O1D-CGD-CBD	-2.80	120.28	124.64
18	B	1223	CLA	O2D-CGD-O1D	-2.80	117.87	123.77
18	4	4009	CLA	O2D-CGD-O1D	-2.80	117.87	123.77
18	B	1213	CLA	C3B-CAB-CBB	-2.80	120.77	126.40
27	3	3501	LUT	C35-C15-C14	-2.80	117.20	123.23
27	3	3502	LUT	C19-C9-C10	-2.79	118.82	122.89
18	A	1124	CLA	CAA-C2A-C3A	-2.79	105.22	112.79
22	B	6005	BCR	C37-C22-C21	-2.79	118.83	122.89
29	4	4505	ZEX	C15-C35-C34	-2.79	117.22	123.23
18	L	1501	CLA	OBD-CAD-CBD	-2.78	121.73	125.94
22	B	6004	BCR	C38-C26-C25	-2.78	121.66	124.62
18	B	1240	CLA	C3B-CAB-CBB	-2.77	120.82	126.40
18	1	1013	CLA	O2D-CGD-O1D	-2.77	117.93	123.77
18	1	1005	CLA	O2D-CGD-O1D	-2.77	117.93	123.77
23	F	5001	LMG	O7-C10-O9	-2.77	117.30	122.92
18	4	4001	CLA	CBC-CAC-C3C	-2.76	103.98	112.38
22	B	6005	BCR	C23-C24-C25	-2.76	119.23	127.24
27	4	4501	LUT	C38-C25-C24	-2.76	117.74	123.75
18	4	4001	CLA	C3B-CAB-CBB	-2.76	120.85	126.40
23	2	2802	LMG	O6-C1-C2	-2.75	104.55	110.28
21	A	5003	LHG	C5-O7-C7	-2.75	111.10	117.91
18	A	1120	CLA	C3B-CAB-CBB	-2.75	120.86	126.40
18	A	1134	CLA	C3B-CAB-CBB	-2.75	120.88	126.40
29	4	4505	ZEX	O23-C23-C22	-2.74	103.52	109.80
18	A	1136	CLA	C3B-CAB-CBB	-2.74	120.88	126.40
22	A	6008	BCR	C34-C9-C10	-2.74	118.90	122.89
18	B	1239	CLA	C3B-CAB-CBB	-2.74	120.89	126.40
22	3	3503	BCR	C23-C24-C25	-2.74	119.29	127.24
27	1	1501	LUT	C10-C11-C12	-2.74	114.66	123.11
22	A	6008	BCR	C37-C22-C21	-2.73	118.91	122.89
22	A	6007	BCR	C3-C4-C5	-2.73	109.34	113.87
18	A	1136	CLA	O1D-CGD-CBD	-2.73	120.38	124.64
18	A	1111	CLA	C3B-CAB-CBB	-2.73	120.90	126.40
18	B	1214	CLA	C6-C5-C3	-2.73	107.87	112.76
18	3	3005	CLA	O1D-CGD-CBD	-2.73	120.40	124.64
18	3	3001	CLA	C1-C2-C3	-2.72	122.00	126.64
23	4	4801	LMG	O2-C2-C3	-2.72	104.23	110.36
22	B	6006	BCR	C36-C18-C17	-2.72	118.94	122.89
18	A	1123	CLA	O2D-CGD-O1D	-2.71	118.06	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1002	CLA	OBD-CAD-C3D	-2.71	123.30	128.09
18	A	1122	CLA	C3B-CAB-CBB	-2.71	120.94	126.40
27	1	1502	LUT	C15-C35-C34	-2.71	117.39	123.23
26	B	8002	LMU	C1-O1'-C1'	-2.71	109.27	114.00
18	B	1235	CLA	C3B-CAB-CBB	-2.71	120.95	126.40
18	1	1002	CLA	O1D-CGD-CBD	-2.71	120.43	124.64
18	B	1239	CLA	O1D-CGD-CBD	-2.70	120.43	124.64
18	A	1013	CLA	C6-C5-C3	-2.70	107.91	112.76
18	A	1112	CLA	O1D-CGD-CBD	-2.70	120.44	124.64
27	3	3502	LUT	C10-C11-C12	-2.70	114.77	123.11
18	B	1202	CLA	O2D-CGD-O1D	-2.70	118.09	123.77
29	4	4505	ZEX	C16-C1-C6	-2.70	106.21	110.33
18	3	3017	CLA	C3B-CAB-CBB	-2.70	120.97	126.40
18	A	1121	CLA	CAA-C2A-C3A	-2.70	105.47	112.79
18	G	1001	CLA	C4-C3-C2	-2.69	118.37	123.58
18	1	1013	CLA	CMD-C2D-C3D	-2.69	119.82	125.09
28	4	4011	CHL	C3B-C4B-NB	-2.69	105.86	110.94
18	4	4003	CLA	C6-C5-C3	-2.69	107.93	112.76
27	4	4502	LUT	C8-C7-C6	-2.69	119.44	127.24
18	B	1212	CLA	O2D-CGD-O1D	-2.68	118.12	123.77
22	A	6011	BCR	C23-C24-C25	-2.68	119.45	127.24
18	A	1130	CLA	C1-C2-C3	-2.68	122.07	126.64
18	A	1117	CLA	O1D-CGD-CBD	-2.68	120.47	124.64
18	A	1013	CLA	CAA-C2A-C3A	-2.68	105.51	112.79
18	B	1217	CLA	O1D-CGD-CBD	-2.68	120.47	124.64
18	4	4005	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
27	3	3501	LUT	C38-C25-C24	-2.68	117.92	123.75
18	A	1102	CLA	C3B-CAB-CBB	-2.68	121.01	126.40
27	2	2502	LUT	C8-C7-C6	-2.68	119.47	127.24
18	A	1130	CLA	O1D-CGD-CBD	-2.68	120.47	124.64
18	1	1001	CLA	O1D-CGD-CBD	-2.68	120.47	124.64
18	A	1125	CLA	C3B-CAB-CBB	-2.68	121.02	126.40
22	L	6019	BCR	C38-C26-C25	-2.68	121.77	124.62
18	B	1223	CLA	OBD-CAD-C3D	-2.67	123.36	128.09
22	L	6020	BCR	C35-C13-C14	-2.67	119.00	122.89
18	B	1234	CLA	C4-C3-C2	-2.67	118.42	123.58
28	2	2013	CHL	C3B-C4B-NB	-2.66	105.92	110.94
18	1	1006	CLA	O1D-CGD-CBD	-2.66	120.50	124.64
27	1	1502	LUT	C38-C25-C24	-2.66	117.96	123.75
18	A	1103	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
18	A	1103	CLA	C3B-CAB-CBB	-2.65	121.07	126.40
18	B	1209	CLA	O2D-CGD-O1D	-2.65	118.20	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1223	CLA	O1D-CGD-CBD	-2.64	120.53	124.64
18	B	1226	CLA	O2D-CGD-O1D	-2.64	118.21	123.77
22	F	6016	BCR	C37-C22-C21	-2.64	119.04	122.89
18	A	1131	CLA	O1D-CGD-CBD	-2.64	120.53	124.64
18	2	2019	CLA	C2C-C1C-CHC	-2.64	120.25	125.24
18	4	4004	CLA	CAA-C2A-C3A	-2.63	105.64	112.79
18	A	1106	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
18	4	4012	CLA	CAA-C2A-C3A	-2.63	105.65	112.79
18	4	4002	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
18	A	1102	CLA	O2D-CGD-O1D	-2.63	118.24	123.77
18	1	1006	CLA	CMD-C2D-C3D	-2.62	119.95	125.09
22	B	6006	BCR	C7-C6-C5	-2.62	115.28	121.36
22	K	2011	BCR	C27-C26-C25	-2.62	119.85	122.73
18	2	2006	CLA	O1D-CGD-CBD	-2.62	120.56	124.64
18	B	1226	CLA	C3B-CAB-CBB	-2.61	121.14	126.40
18	A	1125	CLA	OBD-CAD-C3D	-2.61	123.47	128.09
22	G	2011	BCR	C15-C14-C13	-2.61	123.42	127.22
18	B	1225	CLA	O1D-CGD-CBD	-2.61	120.58	124.64
18	A	1113	CLA	CAA-C2A-C3A	-2.61	105.72	112.79
18	A	1110	CLA	CAA-C2A-C3A	-2.60	105.72	112.79
23	F	5001	LMG	O6-C5-C4	-2.60	104.70	109.67
18	3	3007	CLA	O1D-CGD-CBD	-2.60	120.59	124.64
18	A	1135	CLA	O1D-CGD-CBD	-2.60	120.59	124.64
18	4	4006	CLA	O1D-CGD-CBD	-2.60	120.60	124.64
22	B	6004	BCR	C34-C9-C10	-2.59	119.12	122.89
27	2	2501	LUT	C31-C30-C29	-2.59	123.45	127.22
18	3	3019	CLA	C2A-C3A-C4A	-2.59	101.27	103.96
18	B	1222	CLA	C3B-CAB-CBB	-2.59	121.19	126.40
17	A	1011	CL0	CAA-C2A-C3A	-2.59	105.76	112.79
27	1	1501	LUT	C7-C8-C9	-2.59	122.30	126.21
18	B	1230	CLA	C4-C3-C2	-2.59	118.57	123.58
27	I	6018	LUT	C30-C31-C32	-2.59	115.11	123.11
18	4	4006	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
18	4	4001	CLA	C4-C3-C2	-2.59	118.57	123.58
18	3	3007	CLA	OBD-CAD-C3D	-2.58	123.52	128.09
18	J	1302	CLA	O2D-CGD-O1D	-2.58	118.33	123.77
18	A	1103	CLA	CAA-C2A-C3A	-2.58	105.78	112.79
18	2	2002	CLA	CBA-CAA-C2A	-2.58	107.31	113.96
18	A	1134	CLA	O1D-CGD-CBD	-2.58	120.63	124.64
18	4	4004	CLA	O2D-CGD-O1D	-2.58	118.34	123.77
22	A	6017	BCR	C24-C23-C22	-2.58	122.32	126.21
27	4	4502	LUT	C1-C2-C3	-2.57	107.22	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4016	CLA	CAA-C2A-C3A	-2.57	105.81	112.79
18	A	1237	CLA	O1D-CGD-CBD	-2.57	120.64	124.64
18	A	1106	CLA	C6-C5-C3	-2.57	108.16	112.76
22	A	6011	BCR	C4-C5-C6	-2.56	119.92	122.73
27	I	6018	LUT	C38-C25-C24	-2.55	118.18	123.75
18	3	3004	CLA	CAA-C2A-C3A	-2.55	105.85	112.79
22	B	6010	BCR	C24-C23-C22	-2.55	122.35	126.21
18	B	1208	CLA	O2D-CGD-O1D	-2.55	118.40	123.77
18	4	4016	CLA	CMD-C2D-C3D	-2.55	120.10	125.09
18	B	1211	CLA	OBD-CAD-C3D	-2.55	123.58	128.09
18	A	1140	CLA	O2D-CGD-O1D	-2.55	118.41	123.77
18	B	1231	CLA	O1D-CGD-CBD	-2.55	120.67	124.64
18	3	3013	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
22	B	6005	BCR	C27-C26-C25	-2.55	119.93	122.73
18	1	1003	CLA	CAA-C2A-C3A	-2.54	105.89	112.79
18	A	1129	CLA	O1D-CGD-CBD	-2.54	120.69	124.64
25	B	7101	DGD	CDB-CCB-CBB	-2.54	101.35	114.54
18	3	3012	CLA	O1D-CGD-CBD	-2.54	120.69	124.64
18	F	1302	CLA	O2D-CGD-O1D	-2.54	118.43	123.77
18	B	1235	CLA	O2D-CGD-O1D	-2.53	118.44	123.77
18	F	1301	CLA	O1D-CGD-CBD	-2.53	120.70	124.64
18	A	1126	CLA	C6-C5-C3	-2.53	108.22	112.76
18	H	1000	CLA	O1D-CGD-CBD	-2.53	120.70	124.64
18	3	3002	CLA	CBA-CAA-C2A	-2.53	107.44	113.96
22	J	6012	BCR	C39-C30-C25	-2.53	106.47	110.33
18	A	1135	CLA	O2D-CGD-O1D	-2.52	118.46	123.77
18	1	1008	CLA	OBD-CAD-C3D	-2.52	123.64	128.09
22	3	3503	BCR	C4-C5-C6	-2.52	119.96	122.73
18	B	1218	CLA	O2D-CGD-O1D	-2.52	118.47	123.77
22	A	6003	BCR	C37-C22-C21	-2.52	119.23	122.89
18	2	2009	CLA	O2D-CGD-O1D	-2.52	118.47	123.77
23	4	4801	LMG	O8-C28-O10	-2.52	116.91	123.51
18	3	3019	CLA	C3A-C4A-CHB	-2.52	121.44	123.97
18	B	1021	CLA	CAA-C2A-C3A	-2.51	105.96	112.79
18	L	1501	CLA	CAA-C2A-C3A	-2.51	105.97	112.79
18	1	1007	CLA	OBD-CAD-C3D	-2.51	123.65	128.09
22	J	6013	BCR	C31-C1-C6	-2.51	106.50	110.33
18	3	3002	CLA	CAA-CBA-CGA	-2.51	106.02	113.28
27	2	2502	LUT	C10-C11-C12	-2.51	115.36	123.11
18	A	1125	CLA	O1D-CGD-CBD	-2.51	120.73	124.64
18	B	1227	CLA	CAA-C2A-C3A	-2.51	105.98	112.79
18	4	4006	CLA	C3B-CAB-CBB	-2.51	121.36	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6008	BCR	C35-C13-C14	-2.51	119.24	122.89
18	4	4002	CLA	CBC-CAC-C3C	-2.50	104.77	112.38
18	3	3006	CLA	O1D-CGD-CBD	-2.50	120.75	124.64
18	A	1022	CLA	C6-C5-C3	-2.50	108.28	112.76
23	G	2021	LMG	O8-C28-O10	-2.50	116.96	123.51
18	A	1117	CLA	C3B-CAB-CBB	-2.50	121.38	126.40
22	3	3503	BCR	C30-C25-C26	-2.50	119.16	122.50
18	B	1240	CLA	O2D-CGD-O1D	-2.50	118.52	123.77
18	B	1215	CLA	O1D-CGD-CBD	-2.49	120.76	124.64
18	B	1216	CLA	O1D-CGD-CBD	-2.49	120.76	124.64
18	3	3005	CLA	C4-C3-C2	-2.49	118.76	123.58
18	B	1213	CLA	O1D-CGD-CBD	-2.49	120.76	124.64
18	1	1012	CLA	O1D-CGD-CBD	-2.49	120.76	124.64
18	2	2003	CLA	O1D-CGD-CBD	-2.49	120.77	124.64
18	A	1138	CLA	C3B-CAB-CBB	-2.49	121.40	126.40
18	A	1139	CLA	C6-C5-C3	-2.49	108.30	112.76
22	J	6012	BCR	C35-C13-C14	-2.48	119.27	122.89
18	4	4012	CLA	C6-C5-C3	-2.48	108.31	112.76
18	B	1230	CLA	CAA-CBA-CGA	-2.48	106.10	113.28
18	4	4001	CLA	CMD-C2D-C3D	-2.48	120.24	125.09
18	F	1302	CLA	O1D-CGD-CBD	-2.48	120.78	124.64
18	A	1107	CLA	O2D-CGD-O1D	-2.48	118.55	123.77
22	3	3503	BCR	C1-C6-C5	-2.48	119.19	122.50
18	3	3018	CLA	O1D-CGD-CBD	-2.47	120.79	124.64
18	B	1214	CLA	O1D-CGD-CBD	-2.47	120.79	124.64
18	A	1126	CLA	O1D-CGD-CBD	-2.47	120.80	124.64
18	A	1110	CLA	O1D-CGD-CBD	-2.47	120.80	124.64
18	A	1140	CLA	C3B-CAB-CBB	-2.47	121.44	126.40
18	A	1151	CLA	O1D-CGD-CBD	-2.47	120.80	124.64
22	G	2011	BCR	C8-C7-C6	-2.47	120.08	127.24
22	A	6008	BCR	C28-C27-C26	-2.46	109.78	113.87
18	B	1023	CLA	CAA-C2A-C3A	-2.46	106.11	112.79
18	3	3003	CLA	CHC-C1C-C2C	-2.46	119.49	126.31
18	2	2005	CLA	C4-C3-C2	-2.46	118.82	123.58
18	A	1108	CLA	O1D-CGD-CBD	-2.46	120.81	124.64
23	F	5002	LMG	O8-C28-O10	-2.46	117.06	123.51
23	G	2021	LMG	O4-C4-C3	-2.46	104.81	110.36
18	A	1133	CLA	O1D-CGD-CBD	-2.46	120.81	124.64
18	B	1235	CLA	O1D-CGD-CBD	-2.46	120.82	124.64
18	B	1212	CLA	O1D-CGD-CBD	-2.46	120.82	124.64
18	B	1207	CLA	C3B-CAB-CBB	-2.46	121.46	126.40
23	2	2802	LMG	O1-C7-C8	-2.45	105.15	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1210	CLA	O2D-CGD-O1D	-2.45	118.61	123.77
18	A	1127	CLA	C3B-CAB-CBB	-2.45	121.47	126.40
18	G	1003	CLA	O2D-CGD-O1D	-2.45	118.61	123.77
27	4	4501	LUT	C39-C29-C30	-2.45	119.32	122.89
23	4	4801	LMG	O6-C1-C2	-2.45	105.19	110.28
18	B	1240	CLA	O1D-CGD-CBD	-2.44	120.84	124.64
18	3	3005	CLA	OBD-CAD-C3D	-2.44	123.78	128.09
18	2	2016	CLA	CGD-CBD-CAD	-2.44	102.45	110.70
22	B	6005	BCR	C30-C25-C26	-2.43	119.24	122.50
17	A	1011	CL0	O2D-CGD-O1D	-2.43	118.65	123.77
18	K	1001	CLA	CMD-C2D-C3D	-2.43	120.33	125.09
22	B	6006	BCR	C24-C23-C22	-2.43	122.54	126.21
18	A	1121	CLA	C3B-CAB-CBB	-2.43	121.51	126.40
18	3	3006	CLA	CMD-C2D-C3D	-2.43	120.34	125.09
27	1	1501	LUT	C35-C34-C33	-2.42	123.70	127.22
21	A	7001	LHG	C5-O7-C7	-2.42	111.92	117.91
22	B	6010	BCR	C28-C27-C26	-2.42	109.85	113.87
18	L	1501	CLA	OBD-CAD-C3D	-2.42	123.81	128.09
18	B	1227	CLA	O2D-CGD-O1D	-2.42	118.67	123.77
18	B	1236	CLA	O1D-CGD-CBD	-2.42	120.87	124.64
18	B	1012	CLA	C6-C5-C3	-2.42	108.42	112.76
18	1	1012	CLA	CBC-CAC-C3C	-2.42	105.04	112.38
22	B	6006	BCR	C28-C27-C26	-2.42	109.86	113.87
18	B	1205	CLA	O2D-CGD-O1D	-2.41	118.69	123.77
18	B	1209	CLA	O1D-CGD-CBD	-2.41	120.88	124.64
18	1	1014	CLA	CAA-CBA-CGA	-2.41	106.31	113.28
18	A	1126	CLA	CAA-CBA-CGA	-2.41	106.32	113.28
22	I	6020	BCR	C23-C24-C25	-2.41	120.25	127.24
18	A	1125	CLA	O2D-CGD-O1D	-2.40	118.71	123.77
27	2	2501	LUT	C11-C10-C9	-2.40	123.73	127.22
18	A	1113	CLA	O1D-CGD-CBD	-2.40	120.91	124.64
18	A	1118	CLA	O2D-CGD-O1D	-2.40	118.72	123.77
28	2	2010	CHL	C3A-C4A-CHB	-2.40	119.47	123.00
18	1	1007	CLA	CAA-C2A-C3A	-2.40	106.28	112.79
22	F	6016	BCR	C31-C1-C6	-2.40	106.67	110.33
18	A	1132	CLA	CAA-C2A-C3A	-2.39	106.29	112.79
18	B	1215	CLA	O2D-CGD-O1D	-2.39	118.75	123.77
18	B	1236	CLA	O2D-CGD-O1D	-2.39	118.75	123.77
18	A	1137	CLA	C4-C3-C2	-2.38	118.97	123.58
18	4	4007	CLA	CMD-C2D-C3D	-2.38	120.43	125.09
18	B	1021	CLA	C6-C5-C3	-2.38	108.49	112.76
18	3	3003	CLA	OBD-CAD-CBD	-2.38	122.35	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6002	BCR	C34-C9-C10	-2.38	119.43	122.89
27	2	2502	LUT	C15-C35-C34	-2.38	118.11	123.23
18	A	1139	CLA	O2D-CGD-O1D	-2.38	118.77	123.77
27	I	6018	LUT	C12-C13-C14	-2.38	115.12	118.95
18	A	1124	CLA	O1D-CGD-CBD	-2.38	120.94	124.64
22	A	6008	BCR	C30-C25-C26	-2.37	119.32	122.50
18	B	1021	CLA	CMA-C3A-C2A	-2.37	103.60	113.99
22	A	6002	BCR	C30-C25-C26	-2.37	119.33	122.50
22	A	6002	BCR	C27-C26-C25	-2.37	120.13	122.73
22	A	6008	BCR	C31-C1-C6	-2.36	106.72	110.33
18	J	1302	CLA	OBD-CAD-C3D	-2.36	123.91	128.09
18	B	1212	CLA	CAA-C2A-C3A	-2.36	106.38	112.79
22	F	6016	BCR	C8-C7-C6	-2.36	120.39	127.24
18	2	2004	CLA	CBC-CAC-C3C	-2.36	105.21	112.38
18	B	1221	CLA	C4-C3-C2	-2.36	119.01	123.58
22	A	6011	BCR	C37-C22-C21	-2.36	119.46	122.89
27	1	1502	LUT	C17-C1-C6	-2.36	106.73	110.33
18	2	2012	CLA	C4-C3-C2	-2.35	119.02	123.58
18	B	1216	CLA	O2D-CGD-O1D	-2.35	118.81	123.77
27	2	2501	LUT	C35-C34-C33	-2.35	123.80	127.22
28	4	4010	CHL	C3A-C4A-CHB	-2.35	119.53	123.00
18	A	1116	CLA	O2D-CGD-O1D	-2.34	118.84	123.77
18	A	1101	CLA	C3B-CAB-CBB	-2.34	121.69	126.40
18	3	3017	CLA	O1D-CGD-CBD	-2.34	121.00	124.64
18	B	1207	CLA	O2D-CGD-O1D	-2.34	118.84	123.77
18	3	3005	CLA	O2D-CGD-O1D	-2.34	118.84	123.77
18	A	1121	CLA	O2D-CGD-O1D	-2.34	118.84	123.77
18	A	1110	CLA	O2D-CGD-O1D	-2.34	118.84	123.77
18	3	3008	CLA	O2D-CGD-O1D	-2.34	118.85	123.77
27	4	4502	LUT	C38-C25-C24	-2.34	118.66	123.75
18	A	1109	CLA	O2D-CGD-O1D	-2.34	118.85	123.77
27	1	1502	LUT	C40-C33-C34	-2.34	119.49	122.89
22	B	6005	BCR	C24-C23-C22	-2.34	122.68	126.21
18	A	1114	CLA	O2D-CGD-O1D	-2.34	118.85	123.77
18	A	1127	CLA	O2D-CGD-O1D	-2.34	118.85	123.77
18	3	3010	CLA	O1D-CGD-CBD	-2.33	121.00	124.64
18	B	1023	CLA	O2D-CGD-O1D	-2.33	118.86	123.77
18	B	1225	CLA	O2D-CGD-O1D	-2.33	118.86	123.77
18	B	1234	CLA	O2D-CGD-O1D	-2.33	118.86	123.77
18	3	3010	CLA	CHC-C1C-C2C	-2.33	119.85	126.31
18	4	4008	CLA	OBD-CAD-CBD	-2.33	122.42	125.94
18	3	3018	CLA	CGD-CBD-CAD	-2.33	102.81	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4012	CLA	CHC-C1C-C2C	-2.33	119.86	126.31
18	B	1204	CLA	O2D-CGD-O1D	-2.33	118.87	123.77
18	B	1218	CLA	OBD-CAD-C3D	-2.33	123.98	128.09
22	3	3503	BCR	C39-C30-C25	-2.33	106.78	110.33
22	G	2011	BCR	C38-C26-C25	-2.32	122.15	124.62
18	B	1217	CLA	O2D-CGD-O1D	-2.32	118.88	123.77
18	B	1211	CLA	OBD-CAD-CBD	-2.32	122.43	125.94
18	L	1502	CLA	OBD-CAD-C3D	-2.32	123.98	128.09
23	4	4801	LMG	O7-C10-O9	-2.32	117.35	123.67
18	A	1118	CLA	CAA-C2A-C3A	-2.32	106.48	112.79
18	4	4012	CLA	OBD-CAD-C3D	-2.32	123.99	128.09
18	A	1128	CLA	CAA-C2A-C3A	-2.32	106.49	112.79
18	1	1008	CLA	O2D-CGD-O1D	-2.32	118.89	123.77
18	A	1121	CLA	C4-C3-C2	-2.32	119.09	123.58
18	B	1201	CLA	O2D-CGD-O1D	-2.32	118.90	123.77
18	1	1008	CLA	CHC-C1C-C2C	-2.31	119.90	126.31
18	A	1137	CLA	O2D-CGD-O1D	-2.31	118.90	123.77
18	B	1240	CLA	CAA-CBA-CGA	-2.31	106.60	113.28
18	3	3002	CLA	O2D-CGD-O1D	-2.31	118.91	123.77
18	4	4007	CLA	CHC-C1C-C2C	-2.31	119.91	126.31
18	2	2008	CLA	CAA-C2A-C3A	-2.31	106.52	112.79
18	1	1004	CLA	O2D-CGD-O1D	-2.31	118.91	123.77
18	2	2002	CLA	CBC-CAC-C3C	-2.31	105.37	112.38
18	B	1220	CLA	CAA-CBA-CGA	-2.31	106.61	113.28
18	B	1012	CLA	O1D-CGD-CBD	-2.31	121.05	124.64
18	A	1135	CLA	C3B-CAB-CBB	-2.31	121.76	126.40
18	L	1501	CLA	O2D-CGD-O1D	-2.30	118.92	123.77
18	2	2016	CLA	CAA-CBA-CGA	-2.30	106.62	113.28
18	B	1220	CLA	C6-C5-C3	-2.30	108.63	112.76
22	B	6010	BCR	C39-C30-C25	-2.29	106.83	110.33
18	4	4003	CLA	O2D-CGD-O1D	-2.29	118.95	123.77
18	4	4005	CLA	CHC-C1C-C2C	-2.29	119.97	126.31
18	A	1124	CLA	O2D-CGD-O1D	-2.29	118.95	123.77
18	1	1013	CLA	CHC-C1C-C2C	-2.29	119.97	126.31
25	B	7101	DGD	C3G-C2G-C1G	-2.29	106.75	112.08
18	3	3002	CLA	OBD-CAD-CBD	-2.29	122.49	125.94
22	F	6014	BCR	C30-C25-C26	-2.28	119.44	122.50
18	B	1206	CLA	O2D-CGD-O1D	-2.28	118.96	123.77
18	A	1137	CLA	O1D-CGD-CBD	-2.28	121.08	124.64
18	A	1107	CLA	O1D-CGD-CBD	-2.28	121.08	124.64
25	B	7101	DGD	O2D-C2D-C1D	-2.28	104.95	110.01
22	G	2011	BCR	C39-C30-C25	-2.28	106.85	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1117	CLA	O2D-CGD-O1D	-2.28	118.97	123.77
18	A	1115	CLA	O1D-CGD-CBD	-2.28	121.09	124.64
18	K	1001	CLA	O2D-CGD-O1D	-2.28	118.97	123.77
18	A	1103	CLA	O1D-CGD-CBD	-2.28	121.10	124.64
18	G	1001	CLA	CHC-C1C-C2C	-2.28	120.00	126.31
22	A	6011	BCR	C24-C23-C22	-2.27	122.77	126.21
18	3	3013	CLA	C3B-CAB-CBB	-2.27	121.83	126.40
18	B	1231	CLA	C3B-CAB-CBB	-2.27	121.83	126.40
18	G	1003	CLA	CMD-C2D-C3D	-2.27	120.65	125.09
18	B	1021	CLA	O1D-CGD-CBD	-2.27	121.11	124.64
18	L	1501	CLA	C2A-C1A-CHA	-2.27	120.14	123.80
18	3	3018	CLA	CMD-C2D-C3D	-2.27	120.66	125.09
18	B	1232	CLA	O1D-CGD-CBD	-2.27	121.11	124.64
21	A	7001	LHG	O8-C23-O10	-2.26	117.57	123.51
18	A	1120	CLA	O1D-CGD-CBD	-2.26	121.12	124.64
18	A	1140	CLA	O1D-CGD-CBD	-2.26	121.12	124.64
18	L	1503	CLA	OBD-CAD-C3D	-2.26	124.09	128.09
27	1	1501	LUT	C37-C21-C22	-2.26	105.68	109.51
18	3	3004	CLA	O1D-CGD-CBD	-2.26	121.12	124.64
18	A	1133	CLA	O2D-CGD-O1D	-2.26	119.01	123.77
23	F	5002	LMG	O7-C10-O9	-2.26	117.53	123.67
18	4	4008	CLA	CHC-C1C-C2C	-2.26	120.05	126.31
18	B	1202	CLA	C4-C3-C2	-2.26	119.22	123.58
18	B	1235	CLA	CAA-C2A-C3A	-2.25	106.67	112.79
18	4	4002	CLA	CHC-C1C-C2C	-2.25	120.07	126.31
18	B	1231	CLA	C4-C3-C2	-2.25	119.22	123.58
22	J	6012	BCR	C40-C30-C25	-2.25	106.89	110.33
22	A	6011	BCR	C8-C7-C6	-2.25	120.71	127.24
22	B	6005	BCR	C34-C9-C10	-2.25	119.61	122.89
18	2	2001	CLA	CHC-C1C-C2C	-2.25	120.07	126.31
18	A	1122	CLA	O1D-CGD-CBD	-2.25	121.14	124.64
18	B	1234	CLA	OBD-CAD-C3D	-2.25	124.12	128.09
18	A	1104	CLA	C3B-CAB-CBB	-2.25	121.88	126.40
18	L	1503	CLA	CAA-C2A-C3A	-2.25	106.69	112.79
18	B	1232	CLA	C3B-CAB-CBB	-2.25	121.88	126.40
18	4	4003	CLA	O1D-CGD-CBD	-2.24	121.14	124.64
18	3	3002	CLA	CHC-C1C-C2C	-2.24	120.09	126.31
18	B	1207	CLA	O1D-CGD-CBD	-2.24	121.15	124.64
27	4	4502	LUT	C10-C11-C12	-2.24	116.18	123.11
21	2	2801	LHG	C5-O7-C7	-2.24	112.37	117.91
18	1	1005	CLA	CAA-CBA-CGA	-2.24	106.80	113.28
18	2	2001	CLA	OBD-CAD-CBD	-2.24	122.56	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	5001	LMG	O4-C4-C5	-2.24	103.33	109.23
27	2	2501	LUT	C8-C7-C6	-2.24	120.74	127.24
18	F	1301	CLA	OBD-CAD-C3D	-2.24	124.13	128.09
18	B	1204	CLA	O1D-CGD-CBD	-2.24	121.15	124.64
22	B	6010	BCR	C23-C24-C25	-2.24	120.75	127.24
22	A	6003	BCR	C3-C4-C5	-2.23	110.17	113.87
18	2	2004	CLA	OBD-CAD-CBD	-2.23	122.57	125.94
18	1	1002	CLA	CHD-C4C-C3C	-2.23	121.47	124.91
18	A	1127	CLA	O1D-CGD-CBD	-2.23	121.17	124.64
27	3	3502	LUT	C38-C25-C24	-2.23	118.90	123.75
18	B	1214	CLA	C4-C3-C2	-2.23	119.27	123.58
22	A	6007	BCR	C31-C1-C6	-2.23	106.93	110.33
18	A	1108	CLA	CAA-C2A-C3A	-2.23	106.74	112.79
17	A	1011	CL0	O1D-CGD-CBD	-2.23	121.17	124.64
18	A	1129	CLA	O2D-CGD-O1D	-2.23	119.08	123.77
28	1	1009	CHL	C1D-CHD-C4C	-2.23	124.92	129.34
18	3	3019	CLA	C3A-C2A-C1A	-2.22	101.31	104.48
18	2	2001	CLA	CBC-CAC-C3C	-2.22	105.63	112.38
18	B	1232	CLA	CAA-C2A-C3A	-2.22	106.76	112.79
18	B	1238	CLA	O2D-CGD-O1D	-2.22	119.09	123.77
18	1	1003	CLA	CAA-CBA-CGA	-2.22	106.86	113.28
22	B	6010	BCR	C34-C9-C10	-2.22	119.66	122.89
18	A	1013	CLA	O2D-CGD-O1D	-2.22	119.09	123.77
27	4	4502	LUT	C39-C29-C30	-2.22	119.66	122.89
18	A	1022	CLA	O2D-CGD-O1D	-2.22	119.10	123.77
18	1	1004	CLA	C6-C5-C3	-2.22	108.78	112.76
18	A	1130	CLA	O2D-CGD-O1D	-2.22	119.10	123.77
22	3	3503	BCR	C35-C13-C14	-2.22	119.66	122.89
18	3	3002	CLA	CMD-C2D-C3D	-2.22	120.75	125.09
18	3	3010	CLA	OBD-CAD-C3D	-2.21	124.18	128.09
25	B	7101	DGD	O3E-C3E-C2E	-2.21	105.37	110.36
18	B	1229	CLA	O2D-CGD-O1D	-2.21	119.12	123.77
18	B	1239	CLA	O2D-CGD-O1D	-2.21	119.12	123.77
27	3	3501	LUT	C31-C30-C29	-2.21	124.01	127.22
18	3	3008	CLA	CHD-C4C-C3C	-2.21	121.50	124.91
27	3	3502	LUT	C30-C31-C32	-2.21	116.28	123.11
18	A	1113	CLA	O2D-CGD-O1D	-2.21	119.12	123.77
18	2	2004	CLA	O2D-CGD-O1D	-2.21	119.12	123.77
18	A	1134	CLA	O2D-CGD-O1D	-2.21	119.12	123.77
18	4	4001	CLA	CHC-C1C-C2C	-2.21	120.19	126.31
18	3	3003	CLA	C4-C3-C2	-2.21	119.31	123.58
22	K	2011	BCR	C31-C1-C6	-2.20	106.97	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1222	CLA	O2D-CGD-O1D	-2.20	119.14	123.77
29	4	4505	ZEX	C22-C21-C26	-2.20	107.27	110.58
18	3	3007	CLA	OBD-CAD-CBD	-2.20	122.62	125.94
18	B	1203	CLA	O1D-CGD-CBD	-2.20	121.22	124.64
18	A	1105	CLA	CAA-CBA-CGA	-2.20	106.93	113.28
18	A	1138	CLA	O2D-CGD-O1D	-2.20	119.15	123.77
27	3	3502	LUT	C31-C30-C29	-2.19	124.03	127.22
18	B	1210	CLA	OBD-CAD-C3D	-2.19	124.22	128.09
18	A	1105	CLA	O1D-CGD-CBD	-2.19	121.23	124.64
18	A	1116	CLA	C3B-CAB-CBB	-2.19	122.00	126.40
18	B	1021	CLA	CBA-CAA-C2A	-2.19	108.32	113.96
18	A	1116	CLA	O1D-CGD-CBD	-2.19	121.23	124.64
27	2	2502	LUT	C38-C25-C24	-2.19	118.98	123.75
27	4	4501	LUT	C35-C15-C14	-2.19	118.52	123.23
23	G	2021	LMG	C7-O1-C1	-2.18	109.25	113.81
18	G	1003	CLA	O1D-CGD-CBD	-2.18	121.24	124.64
18	A	1136	CLA	O2D-CGD-O1D	-2.18	119.18	123.77
18	A	1106	CLA	C3B-CAB-CBB	-2.18	122.02	126.40
18	B	1224	CLA	C6-C5-C3	-2.18	108.85	112.76
18	B	1229	CLA	C6-C7-C8	-2.18	108.72	115.46
25	B	7101	DGD	CFB-CEB-CDB	-2.18	103.24	114.54
18	2	2008	CLA	CGD-CBD-CAD	-2.18	103.33	110.70
18	B	1021	CLA	O2D-CGD-O1D	-2.17	119.19	123.77
18	A	1237	CLA	CMD-C2D-C3D	-2.17	120.84	125.09
27	I	6018	LUT	C7-C6-C5	-2.17	116.32	121.36
28	4	4011	CHL	C1-C2-C3	-2.17	122.94	126.64
18	B	1224	CLA	O2D-CGD-O1D	-2.17	119.20	123.77
18	1	1011	CLA	CAA-C2A-C3A	-2.16	106.91	112.79
27	4	4502	LUT	C40-C33-C34	-2.16	119.74	122.89
18	A	1104	CLA	O2D-CGD-O1D	-2.16	119.22	123.77
18	B	1203	CLA	O2D-CGD-O1D	-2.16	119.23	123.77
18	A	1112	CLA	OBD-CAD-C3D	-2.16	124.28	128.09
18	B	1208	CLA	C6-C5-C3	-2.16	108.89	112.76
18	A	1119	CLA	O2D-CGD-O1D	-2.15	119.23	123.77
18	2	2002	CLA	O2D-CGD-O1D	-2.15	119.24	123.77
23	4	4801	LMG	O4-C4-C5	-2.15	103.56	109.23
18	B	1215	CLA	C4-C3-C2	-2.15	119.42	123.58
18	A	1151	CLA	O2D-CGD-O1D	-2.15	119.25	123.77
18	A	1131	CLA	O2D-CGD-O1D	-2.15	119.25	123.77
18	4	4017	CLA	O1D-CGD-CBD	-2.15	121.30	124.64
18	2	2016	CLA	CHD-C4C-C3C	-2.15	121.60	124.91
27	1	1501	LUT	C20-C13-C14	-2.15	119.77	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1119	CLA	O1D-CGD-CBD	-2.14	121.31	124.64
27	1	1502	LUT	C1-C6-C5	-2.14	119.64	122.50
18	2	2008	CLA	CAA-CBA-CGA	-2.14	107.11	113.28
28	1	1009	CHL	C3A-C4A-CHB	-2.13	119.85	123.00
18	1	1007	CLA	CMD-C2D-C3D	-2.13	120.92	125.09
21	A	5003	LHG	O8-C23-O10	-2.13	117.92	123.51
18	2	2001	CLA	C4-C3-C2	-2.13	119.45	123.58
22	A	6002	BCR	C31-C1-C6	-2.13	107.08	110.33
18	A	1133	CLA	C6-C5-C3	-2.13	108.94	112.76
18	4	4006	CLA	OBD-CAD-C3D	-2.13	124.33	128.09
18	A	1111	CLA	O2D-CGD-O1D	-2.13	119.28	123.77
27	4	4502	LUT	C7-C8-C9	-2.13	122.99	126.21
18	3	3007	CLA	CGD-CBD-CHA	-2.13	103.58	110.88
18	A	1120	CLA	O2D-CGD-O1D	-2.13	119.29	123.77
18	B	1012	CLA	O2D-CGD-O1D	-2.13	119.29	123.77
18	B	1205	CLA	CAA-C2A-C3A	-2.13	107.02	112.79
18	A	1126	CLA	C4-C3-C2	-2.13	119.47	123.58
18	3	3019	CLA	C2C-C1C-CHC	-2.13	121.21	125.24
18	B	1219	CLA	O2D-CGD-O1D	-2.13	119.30	123.77
22	K	2011	BCR	C15-C14-C13	-2.12	124.13	127.22
18	1	1003	CLA	O1D-CGD-CBD	-2.12	121.33	124.64
22	I	6020	BCR	C27-C26-C25	-2.12	120.40	122.73
18	2	2008	CLA	O2D-CGD-O1D	-2.12	119.30	123.77
18	3	3008	CLA	CBC-CAC-C3C	-2.12	105.93	112.38
27	3	3501	LUT	C2-C3-C4	-2.12	107.02	110.29
18	1	1003	CLA	CHC-C1C-C2C	-2.12	120.44	126.31
18	B	1215	CLA	C3B-CAB-CBB	-2.12	122.14	126.40
22	B	6004	BCR	C35-C13-C14	-2.12	119.81	122.89
22	B	6004	BCR	C1-C6-C5	-2.12	119.67	122.50
18	A	1137	CLA	C3B-CAB-CBB	-2.11	122.15	126.40
18	A	1108	CLA	O2D-CGD-O1D	-2.11	119.33	123.77
18	4	4005	CLA	O2D-CGD-O1D	-2.11	119.33	123.77
22	G	2011	BCR	C3-C4-C5	-2.11	110.37	113.87
22	A	6011	BCR	C32-C1-C6	-2.11	107.11	110.33
18	A	1115	CLA	O2D-CGD-O1D	-2.11	119.33	123.77
18	4	4017	CLA	C6-C5-C3	-2.10	108.99	112.76
18	A	1102	CLA	O1D-CGD-CBD	-2.10	121.37	124.64
18	3	3007	CLA	CAA-CBA-CGA	-2.10	107.21	113.28
18	B	1023	CLA	O1D-CGD-CBD	-2.10	121.37	124.64
25	B	7101	DGD	CBB-CAB-C9B	-2.10	103.65	114.54
22	F	6016	BCR	C27-C26-C25	-2.09	120.43	122.73
18	G	1002	CLA	O2D-CGD-O1D	-2.09	119.36	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1207	CLA	C4-C3-C2	-2.09	119.53	123.58
18	B	1236	CLA	C4-C3-C2	-2.09	119.53	123.58
18	A	1103	CLA	C6-C5-C3	-2.09	109.01	112.76
18	B	1228	CLA	O2D-CGD-O1D	-2.09	119.36	123.77
18	1	1013	CLA	CBA-CAA-C2A	-2.09	108.56	113.96
18	B	1217	CLA	C3B-CAB-CBB	-2.09	122.19	126.40
18	B	1226	CLA	CHC-C1C-C2C	-2.09	120.52	126.31
27	2	2501	LUT	C10-C11-C12	-2.09	116.66	123.11
25	B	7101	DGD	O6E-C1E-O5D	-2.09	104.98	109.99
18	G	1002	CLA	CMD-C2D-C3D	-2.09	121.01	125.09
18	A	1123	CLA	OBD-CAD-C3D	-2.08	124.41	128.09
18	4	4016	CLA	OBD-CAD-C3D	-2.08	124.41	128.09
18	B	1206	CLA	OBD-CAD-C3D	-2.08	124.41	128.09
18	4	4005	CLA	CHA-C1A-NA	-2.08	121.00	126.21
27	3	3502	LUT	C15-C14-C13	-2.08	124.20	127.22
18	2	2003	CLA	CHC-C1C-C2C	-2.08	120.55	126.31
18	B	1222	CLA	CAA-CBA-CGA	-2.07	107.28	113.28
18	B	1210	CLA	O1D-CGD-CBD	-2.07	121.41	124.64
18	H	1000	CLA	O2D-CGD-O1D	-2.07	119.41	123.77
18	B	1205	CLA	OBD-CAD-C3D	-2.07	124.43	128.09
18	L	1501	CLA	CBC-CAC-C3C	-2.07	106.09	112.38
18	2	2006	CLA	O2D-CGD-O1D	-2.07	119.41	123.77
18	A	1139	CLA	O1D-CGD-CBD	-2.07	121.42	124.64
27	2	2501	LUT	C16-C1-C6	-2.07	107.17	110.33
22	I	6020	BCR	C15-C14-C13	-2.07	124.22	127.22
18	A	1113	CLA	CAA-CBA-CGA	-2.07	107.31	113.28
18	B	1210	CLA	CAA-C2A-C3A	-2.07	107.18	112.79
18	3	3017	CLA	CHA-C1A-NA	-2.07	121.04	126.21
28	4	4010	CHL	C1D-CHD-C4C	-2.06	125.24	129.34
27	1	1502	LUT	C30-C31-C32	-2.06	116.74	123.11
23	F	5001	LMG	C3-C4-C5	-2.06	106.55	110.23
18	B	1229	CLA	C6-C5-C3	-2.06	109.07	112.76
18	A	1105	CLA	O2D-CGD-O1D	-2.06	119.44	123.77
18	2	2009	CLA	CMD-C2D-C3D	-2.06	121.06	125.09
18	1	1008	CLA	CAA-C2A-C3A	-2.06	107.21	112.79
27	4	4503	LUT	C15-C35-C34	-2.06	118.80	123.23
18	B	1202	CLA	O1D-CGD-CBD	-2.05	121.44	124.64
22	K	2011	BCR	C7-C6-C5	-2.05	116.60	121.36
27	1	1501	LUT	C11-C10-C9	-2.05	124.24	127.22
18	B	1206	CLA	C6-C5-C3	-2.05	109.08	112.76
27	2	2502	LUT	C39-C29-C30	-2.05	119.90	122.89
18	K	1001	CLA	CGD-CBD-CHA	-2.05	103.84	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1214	CLA	O2D-CGD-O1D	-2.05	119.45	123.77
22	A	6003	BCR	C34-C9-C10	-2.05	119.91	122.89
18	1	1005	CLA	C4C-C3C-C2C	-2.05	103.67	106.94
18	A	1136	CLA	CAA-C2A-C3A	-2.05	107.23	112.79
18	A	1120	CLA	C4-C3-C2	-2.05	119.62	123.58
18	1	1003	CLA	OBD-CAD-C3D	-2.04	124.48	128.09
18	4	4016	CLA	CHC-C1C-C2C	-2.04	120.64	126.31
27	3	3501	LUT	C30-C31-C32	-2.04	116.79	123.11
22	K	2011	BCR	C4-C5-C6	-2.04	120.48	122.73
18	B	1220	CLA	C4-C3-C2	-2.04	119.63	123.58
18	A	1101	CLA	O1D-CGD-CBD	-2.04	121.46	124.64
23	F	5001	LMG	C7-O1-C1	-2.04	109.55	113.81
25	B	7101	DGD	C5B-C4B-C3B	-2.04	103.93	114.54
18	A	1123	CLA	C4-C3-C2	-2.04	119.63	123.58
18	2	2003	CLA	O2D-CGD-O1D	-2.04	119.47	123.77
18	3	3018	CLA	O2D-CGD-O1D	-2.04	119.47	123.77
18	1	1002	CLA	CBC-CAC-C3C	-2.04	106.18	112.38
27	3	3502	LUT	C39-C29-C30	-2.04	119.92	122.89
18	B	1208	CLA	C4-C3-C2	-2.04	119.64	123.58
18	B	1012	CLA	C6-C7-C8	-2.04	109.16	115.46
18	A	1111	CLA	C6-C5-C3	-2.03	109.11	112.76
18	A	1140	CLA	C4-C3-C2	-2.03	119.64	123.58
18	A	1119	CLA	C4-C3-C2	-2.03	119.64	123.58
18	1	1005	CLA	C4-C3-C2	-2.03	119.65	123.58
22	A	6011	BCR	C40-C30-C25	-2.03	107.23	110.33
18	B	1206	CLA	O1D-CGD-CBD	-2.03	121.48	124.64
18	A	1139	CLA	C4-C3-C2	-2.03	119.66	123.58
18	B	1021	CLA	C4-C3-C2	-2.03	119.66	123.58
18	4	4007	CLA	C4-C3-C2	-2.02	119.66	123.58
18	1	1003	CLA	OBD-CAD-CBD	-2.02	122.88	125.94
18	A	1124	CLA	C4-C3-C2	-2.02	119.67	123.58
18	A	1126	CLA	O2D-CGD-O1D	-2.02	119.52	123.77
22	B	6005	BCR	C3-C4-C5	-2.02	110.52	113.87
18	B	1220	CLA	O2D-CGD-O1D	-2.02	119.52	123.77
18	4	4003	CLA	C4-C3-C2	-2.02	119.67	123.58
22	K	2011	BCR	C30-C25-C26	-2.02	119.80	122.50
18	A	1138	CLA	O1D-CGD-CBD	-2.02	121.50	124.64
23	F	5002	LMG	O6-C1-C2	-2.02	106.09	110.28
18	B	1228	CLA	O1D-CGD-CBD	-2.01	121.50	124.64
21	B	5004	LHG	O7-C7-O9	-2.01	118.83	122.92
18	B	1023	CLA	OBD-CAD-C3D	-2.01	124.54	128.09
18	B	1224	CLA	CAA-C2A-C3A	-2.01	107.33	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2008	CLA	CHD-C4C-C3C	-2.01	121.81	124.91
18	A	1022	CLA	O1D-CGD-CBD	-2.01	121.52	124.64
22	A	6017	BCR	C31-C1-C6	-2.00	107.27	110.33
18	B	1226	CLA	C6-C5-C3	-2.00	109.17	112.76
18	B	1219	CLA	O1D-CGD-CBD	-2.00	121.52	124.64
18	A	1125	CLA	C4-C3-C2	-2.00	119.70	123.58
22	A	6011	BCR	C29-C30-C25	2.00	113.45	110.48
18	3	3008	CLA	CMC-C2C-C3C	2.00	131.66	125.91
18	A	1134	CLA	CAC-C3C-C4C	2.00	127.77	124.82
18	2	2001	CLA	CAC-C3C-C4C	2.00	127.78	124.82
18	2	2007	CLA	CAC-C3C-C4C	2.00	127.78	124.82
18	2	2007	CLA	CMB-C2B-C3B	2.00	129.01	125.09
18	A	1102	CLA	C5-C3-C4	2.00	119.48	114.61
27	1	1502	LUT	C18-C5-C4	2.01	117.91	114.25
18	A	1129	CLA	CAC-C3C-C4C	2.01	127.78	124.82
18	B	1220	CLA	C4-C3-C5	2.01	118.43	115.37
18	2	2002	CLA	C1-O2A-CGA	2.01	123.33	116.21
22	B	6009	BCR	C23-C22-C21	2.01	122.19	118.95
18	B	1206	CLA	CAC-C3C-C4C	2.01	127.79	124.82
18	A	1134	CLA	CMB-C2B-C3B	2.01	129.03	125.09
22	F	6014	BCR	C30-C25-C24	2.02	121.72	115.96
18	A	1237	CLA	CMB-C2B-C3B	2.02	129.03	125.09
28	2	2010	CHL	CMD-C2D-C3D	2.02	129.03	125.09
18	A	1122	CLA	CAC-C3C-C4C	2.02	127.80	124.82
18	A	1115	CLA	C4A-NA-C1A	2.02	108.94	106.38
18	A	1135	CLA	CAC-C3C-C4C	2.02	127.80	124.82
18	A	1116	CLA	C4A-NA-C1A	2.02	108.94	106.38
18	3	3013	CLA	CMB-C2B-C3B	2.02	129.04	125.09
18	B	1208	CLA	CMB-C2B-C3B	2.02	129.04	125.09
18	1	1008	CLA	CMB-C2B-C3B	2.02	129.04	125.09
18	J	1302	CLA	CAC-C3C-C4C	2.02	127.81	124.82
18	1	1004	CLA	CMB-C2B-C3B	2.02	129.05	125.09
18	4	4001	CLA	C3C-C4C-NC	2.03	112.27	110.21
18	A	1128	CLA	CMC-C2C-C1C	2.03	128.01	125.00
18	B	1207	CLA	C4A-NA-C1A	2.03	108.95	106.38
29	4	4505	ZEX	C21-C26-C27	2.03	121.76	115.96
18	B	1239	CLA	CMB-C2B-C3B	2.03	129.06	125.09
18	B	1220	CLA	CMB-C2B-C3B	2.03	129.07	125.09
27	2	2501	LUT	C18-C5-C4	2.03	117.97	114.25
18	A	1101	CLA	C4A-NA-C1A	2.04	108.96	106.38
22	B	6009	BCR	C19-C18-C17	2.04	122.24	118.95
18	A	1137	CLA	C4A-NA-C1A	2.04	108.96	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4002	CLA	CED-O2D-CGD	2.04	120.81	115.97
18	1	1003	CLA	CMB-C2B-C3B	2.04	129.07	125.09
18	B	1202	CLA	CAC-C3C-C4C	2.04	127.83	124.82
18	H	1000	CLA	CED-O2D-CGD	2.04	120.82	115.97
18	A	1138	CLA	CAC-C3C-C4C	2.04	127.83	124.82
18	A	1135	CLA	C4A-NA-C1A	2.04	108.97	106.38
18	B	1209	CLA	C4A-NA-C1A	2.04	108.97	106.38
18	A	1128	CLA	C4A-NA-C1A	2.05	108.97	106.38
18	B	1215	CLA	C4A-NA-C1A	2.05	108.97	106.38
27	2	2502	LUT	C2-C1-C6	2.05	113.66	110.58
18	B	1221	CLA	CAC-C3C-C4C	2.05	127.84	124.82
18	B	1224	CLA	CAC-C3C-C4C	2.05	127.85	124.82
18	A	1107	CLA	C4A-NA-C1A	2.05	108.98	106.38
18	A	1105	CLA	CED-O2D-CGD	2.05	120.85	115.97
18	4	4017	CLA	CAC-C3C-C4C	2.05	127.85	124.82
18	B	1212	CLA	CMB-C2B-C3B	2.05	129.11	125.09
27	3	3501	LUT	C39-C29-C28	2.06	121.44	118.08
18	2	2005	CLA	CMB-C2B-C3B	2.06	129.11	125.09
18	2	2001	CLA	CGD-CBD-CAD	2.06	117.67	110.70
18	B	1218	CLA	C4A-NA-C1A	2.06	108.99	106.38
18	A	1133	CLA	CAC-C3C-C4C	2.06	127.86	124.82
18	L	1503	CLA	C5-C3-C4	2.06	119.62	114.61
18	B	1227	CLA	C4A-NA-C1A	2.06	108.99	106.38
18	4	4017	CLA	CMB-C2B-C3B	2.06	129.12	125.09
18	J	1302	CLA	C5-C3-C4	2.06	119.62	114.61
18	B	1218	CLA	CMB-C2B-C3B	2.06	129.12	125.09
18	A	1133	CLA	C4A-NA-C1A	2.07	109.00	106.38
18	A	1151	CLA	C4A-NA-C1A	2.07	109.00	106.38
18	4	4001	CLA	CED-O2D-CGD	2.07	120.89	115.97
22	A	6003	BCR	C38-C26-C27	2.07	117.47	113.47
22	F	6014	BCR	C29-C28-C27	2.07	116.66	111.42
18	A	1137	CLA	CMB-C2B-C3B	2.07	129.14	125.09
18	B	1230	CLA	CMB-C2B-C3B	2.07	129.14	125.09
18	A	1117	CLA	CAC-C3C-C4C	2.07	127.88	124.82
18	A	1110	CLA	C4A-NA-C1A	2.07	109.01	106.38
18	1	1014	CLA	C1-O2A-CGA	2.07	123.57	116.21
26	B	8001	LMU	O5'-C1'-C2'	2.07	114.59	110.28
18	B	1217	CLA	C4A-NA-C1A	2.07	109.01	106.38
18	J	1302	CLA	CMB-C2B-C3B	2.08	129.15	125.09
22	3	3503	BCR	C38-C26-C27	2.08	117.49	113.47
18	B	1220	CLA	CAC-C3C-C4C	2.08	127.89	124.82
18	4	4002	CLA	CMB-C2B-C3B	2.08	129.16	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1225	CLA	CMB-C2B-C3B	2.08	129.16	125.09
18	A	1106	CLA	C4A-NA-C1A	2.08	109.02	106.38
18	A	1237	CLA	CAC-C3C-C4C	2.08	127.90	124.82
23	B	5005	LMG	O1-C1-C2	2.08	110.56	108.00
18	B	1214	CLA	C4A-NA-C1A	2.08	109.02	106.38
18	B	1201	CLA	C5-C3-C4	2.09	119.68	114.61
18	A	1114	CLA	C4A-NA-C1A	2.09	109.02	106.38
18	4	4008	CLA	CMB-C2B-C3B	2.09	129.17	125.09
18	A	1129	CLA	C5-C3-C4	2.09	119.68	114.61
18	B	1236	CLA	C4A-NA-C1A	2.09	109.03	106.38
18	1	1006	CLA	CMB-C2B-C3B	2.09	129.18	125.09
18	A	1130	CLA	C5-C3-C4	2.09	119.69	114.61
22	F	6016	BCR	C35-C13-C12	2.09	121.50	118.08
18	B	1232	CLA	CMB-C2B-C3B	2.09	129.18	125.09
18	A	1103	CLA	CAC-C3C-C4C	2.09	127.91	124.82
18	B	1204	CLA	C4A-NA-C1A	2.09	109.03	106.38
18	B	1239	CLA	C4A-NA-C1A	2.09	109.03	106.38
22	A	6008	BCR	C30-C25-C24	2.10	121.95	115.96
18	4	4016	CLA	CED-O2D-CGD	2.10	120.95	115.97
18	B	1203	CLA	CMB-C2B-C3B	2.10	129.19	125.09
18	B	1219	CLA	C4A-NA-C1A	2.10	109.05	106.38
18	A	1131	CLA	CMB-C2B-C3B	2.10	129.20	125.09
18	A	1138	CLA	C4A-NA-C1A	2.10	109.05	106.38
18	A	1237	CLA	C4A-NA-C1A	2.10	109.05	106.38
18	4	4016	CLA	CMB-C2B-C3B	2.11	129.21	125.09
22	L	6020	BCR	C12-C13-C14	2.11	122.35	118.95
18	B	1205	CLA	C4A-NA-C1A	2.11	109.05	106.38
18	B	1213	CLA	C4A-NA-C1A	2.11	109.05	106.38
18	1	1012	CLA	CMB-C2B-C3B	2.11	129.22	125.09
18	3	3010	CLA	C3C-C4C-NC	2.11	112.35	110.21
18	A	1105	CLA	CMB-C2B-C3B	2.11	129.22	125.09
18	A	1139	CLA	C4A-NA-C1A	2.11	109.06	106.38
22	J	6012	BCR	C38-C26-C27	2.11	117.56	113.47
22	3	3503	BCR	C29-C28-C27	2.11	116.78	111.42
18	H	1000	CLA	CAC-C3C-C4C	2.12	127.94	124.82
18	2	2009	CLA	C5-C3-C4	2.12	119.75	114.61
22	I	6020	BCR	C33-C5-C4	2.12	117.56	113.47
18	A	1117	CLA	C4A-NA-C1A	2.12	109.07	106.38
18	J	1302	CLA	C4A-NA-C1A	2.12	109.07	106.38
18	A	1139	CLA	CMB-C2B-C3B	2.12	129.24	125.09
18	4	4005	CLA	CAC-C3C-C4C	2.12	127.95	124.82
18	A	1121	CLA	C4A-NA-C1A	2.12	109.07	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2009	CLA	CMB-C2B-C3B	2.12	129.24	125.09
18	A	1151	CLA	C5-C3-C4	2.12	119.77	114.61
18	L	1501	CLA	C5-C3-C4	2.13	119.78	114.61
18	F	1302	CLA	CMB-C2B-C3B	2.13	129.25	125.09
22	F	6016	BCR	C23-C22-C21	2.13	122.39	118.95
17	A	1011	CL0	C4A-NA-C1A	2.13	109.08	106.38
22	G	2011	BCR	C1-C6-C7	2.13	122.06	115.96
18	B	1234	CLA	C4A-NA-C1A	2.14	109.09	106.38
18	A	1140	CLA	CMB-C2B-C3B	2.14	129.27	125.09
18	A	1112	CLA	CMB-C2B-C3B	2.14	129.27	125.09
18	1	1002	CLA	CMB-C2B-C3B	2.14	129.27	125.09
22	J	6012	BCR	C23-C22-C21	2.14	122.40	118.95
18	1	1003	CLA	C3C-C4C-NC	2.14	112.38	110.21
18	F	1302	CLA	C5-C3-C4	2.14	119.82	114.61
18	B	1223	CLA	CMB-C2B-C3B	2.14	129.28	125.09
18	B	1205	CLA	CMB-C2B-C3B	2.15	129.29	125.09
18	4	4001	CLA	CMB-C2B-C3B	2.15	129.29	125.09
18	A	1130	CLA	C4A-NA-C1A	2.15	109.11	106.38
18	B	1012	CLA	CMB-C2B-C3B	2.15	129.30	125.09
18	3	3019	CLA	C2B-C3B-C4B	2.15	108.17	106.29
18	A	1120	CLA	CMB-C2B-C3B	2.15	129.30	125.09
27	I	6018	LUT	C1-C6-C7	2.16	122.12	115.96
18	A	1125	CLA	CMB-C2B-C3B	2.16	129.31	125.09
18	A	1113	CLA	CMB-C2B-C3B	2.16	129.31	125.09
22	B	6006	BCR	C1-C6-C7	2.16	122.12	115.96
18	A	1107	CLA	CMB-C2B-C3B	2.16	129.31	125.09
18	B	1012	CLA	C4A-NA-C1A	2.16	109.12	106.38
18	A	1134	CLA	C4A-NA-C1A	2.16	109.12	106.38
22	G	2011	BCR	C30-C25-C24	2.16	122.14	115.96
18	A	1113	CLA	CMC-C2C-C1C	2.17	128.21	125.00
18	4	4006	CLA	C5-C3-C4	2.17	119.88	114.61
18	B	1235	CLA	CMB-C2B-C3B	2.17	129.33	125.09
22	L	6020	BCR	C33-C5-C4	2.17	117.67	113.47
18	L	1502	CLA	CBA-CAA-C2A	2.17	119.56	113.96
18	B	1223	CLA	C4A-NA-C1A	2.17	109.14	106.38
18	H	1000	CLA	C4A-NA-C1A	2.17	109.14	106.38
23	2	2802	LMG	C3-C4-C5	2.17	114.10	110.23
18	B	1222	CLA	C4A-NA-C1A	2.17	109.14	106.38
18	B	1203	CLA	C4A-NA-C1A	2.17	109.14	106.38
18	B	1209	CLA	CAC-C3C-C4C	2.18	128.03	124.82
18	A	1136	CLA	CMB-C2B-C3B	2.18	129.34	125.09
18	A	1111	CLA	C4A-NA-C1A	2.18	109.14	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1118	CLA	CMB-C2B-C3B	2.18	129.35	125.09
22	B	6004	BCR	C1-C6-C7	2.19	122.20	115.96
22	L	6020	BCR	C2-C1-C6	2.19	113.73	110.48
28	2	2010	CHL	C4B-CHC-C1C	2.19	131.08	125.40
18	A	1129	CLA	CMB-C2B-C3B	2.19	129.37	125.09
18	2	2006	CLA	CMB-C2B-C3B	2.19	129.37	125.09
18	4	4003	CLA	CAC-C3C-C4C	2.19	128.05	124.82
18	A	1114	CLA	CAC-C3C-C4C	2.19	128.05	124.82
18	A	1131	CLA	C4A-NA-C1A	2.19	109.16	106.38
22	B	6004	BCR	C30-C25-C24	2.20	122.23	115.96
18	A	1116	CLA	CMB-C2B-C3B	2.20	129.38	125.09
18	G	1003	CLA	CMB-C2B-C3B	2.20	129.38	125.09
18	A	1136	CLA	C4A-NA-C1A	2.20	109.17	106.38
18	B	1217	CLA	CMB-C2B-C3B	2.20	129.39	125.09
18	A	1113	CLA	C4A-NA-C1A	2.20	109.17	106.38
22	J	6013	BCR	C38-C26-C27	2.20	117.73	113.47
18	A	1126	CLA	CAC-C3C-C4C	2.20	128.07	124.82
22	A	6011	BCR	C38-C26-C27	2.21	117.74	113.47
18	B	1201	CLA	CAC-C3C-C4C	2.21	128.07	124.82
18	B	1240	CLA	CMB-C2B-C3B	2.21	129.41	125.09
18	A	1013	CLA	C4A-NA-C1A	2.21	109.19	106.38
18	A	1127	CLA	C4A-NA-C1A	2.21	109.19	106.38
18	B	1236	CLA	CMB-C2B-C3B	2.21	129.42	125.09
18	4	4006	CLA	CMB-C2B-C3B	2.21	129.42	125.09
18	A	1101	CLA	CAC-C3C-C4C	2.22	128.09	124.82
22	B	6006	BCR	C38-C26-C27	2.22	117.75	113.47
18	A	1103	CLA	CMB-C2B-C3B	2.22	129.42	125.09
18	A	1109	CLA	C4A-NA-C1A	2.22	109.19	106.38
18	A	1121	CLA	CMB-C2B-C3B	2.22	129.42	125.09
18	B	1214	CLA	CMB-C2B-C3B	2.22	129.42	125.09
18	B	1240	CLA	C4A-NA-C1A	2.22	109.19	106.38
18	3	3008	CLA	CMC-C2C-C1C	2.22	128.29	125.00
18	K	1001	CLA	C3C-C4C-NC	2.22	112.46	110.21
18	3	3006	CLA	C5-C3-C4	2.22	120.02	114.61
22	B	6005	BCR	C23-C22-C21	2.23	122.54	118.95
18	3	3001	CLA	C4A-NA-C1A	2.23	109.21	106.38
18	2	2012	CLA	CAC-C3C-C4C	2.23	128.11	124.82
18	2	2001	CLA	C3C-C4C-NC	2.23	112.47	110.21
18	A	1126	CLA	C4A-NA-C1A	2.23	109.21	106.38
22	L	6019	BCR	C2-C1-C6	2.23	113.80	110.48
22	K	2011	BCR	C35-C13-C12	2.23	121.73	118.08
18	3	3018	CLA	C5-C3-C4	2.24	120.05	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1123	CLA	CAC-C3C-C4C	2.24	128.13	124.82
18	1	1006	CLA	C3C-C4C-NC	2.24	112.48	110.21
22	L	6020	BCR	C29-C28-C27	2.24	117.09	111.42
22	B	6006	BCR	C19-C18-C17	2.24	122.57	118.95
18	B	1211	CLA	CMB-C2B-C3B	2.24	129.48	125.09
18	B	1226	CLA	CAC-C3C-C4C	2.25	128.13	124.82
18	B	1236	CLA	C4-C3-C5	2.25	118.79	115.37
18	A	1124	CLA	CMB-C2B-C3B	2.25	129.49	125.09
18	B	1220	CLA	CED-O2D-CGD	2.25	121.32	115.97
18	4	4009	CLA	C5-C3-C4	2.25	120.08	114.61
27	4	4502	LUT	C28-C29-C30	2.25	122.59	118.95
18	B	1229	CLA	C4A-NA-C1A	2.25	109.24	106.38
22	L	6019	BCR	C23-C22-C21	2.26	122.59	118.95
26	B	8001	LMU	O1B-C4'-C3'	2.26	113.07	107.18
27	I	6018	LUT	C40-C33-C32	2.26	121.77	118.08
18	B	1228	CLA	C4A-NA-C1A	2.26	109.24	106.38
18	A	1104	CLA	CMB-C2B-C3B	2.26	129.50	125.09
18	A	1140	CLA	C4A-NA-C1A	2.26	109.25	106.38
18	B	1231	CLA	CMB-C2B-C3B	2.26	129.51	125.09
18	1	1014	CLA	CMC-C2C-C1C	2.26	128.35	125.00
18	1	1006	CLA	C5-C3-C4	2.26	120.11	114.61
18	L	1503	CLA	CAC-C3C-C4C	2.26	128.16	124.82
18	B	1201	CLA	C4A-NA-C1A	2.26	109.25	106.38
18	A	1109	CLA	CMB-C2B-C3B	2.27	129.52	125.09
18	B	1211	CLA	C4A-NA-C1A	2.27	109.26	106.38
18	4	4012	CLA	C3C-C4C-NC	2.27	112.51	110.21
18	4	4003	CLA	CMB-C2B-C3B	2.27	129.53	125.09
18	L	1501	CLA	C3C-C4C-NC	2.28	112.52	110.21
18	A	1125	CLA	C4A-NA-C1A	2.28	109.27	106.38
18	A	1151	CLA	CMB-C2B-C3B	2.28	129.54	125.09
18	A	1115	CLA	CMB-C2B-C3B	2.28	129.55	125.09
18	B	1226	CLA	C3C-C4C-NC	2.28	112.52	110.21
18	B	1222	CLA	CED-O2D-CGD	2.28	121.39	115.97
28	4	4010	CHL	C1-O2A-CGA	2.28	124.32	116.21
18	3	3012	CLA	C5-C3-C4	2.29	120.17	114.61
22	A	6017	BCR	C2-C1-C6	2.29	113.88	110.48
18	A	1120	CLA	C4A-NA-C1A	2.29	109.28	106.38
18	3	3018	CLA	C3C-C4C-NC	2.29	112.53	110.21
18	3	3006	CLA	C4A-NA-C1A	2.30	109.29	106.38
22	G	2011	BCR	C29-C28-C27	2.30	117.23	111.42
18	3	3002	CLA	C3C-C4C-NC	2.30	112.54	110.21
18	3	3007	CLA	CMB-C2B-C3B	2.30	129.59	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1221	CLA	CMB-C2B-C3B	2.30	129.59	125.09
18	A	1110	CLA	CBA-CAA-C2A	2.30	119.89	113.96
18	B	1204	CLA	CMB-C2B-C3B	2.30	129.59	125.09
18	2	2016	CLA	C5-C3-C4	2.30	120.21	114.61
23	2	2802	LMG	O8-C28-C29	2.30	118.94	111.85
18	2	2001	CLA	CAA-CBA-CGA	2.31	119.94	113.28
18	B	1225	CLA	C4A-NA-C1A	2.31	109.31	106.38
26	B	8001	LMU	C1B-C2B-C3B	2.31	114.56	109.98
18	A	1113	CLA	CAC-C3C-C4C	2.31	128.23	124.82
18	A	1122	CLA	C4A-NA-C1A	2.31	109.31	106.38
18	A	1111	CLA	CAC-C3C-C4C	2.31	128.24	124.82
18	1	1003	CLA	CAC-C3C-C4C	2.32	128.24	124.82
18	3	3017	CLA	C4A-NA-C1A	2.32	109.32	106.38
23	4	4801	LMG	O8-C28-C29	2.32	119.00	111.85
18	L	1502	CLA	C4A-NA-C1A	2.32	109.33	106.38
29	4	4505	ZEX	C20-C13-C12	2.32	121.88	118.08
18	B	1228	CLA	CED-O2D-CGD	2.32	121.49	115.97
18	B	1224	CLA	C4A-NA-C1A	2.32	109.33	106.38
22	A	6007	BCR	C33-C5-C4	2.33	117.97	113.47
18	L	1503	CLA	CMB-C2B-C3B	2.33	129.64	125.09
18	3	3004	CLA	C3C-C4C-NC	2.33	112.57	110.21
18	3	3017	CLA	CAC-C3C-C4C	2.33	128.25	124.82
18	L	1502	CLA	C4-C3-C5	2.33	118.92	115.37
18	B	1229	CLA	CMB-C2B-C3B	2.33	129.66	125.09
18	B	1221	CLA	C4A-NA-C1A	2.34	109.35	106.38
27	2	2501	LUT	C2-C1-C6	2.34	114.10	110.58
22	L	6019	BCR	C29-C28-C27	2.34	117.35	111.42
18	B	1208	CLA	C4-C3-C5	2.34	118.94	115.37
18	A	1103	CLA	C4A-NA-C1A	2.35	109.36	106.38
27	3	3502	LUT	C2-C1-C6	2.35	114.11	110.58
22	A	6003	BCR	C33-C5-C4	2.35	118.01	113.47
18	A	1118	CLA	C4A-NA-C1A	2.35	109.36	106.38
18	2	2008	CLA	CMB-C2B-C3B	2.35	129.69	125.09
18	2	2012	CLA	CMC-C2C-C1C	2.35	128.49	125.00
18	A	1108	CLA	CED-O2D-CGD	2.36	121.56	115.97
27	I	6018	LUT	C20-C13-C12	2.36	121.94	118.08
22	A	6011	BCR	C8-C9-C10	2.36	122.76	118.95
18	1	1005	CLA	CAC-C3C-C4C	2.36	128.30	124.82
18	4	4004	CLA	C4A-NA-C1A	2.36	109.38	106.38
18	2	2001	CLA	CMB-C2B-C3B	2.37	129.72	125.09
18	B	1212	CLA	C4A-NA-C1A	2.37	109.38	106.38
18	3	3001	CLA	O2D-CGD-CBD	2.37	114.63	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	2011	BCR	C1-C6-C7	2.37	122.73	115.96
18	4	4004	CLA	CMC-C2C-C1C	2.37	128.52	125.00
22	B	6006	BCR	C33-C5-C4	2.38	118.06	113.47
18	B	1207	CLA	CMB-C2B-C3B	2.38	129.73	125.09
27	4	4501	LUT	C19-C9-C8	2.38	121.97	118.08
18	A	1123	CLA	C4A-NA-C1A	2.38	109.39	106.38
18	2	2001	CLA	CMC-C2C-C1C	2.38	128.53	125.00
18	2	2019	CLA	C2B-C3B-C4B	2.38	108.37	106.29
18	3	3007	CLA	C3C-C4C-NC	2.39	112.63	110.21
18	B	1023	CLA	CED-O2D-CGD	2.39	121.64	115.97
18	L	1501	CLA	CMB-C2B-C3B	2.39	129.76	125.09
28	4	4010	CHL	C2A-C3A-C4A	2.39	106.15	101.50
18	A	1102	CLA	C4A-NA-C1A	2.39	109.41	106.38
18	4	4006	CLA	CAC-C3C-C4C	2.39	128.35	124.82
18	4	4001	CLA	CMC-C2C-C1C	2.39	128.54	125.00
18	1	1004	CLA	C4-C3-C5	2.40	119.03	115.37
18	G	1001	CLA	CMB-C2B-C3B	2.40	129.79	125.09
18	A	1135	CLA	CMB-C2B-C3B	2.41	129.79	125.09
22	J	6012	BCR	C8-C9-C10	2.41	122.84	118.95
18	A	1129	CLA	C4A-NA-C1A	2.41	109.44	106.38
18	G	1003	CLA	C4A-NA-C1A	2.42	109.45	106.38
18	2	2003	CLA	CMB-C2B-C3B	2.42	129.83	125.09
18	B	1206	CLA	CMB-C2B-C3B	2.43	129.83	125.09
28	1	1009	CHL	C4B-CHC-C1C	2.43	131.71	125.40
18	B	1224	CLA	CMC-C2C-C1C	2.43	128.60	125.00
18	A	1111	CLA	CMB-C2B-C3B	2.43	129.85	125.09
18	B	1234	CLA	CMC-C2C-C1C	2.44	128.61	125.00
18	B	1228	CLA	CMC-C2C-C1C	2.45	128.62	125.00
18	B	1023	CLA	C4A-NA-C1A	2.45	109.48	106.38
22	A	6008	BCR	C33-C5-C4	2.45	118.21	113.47
18	B	1224	CLA	CMB-C2B-C3B	2.45	129.88	125.09
18	B	1206	CLA	C4A-NA-C1A	2.46	109.50	106.38
18	1	1011	CLA	C4A-NA-C1A	2.46	109.50	106.38
22	K	2011	BCR	C23-C22-C21	2.47	122.93	118.95
22	F	6016	BCR	C38-C26-C27	2.47	118.25	113.47
18	B	1234	CLA	CMB-C2B-C3B	2.48	129.93	125.09
18	B	1023	CLA	CMB-C2B-C3B	2.48	129.93	125.09
18	2	2009	CLA	C4A-NA-C1A	2.48	109.52	106.38
28	2	2010	CHL	C1-O2A-CGA	2.48	125.02	116.21
21	2	2801	LHG	O8-C23-C24	2.48	119.49	111.85
18	B	1021	CLA	C4A-NA-C1A	2.49	109.53	106.38
18	3	3006	CLA	C3C-C4C-NC	2.49	112.73	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2004	CLA	CMB-C2B-C3B	2.49	129.96	125.09
18	B	1211	CLA	CMC-C2C-C1C	2.49	128.69	125.00
18	3	3007	CLA	CAC-C3C-C4C	2.49	128.50	124.82
18	B	1221	CLA	C4-C3-C5	2.49	119.17	115.37
27	3	3502	LUT	C1-C6-C7	2.49	123.08	115.96
18	1	1012	CLA	C3C-C4C-NC	2.49	112.74	110.21
18	4	4016	CLA	CAC-C3C-C4C	2.49	128.50	124.82
18	B	1023	CLA	CMC-C2C-C1C	2.49	128.70	125.00
18	B	1202	CLA	C4-C3-C5	2.50	119.17	115.37
18	3	3004	CLA	CMC-C2C-C1C	2.50	128.70	125.00
18	2	2003	CLA	CAC-C3C-C4C	2.50	128.51	124.82
18	1	1011	CLA	C3C-C4C-NC	2.50	112.74	110.21
18	1	1011	CLA	CAC-C3C-C4C	2.50	128.51	124.82
22	B	6004	BCR	C23-C22-C21	2.50	122.99	118.95
27	3	3501	LUT	C2-C1-C6	2.50	114.35	110.58
18	B	1235	CLA	C4A-NA-C1A	2.50	109.55	106.38
22	G	2011	BCR	C38-C26-C27	2.51	118.32	113.47
22	3	3503	BCR	C1-C6-C7	2.52	123.15	115.96
18	3	3007	CLA	C4A-NA-C1A	2.52	109.57	106.38
18	B	1230	CLA	C4A-NA-C1A	2.52	109.57	106.38
18	3	3017	CLA	CED-O2D-CGD	2.52	121.95	115.97
18	2	2012	CLA	C6-C5-C3	2.52	117.29	112.76
18	4	4017	CLA	C4-C3-C5	2.52	119.21	115.37
18	A	1126	CLA	CMB-C2B-C3B	2.52	130.02	125.09
22	A	6008	BCR	C19-C18-C17	2.52	123.03	118.95
18	B	1219	CLA	CMB-C2B-C3B	2.53	130.03	125.09
18	B	1227	CLA	CMB-C2B-C3B	2.53	130.03	125.09
18	B	1202	CLA	CMB-C2B-C3B	2.53	130.03	125.09
22	L	6019	BCR	C40-C30-C25	2.53	114.20	110.33
18	2	2002	CLA	CAC-C3C-C4C	2.54	128.57	124.82
18	3	3002	CLA	C4A-NA-C1A	2.54	109.60	106.38
22	B	6010	BCR	C38-C26-C27	2.54	118.38	113.47
18	1	1003	CLA	CMC-C2C-C1C	2.54	128.77	125.00
18	B	1201	CLA	CMB-C2B-C3B	2.55	130.08	125.09
22	B	6006	BCR	C35-C13-C12	2.55	122.25	118.08
18	A	1110	CLA	CMB-C2B-C3B	2.55	130.08	125.09
18	1	1011	CLA	C5-C3-C4	2.56	120.82	114.61
18	4	4017	CLA	C4A-NA-C1A	2.56	109.62	106.38
18	2	2005	CLA	C4A-NA-C1A	2.56	109.62	106.38
18	F	1302	CLA	C4A-NA-C1A	2.56	109.63	106.38
18	G	1002	CLA	C4A-NA-C1A	2.56	109.63	106.38
18	A	1132	CLA	CMB-C2B-C3B	2.56	130.10	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1202	CLA	CMC-C2C-C1C	2.56	128.80	125.00
22	A	6017	BCR	C33-C5-C4	2.56	118.43	113.47
18	3	3004	CLA	C4A-NA-C1A	2.57	109.64	106.38
18	1	1012	CLA	CMC-C2C-C1C	2.57	128.81	125.00
18	B	1226	CLA	CMC-C2C-C1C	2.57	128.81	125.00
18	A	1139	CLA	C4-C3-C5	2.57	119.28	115.37
18	A	1119	CLA	CMB-C2B-C3B	2.57	130.12	125.09
18	A	1138	CLA	CMB-C2B-C3B	2.57	130.12	125.09
18	G	1001	CLA	C3C-C4C-NC	2.58	112.82	110.21
22	K	2011	BCR	C33-C5-C4	2.58	118.46	113.47
18	4	4016	CLA	CMC-C2C-C1C	2.58	128.82	125.00
18	B	1223	CLA	C4-C3-C5	2.58	119.31	115.37
18	4	4002	CLA	CMC-C2C-C1C	2.59	128.83	125.00
18	G	1003	CLA	C4-C3-C5	2.59	119.32	115.37
18	A	1127	CLA	CMB-C2B-C3B	2.59	130.16	125.09
18	B	1210	CLA	CMC-C2C-C1C	2.59	128.84	125.00
22	J	6013	BCR	C1-C6-C7	2.59	123.37	115.96
18	G	1003	CLA	C3C-C4C-NC	2.59	112.84	110.21
18	F	1301	CLA	C4A-NA-C1A	2.60	109.67	106.38
18	B	1223	CLA	CMC-C2C-C1C	2.60	128.85	125.00
22	L	6019	BCR	C33-C5-C4	2.60	118.50	113.47
18	1	1003	CLA	C4A-NA-C1A	2.60	109.68	106.38
26	B	8002	LMU	C1'-O5'-C5'	2.60	118.85	113.74
18	4	4016	CLA	C3C-C4C-NC	2.60	112.85	110.21
18	3	3010	CLA	C4A-NA-C1A	2.61	109.69	106.38
18	B	1207	CLA	CAC-C3C-C4C	2.61	128.67	124.82
18	A	1110	CLA	CMC-C2C-C1C	2.61	128.87	125.00
18	4	4006	CLA	C4A-NA-C1A	2.61	109.69	106.38
18	A	1138	CLA	C3C-C4C-NC	2.62	112.86	110.21
22	F	6016	BCR	C19-C18-C17	2.62	123.18	118.95
18	2	2001	CLA	CGD-CBD-CHA	2.62	119.87	110.88
18	4	4008	CLA	CAC-C3C-C4C	2.62	128.69	124.82
18	3	3008	CLA	CMB-C2B-C3B	2.62	130.22	125.09
27	2	2502	LUT	C37-C21-C36	2.62	111.79	107.88
18	A	1123	CLA	CMB-C2B-C3B	2.63	130.22	125.09
18	B	1205	CLA	C4-C3-C5	2.63	119.37	115.37
18	3	3012	CLA	CMC-C2C-C1C	2.63	128.90	125.00
22	A	6007	BCR	C23-C22-C21	2.63	123.19	118.95
18	K	1001	CLA	CMC-C2C-C1C	2.63	128.90	125.00
18	2	2005	CLA	C3C-C4C-NC	2.64	112.88	110.21
18	4	4003	CLA	C3C-C4C-NC	2.64	112.88	110.21
18	A	1127	CLA	CMC-C2C-C1C	2.64	128.91	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1012	CLA	C4A-NA-C1A	2.64	109.73	106.38
29	4	4505	ZEX	C18-C5-C4	2.64	119.08	114.25
18	G	1002	CLA	C3C-C4C-NC	2.64	112.89	110.21
18	L	1503	CLA	C4A-NA-C1A	2.65	109.73	106.38
18	A	1107	CLA	C4-C3-C5	2.65	119.40	115.37
28	4	4013	CHL	C4B-CHC-C1C	2.65	132.28	125.40
18	B	1204	CLA	CMC-C2C-C1C	2.65	128.92	125.00
22	J	6012	BCR	C35-C13-C12	2.65	122.42	118.08
18	2	2009	CLA	C3C-C4C-NC	2.65	112.90	110.21
18	4	4016	CLA	C4A-NA-C1A	2.66	109.75	106.38
18	3	3018	CLA	CAC-C3C-C4C	2.66	128.75	124.82
18	B	1210	CLA	CAC-C3C-C4C	2.66	128.75	124.82
18	B	1220	CLA	CMC-C2C-C1C	2.66	128.94	125.00
22	F	6014	BCR	C34-C9-C8	2.66	122.43	118.08
18	3	3002	CLA	CMC-C2C-C1C	2.66	128.95	125.00
18	B	1222	CLA	CMB-C2B-C3B	2.66	130.30	125.09
22	A	6017	BCR	C38-C26-C27	2.67	118.63	113.47
18	B	1205	CLA	CMC-C2C-C1C	2.67	128.95	125.00
22	F	6016	BCR	C2-C1-C6	2.67	114.46	110.48
18	A	1102	CLA	CMB-C2B-C3B	2.68	130.32	125.09
27	1	1502	LUT	C40-C33-C32	2.68	122.46	118.08
18	A	1136	CLA	CMC-C2C-C1C	2.68	128.97	125.00
18	A	1126	CLA	C4-C3-C5	2.69	119.46	115.37
18	B	1210	CLA	C4-C3-C5	2.69	119.47	115.37
18	A	1117	CLA	CMB-C2B-C3B	2.69	130.36	125.09
18	3	3010	CLA	CMC-C2C-C1C	2.69	128.99	125.00
18	A	1122	CLA	CMC-C2C-C1C	2.69	128.99	125.00
18	A	1106	CLA	C4-C3-C5	2.70	119.48	115.37
18	1	1004	CLA	C4A-NA-C1A	2.70	109.80	106.38
22	B	6010	BCR	C33-C5-C4	2.70	118.69	113.47
17	A	1011	CL0	C4-C3-C5	2.70	119.48	115.37
18	B	1214	CLA	C4-C3-C5	2.70	119.48	115.37
18	1	1001	CLA	CMC-C2C-C1C	2.70	129.00	125.00
18	2	2006	CLA	C4A-NA-C1A	2.70	109.81	106.38
18	H	1000	CLA	CMC-C2C-C1C	2.70	129.00	125.00
18	2	2002	CLA	C3C-C4C-NC	2.71	112.95	110.21
18	1	1004	CLA	CMC-C2C-C1C	2.71	129.01	125.00
18	4	4005	CLA	CMC-C2C-C1C	2.71	129.02	125.00
18	4	4002	CLA	C4A-NA-C1A	2.72	109.83	106.38
18	A	1022	CLA	CMC-C2C-C1C	2.72	129.04	125.00
18	1	1004	CLA	C3C-C4C-NC	2.73	112.97	110.21
21	2	2801	LHG	O7-C7-C8	2.73	120.55	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1112	CLA	CMC-C2C-C1C	2.73	129.05	125.00
18	B	1211	CLA	C3C-C4C-NC	2.73	112.98	110.21
18	A	1101	CLA	CMC-C2C-C1C	2.74	129.06	125.00
18	A	1101	CLA	C3C-C4C-NC	2.74	112.99	110.21
18	2	2019	CLA	C3C-C4C-NC	2.74	112.57	110.09
18	A	1140	CLA	CMC-C2C-C1C	2.74	129.06	125.00
18	B	1207	CLA	C4-C3-C5	2.74	119.55	115.37
18	3	3017	CLA	C3C-C4C-NC	2.74	112.99	110.21
18	3	3018	CLA	C4A-NA-C1A	2.74	109.86	106.38
18	2	2001	CLA	C4A-NA-C1A	2.75	109.86	106.38
18	2	2004	CLA	C4-C3-C5	2.75	119.55	115.37
18	A	1114	CLA	CMC-C2C-C1C	2.75	129.08	125.00
18	A	1138	CLA	CMC-C2C-C1C	2.75	129.08	125.00
18	4	4007	CLA	C3C-C4C-NC	2.75	113.00	110.21
22	B	6009	BCR	C38-C26-C27	2.76	118.80	113.47
22	F	6014	BCR	C19-C18-C17	2.76	123.40	118.95
18	B	1232	CLA	CMC-C2C-C1C	2.76	129.09	125.00
18	2	2006	CLA	C3C-C4C-NC	2.76	113.01	110.21
18	B	1209	CLA	CMC-C2C-C1C	2.76	129.09	125.00
22	A	6017	BCR	C8-C9-C10	2.76	123.41	118.95
18	G	1001	CLA	C4A-NA-C1A	2.77	109.89	106.38
18	A	1119	CLA	CMC-C2C-C1C	2.77	129.10	125.00
18	B	1238	CLA	CMB-C2B-C3B	2.77	130.50	125.09
18	A	1136	CLA	C4-C3-C5	2.77	119.59	115.37
18	2	2006	CLA	CMC-C2C-C1C	2.77	129.10	125.00
18	A	1134	CLA	C4-C3-C5	2.77	119.59	115.37
22	A	6017	BCR	C12-C13-C14	2.77	123.43	118.95
22	B	6009	BCR	C33-C5-C4	2.78	118.84	113.47
18	B	1228	CLA	C4-C3-C5	2.78	119.61	115.37
18	A	1119	CLA	C4-C3-C5	2.78	119.61	115.37
18	A	1132	CLA	C4-C3-C5	2.78	119.61	115.37
18	A	1237	CLA	C4-C3-C5	2.78	119.61	115.37
18	4	4005	CLA	C4-C3-C5	2.78	119.61	115.37
28	4	4010	CHL	CAA-CBA-CGA	2.78	121.32	113.28
18	A	1109	CLA	CMC-C2C-C1C	2.78	129.13	125.00
18	B	1234	CLA	C4-C3-C5	2.79	119.61	115.37
18	B	1214	CLA	CMC-C2C-C1C	2.79	129.13	125.00
18	4	4017	CLA	CMC-C2C-C1C	2.79	129.13	125.00
18	A	1108	CLA	CMB-C2B-C3B	2.79	130.54	125.09
18	A	1111	CLA	C4-C3-C5	2.79	119.62	115.37
22	3	3503	BCR	C23-C22-C21	2.79	123.45	118.95
28	3	3011	CHL	C4B-CHC-C1C	2.79	132.66	125.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1134	CLA	CMC-C2C-C1C	2.79	129.14	125.00
23	4	4801	LMG	O1-C1-C2	2.79	111.44	108.00
18	4	4003	CLA	C4A-NA-C1A	2.79	109.92	106.38
28	2	2011	CHL	C4B-CHC-C1C	2.79	132.66	125.40
18	B	1239	CLA	C4-C3-C5	2.79	119.63	115.37
18	A	1123	CLA	C4-C3-C5	2.80	119.63	115.37
18	B	1229	CLA	CMC-C2C-C1C	2.80	129.15	125.00
18	B	1240	CLA	C4-C3-C5	2.80	119.63	115.37
18	1	1008	CLA	CAC-C3C-C4C	2.80	128.95	124.82
18	A	1138	CLA	CED-O2D-CGD	2.80	122.62	115.97
18	F	1302	CLA	C3C-C4C-NC	2.80	113.05	110.21
18	B	1021	CLA	C4-C3-C5	2.80	119.64	115.37
18	4	4004	CLA	C3C-C4C-NC	2.80	113.05	110.21
18	4	4009	CLA	C4A-NA-C1A	2.80	109.94	106.38
18	1	1005	CLA	C4A-NA-C1A	2.81	109.94	106.38
18	B	1214	CLA	C3C-C4C-NC	2.81	113.05	110.21
18	B	1218	CLA	C3C-C4C-NC	2.81	113.06	110.21
18	A	1117	CLA	CMC-C2C-C1C	2.81	129.17	125.00
18	B	1212	CLA	C4-C3-C5	2.81	119.66	115.37
18	A	1106	CLA	CMB-C2B-C3B	2.81	130.59	125.09
18	B	1231	CLA	C3C-C4C-NC	2.81	113.06	110.21
18	2	2007	CLA	CMC-C2C-C1C	2.81	129.17	125.00
18	B	1021	CLA	CMB-C2B-C3B	2.82	130.60	125.09
18	B	1228	CLA	CMB-C2B-C3B	2.82	130.61	125.09
18	A	1132	CLA	C3C-C4C-NC	2.82	113.07	110.21
28	1	1010	CHL	C4B-CHC-C1C	2.83	132.75	125.40
18	A	1115	CLA	C3C-C4C-NC	2.83	113.08	110.21
18	B	1205	CLA	C3C-C4C-NC	2.83	113.08	110.21
21	1	1801	LHG	O8-C23-C24	2.83	120.56	111.85
18	2	2007	CLA	C4A-NA-C1A	2.83	109.97	106.38
18	2	2009	CLA	CMC-C2C-C1C	2.83	129.19	125.00
18	A	1013	CLA	CMC-C2C-C1C	2.84	129.20	125.00
18	A	1115	CLA	CMC-C2C-C1C	2.84	129.20	125.00
18	G	1002	CLA	CAC-C3C-C4C	2.84	129.01	124.82
18	3	3017	CLA	CMB-C2B-C3B	2.84	130.64	125.09
18	3	3007	CLA	CMC-C2C-C1C	2.84	129.21	125.00
18	B	1211	CLA	C4-C3-C5	2.84	119.70	115.37
27	4	4501	LUT	C2-C1-C6	2.84	114.86	110.58
23	B	5005	LMG	O8-C28-C29	2.84	120.60	111.85
18	B	1215	CLA	CMB-C2B-C3B	2.84	130.65	125.09
22	K	2011	BCR	C38-C26-C27	2.84	118.97	113.47
23	2	2802	LMG	O1-C1-C2	2.84	111.50	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	5003	LHG	O8-C23-C24	2.85	120.62	111.85
18	B	1224	CLA	C3C-C4C-NC	2.85	113.10	110.21
18	A	1118	CLA	CMC-C2C-C1C	2.85	129.22	125.00
18	B	1217	CLA	CMC-C2C-C1C	2.85	129.22	125.00
18	B	1212	CLA	CMC-C2C-C1C	2.85	129.23	125.00
18	A	1101	CLA	CMB-C2B-C3B	2.85	130.67	125.09
18	A	1126	CLA	CMC-C2C-C1C	2.85	129.23	125.00
18	A	1135	CLA	CMC-C2C-C1C	2.85	129.23	125.00
18	1	1003	CLA	C4-C3-C5	2.86	119.72	115.37
18	3	3003	CLA	C4-C3-C5	2.86	119.72	115.37
18	A	1124	CLA	C4-C3-C5	2.86	119.72	115.37
18	B	1202	CLA	C4A-NA-C1A	2.86	110.01	106.38
18	A	1138	CLA	C4-C3-C5	2.86	119.73	115.37
18	A	1125	CLA	CMC-C2C-C1C	2.86	129.24	125.00
18	A	1105	CLA	CMC-C2C-C1C	2.86	129.24	125.00
18	B	1206	CLA	CMC-C2C-C1C	2.86	129.24	125.00
18	1	1005	CLA	CMC-C2C-C1C	2.87	129.25	125.00
18	A	1109	CLA	C3C-C4C-NC	2.87	113.12	110.21
18	1	1013	CLA	CMC-C2C-C1C	2.87	129.25	125.00
18	B	1226	CLA	C4-C3-C5	2.87	119.74	115.37
18	A	1111	CLA	CMC-C2C-C1C	2.87	129.25	125.00
18	B	1229	CLA	C4-C3-C5	2.87	119.75	115.37
18	4	4012	CLA	C4A-NA-C1A	2.87	110.02	106.38
18	2	2007	CLA	C3C-C4C-NC	2.87	113.12	110.21
18	B	1219	CLA	C4-C3-C5	2.88	119.75	115.37
18	1	1013	CLA	CAC-C3C-C4C	2.88	129.06	124.82
18	2	2006	CLA	C4-C3-C5	2.88	119.75	115.37
18	4	4004	CLA	C4-C3-C5	2.88	119.75	115.37
18	B	1219	CLA	CMC-C2C-C1C	2.88	129.27	125.00
18	2	2012	CLA	C4A-NA-C1A	2.88	110.03	106.38
18	2	2005	CLA	CMC-C2C-C1C	2.88	129.27	125.00
18	B	1227	CLA	C3C-C4C-NC	2.89	113.14	110.21
27	3	3502	LUT	C18-C5-C4	2.89	119.53	114.25
22	I	6020	BCR	C38-C26-C27	2.90	119.07	113.47
18	A	1124	CLA	CMC-C2C-C1C	2.90	129.29	125.00
18	A	1121	CLA	CMC-C2C-C1C	2.90	129.29	125.00
22	A	6002	BCR	C23-C22-C21	2.90	123.63	118.95
18	3	3013	CLA	C3C-C4C-NC	2.90	113.15	110.21
18	B	1204	CLA	C3C-C4C-NC	2.90	113.15	110.21
18	B	1012	CLA	CMC-C2C-C1C	2.91	129.31	125.00
18	3	3018	CLA	CMC-C2C-C1C	2.91	129.31	125.00
18	F	1302	CLA	CMC-C2C-C1C	2.91	129.32	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1116	CLA	CMC-C2C-C1C	2.91	129.32	125.00
18	4	4012	CLA	CMC-C2C-C1C	2.91	129.32	125.00
18	4	4007	CLA	CMC-C2C-C1C	2.92	129.32	125.00
18	A	1132	CLA	CMC-C2C-C1C	2.92	129.32	125.00
18	J	1302	CLA	CMC-C2C-C1C	2.92	129.32	125.00
18	A	1107	CLA	C3C-C4C-NC	2.92	113.17	110.21
22	B	6004	BCR	C38-C26-C27	2.92	119.11	113.47
18	B	1235	CLA	C4-C3-C5	2.92	119.83	115.37
18	4	4003	CLA	CMC-C2C-C1C	2.93	129.34	125.00
18	4	4003	CLA	C4-C3-C5	2.93	119.84	115.37
18	4	4001	CLA	C4A-NA-C1A	2.94	110.10	106.38
22	L	6019	BCR	C8-C9-C10	2.94	123.69	118.95
18	A	1013	CLA	CMB-C2B-C3B	2.94	130.83	125.09
22	A	6011	BCR	C33-C5-C4	2.94	119.15	113.47
18	F	1301	CLA	CMC-C2C-C1C	2.94	129.35	125.00
18	2	2001	CLA	C4-C3-C5	2.94	119.85	115.37
18	B	1217	CLA	C3C-C4C-NC	2.94	113.19	110.21
27	3	3501	LUT	C18-C5-C4	2.94	119.62	114.25
18	B	1220	CLA	C3C-C4C-NC	2.94	113.19	110.21
18	A	1117	CLA	C4-C3-C5	2.94	119.86	115.37
18	B	1201	CLA	C3C-C4C-NC	2.94	113.19	110.21
22	L	6020	BCR	C8-C9-C10	2.95	123.71	118.95
18	A	1122	CLA	C3C-C4C-NC	2.95	113.20	110.21
18	3	3001	CLA	CMC-C2C-C1C	2.96	129.38	125.00
18	A	1013	CLA	C3C-C4C-NC	2.96	113.21	110.21
18	A	1129	CLA	CMC-C2C-C1C	2.96	129.39	125.00
18	B	1203	CLA	CMC-C2C-C1C	2.96	129.39	125.00
18	A	1133	CLA	C4-C3-C5	2.96	119.89	115.37
18	A	1130	CLA	CMC-C2C-C1C	2.97	129.40	125.00
18	B	1239	CLA	C3C-C4C-NC	2.97	113.22	110.21
18	A	1128	CLA	C3C-C4C-NC	2.97	113.22	110.21
18	A	1121	CLA	C3C-C4C-NC	2.97	113.22	110.21
18	A	1108	CLA	C3C-C4C-NC	2.97	113.22	110.21
18	A	1108	CLA	CMC-C2C-C1C	2.97	129.41	125.00
18	A	1131	CLA	CMC-C2C-C1C	2.98	129.41	125.00
18	3	3006	CLA	CMC-C2C-C1C	2.98	129.41	125.00
18	A	1104	CLA	CMC-C2C-C1C	2.98	129.41	125.00
18	B	1206	CLA	C4-C3-C5	2.98	119.91	115.37
18	B	1225	CLA	CMC-C2C-C1C	2.98	129.41	125.00
18	A	1118	CLA	C3C-C4C-NC	2.98	113.23	110.21
18	A	1125	CLA	C4-C3-C5	2.98	119.91	115.37
18	A	1110	CLA	C3C-C4C-NC	2.98	113.23	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6008	BCR	C38-C26-C27	2.98	119.24	113.47
18	A	1103	CLA	C4-C3-C5	2.98	119.91	115.37
18	B	1209	CLA	C3C-C4C-NC	2.98	113.23	110.21
18	A	1137	CLA	C4-C3-C5	2.99	119.92	115.37
18	A	1237	CLA	C3C-C4C-NC	2.99	113.24	110.21
18	B	1023	CLA	C4-C3-C5	2.99	119.93	115.37
18	A	1124	CLA	C3C-C4C-NC	2.99	113.24	110.21
28	4	4011	CHL	C4B-CHC-C1C	2.99	133.18	125.40
18	3	3003	CLA	O2A-CGA-CBA	2.99	121.06	111.85
18	F	1301	CLA	C3C-C4C-NC	3.00	113.25	110.21
18	A	1128	CLA	CMB-C2B-C3B	3.00	130.95	125.09
18	A	1103	CLA	C3C-C4C-NC	3.00	113.25	110.21
18	A	1106	CLA	C3C-C4C-NC	3.00	113.25	110.21
18	A	1134	CLA	C3C-C4C-NC	3.00	113.25	110.21
18	1	1007	CLA	C3C-C4C-NC	3.00	113.25	110.21
18	B	1226	CLA	CMB-C2B-C3B	3.00	130.96	125.09
18	A	1127	CLA	C4-C3-C5	3.00	119.94	115.37
18	2	2008	CLA	CMC-C2C-C1C	3.00	129.45	125.00
18	A	1106	CLA	CMC-C2C-C1C	3.00	129.45	125.00
18	B	1208	CLA	C3C-C4C-NC	3.00	113.25	110.21
18	G	1001	CLA	CAC-C3C-C4C	3.01	129.26	124.82
18	A	1133	CLA	CMC-C2C-C1C	3.01	129.46	125.00
18	3	3005	CLA	C4A-NA-C1A	3.01	110.19	106.38
18	B	1221	CLA	C3C-C4C-NC	3.01	113.26	110.21
18	B	1210	CLA	C3C-C4C-NC	3.01	113.26	110.21
18	B	1215	CLA	CMC-C2C-C1C	3.01	129.46	125.00
18	A	1102	CLA	CMC-C2C-C1C	3.01	129.47	125.00
18	B	1239	CLA	CMC-C2C-C1C	3.02	129.47	125.00
18	2	2004	CLA	CMC-C2C-C1C	3.02	129.47	125.00
18	B	1208	CLA	CMC-C2C-C1C	3.02	129.47	125.00
18	A	1139	CLA	C3C-C4C-NC	3.02	113.27	110.21
18	2	2007	CLA	C4-C3-C5	3.02	119.97	115.37
18	3	3013	CLA	CMC-C2C-C1C	3.02	129.48	125.00
18	A	1116	CLA	C3C-C4C-NC	3.02	113.27	110.21
18	A	1101	CLA	C4-C3-C5	3.03	119.98	115.37
22	A	6007	BCR	C38-C26-C27	3.03	119.32	113.47
18	G	1003	CLA	CMC-C2C-C1C	3.03	129.49	125.00
18	A	1120	CLA	CMC-C2C-C1C	3.03	129.49	125.00
18	B	1213	CLA	C3C-C4C-NC	3.03	113.28	110.21
18	A	1013	CLA	C4-C3-C5	3.03	119.99	115.37
18	2	2003	CLA	C4-C3-C5	3.03	119.99	115.37
18	A	1130	CLA	C3C-C4C-NC	3.03	113.28	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1128	CLA	C4-C3-C5	3.04	119.99	115.37
29	4	4505	ZEX	C2-C1-C6	3.04	115.15	110.58
18	B	1238	CLA	CMC-C2C-C1C	3.04	129.50	125.00
18	4	4001	CLA	C4-C3-C5	3.04	120.00	115.37
18	A	1116	CLA	C4-C3-C5	3.04	120.00	115.37
18	1	1007	CLA	CMC-C2C-C1C	3.04	129.50	125.00
18	1	1001	CLA	C4A-NA-C1A	3.04	110.23	106.38
18	A	1117	CLA	C3C-C4C-NC	3.04	113.29	110.21
18	B	1238	CLA	C4-C3-C5	3.04	120.00	115.37
22	B	6010	BCR	C19-C18-C17	3.04	123.85	118.95
18	B	1215	CLA	C4-C3-C5	3.05	120.01	115.37
18	A	1113	CLA	C3C-C4C-NC	3.05	113.30	110.21
18	1	1008	CLA	C3C-C4C-NC	3.05	113.30	110.21
18	3	3002	CLA	CAC-C3C-C4C	3.05	129.32	124.82
18	B	1228	CLA	C3C-C4C-NC	3.05	113.30	110.21
18	B	1021	CLA	C3C-C4C-NC	3.06	113.31	110.21
18	B	1218	CLA	CMC-C2C-C1C	3.06	129.53	125.00
18	B	1222	CLA	CMC-C2C-C1C	3.06	129.53	125.00
18	H	1000	CLA	C3C-C4C-NC	3.06	113.31	110.21
18	A	1131	CLA	C4-C3-C5	3.06	120.04	115.37
28	2	2013	CHL	C4B-CHC-C1C	3.06	133.37	125.40
18	B	1234	CLA	C3C-C4C-NC	3.06	113.32	110.21
18	A	1237	CLA	CMC-C2C-C1C	3.07	129.54	125.00
18	B	1216	CLA	CMB-C2B-C3B	3.07	131.09	125.09
18	B	1221	CLA	CMC-C2C-C1C	3.07	129.55	125.00
18	B	1203	CLA	C4-C3-C5	3.07	120.04	115.37
18	2	2012	CLA	C3C-C4C-NC	3.07	113.33	110.21
18	3	3012	CLA	C3C-C4C-NC	3.08	113.33	110.21
18	A	1111	CLA	C3C-C4C-NC	3.08	113.33	110.21
22	F	6016	BCR	C34-C9-C8	3.08	123.12	118.08
18	4	4006	CLA	CMC-C2C-C1C	3.08	129.57	125.00
18	1	1013	CLA	C4A-NA-C1A	3.08	110.29	106.38
18	G	1001	CLA	CMC-C2C-C1C	3.09	129.57	125.00
18	A	1112	CLA	C3C-C4C-NC	3.09	113.34	110.21
18	B	1230	CLA	CMC-C2C-C1C	3.09	129.58	125.00
18	2	2019	CLA	C2D-C1D-ND	3.10	114.48	110.22
18	B	1213	CLA	CMB-C2B-C3B	3.10	131.15	125.09
18	A	1126	CLA	C3C-C4C-NC	3.10	113.35	110.21
22	L	6020	BCR	C23-C22-C21	3.10	123.95	118.95
18	A	1131	CLA	C3C-C4C-NC	3.10	113.35	110.21
18	B	1213	CLA	CMC-C2C-C1C	3.11	129.60	125.00
18	1	1008	CLA	CMC-C2C-C1C	3.11	129.60	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1002	CLA	C3C-C4C-NC	3.11	113.36	110.21
18	3	3012	CLA	C4A-NA-C1A	3.11	110.32	106.38
18	B	1202	CLA	C3C-C4C-NC	3.11	113.36	110.21
18	A	1137	CLA	CMC-C2C-C1C	3.11	129.62	125.00
18	4	4017	CLA	C3C-C4C-NC	3.12	113.37	110.21
18	B	1232	CLA	C4-C3-C5	3.12	120.12	115.37
18	A	1114	CLA	C3C-C4C-NC	3.12	113.37	110.21
18	B	1232	CLA	C3C-C4C-NC	3.12	113.38	110.21
18	4	4012	CLA	CAC-C3C-C4C	3.12	129.43	124.82
18	4	4009	CLA	C3C-C4C-NC	3.13	113.38	110.21
18	1	1014	CLA	C4A-NA-C1A	3.13	110.35	106.38
18	2	2002	CLA	O2A-CGA-CBA	3.13	123.94	112.34
18	B	1231	CLA	CMC-C2C-C1C	3.13	129.65	125.00
18	G	1002	CLA	CMC-C2C-C1C	3.13	129.65	125.00
18	B	1238	CLA	C3C-C4C-NC	3.14	113.39	110.21
18	A	1130	CLA	CMB-C2B-C3B	3.14	131.22	125.09
18	B	1203	CLA	C3C-C4C-NC	3.14	113.39	110.21
18	3	3019	CLA	C2D-C1D-ND	3.14	114.53	110.22
18	A	1119	CLA	C3C-C4C-NC	3.14	113.39	110.21
22	A	6003	BCR	C19-C18-C17	3.14	124.02	118.95
18	B	1209	CLA	CMB-C2B-C3B	3.14	131.24	125.09
18	J	1302	CLA	C3C-C4C-NC	3.15	113.40	110.21
18	3	3006	CLA	CMB-C2B-C3B	3.15	131.24	125.09
17	A	1011	CL0	CMC-C2C-C1C	3.15	129.67	125.00
18	B	1023	CLA	CAC-C3C-C4C	3.15	129.47	124.82
18	A	1120	CLA	C3C-C4C-NC	3.15	113.40	110.21
18	B	1224	CLA	C4-C3-C5	3.15	120.17	115.37
18	L	1503	CLA	C3C-C4C-NC	3.16	113.41	110.21
18	A	1104	CLA	C4-C3-C5	3.16	120.19	115.37
18	3	3003	CLA	C4A-NA-C1A	3.16	110.39	106.38
18	A	1133	CLA	C3C-C4C-NC	3.16	113.41	110.21
18	A	1109	CLA	C4-C3-C5	3.16	120.19	115.37
22	L	6020	BCR	C38-C26-C27	3.17	119.59	113.47
18	B	1216	CLA	CMC-C2C-C1C	3.17	129.69	125.00
18	4	4006	CLA	C3C-C4C-NC	3.17	113.42	110.21
18	G	1002	CLA	O2A-CGA-CBA	3.17	124.08	112.34
18	1	1013	CLA	O2A-CGA-CBA	3.17	124.09	112.34
18	A	1135	CLA	C3C-C4C-NC	3.17	113.42	110.21
18	A	1123	CLA	CMC-C2C-C1C	3.17	129.70	125.00
18	A	1136	CLA	C3C-C4C-NC	3.18	113.43	110.21
18	A	1107	CLA	CMC-C2C-C1C	3.18	129.71	125.00
18	4	4008	CLA	O2A-CGA-CBA	3.18	124.12	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4005	CLA	C4A-NA-C1A	3.18	110.42	106.38
18	B	1215	CLA	C3C-C4C-NC	3.18	113.43	110.21
18	A	1105	CLA	C3C-C4C-NC	3.18	113.44	110.21
18	3	3002	CLA	O2A-CGA-CBA	3.19	124.14	112.34
18	1	1012	CLA	O2A-CGA-CBA	3.19	121.65	111.85
18	B	1240	CLA	CMC-C2C-C1C	3.19	129.72	125.00
18	A	1115	CLA	O2A-CGA-CBA	3.19	124.16	112.34
18	B	1023	CLA	C3C-C4C-NC	3.19	113.44	110.21
18	A	1127	CLA	C3C-C4C-NC	3.19	113.44	110.21
18	A	1103	CLA	CMC-C2C-C1C	3.19	129.73	125.00
18	B	1240	CLA	C3C-C4C-NC	3.19	113.45	110.21
18	B	1227	CLA	C4-C3-C5	3.20	120.25	115.37
18	A	1140	CLA	C3C-C4C-NC	3.21	113.46	110.21
18	2	2002	CLA	C4A-NA-C1A	3.21	110.46	106.38
22	B	6004	BCR	C33-C5-C4	3.22	119.69	113.47
18	3	3010	CLA	CAC-C3C-C4C	3.22	129.57	124.82
18	B	1216	CLA	C4-C3-C5	3.22	120.28	115.37
18	A	1114	CLA	O2A-CGA-CBA	3.23	124.29	112.34
18	B	1207	CLA	C3C-C4C-NC	3.23	113.48	110.21
18	B	1206	CLA	C3C-C4C-NC	3.23	113.49	110.21
18	K	1001	CLA	O2A-CGA-CBA	3.23	124.32	112.34
27	4	4501	LUT	C18-C5-C4	3.23	120.16	114.25
18	1	1007	CLA	O2A-CGA-CBA	3.24	124.33	112.34
18	A	1022	CLA	C4-C3-C5	3.24	120.30	115.37
18	A	1108	CLA	O2A-CGA-CBA	3.25	124.37	112.34
22	J	6013	BCR	C8-C9-C10	3.25	124.19	118.95
18	2	2002	CLA	CMC-C2C-C1C	3.25	129.81	125.00
22	A	6007	BCR	C19-C18-C17	3.26	124.20	118.95
18	4	4016	CLA	O2A-CGA-CBA	3.26	124.43	112.34
18	B	1012	CLA	C4-C3-C5	3.26	120.34	115.37
18	B	1209	CLA	O2A-CGA-CBA	3.27	124.44	112.34
18	B	1235	CLA	C3C-C4C-NC	3.27	113.52	110.21
18	1	1002	CLA	O2A-CGA-CBA	3.27	124.45	112.34
18	A	1137	CLA	C3C-C4C-NC	3.27	113.53	110.21
22	B	6010	BCR	C1-C6-C7	3.28	125.32	115.96
18	3	3003	CLA	C3C-C4C-NC	3.28	113.53	110.21
18	B	1235	CLA	CMC-C2C-C1C	3.28	129.86	125.00
18	B	1217	CLA	O2A-CGA-CBA	3.28	124.49	112.34
18	B	1225	CLA	C3C-C4C-NC	3.28	113.54	110.21
18	A	1118	CLA	O2A-CGA-CBA	3.29	124.51	112.34
18	B	1236	CLA	CMC-C2C-C1C	3.29	129.88	125.00
23	G	2021	LMG	O8-C28-C29	3.29	121.97	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1219	CLA	C3C-C4C-NC	3.29	113.55	110.21
18	L	1502	CLA	C3C-C4C-NC	3.29	113.55	110.21
18	B	1240	CLA	O2A-CGA-CBA	3.29	121.99	111.85
18	A	1112	CLA	C4-C3-C5	3.30	120.39	115.37
18	A	1113	CLA	O2A-CGA-CBA	3.30	124.56	112.34
18	4	4002	CLA	C3C-C4C-NC	3.30	113.56	110.21
18	B	1212	CLA	C3C-C4C-NC	3.30	113.56	110.21
18	A	1123	CLA	C3C-C4C-NC	3.31	113.56	110.21
18	B	1236	CLA	C3C-C4C-NC	3.31	113.56	110.21
18	2	2005	CLA	C4-C3-C5	3.31	120.41	115.37
18	A	1120	CLA	C4-C3-C5	3.32	120.42	115.37
18	B	1216	CLA	C3C-C4C-NC	3.32	113.57	110.21
18	L	1501	CLA	CMC-C2C-C1C	3.32	129.92	125.00
18	3	3019	CLA	CAD-C3D-C2D	3.33	140.83	132.73
18	A	1139	CLA	CMC-C2C-C1C	3.33	129.94	125.00
18	A	1121	CLA	C4-C3-C5	3.35	120.47	115.37
18	B	1230	CLA	C3C-C4C-NC	3.35	113.60	110.21
18	1	1006	CLA	CAC-C3C-C4C	3.35	129.76	124.82
18	3	3019	CLA	C2C-C1C-NC	3.35	116.53	109.39
18	B	1227	CLA	CMC-C2C-C1C	3.35	129.97	125.00
18	B	1021	CLA	CMC-C2C-C1C	3.35	129.97	125.00
18	3	3013	CLA	O2A-CGA-CBA	3.36	124.77	112.34
22	J	6013	BCR	C29-C30-C25	3.36	115.47	110.48
22	A	6002	BCR	C38-C26-C27	3.36	119.97	113.47
18	1	1008	CLA	O2A-CGA-CBA	3.36	124.80	112.34
18	K	1001	CLA	C4A-NA-C1A	3.37	110.66	106.38
18	A	1104	CLA	C3C-C4C-NC	3.38	113.63	110.21
22	J	6012	BCR	C19-C18-C17	3.38	124.40	118.95
18	B	1222	CLA	C4-C3-C5	3.38	120.52	115.37
18	L	1502	CLA	CMC-C2C-C1C	3.38	130.01	125.00
18	1	1008	CLA	C4A-NA-C1A	3.38	110.67	106.38
22	J	6012	BCR	C33-C5-C4	3.38	120.01	113.47
18	1	1002	CLA	CMC-C2C-C1C	3.39	130.02	125.00
18	2	2008	CLA	C3C-C4C-NC	3.41	113.66	110.21
18	3	3005	CLA	C4-C3-C5	3.41	120.57	115.37
18	1	1002	CLA	C4A-NA-C1A	3.41	110.71	106.38
27	I	6018	LUT	C2-C3-C4	3.42	115.56	110.29
18	H	1000	CLA	O2A-CGA-CBA	3.43	125.03	112.34
18	B	1231	CLA	C4-C3-C5	3.43	120.59	115.37
18	B	1201	CLA	CMC-C2C-C1C	3.43	130.08	125.00
18	A	1022	CLA	C3C-C4C-NC	3.43	113.69	110.21
22	A	6011	BCR	C35-C13-C12	3.43	123.69	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4008	CLA	CMC-C2C-C1C	3.43	130.09	125.00
22	F	6014	BCR	C23-C22-C21	3.44	124.49	118.95
18	4	4001	CLA	O2D-CGD-CBD	3.44	116.18	111.22
18	A	1102	CLA	C3C-C4C-NC	3.44	113.69	110.21
18	3	3017	CLA	CMC-C2C-C1C	3.44	130.10	125.00
22	B	6005	BCR	C38-C26-C27	3.44	120.12	113.47
18	4	4009	CLA	CMC-C2C-C1C	3.44	130.10	125.00
18	4	4006	CLA	O2A-CGA-CBA	3.45	122.46	111.85
18	B	1213	CLA	C4-C3-C5	3.45	120.63	115.37
18	4	4007	CLA	C4A-NA-C1A	3.46	110.77	106.38
18	B	1222	CLA	C3C-C4C-NC	3.46	113.72	110.21
22	L	6019	BCR	C19-C18-C17	3.47	124.54	118.95
18	A	1129	CLA	C3C-C4C-NC	3.47	113.72	110.21
18	3	3010	CLA	CMB-C2B-C3B	3.48	131.90	125.09
18	2	2003	CLA	CMC-C2C-C1C	3.48	130.16	125.00
18	A	1140	CLA	C4-C3-C5	3.50	120.70	115.37
18	2	2003	CLA	C3C-C4C-NC	3.50	113.76	110.21
18	3	3017	CLA	O2A-CGA-CBA	3.51	125.34	112.34
18	B	1207	CLA	CMC-C2C-C1C	3.52	130.21	125.00
23	J	5001	LMG	O8-C28-C29	3.52	122.69	111.85
18	1	1007	CLA	C4A-NA-C1A	3.53	110.86	106.38
18	A	1151	CLA	C3C-C4C-NC	3.54	113.79	110.21
18	B	1227	CLA	O2A-CGA-CBA	3.54	122.75	111.85
22	B	6006	BCR	C8-C9-C10	3.55	124.67	118.95
18	1	1011	CLA	CMC-C2C-C1C	3.55	130.26	125.00
18	2	2019	CLA	C2C-C1C-NC	3.55	116.96	109.39
18	1	1014	CLA	C3C-C4C-NC	3.56	113.82	110.21
18	B	1207	CLA	O2A-CGA-CBA	3.56	122.82	111.85
17	A	1011	CL0	C3C-C4C-NC	3.57	113.82	110.21
23	F	5002	LMG	O8-C28-C29	3.57	122.83	111.85
18	2	2008	CLA	C4A-NA-C1A	3.57	110.91	106.38
22	3	3503	BCR	C8-C9-C10	3.58	124.72	118.95
22	G	2011	BCR	C8-C9-C10	3.58	124.72	118.95
18	2	2019	CLA	CAD-C3D-C2D	3.58	141.45	132.73
18	A	1103	CLA	O2A-CGA-CBA	3.59	122.91	111.85
18	A	1117	CLA	O2A-CGA-CBA	3.60	122.93	111.85
22	J	6012	BCR	C29-C30-C25	3.61	115.85	110.48
18	4	4005	CLA	C3C-C4C-NC	3.63	113.89	110.21
18	2	2019	CLA	C2B-C1B-NB	3.64	113.35	110.09
18	B	1221	CLA	O2A-CGA-CBA	3.64	123.04	111.85
18	A	1013	CLA	O2A-CGA-CBA	3.64	123.05	111.85
23	G	2021	LMG	O7-C10-C11	3.64	119.19	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4001	CLA	CGD-CBD-CHA	3.64	123.38	110.88
18	B	1223	CLA	C3C-C4C-NC	3.65	113.90	110.21
18	2	2001	CLA	CBA-CAA-C2A	3.65	123.36	113.96
22	A	6017	BCR	C23-C22-C21	3.65	124.84	118.95
18	L	1501	CLA	O2A-CGA-CBA	3.66	123.11	111.85
22	K	2011	BCR	C19-C18-C17	3.66	124.86	118.95
18	B	1225	CLA	C4-C3-C5	3.68	120.97	115.37
21	A	7001	LHG	O8-C23-C24	3.68	123.17	111.85
18	3	3005	CLA	C3C-C4C-NC	3.68	113.94	110.21
18	A	1138	CLA	O2A-CGA-CBA	3.69	123.19	111.85
18	3	3008	CLA	C3C-C4C-NC	3.69	113.95	110.21
18	4	4012	CLA	O2A-CGA-CBA	3.70	123.24	111.85
18	B	1012	CLA	C3C-C4C-NC	3.70	113.96	110.21
18	A	1102	CLA	O2A-CGA-CBA	3.71	123.26	111.85
18	1	1011	CLA	O2A-CGA-CBA	3.72	123.30	111.85
18	L	1503	CLA	CMC-C2C-C1C	3.73	130.53	125.00
18	B	1231	CLA	O2A-CGA-CBA	3.74	123.35	111.85
18	2	2003	CLA	C4A-NA-C1A	3.74	111.13	106.38
18	L	1502	CLA	O2A-CGA-CBA	3.75	123.40	111.85
18	3	3010	CLA	C4-C3-C5	3.76	121.10	115.37
18	B	1204	CLA	O2A-CGA-CBA	3.76	123.44	111.85
18	4	4003	CLA	O2A-CGA-CBA	3.77	123.44	111.85
18	B	1216	CLA	O2A-CGA-CBA	3.77	123.45	111.85
18	A	1125	CLA	C3C-C4C-NC	3.77	114.03	110.21
18	2	2005	CLA	O2A-CGA-CBA	3.77	123.46	111.85
22	G	2011	BCR	C23-C22-C21	3.77	125.04	118.95
18	3	3005	CLA	CMC-C2C-C1C	3.77	130.59	125.00
18	A	1139	CLA	O2A-CGA-CBA	3.78	123.49	111.85
18	B	1213	CLA	O2A-CGA-CBA	3.79	123.50	111.85
18	B	1229	CLA	C3C-C4C-NC	3.79	114.05	110.21
18	1	1014	CLA	O2A-CGA-CBA	3.79	126.39	112.34
18	3	3019	CLA	C3C-C4C-NC	3.80	113.53	110.09
22	J	6013	BCR	C33-C5-C4	3.80	120.82	113.47
23	2	2802	LMG	O7-C10-C11	3.80	119.54	111.53
27	I	6018	LUT	C18-C5-C4	3.82	121.23	114.25
18	3	3019	CLA	C2B-C1B-NB	3.83	113.53	110.09
18	4	4004	CLA	O2A-CGA-CBA	3.84	123.66	111.85
22	J	6012	BCR	C2-C1-C6	3.84	116.19	110.48
18	B	1212	CLA	O2A-CGA-CBA	3.84	123.67	111.85
18	4	4008	CLA	C4A-NA-C1A	3.84	111.25	106.38
18	B	1218	CLA	C4-C3-C5	3.85	121.23	115.37
22	G	2011	BCR	C33-C5-C4	3.85	120.92	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3006	CLA	O2A-CGA-CBA	3.85	123.71	111.85
18	B	1203	CLA	O2A-CGA-CBA	3.86	123.72	111.85
18	B	1234	CLA	O2A-CGA-CBA	3.86	123.73	111.85
18	A	1022	CLA	O2A-CGA-CBA	3.86	123.74	111.85
22	J	6013	BCR	C23-C22-C21	3.87	125.19	118.95
18	2	2008	CLA	O2A-CGA-CBA	3.89	123.81	111.85
22	A	6002	BCR	C19-C18-C17	3.89	125.23	118.95
18	A	1122	CLA	C4-C3-C5	3.89	121.30	115.37
18	A	1125	CLA	O2A-CGA-CBA	3.90	123.84	111.85
18	B	1201	CLA	O2A-CGA-CBA	3.90	123.86	111.85
18	A	1128	CLA	O2A-CGA-CBA	3.91	123.87	111.85
18	G	1001	CLA	C4-C3-C5	3.91	121.32	115.37
18	A	1105	CLA	O2A-CGA-CBA	3.92	123.91	111.85
18	3	3012	CLA	O2A-CGA-CBA	3.95	124.02	111.85
18	4	4002	CLA	O2D-CGD-CBD	3.96	116.93	111.22
18	2	2012	CLA	C4-C3-C5	3.97	121.41	115.37
18	A	1111	CLA	O2A-CGA-CBA	3.97	124.08	111.85
18	B	1239	CLA	O2A-CGA-CBA	3.97	124.08	111.85
21	A	7001	LHG	O7-C7-C8	3.98	119.90	111.53
18	4	4001	CLA	O2A-CGA-CBA	3.98	124.11	111.85
22	3	3503	BCR	C19-C18-C17	3.99	125.38	118.95
18	3	3008	CLA	O2A-C1-C2	3.99	122.31	109.14
18	1	1005	CLA	C3C-C4C-NC	3.99	114.25	110.21
18	A	1135	CLA	O2A-CGA-CBA	3.99	124.14	111.85
18	B	1202	CLA	O2A-CGA-CBA	4.00	124.16	111.85
22	F	6014	BCR	C2-C1-C6	4.01	116.44	110.48
18	4	4002	CLA	O2A-CGA-CBA	4.01	124.20	111.85
18	B	1228	CLA	O2A-CGA-CBA	4.02	124.22	111.85
18	2	2016	CLA	O2A-CGA-CBA	4.02	124.22	111.85
18	B	1023	CLA	O2A-CGA-CBA	4.02	124.22	111.85
18	A	1109	CLA	O2A-CGA-CBA	4.02	124.23	111.85
18	2	2012	CLA	O2A-CGA-CBA	4.03	124.24	111.85
18	1	1005	CLA	O2A-CGA-CBA	4.03	124.26	111.85
18	A	1112	CLA	O2A-CGA-CBA	4.04	124.28	111.85
18	1	1001	CLA	C3C-C4C-NC	4.04	114.30	110.21
18	A	1130	CLA	O2A-CGA-CBA	4.04	124.29	111.85
18	A	1129	CLA	O2A-CGA-CBA	4.05	124.31	111.85
18	3	3007	CLA	O2A-CGA-CBA	4.05	124.32	111.85
18	B	1220	CLA	O2A-CGA-CBA	4.05	124.32	111.85
18	3	3018	CLA	O2A-CGA-CBA	4.05	124.32	111.85
18	A	1104	CLA	O2A-CGA-CBA	4.07	124.38	111.85
18	B	1021	CLA	O2A-CGA-CBA	4.07	124.38	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1120	CLA	O2A-CGA-CBA	4.07	124.38	111.85
22	3	3503	BCR	C33-C5-C4	4.07	121.35	113.47
18	B	1232	CLA	O2A-CGA-CBA	4.07	124.39	111.85
18	A	1137	CLA	O2A-CGA-CBA	4.07	124.39	111.85
18	3	3005	CLA	O2A-CGA-CBA	4.08	124.40	111.85
18	A	1123	CLA	O2A-CGA-CBA	4.08	124.41	111.85
18	A	1126	CLA	O2A-CGA-CBA	4.08	124.42	111.85
18	B	1208	CLA	O2A-CGA-CBA	4.08	124.42	111.85
18	A	1237	CLA	O2A-CGA-CBA	4.09	124.42	111.85
18	B	1206	CLA	O2A-CGA-CBA	4.09	124.43	111.85
18	4	4007	CLA	O2A-CGA-CBA	4.09	124.43	111.85
18	A	1151	CLA	O2A-CGA-CBA	4.09	124.44	111.85
18	B	1219	CLA	O2A-CGA-CBA	4.09	124.45	111.85
18	A	1101	CLA	O2A-CGA-CBA	4.10	124.47	111.85
18	A	1140	CLA	O2A-CGA-CBA	4.11	124.50	111.85
18	3	3001	CLA	O2A-CGA-CBA	4.11	124.50	111.85
18	B	1236	CLA	O2A-CGA-CBA	4.11	124.51	111.85
18	A	1131	CLA	O2A-CGA-CBA	4.12	124.52	111.85
18	A	1119	CLA	O2A-CGA-CBA	4.12	124.53	111.85
18	A	1110	CLA	O2A-CGA-CBA	4.12	124.54	111.85
18	B	1012	CLA	O2A-CGA-CBA	4.13	124.55	111.85
22	J	6013	BCR	C19-C18-C17	4.13	125.61	118.95
18	B	1205	CLA	O2A-CGA-CBA	4.14	124.59	111.85
18	A	1106	CLA	O2A-CGA-CBA	4.14	124.60	111.85
18	2	2006	CLA	O2A-CGA-CBA	4.14	124.61	111.85
20	B	5002	PQN	C14-C13-C15	4.15	121.69	115.37
18	G	1003	CLA	O2A-CGA-CBA	4.15	124.62	111.85
18	B	1225	CLA	O2A-CGA-CBA	4.16	124.64	111.85
18	B	1223	CLA	O2A-CGA-CBA	4.17	124.68	111.85
18	B	1210	CLA	O2A-CGA-CBA	4.17	124.69	111.85
22	I	6020	BCR	C19-C18-C17	4.17	125.68	118.95
18	2	2003	CLA	O2A-CGA-CBA	4.18	124.70	111.85
22	B	6005	BCR	C19-C18-C17	4.18	125.69	118.95
18	2	2001	CLA	O2D-CGD-CBD	4.19	117.26	111.22
18	4	4005	CLA	O2A-CGA-CBA	4.21	124.80	111.85
18	2	2009	CLA	O2A-CGA-CBA	4.21	124.80	111.85
18	4	4008	CLA	C3C-C4C-NC	4.22	114.48	110.21
18	A	1132	CLA	O2A-CGA-CBA	4.22	124.83	111.85
18	L	1503	CLA	O2A-CGA-CBA	4.22	124.83	111.85
18	B	1238	CLA	O2A-CGA-CBA	4.22	124.84	111.85
18	B	1222	CLA	O2A-CGA-CBA	4.22	124.84	111.85
18	A	1136	CLA	O2A-CGA-CBA	4.23	124.88	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	5005	LMG	O7-C10-C11	4.25	120.48	111.53
18	4	4017	CLA	O2A-CGA-CBA	4.25	124.93	111.85
18	A	1121	CLA	O2A-CGA-CBA	4.25	124.94	111.85
18	B	1211	CLA	O2A-CGA-CBA	4.26	124.95	111.85
18	2	2007	CLA	O2A-CGA-CBA	4.26	124.97	111.85
18	B	1230	CLA	O2A-CGA-CBA	4.27	124.99	111.85
18	2	2016	CLA	CMC-C2C-C1C	4.28	131.35	125.00
18	A	1116	CLA	O2A-CGA-CBA	4.29	125.04	111.85
18	2	2016	CLA	C4A-NA-C1A	4.30	111.83	106.38
18	1	1001	CLA	O2A-CGA-CBA	4.30	125.08	111.85
18	F	1302	CLA	O2A-CGA-CBA	4.31	125.11	111.85
18	A	1127	CLA	O2A-CGA-CBA	4.31	125.12	111.85
18	4	4009	CLA	O2A-CGA-CBA	4.33	125.16	111.85
18	A	1134	CLA	O2A-CGA-CBA	4.34	125.20	111.85
18	3	3008	CLA	O2A-CGA-CBA	4.34	125.21	111.85
18	1	1006	CLA	CMC-C2C-C1C	4.34	131.44	125.00
18	3	3010	CLA	O2A-CGA-CBA	4.35	125.24	111.85
18	B	1235	CLA	O2A-CGA-CBA	4.36	125.27	111.85
18	A	1107	CLA	O2A-CGA-CBA	4.36	125.28	111.85
18	B	1226	CLA	O2A-CGA-CBA	4.37	125.31	111.85
18	2	2016	CLA	C3C-C4C-NC	4.38	114.64	110.21
18	2	2004	CLA	O2A-CGA-CBA	4.38	125.32	111.85
20	A	5001	PQN	C14-C13-C15	4.39	122.05	115.37
18	A	1122	CLA	O2A-CGA-CBA	4.39	125.36	111.85
17	A	1011	CL0	O2A-CGA-CBA	4.43	125.47	111.85
18	3	3008	CLA	C4A-NA-C1A	4.43	112.00	106.38
18	B	1215	CLA	O2A-CGA-CBA	4.45	125.53	111.85
18	B	1218	CLA	O2A-CGA-CBA	4.45	125.55	111.85
18	3	3004	CLA	O2A-CGA-CBA	4.46	125.57	111.85
18	B	1214	CLA	O2A-CGA-CBA	4.47	125.61	111.85
18	B	1229	CLA	O2A-CGA-CBA	4.49	125.67	111.85
21	A	5003	LHG	O7-C7-C8	4.49	120.99	111.53
18	2	2001	CLA	O2A-CGA-CBA	4.49	125.68	111.85
18	A	1133	CLA	O2A-CGA-CBA	4.52	125.77	111.85
27	4	4503	LUT	C38-C25-C26	4.55	119.44	116.04
18	B	1205	CLA	O2D-CGD-CBD	4.55	117.78	111.22
18	1	1008	CLA	O2D-CGD-CBD	4.57	117.81	111.22
18	G	1001	CLA	O2A-CGA-CBA	4.58	125.95	111.85
18	3	3003	CLA	O2D-CGD-CBD	4.60	117.86	111.22
18	B	1224	CLA	O2A-CGA-CBA	4.61	126.03	111.85
22	L	6020	BCR	C19-C18-C17	4.63	126.41	118.95
18	J	1302	CLA	O2A-CGA-CBA	4.65	126.17	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4016	CLA	O2D-CGD-CBD	4.66	117.95	111.22
18	B	1230	CLA	C4-C3-C5	4.67	122.49	115.37
23	F	5002	LMG	O7-C10-C11	4.68	121.40	111.53
18	4	4006	CLA	O2D-CGD-CBD	4.69	117.99	111.22
18	3	3017	CLA	O2D-CGD-CBD	4.70	118.01	111.22
18	A	1124	CLA	O2A-CGA-CBA	4.71	126.34	111.85
18	1	1004	CLA	O2A-CGA-CBA	4.71	126.36	111.85
22	B	6004	BCR	C19-C18-C17	4.76	126.62	118.95
22	B	6006	BCR	C39-C30-C25	4.76	117.61	110.33
18	1	1003	CLA	O2A-CGA-CBA	4.76	126.51	111.85
21	1	1801	LHG	O7-C7-C8	4.78	121.59	111.53
18	2	2002	CLA	O2D-CGD-CBD	4.78	118.11	111.22
18	3	3012	CLA	O2D-CGD-CBD	4.81	118.16	111.22
18	1	1006	CLA	O2A-CGA-CBA	4.85	126.79	111.85
18	4	4012	CLA	O2D-CGD-CBD	4.86	118.23	111.22
18	3	3013	CLA	O2D-CGD-CBD	4.88	118.26	111.22
18	1	1012	CLA	O2D-CGD-CBD	4.89	118.27	111.22
18	1	1001	CLA	O2D-CGD-CBD	4.91	118.31	111.22
18	2	2005	CLA	O2D-CGD-CBD	4.92	118.31	111.22
22	I	6020	BCR	C20-C19-C18	4.94	140.82	126.34
18	2	2009	CLA	O2D-CGD-CBD	4.95	118.36	111.22
18	3	3008	CLA	O2D-CGD-CBD	4.97	118.39	111.22
22	G	2011	BCR	C19-C18-C17	5.00	127.02	118.95
22	A	6017	BCR	C20-C19-C18	5.01	141.02	126.34
18	K	1001	CLA	O2D-CGD-CBD	5.04	118.49	111.22
18	A	1013	CLA	O2D-CGD-CBD	5.05	118.50	111.22
21	B	5004	LHG	O7-C7-C8	5.06	120.72	111.09
22	B	6004	BCR	C20-C19-C18	5.06	141.17	126.34
18	B	1220	CLA	O2D-CGD-CBD	5.08	118.56	111.22
18	B	1232	CLA	O2D-CGD-CBD	5.16	118.66	111.22
27	2	2502	LUT	C38-C25-C26	5.22	119.94	116.04
18	L	1503	CLA	O2D-CGD-CBD	5.22	118.75	111.22
18	B	1201	CLA	O2D-CGD-CBD	5.25	118.79	111.22
18	1	1003	CLA	O2D-CGD-CBD	5.25	118.80	111.22
18	4	4009	CLA	O2D-CGD-CBD	5.28	118.84	111.22
18	A	1109	CLA	O2D-CGD-CBD	5.28	118.84	111.22
23	F	5001	LMG	O7-C10-C11	5.31	121.20	111.09
18	3	3010	CLA	O2D-CGD-CBD	5.32	118.89	111.22
18	B	1222	CLA	O2D-CGD-CBD	5.32	118.90	111.22
18	3	3007	CLA	O2D-CGD-CBD	5.38	118.98	111.22
18	1	1002	CLA	O2D-CGD-CBD	5.39	118.99	111.22
18	3	3019	CLA	CBD-CAD-C3D	5.39	108.55	104.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3006	CLA	O2D-CGD-CBD	5.40	119.02	111.22
18	B	1213	CLA	O2D-CGD-CBD	5.40	119.02	111.22
22	A	6017	BCR	C19-C18-C17	5.43	127.70	118.95
18	2	2019	CLA	CBD-CAD-C3D	5.43	108.58	104.28
18	B	1228	CLA	O2D-CGD-CBD	5.48	119.13	111.22
18	2	2012	CLA	O2D-CGD-CBD	5.49	119.14	111.22
18	2	2007	CLA	O2D-CGD-CBD	5.49	119.15	111.22
18	1	1006	CLA	O2D-CGD-CBD	5.51	119.18	111.22
18	B	1219	CLA	O2D-CGD-CBD	5.52	119.18	111.22
23	4	4801	LMG	O7-C10-C11	5.53	123.17	111.53
23	J	5001	LMG	O7-C10-C11	5.56	123.24	111.53
18	A	1104	CLA	O2D-CGD-CBD	5.57	119.25	111.22
27	1	1501	LUT	C38-C25-C26	5.57	120.20	116.04
18	A	1122	CLA	O2D-CGD-CBD	5.59	119.28	111.22
18	3	3004	CLA	O2D-CGD-CBD	5.59	119.29	111.22
22	G	2011	BCR	C20-C19-C18	5.59	142.74	126.34
18	A	1138	CLA	O2D-CGD-CBD	5.62	119.33	111.22
18	2	2004	CLA	C2C-C1C-NC	5.62	114.09	110.22
18	A	1105	CLA	O2D-CGD-CBD	5.62	119.33	111.22
18	1	1005	CLA	O2D-CGD-CBD	5.64	119.36	111.22
18	A	1022	CLA	O2D-CGD-CBD	5.66	119.38	111.22
27	I	6018	LUT	C38-C25-C26	5.69	120.30	116.04
18	A	1119	CLA	O2D-CGD-CBD	5.71	119.45	111.22
27	3	3502	LUT	C38-C25-C26	5.73	120.33	116.04
18	B	1231	CLA	O2D-CGD-CBD	5.77	119.54	111.22
18	B	1206	CLA	O2D-CGD-CBD	5.77	119.55	111.22
18	B	1203	CLA	O2D-CGD-CBD	5.78	119.56	111.22
18	F	1301	CLA	O2D-CGD-CBD	5.79	119.57	111.22
18	A	1115	CLA	O2D-CGD-CBD	5.79	119.57	111.22
18	A	1120	CLA	O2D-CGD-CBD	5.80	119.59	111.22
18	B	1012	CLA	O2D-CGD-CBD	5.83	119.63	111.22
18	A	1126	CLA	O2D-CGD-CBD	5.87	119.69	111.22
22	B	6005	BCR	C20-C19-C18	5.87	143.55	126.34
18	B	1021	CLA	O2D-CGD-CBD	5.87	119.70	111.22
18	3	3018	CLA	O2D-CGD-CBD	5.89	119.72	111.22
18	2	2003	CLA	O2D-CGD-CBD	5.90	119.73	111.22
18	B	1214	CLA	O2D-CGD-CBD	5.91	119.75	111.22
18	A	1237	CLA	O2D-CGD-CBD	5.91	119.75	111.22
18	B	1023	CLA	O2D-CGD-CBD	5.92	119.76	111.22
18	A	1139	CLA	O2D-CGD-CBD	5.96	119.81	111.22
22	3	3503	BCR	C20-C19-C18	5.97	143.85	126.34
18	1	1007	CLA	O2D-CGD-CBD	5.98	119.85	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1108	CLA	O2D-CGD-CBD	5.99	119.86	111.22
18	H	1000	CLA	O2D-CGD-CBD	6.01	119.89	111.22
18	1	1011	CLA	O2D-CGD-CBD	6.02	119.90	111.22
18	4	4003	CLA	O2D-CGD-CBD	6.02	119.90	111.22
18	4	4007	CLA	O2D-CGD-CBD	6.03	119.93	111.22
18	A	1116	CLA	O2D-CGD-CBD	6.03	119.93	111.22
18	B	1210	CLA	O2D-CGD-CBD	6.04	119.94	111.22
18	B	1226	CLA	O2D-CGD-CBD	6.05	119.95	111.22
18	A	1151	CLA	O2D-CGD-CBD	6.05	119.95	111.22
18	A	1127	CLA	O2D-CGD-CBD	6.06	119.97	111.22
18	B	1204	CLA	O2D-CGD-CBD	6.07	119.97	111.22
18	A	1113	CLA	O2D-CGD-CBD	6.07	119.97	111.22
22	A	6007	BCR	C20-C19-C18	6.07	144.13	126.34
18	J	1302	CLA	O2D-CGD-CBD	6.08	119.99	111.22
18	B	1207	CLA	O2D-CGD-CBD	6.09	120.01	111.22
18	A	1137	CLA	O2D-CGD-CBD	6.09	120.01	111.22
18	2	2006	CLA	O2D-CGD-CBD	6.10	120.02	111.22
27	3	3501	LUT	C38-C25-C26	6.13	120.62	116.04
22	B	6010	BCR	C20-C19-C18	6.15	144.35	126.34
18	A	1124	CLA	O2D-CGD-CBD	6.16	120.10	111.22
18	G	1003	CLA	O2D-CGD-CBD	6.19	120.15	111.22
18	A	1133	CLA	O2D-CGD-CBD	6.20	120.17	111.22
17	A	1011	CL0	O2D-CGD-CBD	6.21	120.18	111.22
18	A	1129	CLA	O2D-CGD-CBD	6.22	120.19	111.22
18	A	1131	CLA	O2D-CGD-CBD	6.24	120.22	111.22
27	4	4501	LUT	C38-C25-C26	6.25	120.72	116.04
18	A	1134	CLA	O2D-CGD-CBD	6.26	120.25	111.22
27	1	1502	LUT	C38-C25-C26	6.29	120.74	116.04
22	A	6002	BCR	C20-C19-C18	6.29	144.78	126.34
18	1	1014	CLA	O2D-CGD-CBD	6.33	120.35	111.22
18	A	1110	CLA	O2D-CGD-CBD	6.33	120.36	111.22
18	A	1107	CLA	O2D-CGD-CBD	6.34	120.36	111.22
18	L	1502	CLA	O2D-CGD-CBD	6.34	120.37	111.22
18	1	1013	CLA	O2D-CGD-CBD	6.35	120.38	111.22
18	B	1236	CLA	O2D-CGD-CBD	6.35	120.38	111.22
18	A	1102	CLA	O2D-CGD-CBD	6.35	120.39	111.22
18	A	1130	CLA	O2D-CGD-CBD	6.38	120.42	111.22
18	B	1216	CLA	O2D-CGD-CBD	6.38	120.42	111.22
18	A	1136	CLA	O2D-CGD-CBD	6.38	120.43	111.22
18	B	1239	CLA	O2D-CGD-CBD	6.39	120.44	111.22
18	G	1001	CLA	O2D-CGD-CBD	6.40	120.46	111.22
18	B	1202	CLA	O2D-CGD-CBD	6.41	120.47	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1140	CLA	O2D-CGD-CBD	6.42	120.48	111.22
18	B	1215	CLA	O2D-CGD-CBD	6.43	120.49	111.22
18	4	4008	CLA	O2D-CGD-CBD	6.46	120.54	111.22
18	A	1125	CLA	O2D-CGD-CBD	6.47	120.55	111.22
18	B	1224	CLA	O2D-CGD-CBD	6.47	120.56	111.22
18	B	1225	CLA	O2D-CGD-CBD	6.48	120.56	111.22
18	A	1117	CLA	O2D-CGD-CBD	6.48	120.56	111.22
22	L	6020	BCR	C20-C19-C18	6.50	145.39	126.34
18	B	1240	CLA	O2D-CGD-CBD	6.50	120.60	111.22
18	B	1217	CLA	O2D-CGD-CBD	6.54	120.65	111.22
18	B	1238	CLA	O2D-CGD-CBD	6.55	120.67	111.22
22	K	2011	BCR	C20-C19-C18	6.57	145.58	126.34
18	A	1111	CLA	O2D-CGD-CBD	6.58	120.72	111.22
18	A	1103	CLA	O2D-CGD-CBD	6.59	120.72	111.22
22	A	6003	BCR	C20-C19-C18	6.60	145.68	126.34
18	B	1235	CLA	O2D-CGD-CBD	6.60	120.74	111.22
27	2	2501	LUT	C38-C25-C26	6.60	120.98	116.04
18	L	1501	CLA	C2C-C1C-NC	6.60	114.76	110.22
18	3	3005	CLA	O2D-CGD-CBD	6.61	120.76	111.22
18	F	1302	CLA	O2D-CGD-CBD	6.63	120.79	111.22
18	3	3002	CLA	O2D-CGD-CBD	6.66	120.84	111.22
18	2	2008	CLA	O2D-CGD-CBD	6.67	120.84	111.22
18	B	1229	CLA	O2D-CGD-CBD	6.69	120.87	111.22
18	B	1234	CLA	O2D-CGD-CBD	6.70	120.89	111.22
18	B	1211	CLA	C2C-C1C-NC	6.71	114.84	110.22
22	A	6008	BCR	C20-C19-C18	6.71	146.01	126.34
18	4	4017	CLA	O2D-CGD-CBD	6.72	120.92	111.22
18	B	1209	CLA	O2D-CGD-CBD	6.72	120.92	111.22
18	A	1121	CLA	O2D-CGD-CBD	6.73	120.93	111.22
18	A	1135	CLA	O2D-CGD-CBD	6.74	120.94	111.22
18	4	4005	CLA	O2D-CGD-CBD	6.74	120.95	111.22
18	A	1114	CLA	O2D-CGD-CBD	6.75	120.96	111.22
18	B	1212	CLA	O2D-CGD-CBD	6.82	121.06	111.22
22	J	6013	BCR	C20-C19-C18	6.82	146.34	126.34
22	J	6012	BCR	C20-C19-C18	6.89	146.53	126.34
18	1	1004	CLA	O2D-CGD-CBD	6.91	121.19	111.22
18	A	1101	CLA	O2D-CGD-CBD	6.92	121.21	111.22
22	B	6006	BCR	C20-C19-C18	6.95	146.71	126.34
18	1	1011	CLA	C2C-C1C-NC	6.97	115.02	110.22
18	B	1230	CLA	C2C-C1C-NC	7.01	115.04	110.22
18	B	1227	CLA	O2D-CGD-CBD	7.04	121.38	111.22
18	A	1118	CLA	O2D-CGD-CBD	7.08	121.44	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1208	CLA	O2D-CGD-CBD	7.13	121.50	111.22
22	F	6014	BCR	C20-C19-C18	7.14	147.27	126.34
18	B	1218	CLA	O2D-CGD-CBD	7.14	121.53	111.22
22	A	6011	BCR	C20-C19-C18	7.19	147.41	126.34
18	B	1223	CLA	O2D-CGD-CBD	7.19	121.59	111.22
18	A	1013	CLA	C2C-C1C-NC	7.20	115.17	110.22
18	4	4004	CLA	C2C-C1C-NC	7.23	115.19	110.22
22	B	6009	BCR	C20-C19-C18	7.23	147.52	126.34
18	B	1231	CLA	C2C-C1C-NC	7.26	115.21	110.22
18	A	1112	CLA	O2D-CGD-CBD	7.33	121.80	111.22
18	1	1002	CLA	C2C-C1C-NC	7.33	115.27	110.22
18	A	1123	CLA	O2D-CGD-CBD	7.35	121.83	111.22
18	4	4004	CLA	O2D-CGD-CBD	7.38	121.87	111.22
18	A	1132	CLA	O2D-CGD-CBD	7.39	121.88	111.22
18	L	1502	CLA	C2C-C1C-NC	7.42	115.32	110.22
18	A	1106	CLA	O2D-CGD-CBD	7.42	121.93	111.22
18	B	1213	CLA	C2C-C1C-NC	7.45	115.34	110.22
18	G	1002	CLA	O2D-CGD-CBD	7.45	121.98	111.22
27	4	4502	LUT	C38-C25-C26	7.49	121.64	116.04
18	2	2012	CLA	C2C-C1C-NC	7.51	115.39	110.22
18	1	1001	CLA	C2C-C1C-NC	7.54	115.41	110.22
22	L	6019	BCR	C20-C19-C18	7.55	148.48	126.34
18	B	1201	CLA	C2C-C1C-NC	7.60	115.45	110.22
18	B	1023	CLA	C2C-C1C-NC	7.60	115.45	110.22
18	3	3017	CLA	C2C-C1C-NC	7.61	115.45	110.22
18	A	1140	CLA	C2C-C1C-NC	7.63	115.47	110.22
18	A	1138	CLA	C2C-C1C-NC	7.63	115.47	110.22
18	3	3012	CLA	C2C-C1C-NC	7.63	115.47	110.22
18	B	1234	CLA	C2C-C1C-NC	7.67	115.50	110.22
18	B	1227	CLA	C2C-C1C-NC	7.69	115.51	110.22
18	4	4003	CLA	C2C-C1C-NC	7.69	115.51	110.22
18	A	1110	CLA	C2C-C1C-NC	7.71	115.52	110.22
18	3	3001	CLA	C2C-C1C-NC	7.72	115.53	110.22
18	1	1004	CLA	C2C-C1C-NC	7.74	115.55	110.22
18	3	3013	CLA	C2C-C1C-NC	7.75	115.55	110.22
18	1	1014	CLA	C2C-C1C-NC	7.75	115.55	110.22
18	2	2002	CLA	C2C-C1C-NC	7.75	115.56	110.22
18	B	1228	CLA	C2C-C1C-NC	7.78	115.57	110.22
18	B	1236	CLA	C2C-C1C-NC	7.81	115.59	110.22
18	B	1235	CLA	C2C-C1C-NC	7.82	115.60	110.22
18	L	1501	CLA	O2D-CGD-CBD	7.83	122.52	111.22
18	3	3006	CLA	C2C-C1C-NC	7.83	115.61	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	1302	CLA	C2C-C1C-NC	7.83	115.61	110.22
18	A	1102	CLA	C2C-C1C-NC	7.84	115.61	110.22
18	2	2005	CLA	C2C-C1C-NC	7.84	115.61	110.22
18	B	1021	CLA	C2C-C1C-NC	7.85	115.62	110.22
18	A	1128	CLA	O2D-CGD-CBD	7.85	122.55	111.22
18	A	1125	CLA	C2C-C1C-NC	7.86	115.62	110.22
18	B	1208	CLA	C2C-C1C-NC	7.86	115.63	110.22
18	L	1503	CLA	C2C-C1C-NC	7.86	115.63	110.22
18	B	1238	CLA	C2C-C1C-NC	7.87	115.64	110.22
18	A	1131	CLA	C2C-C1C-NC	7.90	115.65	110.22
18	G	1003	CLA	C2C-C1C-NC	7.90	115.66	110.22
18	3	3007	CLA	C2C-C1C-NC	7.90	115.66	110.22
18	B	1220	CLA	C2C-C1C-NC	7.91	115.67	110.22
18	A	1107	CLA	C2C-C1C-NC	7.93	115.67	110.22
18	4	4017	CLA	C2C-C1C-NC	7.93	115.67	110.22
18	B	1203	CLA	C2C-C1C-NC	7.93	115.68	110.22
18	B	1207	CLA	C2C-C1C-NC	7.94	115.68	110.22
18	2	2008	CLA	C2C-C1C-NC	7.94	115.68	110.22
18	2	2006	CLA	C2C-C1C-NC	7.96	115.69	110.22
18	4	4009	CLA	C2C-C1C-NC	7.96	115.70	110.22
18	B	1205	CLA	C2C-C1C-NC	7.96	115.70	110.22
18	A	1120	CLA	C2C-C1C-NC	7.97	115.70	110.22
18	B	1229	CLA	C2C-C1C-NC	7.99	115.72	110.22
18	A	1108	CLA	C2C-C1C-NC	8.00	115.72	110.22
22	F	6016	BCR	C20-C19-C18	8.00	149.79	126.34
18	B	1232	CLA	C2C-C1C-NC	8.00	115.73	110.22
18	B	1221	CLA	C2C-C1C-NC	8.02	115.74	110.22
18	B	1222	CLA	C2C-C1C-NC	8.02	115.74	110.22
18	A	1103	CLA	C2C-C1C-NC	8.03	115.75	110.22
18	4	4016	CLA	C2C-C1C-NC	8.04	115.75	110.22
18	A	1132	CLA	C2C-C1C-NC	8.06	115.76	110.22
18	1	1005	CLA	C2C-C1C-NC	8.06	115.76	110.22
18	A	1104	CLA	C2C-C1C-NC	8.06	115.76	110.22
18	4	4006	CLA	C2C-C1C-NC	8.10	115.79	110.22
18	1	1006	CLA	C2C-C1C-NC	8.10	115.79	110.22
18	B	1012	CLA	C2C-C1C-NC	8.10	115.79	110.22
18	A	1121	CLA	C2C-C1C-NC	8.11	115.80	110.22
18	B	1218	CLA	C2C-C1C-NC	8.11	115.80	110.22
18	A	1130	CLA	C2C-C1C-NC	8.11	115.80	110.22
18	B	1204	CLA	C2C-C1C-NC	8.12	115.81	110.22
18	1	1012	CLA	C2C-C1C-NC	8.12	115.81	110.22
18	B	1216	CLA	C2C-C1C-NC	8.12	115.81	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1136	CLA	C2C-C1C-NC	8.12	115.81	110.22
18	F	1301	CLA	C2C-C1C-NC	8.13	115.81	110.22
18	A	1111	CLA	C2C-C1C-NC	8.14	115.82	110.22
18	B	1225	CLA	C2C-C1C-NC	8.15	115.83	110.22
18	B	1212	CLA	C2C-C1C-NC	8.15	115.83	110.22
18	B	1221	CLA	O2D-CGD-CBD	8.15	122.98	111.22
18	A	1237	CLA	C2C-C1C-NC	8.15	115.83	110.22
18	B	1210	CLA	C2C-C1C-NC	8.16	115.83	110.22
18	A	1115	CLA	C2C-C1C-NC	8.16	115.84	110.22
18	A	1122	CLA	C2C-C1C-NC	8.16	115.84	110.22
18	1	1007	CLA	C2C-C1C-NC	8.18	115.85	110.22
18	B	1240	CLA	C2C-C1C-NC	8.19	115.86	110.22
18	A	1109	CLA	C2C-C1C-NC	8.19	115.86	110.22
18	B	1211	CLA	O2D-CGD-CBD	8.20	123.05	111.22
18	A	1105	CLA	C2C-C1C-NC	8.20	115.86	110.22
18	A	1129	CLA	C2C-C1C-NC	8.20	115.86	110.22
18	A	1124	CLA	C2C-C1C-NC	8.22	115.87	110.22
18	B	1223	CLA	C2C-C1C-NC	8.22	115.88	110.22
18	B	1215	CLA	C2C-C1C-NC	8.22	115.88	110.22
18	A	1126	CLA	C2C-C1C-NC	8.23	115.88	110.22
18	A	1106	CLA	C2C-C1C-NC	8.26	115.90	110.22
18	B	1219	CLA	C2C-C1C-NC	8.27	115.91	110.22
18	2	2007	CLA	C2C-C1C-NC	8.27	115.91	110.22
18	A	1112	CLA	C2C-C1C-NC	8.27	115.91	110.22
18	2	2004	CLA	O2D-CGD-CBD	8.28	123.17	111.22
18	A	1101	CLA	C2C-C1C-NC	8.29	115.92	110.22
18	B	1214	CLA	C2C-C1C-NC	8.29	115.92	110.22
18	A	1022	CLA	C2C-C1C-NC	8.33	115.95	110.22
18	2	2009	CLA	C2C-C1C-NC	8.34	115.96	110.22
18	A	1137	CLA	C2C-C1C-NC	8.37	115.97	110.22
18	A	1117	CLA	C2C-C1C-NC	8.37	115.98	110.22
18	B	1239	CLA	C2C-C1C-NC	8.37	115.98	110.22
18	3	3018	CLA	C2C-C1C-NC	8.39	115.99	110.22
18	A	1116	CLA	C2C-C1C-NC	8.39	115.99	110.22
18	A	1113	CLA	C2C-C1C-NC	8.42	116.01	110.22
17	A	1011	CL0	C2C-C1C-NC	8.42	116.02	110.22
18	2	2003	CLA	C2C-C1C-NC	8.44	116.03	110.22
18	G	1002	CLA	C2C-C1C-NC	8.44	116.03	110.22
18	3	3004	CLA	C2C-C1C-NC	8.45	116.03	110.22
18	B	1217	CLA	C2C-C1C-NC	8.45	116.03	110.22
18	A	1118	CLA	C2C-C1C-NC	8.49	116.06	110.22
18	A	1139	CLA	C2C-C1C-NC	8.51	116.07	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1127	CLA	C2C-C1C-NC	8.55	116.10	110.22
18	B	1209	CLA	C2C-C1C-NC	8.55	116.10	110.22
18	B	1230	CLA	O2D-CGD-CBD	8.56	123.56	111.22
18	B	1202	CLA	C2C-C1C-NC	8.58	116.12	110.22
22	G	2011	BCR	C11-C10-C9	8.58	139.70	127.22
18	1	1003	CLA	C2C-C1C-NC	8.58	116.12	110.22
18	A	1134	CLA	C2C-C1C-NC	8.60	116.14	110.22
18	A	1119	CLA	C2C-C1C-NC	8.60	116.14	110.22
18	A	1133	CLA	C2C-C1C-NC	8.61	116.14	110.22
18	J	1302	CLA	C2C-C1C-NC	8.61	116.15	110.22
18	A	1128	CLA	C2C-C1C-NC	8.62	116.15	110.22
18	3	3010	CLA	C2C-C1C-NC	8.64	116.16	110.22
18	4	4012	CLA	C2C-C1C-NC	8.65	116.17	110.22
18	3	3002	CLA	C2C-C1C-NC	8.68	116.19	110.22
18	A	1123	CLA	C2C-C1C-NC	8.69	116.20	110.22
18	A	1135	CLA	C2C-C1C-NC	8.70	116.20	110.22
18	B	1224	CLA	C2C-C1C-NC	8.71	116.21	110.22
22	G	2011	BCR	C11-C12-C13	8.72	151.91	126.34
18	3	3005	CLA	C2C-C1C-NC	8.73	116.22	110.22
18	K	1001	CLA	C2C-C1C-NC	8.77	116.26	110.22
18	G	1001	CLA	C2C-C1C-NC	8.80	116.28	110.22
18	4	4007	CLA	C2C-C1C-NC	8.83	116.30	110.22
18	4	4001	CLA	C2C-C1C-NC	8.86	116.31	110.22
18	H	1000	CLA	C2C-C1C-NC	8.86	116.32	110.22
18	A	1151	CLA	C2C-C1C-NC	8.88	116.33	110.22
18	2	2016	CLA	O2D-CGD-CBD	8.90	124.06	111.22
18	B	1226	CLA	C2C-C1C-NC	8.92	116.36	110.22
18	A	1114	CLA	C2C-C1C-NC	8.97	116.39	110.22
22	L	6020	BCR	C11-C12-C13	8.99	152.69	126.34
18	1	1008	CLA	C2C-C1C-NC	9.03	116.43	110.22
18	4	4005	CLA	C2C-C1C-NC	9.05	116.45	110.22
18	2	2016	CLA	C2C-C1C-NC	9.07	116.46	110.22
18	1	1013	CLA	C2C-C1C-NC	9.21	116.56	110.22
18	B	1206	CLA	C2C-C1C-NC	9.24	116.57	110.22
22	B	6004	BCR	C11-C12-C13	9.27	153.52	126.34
22	A	6007	BCR	C11-C12-C13	9.28	153.53	126.34
18	4	4002	CLA	C2C-C1C-NC	9.33	116.64	110.22
18	2	2001	CLA	C2C-C1C-NC	9.34	116.64	110.22
22	3	3503	BCR	C11-C10-C9	9.44	140.95	127.22
22	3	3503	BCR	C11-C12-C13	9.59	154.46	126.34
22	J	6012	BCR	C11-C12-C13	9.64	154.59	126.34
22	K	2011	BCR	C11-C12-C13	9.64	154.59	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6008	BCR	C11-C12-C13	9.68	154.72	126.34
22	B	6010	BCR	C11-C12-C13	9.69	154.74	126.34
22	A	6017	BCR	C11-C12-C13	9.69	154.75	126.34
18	4	4008	CLA	C2C-C1C-NC	9.80	116.96	110.22
22	B	6004	BCR	C11-C10-C9	9.88	141.58	127.22
22	F	6016	BCR	C11-C12-C13	10.02	155.71	126.34
22	F	6014	BCR	C11-C12-C13	10.05	155.81	126.34
22	A	6003	BCR	C11-C12-C13	10.21	156.26	126.34
22	J	6013	BCR	C11-C12-C13	10.35	156.68	126.34
22	B	6009	BCR	C11-C12-C13	10.38	156.78	126.34
22	I	6020	BCR	C11-C12-C13	10.40	156.83	126.34
18	3	3008	CLA	C2C-C1C-NC	10.47	117.42	110.22
22	L	6019	BCR	C11-C12-C13	10.51	157.16	126.34
22	A	6002	BCR	C11-C12-C13	10.56	157.30	126.34
22	B	6009	BCR	C11-C10-C9	10.65	142.70	127.22
22	B	6005	BCR	C11-C12-C13	10.65	157.56	126.34
18	3	3003	CLA	C2C-C1C-NC	10.87	117.70	110.22
22	K	2011	BCR	C11-C10-C9	10.88	143.04	127.22
22	K	2011	BCR	C21-C20-C19	10.92	156.81	123.11
22	B	6006	BCR	C21-C20-C19	11.09	157.33	123.11
22	L	6019	BCR	C11-C10-C9	11.21	143.51	127.22
22	F	6014	BCR	C16-C15-C14	11.30	147.62	123.23
22	B	6010	BCR	C11-C10-C9	11.31	143.66	127.22
22	L	6020	BCR	C11-C10-C9	11.50	143.94	127.22
22	B	6006	BCR	C11-C12-C13	11.51	160.07	126.34
22	J	6012	BCR	C16-C15-C14	11.71	148.49	123.23
22	A	6002	BCR	C16-C15-C14	11.71	148.49	123.23
22	A	6011	BCR	C11-C12-C13	11.79	160.88	126.34
22	B	6009	BCR	C16-C15-C14	11.91	148.92	123.23
22	F	6016	BCR	C16-C15-C14	12.02	149.15	123.23
22	B	6006	BCR	C16-C15-C14	12.05	149.23	123.23
22	A	6003	BCR	C16-C15-C14	12.06	149.24	123.23
22	A	6011	BCR	C21-C20-C19	12.13	160.56	123.11
22	F	6016	BCR	C21-C20-C19	12.19	160.73	123.11
22	A	6011	BCR	C16-C15-C14	12.19	149.53	123.23
22	B	6010	BCR	C16-C15-C14	12.30	149.76	123.23
22	J	6013	BCR	C16-C15-C14	12.31	149.78	123.23
22	B	6005	BCR	C16-C15-C14	12.40	149.99	123.23
22	K	2011	BCR	C16-C15-C14	12.43	150.05	123.23
22	A	6003	BCR	C11-C10-C9	12.44	145.30	127.22
22	I	6020	BCR	C16-C15-C14	12.51	150.22	123.23
22	A	6008	BCR	C11-C10-C9	12.56	145.48	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	6007	BCR	C16-C15-C14	12.58	150.38	123.23
22	B	6009	BCR	C21-C20-C19	12.71	162.34	123.11
22	J	6013	BCR	C11-C10-C9	12.73	145.73	127.22
22	G	2011	BCR	C16-C15-C14	12.77	150.78	123.23
22	L	6019	BCR	C16-C15-C14	12.78	150.81	123.23
22	L	6020	BCR	C21-C20-C19	12.90	162.95	123.11
22	B	6005	BCR	C11-C10-C9	12.95	146.05	127.22
22	L	6019	BCR	C21-C20-C19	13.07	163.46	123.11
22	A	6007	BCR	C11-C10-C9	13.11	146.28	127.22
22	J	6013	BCR	C21-C20-C19	13.11	163.58	123.11
22	A	6008	BCR	C21-C20-C19	13.12	163.62	123.11
22	F	6016	BCR	C11-C10-C9	13.16	146.34	127.22
22	B	6004	BCR	C16-C15-C14	13.16	151.61	123.23
22	J	6012	BCR	C21-C20-C19	13.23	163.94	123.11
22	A	6017	BCR	C11-C10-C9	13.26	146.49	127.22
22	F	6014	BCR	C21-C20-C19	13.28	164.10	123.11
22	A	6003	BCR	C21-C20-C19	13.31	164.18	123.11
22	3	3503	BCR	C21-C20-C19	13.36	164.34	123.11
22	G	2011	BCR	C21-C20-C19	13.45	164.64	123.11
22	A	6017	BCR	C15-C16-C17	13.50	152.35	123.23
22	B	6010	BCR	C21-C20-C19	13.58	165.04	123.11
22	A	6002	BCR	C21-C20-C19	13.72	165.45	123.11
22	A	6002	BCR	C11-C10-C9	13.85	147.36	127.22
22	L	6020	BCR	C16-C15-C14	13.90	153.22	123.23
22	3	3503	BCR	C16-C15-C14	13.92	153.26	123.23
22	F	6014	BCR	C11-C10-C9	14.00	147.57	127.22
22	A	6007	BCR	C21-C20-C19	14.00	166.34	123.11
22	B	6005	BCR	C21-C20-C19	14.06	166.53	123.11
22	I	6020	BCR	C21-C20-C19	14.32	167.30	123.11
22	I	6020	BCR	C11-C10-C9	14.38	148.12	127.22
22	A	6008	BCR	C16-C15-C14	14.53	154.59	123.23
22	J	6012	BCR	C11-C10-C9	14.60	148.44	127.22
22	B	6004	BCR	C21-C20-C19	14.60	168.18	123.11
22	K	2011	BCR	C15-C16-C17	14.76	155.08	123.23
22	B	6005	BCR	C15-C16-C17	14.82	155.21	123.23
22	A	6017	BCR	C21-C20-C19	14.84	168.93	123.11
22	I	6020	BCR	C15-C16-C17	14.84	155.26	123.23
22	G	2011	BCR	C15-C16-C17	15.06	155.72	123.23
22	A	6011	BCR	C11-C10-C9	15.13	149.22	127.22
22	B	6004	BCR	C15-C16-C17	15.39	156.44	123.23
22	A	6011	BCR	C10-C11-C12	15.84	172.00	123.11
22	B	6006	BCR	C11-C10-C9	15.90	150.33	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	6004	BCR	C10-C11-C12	15.95	172.34	123.11
22	B	6006	BCR	C10-C11-C12	16.19	173.10	123.11
22	A	6017	BCR	C10-C11-C12	16.86	175.16	123.11
22	B	6010	BCR	C10-C11-C12	16.88	175.24	123.11
22	B	6009	BCR	C10-C11-C12	16.92	175.35	123.11
22	I	6020	BCR	C10-C11-C12	17.01	175.61	123.11
22	A	6017	BCR	C16-C15-C14	17.07	160.05	123.23
22	J	6013	BCR	C16-C17-C18	17.14	152.14	127.22
22	A	6008	BCR	C10-C11-C12	17.19	176.19	123.11
22	A	6002	BCR	C10-C11-C12	17.20	176.19	123.11
22	3	3503	BCR	C10-C11-C12	17.26	176.40	123.11
22	A	6011	BCR	C15-C16-C17	17.27	160.50	123.23
22	B	6005	BCR	C10-C11-C12	17.28	176.46	123.11
22	J	6012	BCR	C10-C11-C12	17.29	176.49	123.11
22	F	6014	BCR	C10-C11-C12	17.33	176.62	123.11
22	A	6017	BCR	C20-C21-C22	17.37	152.47	127.22
22	A	6003	BCR	C10-C11-C12	17.50	177.14	123.11
22	J	6013	BCR	C10-C11-C12	17.52	177.20	123.11
22	A	6002	BCR	C16-C17-C18	17.57	152.76	127.22
22	A	6008	BCR	C15-C16-C17	17.59	161.17	123.23
22	A	6007	BCR	C10-C11-C12	17.61	177.47	123.11
22	F	6016	BCR	C10-C11-C12	17.69	177.72	123.11
22	F	6016	BCR	C15-C16-C17	17.72	161.46	123.23
22	L	6019	BCR	C10-C11-C12	17.72	177.82	123.11
22	3	3503	BCR	C15-C16-C17	17.88	161.80	123.23
22	I	6020	BCR	C20-C21-C22	17.95	153.32	127.22
22	L	6020	BCR	C10-C11-C12	18.07	178.90	123.11
22	G	2011	BCR	C10-C11-C12	18.41	179.94	123.11
22	K	2011	BCR	C10-C11-C12	18.42	179.97	123.11
22	3	3503	BCR	C16-C17-C18	18.71	154.41	127.22
22	L	6020	BCR	C15-C16-C17	18.82	163.82	123.23
22	J	6013	BCR	C20-C21-C22	18.88	154.66	127.22
22	L	6019	BCR	C15-C16-C17	18.90	164.00	123.23
22	A	6002	BCR	C20-C21-C22	19.07	154.94	127.22
22	L	6020	BCR	C16-C17-C18	19.08	154.95	127.22
22	A	6007	BCR	C15-C16-C17	19.19	164.63	123.23
22	B	6006	BCR	C15-C16-C17	19.19	164.64	123.23
22	G	2011	BCR	C20-C21-C22	19.22	155.16	127.22
22	A	6007	BCR	C20-C21-C22	19.24	155.18	127.22
22	B	6010	BCR	C15-C16-C17	19.30	164.87	123.23
22	J	6012	BCR	C16-C17-C18	19.30	155.28	127.22
22	A	6003	BCR	C16-C17-C18	19.31	155.29	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	6004	BCR	C20-C21-C22	19.31	155.30	127.22
22	J	6012	BCR	C15-C16-C17	19.35	164.97	123.23
22	B	6009	BCR	C16-C17-C18	19.41	155.43	127.22
22	B	6009	BCR	C15-C16-C17	19.44	165.16	123.23
22	J	6012	BCR	C20-C21-C22	19.53	155.61	127.22
22	B	6006	BCR	C16-C17-C18	19.54	155.62	127.22
22	L	6019	BCR	C16-C17-C18	19.61	155.72	127.22
22	B	6010	BCR	C16-C17-C18	19.64	155.77	127.22
22	A	6003	BCR	C15-C16-C17	19.66	165.65	123.23
22	A	6007	BCR	C16-C17-C18	19.77	155.96	127.22
22	A	6008	BCR	C16-C17-C18	19.78	155.97	127.22
22	F	6014	BCR	C15-C16-C17	19.81	165.97	123.23
22	3	3503	BCR	C20-C21-C22	19.85	156.07	127.22
22	B	6009	BCR	C20-C21-C22	20.02	156.32	127.22
22	L	6020	BCR	C20-C21-C22	20.04	156.36	127.22
22	B	6005	BCR	C20-C21-C22	20.10	156.43	127.22
22	A	6002	BCR	C15-C16-C17	20.18	166.77	123.23
22	A	6003	BCR	C20-C21-C22	20.36	156.82	127.22
22	F	6014	BCR	C20-C21-C22	20.45	156.95	127.22
22	J	6013	BCR	C15-C16-C17	20.50	167.46	123.23
22	A	6008	BCR	C20-C21-C22	20.52	157.06	127.22
22	L	6019	BCR	C20-C21-C22	20.59	157.16	127.22
22	K	2011	BCR	C20-C21-C22	20.99	157.73	127.22
22	A	6011	BCR	C20-C21-C22	21.29	158.17	127.22
22	F	6016	BCR	C20-C21-C22	21.64	158.67	127.22
22	F	6014	BCR	C16-C17-C18	21.99	159.18	127.22
22	B	6010	BCR	C20-C21-C22	22.59	160.06	127.22
22	A	6011	BCR	C16-C17-C18	23.15	160.87	127.22
22	F	6016	BCR	C16-C17-C18	23.34	161.15	127.22
22	B	6006	BCR	C20-C21-C22	24.60	162.98	127.22
22	B	6004	BCR	C16-C17-C18	26.55	165.82	127.22
22	I	6020	BCR	C16-C17-C18	26.72	166.06	127.22
22	K	2011	BCR	C16-C17-C18	27.16	166.70	127.22
22	B	6005	BCR	C16-C17-C18	27.27	166.86	127.22
22	G	2011	BCR	C16-C17-C18	27.51	167.20	127.22
22	A	6017	BCR	C16-C17-C18	29.37	169.91	127.22

All (425) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1132	CLA	NC
18	A	1132	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	1132	CLA	NA
18	B	1220	CLA	NC
18	B	1220	CLA	NA
18	B	1201	CLA	NC
18	B	1201	CLA	ND
18	B	1201	CLA	NA
18	4	4001	CLA	NC
18	4	4001	CLA	ND
18	4	4001	CLA	NA
18	1	1005	CLA	NC
18	1	1005	CLA	ND
18	1	1005	CLA	NA
18	3	3004	CLA	NC
18	3	3004	CLA	ND
18	3	3004	CLA	NA
18	B	1222	CLA	NC
18	B	1222	CLA	ND
18	B	1222	CLA	NA
18	B	1240	CLA	ND
18	B	1240	CLA	NA
18	B	1225	CLA	NC
18	B	1225	CLA	ND
18	B	1225	CLA	NA
18	1	1003	CLA	NC
18	1	1003	CLA	ND
18	1	1003	CLA	NA
18	4	4009	CLA	NC
18	4	4009	CLA	ND
18	4	4009	CLA	NA
18	A	1013	CLA	NC
18	A	1013	CLA	ND
18	A	1013	CLA	NA
18	J	1302	CLA	NC
18	J	1302	CLA	ND
18	J	1302	CLA	NA
18	A	1126	CLA	NC
18	A	1126	CLA	ND
18	A	1126	CLA	NA
18	A	1111	CLA	ND
18	A	1111	CLA	NA
18	1	1013	CLA	NC
18	1	1013	CLA	ND

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Mol	Chain	Res	Type	Atom
18	1	1013	CLA	NA
18	A	1114	CLA	NC
18	A	1114	CLA	ND
18	A	1114	CLA	NA
18	2	2001	CLA	NC
18	2	2001	CLA	ND
18	2	2001	CLA	NA
18	A	1237	CLA	NC
18	A	1237	CLA	ND
18	A	1237	CLA	NA
18	A	1121	CLA	NC
18	A	1121	CLA	ND
18	A	1121	CLA	NA
18	2	2004	CLA	NC
18	2	2004	CLA	ND
18	2	2004	CLA	NA
18	3	3008	CLA	NC
18	3	3008	CLA	ND
18	3	3008	CLA	NA
18	G	1003	CLA	NC
18	G	1003	CLA	ND
18	G	1003	CLA	NA
27	2	2502	LUT	C26
27	2	2501	LUT	C26
18	3	3002	CLA	NC
18	3	3002	CLA	ND
18	3	3002	CLA	NA
18	A	1137	CLA	NC
18	A	1137	CLA	ND
18	A	1137	CLA	NA
18	3	3013	CLA	NC
18	3	3013	CLA	ND
18	3	3013	CLA	NA
18	2	2009	CLA	NC
18	2	2009	CLA	ND
18	2	2009	CLA	NA
18	2	2008	CLA	NC
18	2	2008	CLA	ND
18	2	2008	CLA	NA
18	B	1228	CLA	NC
18	B	1228	CLA	ND
18	B	1228	CLA	NA

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Mol	Chain	Res	Type	Atom
18	A	1112	CLA	ND
18	A	1112	CLA	NA
18	A	1118	CLA	NC
18	A	1118	CLA	ND
18	A	1118	CLA	NA
18	A	1139	CLA	NC
18	A	1139	CLA	ND
18	A	1139	CLA	NA
27	3	3502	LUT	C26
18	A	1130	CLA	NC
18	A	1130	CLA	NA
18	4	4003	CLA	NC
18	4	4003	CLA	ND
18	4	4003	CLA	NA
18	A	1107	CLA	NC
18	A	1107	CLA	ND
18	A	1107	CLA	NA
18	2	2019	CLA	NC
18	2	2019	CLA	ND
18	2	2019	CLA	NA
18	B	1221	CLA	NC
18	B	1221	CLA	ND
18	B	1221	CLA	NA
18	4	4016	CLA	NC
18	4	4016	CLA	ND
18	4	4016	CLA	NA
27	1	1502	LUT	C26
18	B	1208	CLA	NC
18	B	1208	CLA	ND
18	B	1208	CLA	NA
18	A	1116	CLA	NC
18	A	1116	CLA	ND
18	A	1116	CLA	NA
18	B	1204	CLA	ND
18	B	1204	CLA	NA
18	2	2006	CLA	NC
18	2	2006	CLA	ND
18	2	2006	CLA	NA
18	2	2012	CLA	NC
18	2	2012	CLA	ND
18	2	2012	CLA	NA
27	4	4502	LUT	C26

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Mol	Chain	Res	Type	Atom
18	2	2003	CLA	NC
18	2	2003	CLA	ND
18	2	2003	CLA	NA
18	1	1001	CLA	NC
18	1	1001	CLA	ND
18	1	1001	CLA	NA
18	4	4007	CLA	NC
18	4	4007	CLA	ND
18	4	4007	CLA	NA
18	A	1123	CLA	ND
18	A	1123	CLA	NA
18	A	1115	CLA	NC
18	A	1115	CLA	ND
18	A	1115	CLA	NA
18	H	1000	CLA	NC
18	H	1000	CLA	ND
18	H	1000	CLA	NA
18	A	1134	CLA	ND
18	A	1134	CLA	NA
18	3	3010	CLA	NC
18	3	3010	CLA	ND
18	3	3010	CLA	NA
27	4	4503	LUT	C26
18	1	1006	CLA	NC
18	1	1006	CLA	ND
18	1	1006	CLA	NA
18	2	2005	CLA	NC
18	2	2005	CLA	ND
18	2	2005	CLA	NA
18	A	1022	CLA	ND
18	A	1022	CLA	NA
18	B	1232	CLA	NC
18	B	1232	CLA	ND
18	B	1232	CLA	NA
18	A	1129	CLA	ND
18	A	1129	CLA	NA
18	F	1301	CLA	NC
18	F	1301	CLA	ND
18	F	1301	CLA	NA
18	L	1502	CLA	NC
18	L	1502	CLA	ND
18	L	1502	CLA	NA

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Mol	Chain	Res	Type	Atom
27	1	1501	LUT	C26
18	2	2007	CLA	NC
18	2	2007	CLA	ND
18	2	2007	CLA	NA
18	3	3007	CLA	NC
18	3	3007	CLA	ND
18	3	3007	CLA	NA
18	2	2002	CLA	NC
18	2	2002	CLA	ND
18	2	2002	CLA	NA
18	B	1223	CLA	NC
18	B	1223	CLA	NA
18	A	1133	CLA	NC
18	A	1133	CLA	NA
18	A	1151	CLA	NC
18	A	1151	CLA	ND
18	A	1151	CLA	NA
18	B	1238	CLA	NC
18	B	1238	CLA	ND
18	B	1238	CLA	NA
18	A	1104	CLA	NC
18	A	1104	CLA	ND
18	A	1104	CLA	NA
18	B	1023	CLA	NC
18	B	1023	CLA	ND
18	B	1023	CLA	NA
18	3	3018	CLA	NC
18	3	3018	CLA	ND
18	3	3018	CLA	NA
18	3	3019	CLA	NC
18	3	3019	CLA	ND
18	3	3019	CLA	NA
18	B	1202	CLA	ND
18	B	1202	CLA	NA
18	B	1229	CLA	NC
18	B	1229	CLA	ND
18	B	1229	CLA	NA
18	A	1135	CLA	ND
18	A	1135	CLA	NA
18	A	1102	CLA	NC
18	A	1102	CLA	ND
18	A	1102	CLA	NA

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Mol	Chain	Res	Type	Atom
18	A	1127	CLA	NC
18	A	1127	CLA	ND
18	A	1127	CLA	NA
18	3	3017	CLA	NC
18	3	3017	CLA	ND
18	3	3017	CLA	NA
18	4	4005	CLA	NC
18	4	4005	CLA	ND
18	4	4005	CLA	NA
17	A	1011	CL0	NC
17	A	1011	CL0	ND
17	A	1011	CL0	NA
18	4	4008	CLA	NC
18	4	4008	CLA	ND
18	4	4008	CLA	NA
18	4	4004	CLA	NC
18	4	4004	CLA	ND
18	4	4004	CLA	NA
18	B	1227	CLA	NC
18	B	1227	CLA	ND
18	B	1227	CLA	NA
18	B	1230	CLA	NC
18	B	1230	CLA	ND
18	B	1230	CLA	NA
18	A	1120	CLA	NC
18	A	1120	CLA	ND
18	A	1120	CLA	NA
18	A	1108	CLA	NC
18	A	1108	CLA	ND
18	A	1108	CLA	NA
18	4	4002	CLA	NC
18	4	4002	CLA	ND
18	4	4002	CLA	NA
18	A	1125	CLA	NC
18	A	1125	CLA	ND
18	A	1125	CLA	NA
18	B	1206	CLA	ND
18	B	1206	CLA	NA
18	A	1117	CLA	ND
18	A	1117	CLA	NA
18	B	1207	CLA	NC
18	B	1207	CLA	NA

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Mol	Chain	Res	Type	Atom
18	B	1235	CLA	ND
18	B	1235	CLA	NA
18	A	1140	CLA	NC
18	A	1140	CLA	ND
18	A	1140	CLA	NA
18	1	1004	CLA	NC
18	1	1004	CLA	ND
18	1	1004	CLA	NA
18	A	1110	CLA	NC
18	A	1110	CLA	ND
18	A	1110	CLA	NA
18	B	1211	CLA	NC
18	B	1211	CLA	ND
18	B	1211	CLA	NA
18	2	2016	CLA	NC
18	2	2016	CLA	ND
18	2	2016	CLA	NA
27	4	4501	LUT	C26
18	3	3005	CLA	NC
18	3	3005	CLA	ND
18	3	3005	CLA	NA
18	B	1214	CLA	NC
18	B	1214	CLA	ND
18	B	1214	CLA	NA
18	L	1503	CLA	NC
18	L	1503	CLA	ND
18	L	1503	CLA	NA
18	A	1131	CLA	NC
18	A	1131	CLA	ND
18	A	1131	CLA	NA
18	B	1231	CLA	NC
18	B	1231	CLA	ND
18	B	1231	CLA	NA
18	B	1234	CLA	NC
18	B	1234	CLA	ND
18	B	1234	CLA	NA
27	I	6018	LUT	C26
18	3	3006	CLA	NC
18	3	3006	CLA	ND
18	3	3006	CLA	NA
18	3	3003	CLA	NC
18	3	3003	CLA	ND

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Mol	Chain	Res	Type	Atom
18	3	3003	CLA	NA
18	B	1209	CLA	NC
18	B	1209	CLA	ND
18	B	1209	CLA	NA
18	1	1014	CLA	NC
18	1	1014	CLA	ND
18	1	1014	CLA	NA
18	B	1236	CLA	ND
18	B	1236	CLA	NA
18	3	3012	CLA	NC
18	3	3012	CLA	ND
18	3	3012	CLA	NA
18	1	1011	CLA	NC
18	1	1011	CLA	ND
18	1	1011	CLA	NA
18	B	1219	CLA	NC
18	B	1219	CLA	ND
18	B	1219	CLA	NA
18	B	1218	CLA	NC
18	B	1218	CLA	ND
18	B	1218	CLA	NA
18	A	1109	CLA	NC
18	A	1109	CLA	ND
18	A	1109	CLA	NA
18	B	1203	CLA	ND
18	B	1203	CLA	NA
18	1	1012	CLA	NC
18	1	1012	CLA	ND
18	1	1012	CLA	NA
18	A	1106	CLA	NC
18	A	1106	CLA	ND
18	A	1106	CLA	NA
18	G	1002	CLA	NC
18	G	1002	CLA	ND
18	G	1002	CLA	NA
18	A	1103	CLA	ND
18	A	1103	CLA	NA
18	B	1224	CLA	NC
18	B	1224	CLA	ND
18	B	1224	CLA	NA
18	4	4006	CLA	NC
18	4	4006	CLA	ND

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Mol	Chain	Res	Type	Atom
18	4	4006	CLA	NA
18	F	1302	CLA	NC
18	F	1302	CLA	ND
18	F	1302	CLA	NA
18	4	4017	CLA	NC
18	4	4017	CLA	ND
18	4	4017	CLA	NA
18	A	1122	CLA	NC
18	A	1122	CLA	ND
18	A	1122	CLA	NA
27	3	3501	LUT	C26
18	B	1239	CLA	NC
18	B	1239	CLA	ND
18	B	1239	CLA	NA
18	B	1216	CLA	NC
18	B	1216	CLA	ND
18	B	1216	CLA	NA
18	1	1007	CLA	NC
18	1	1007	CLA	ND
18	1	1007	CLA	NA
18	A	1124	CLA	NC
18	A	1124	CLA	ND
18	A	1124	CLA	NA
18	1	1008	CLA	NC
18	1	1008	CLA	ND
18	1	1008	CLA	NA
18	A	1113	CLA	ND
18	A	1113	CLA	NA
18	1	1002	CLA	NC
18	1	1002	CLA	ND
18	1	1002	CLA	NA
18	B	1213	CLA	NC
18	B	1213	CLA	NA
18	A	1105	CLA	NC
18	A	1105	CLA	ND
18	A	1105	CLA	NA
18	L	1501	CLA	NC
18	L	1501	CLA	ND
18	L	1501	CLA	NA
18	A	1136	CLA	NC
18	A	1136	CLA	ND
18	A	1136	CLA	NA

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Mol	Chain	Res	Type	Atom
18	B	1021	CLA	NC
18	B	1021	CLA	ND
18	B	1021	CLA	NA
18	B	1215	CLA	ND
18	B	1215	CLA	NA
18	A	1128	CLA	NC
18	A	1128	CLA	ND
18	A	1128	CLA	NA
18	3	3001	CLA	NC
18	3	3001	CLA	ND
18	3	3001	CLA	NA
18	4	4012	CLA	NC
18	4	4012	CLA	ND
18	4	4012	CLA	NA
18	A	1119	CLA	NC
18	A	1119	CLA	ND
18	A	1119	CLA	NA
18	B	1217	CLA	NC
18	B	1217	CLA	ND
18	B	1217	CLA	NA
18	A	1101	CLA	ND
18	A	1101	CLA	NA
18	A	1138	CLA	NC
18	A	1138	CLA	ND
18	A	1138	CLA	NA
18	B	1212	CLA	NC
18	B	1212	CLA	ND
18	B	1212	CLA	NA
18	K	1001	CLA	NC
18	K	1001	CLA	ND
18	K	1001	CLA	NA
18	B	1012	CLA	ND
18	B	1012	CLA	NA
18	G	1001	CLA	NC
18	G	1001	CLA	ND
18	G	1001	CLA	NA
18	B	1205	CLA	NC
18	B	1205	CLA	ND
18	B	1205	CLA	NA
18	B	1210	CLA	NC
18	B	1210	CLA	ND
18	B	1210	CLA	NA

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Mol	Chain	Res	Type	Atom
18	B	1226	CLA	NC
18	B	1226	CLA	ND
18	B	1226	CLA	NA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	4	4801	LMG	C7-O1-C1-O6
27	3	3502	LUT	C28-C27-C26-C21
18	G	1001	CLA	CED-O2D-CGD-CBD
21	1	1801	LHG	C5-O7-C7-O9
21	1	1801	LHG	C5-O7-C7-C8

There are no ring outliers.

205 monomers are involved in 1953 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	1001	CLA	48	0
18	1	1002	CLA	21	0
18	1	1003	CLA	32	0
18	1	1004	CLA	26	0
18	1	1005	CLA	15	0
18	1	1006	CLA	11	0
18	1	1007	CLA	10	0
18	1	1008	CLA	34	0
28	1	1009	CHL	27	0
28	1	1010	CHL	8	0
18	1	1011	CLA	18	0
18	1	1012	CLA	16	0
18	1	1013	CLA	16	0
18	1	1014	CLA	14	0
27	1	1501	LUT	31	0
27	1	1502	LUT	17	0
21	1	1801	LHG	15	0
18	2	2001	CLA	33	0
18	2	2002	CLA	38	0
18	2	2003	CLA	30	0
18	2	2004	CLA	23	0
18	2	2005	CLA	24	0
18	2	2006	CLA	22	0
18	2	2007	CLA	26	0
18	2	2008	CLA	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	2009	CLA	15	0
28	2	2010	CHL	18	0
28	2	2011	CHL	6	0
18	2	2012	CLA	24	0
28	2	2013	CHL	18	0
18	2	2016	CLA	36	0
27	2	2501	LUT	23	0
27	2	2502	LUT	32	0
21	2	2801	LHG	6	0
23	2	2802	LMG	9	0
18	3	3001	CLA	24	0
18	3	3002	CLA	10	0
18	3	3003	CLA	51	0
18	3	3004	CLA	20	0
18	3	3005	CLA	18	0
18	3	3006	CLA	36	0
18	3	3007	CLA	8	0
18	3	3008	CLA	19	0
18	3	3010	CLA	34	0
28	3	3011	CHL	22	0
18	3	3012	CLA	32	0
18	3	3013	CLA	23	0
18	3	3017	CLA	11	0
18	3	3018	CLA	19	0
18	3	3019	CLA	1	0
27	3	3501	LUT	38	0
27	3	3502	LUT	24	0
22	3	3503	BCR	21	0
18	4	4001	CLA	25	0
18	4	4002	CLA	11	0
18	4	4003	CLA	13	0
18	4	4004	CLA	19	0
18	4	4005	CLA	16	0
18	4	4006	CLA	21	0
18	4	4007	CLA	20	0
18	4	4008	CLA	15	0
18	4	4009	CLA	9	0
28	4	4010	CHL	8	0
28	4	4011	CHL	20	0
18	4	4012	CLA	28	0
28	4	4013	CHL	19	0
18	4	4016	CLA	24	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	4017	CLA	11	0
27	4	4501	LUT	21	0
27	4	4502	LUT	31	0
27	4	4503	LUT	32	0
29	4	4505	ZEX	12	0
23	4	4801	LMG	6	0
17	A	1011	CL0	6	0
18	A	1013	CLA	8	0
18	A	1022	CLA	7	0
18	A	1101	CLA	6	0
18	A	1102	CLA	4	0
18	A	1103	CLA	6	0
18	A	1104	CLA	4	0
18	A	1105	CLA	3	0
18	A	1106	CLA	9	0
18	A	1107	CLA	3	0
18	A	1108	CLA	3	0
18	A	1109	CLA	8	0
18	A	1110	CLA	10	0
18	A	1111	CLA	8	0
18	A	1112	CLA	13	0
18	A	1113	CLA	2	0
18	A	1114	CLA	3	0
18	A	1115	CLA	3	0
18	A	1116	CLA	7	0
18	A	1117	CLA	4	0
18	A	1118	CLA	3	0
18	A	1119	CLA	7	0
18	A	1120	CLA	3	0
18	A	1121	CLA	4	0
18	A	1122	CLA	6	0
18	A	1123	CLA	4	0
18	A	1124	CLA	4	0
18	A	1125	CLA	3	0
18	A	1126	CLA	10	0
18	A	1127	CLA	6	0
18	A	1128	CLA	11	0
18	A	1129	CLA	1	0
18	A	1130	CLA	4	0
18	A	1131	CLA	3	0
18	A	1132	CLA	7	0
18	A	1133	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1134	CLA	2	0
18	A	1135	CLA	4	0
18	A	1136	CLA	7	0
18	A	1137	CLA	3	0
18	A	1138	CLA	4	0
18	A	1139	CLA	5	0
18	A	1140	CLA	5	0
18	A	1151	CLA	4	0
18	A	1237	CLA	5	0
19	A	3001	SF4	1	0
20	A	5001	PQN	3	0
21	A	5003	LHG	5	0
22	A	6002	BCR	4	0
22	A	6003	BCR	2	0
22	A	6007	BCR	3	0
22	A	6008	BCR	2	0
22	A	6011	BCR	5	0
22	A	6017	BCR	5	0
21	A	7001	LHG	7	0
18	B	1012	CLA	6	0
18	B	1021	CLA	9	0
18	B	1023	CLA	5	0
18	B	1201	CLA	2	0
18	B	1202	CLA	7	0
18	B	1203	CLA	3	0
18	B	1204	CLA	10	0
18	B	1205	CLA	8	0
18	B	1206	CLA	6	0
18	B	1207	CLA	12	0
18	B	1208	CLA	7	0
18	B	1209	CLA	3	0
18	B	1210	CLA	9	0
18	B	1211	CLA	7	0
18	B	1212	CLA	5	0
18	B	1213	CLA	6	0
18	B	1214	CLA	3	0
18	B	1215	CLA	4	0
18	B	1216	CLA	7	0
18	B	1217	CLA	1	0
18	B	1218	CLA	11	0
18	B	1219	CLA	2	0
18	B	1220	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1221	CLA	14	0
18	B	1222	CLA	8	0
18	B	1223	CLA	4	0
18	B	1224	CLA	7	0
18	B	1225	CLA	4	0
18	B	1226	CLA	7	0
18	B	1227	CLA	8	0
18	B	1228	CLA	1	0
18	B	1229	CLA	6	0
18	B	1230	CLA	8	0
18	B	1231	CLA	3	0
18	B	1232	CLA	3	0
18	B	1234	CLA	8	0
18	B	1235	CLA	5	0
18	B	1236	CLA	5	0
18	B	1238	CLA	9	0
18	B	1239	CLA	5	0
18	B	1240	CLA	10	0
20	B	5002	PQN	5	0
21	B	5004	LHG	1	0
23	B	5005	LMG	3	0
22	B	6004	BCR	10	0
22	B	6005	BCR	2	0
22	B	6006	BCR	5	0
22	B	6009	BCR	6	0
22	B	6010	BCR	1	0
25	B	7101	DGD	4	0
26	B	8001	LMU	1	0
26	B	8002	LMU	3	0
18	F	1301	CLA	6	0
18	F	1302	CLA	14	0
23	F	5001	LMG	7	0
23	F	5002	LMG	6	0
22	F	6014	BCR	8	0
22	F	6016	BCR	11	0
18	G	1001	CLA	36	0
18	G	1002	CLA	26	0
18	G	1003	CLA	30	0
22	G	2011	BCR	29	0
23	G	2021	LMG	20	0
18	H	1000	CLA	4	0
27	I	6018	LUT	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	I	6020	BCR	3	0
18	J	1302	CLA	7	0
23	J	5001	LMG	9	0
22	J	6012	BCR	7	0
22	J	6013	BCR	8	0
18	K	1001	CLA	12	0
22	K	2011	BCR	17	0
18	L	1501	CLA	15	0
18	L	1502	CLA	13	0
18	L	1503	CLA	11	0
22	L	6019	BCR	22	0
22	L	6020	BCR	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	742/758 (97%)	0.36	47 (6%) 23 14	56, 92, 150, 244	0
2	B	732/733 (99%)	0.30	43 (5%) 26 16	61, 89, 126, 157	0
3	I	29/30 (96%)	0.53	4 (13%) 4 2	89, 114, 148, 153	0
4	J	41/42 (97%)	0.17	3 (7%) 18 10	70, 80, 116, 164	0
5	F	150/154 (97%)	0.08	6 (4%) 42 30	66, 90, 122, 157	0
6	G	91/97 (93%)	0.49	11 (12%) 6 3	98, 129, 174, 184	0
7	L	160/167 (95%)	0.68	24 (15%) 3 2	86, 123, 172, 197	0
8	C	80/81 (98%)	0.10	4 (5%) 32 21	66, 81, 96, 106	0
9	D	141/147 (95%)	0.56	20 (14%) 4 2	77, 97, 120, 139	0
10	E	66/66 (100%)	0.35	7 (10%) 8 4	65, 91, 136, 183	0
11	H	84/90 (93%)	0.33	11 (13%) 5 2	103, 138, 178, 234	0
12	K	57/129 (44%)	1.58	19 (33%) 0 0	147, 215, 286, 324	0
13	2	207/269 (76%)	0.61	32 (15%) 3 1	85, 130, 180, 270	0
14	4	198/252 (78%)	0.60	26 (13%) 5 2	84, 121, 193, 274	0
15	1	194/202 (96%)	0.86	39 (20%) 1 1	95, 147, 225, 289	0
16	3	215/275 (78%)	0.73	31 (14%) 3 2	111, 179, 317, 368	0
All	All	3187/3492 (91%)	0.46	327 (10%) 9 4	56, 106, 205, 368	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	1	103	GLY	12.8
16	3	145	ALA	11.1
15	1	172	LYS	9.6
2	B	82	PHE	8.3
9	D	206	LYS	7.4

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Mol	Chain	Res	Type	RSRZ
7	L	211	TYR	7.4
9	D	196	VAL	7.3
2	B	491	ASN	7.2
1	A	250	LEU	7.0
16	3	132	THR	7.0
16	3	87	GLU	6.8
11	H	132	PRO	6.6
16	3	217	GLU	6.4
15	1	162	GLY	6.3
16	3	121	TYR	6.2
15	1	176	LYS	6.0
12	K	77	MET	5.9
16	3	125	VAL	5.8
2	B	490	ARG	5.7
3	I	4	LEU	5.7
2	B	214	ASP	5.7
1	A	115	HIS	5.7
15	1	100	LEU	5.6
12	K	122	THR	5.5
6	G	108	ALA	5.5
1	A	257	GLN	5.5
7	L	123	THR	5.5
2	B	159	PRO	5.5
1	A	502	THR	5.4
1	A	277	TYR	5.4
7	L	212	TYR	5.4
9	D	208	PRO	5.4
15	1	54	SER	5.4
1	A	263	ALA	5.3
2	B	161	TRP	5.3
9	D	207	GLN	5.2
15	1	219	ALA	5.2
1	A	517	GLY	5.1
1	A	264	GLU	5.1
13	2	127	THR	5.1
6	G	109	LYS	5.0
9	D	200	GLU	5.0
15	1	60	GLY	4.9
14	4	133	GLU	4.9
6	G	147	ASP	4.8
14	4	118	ILE	4.8
16	3	144	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
10	E	91	VAL	4.7
15	1	102	LEU	4.6
1	A	260	PRO	4.6
13	2	185	ASN	4.5
16	3	124	LYS	4.5
15	1	175	LYS	4.5
14	4	195	ALA	4.5
16	3	253	TYR	4.5
1	A	276	LYS	4.4
2	B	482	ASN	4.4
7	L	172	GLN	4.4
15	1	99	ALA	4.4
1	A	518	GLY	4.4
12	K	88	SER	4.3
15	1	123	GLY	4.3
7	L	205	TYR	4.3
16	3	89	THR	4.3
9	D	211	LEU	4.3
15	1	161	PRO	4.2
15	1	173	ASP	4.2
1	A	259	TYR	4.2
16	3	96	ARG	4.2
14	4	178	PRO	4.2
7	L	171	LYS	4.1
15	1	125	PRO	4.1
9	D	76	ASP	4.1
15	1	174	PRO	4.1
2	B	552	ASP	4.1
11	H	117	THR	4.1
7	L	131	SER	4.1
9	D	197	SER	4.0
15	1	171	SER	4.0
6	G	107	ARG	4.0
6	G	110	GLU	3.9
1	A	23	ASP	3.9
12	K	125	CYS	3.9
16	3	77	GLY	3.9
12	K	140	LEU	3.9
12	K	136	VAL	3.9
2	B	210	ASN	3.8
12	K	87	PRO	3.8
15	1	218	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
16	3	184	LYS	3.8
1	A	42	ARG	3.8
3	I	5	PRO	3.8
1	A	279	ASP	3.8
15	1	96	VAL	3.8
4	J	7	TYR	3.7
13	2	264	ALA	3.7
1	A	271	THR	3.7
14	4	225	THR	3.7
2	B	295	PHE	3.7
11	H	75	PRO	3.6
14	4	120	ILE	3.6
16	3	129	PRO	3.6
14	4	52	LYS	3.6
11	H	113	TYR	3.6
1	A	261	SER	3.6
12	K	134	VAL	3.6
14	4	198	LEU	3.6
2	B	487	ASN	3.6
7	L	173	PRO	3.6
10	E	71	GLY	3.5
3	I	32	LEU	3.5
5	F	189	LYS	3.5
11	H	131	LEU	3.5
14	4	119	GLY	3.5
14	4	238	SER	3.5
8	C	32	GLY	3.4
1	A	46	LYS	3.4
2	B	212	PHE	3.4
7	L	174	ASP	3.4
13	2	178	ASN	3.4
13	2	78	ASP	3.4
14	4	121	ILE	3.4
2	B	360	PHE	3.4
15	1	157	LYS	3.4
1	A	525	ASN	3.4
13	2	134	THR	3.4
9	D	190	ARG	3.4
10	E	98	ASN	3.3
15	1	233	PRO	3.3
11	H	135	LEU	3.3
13	2	184	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
13	2	77	LEU	3.3
13	2	133	LEU	3.3
1	A	240	LYS	3.2
7	L	116	LYS	3.2
12	K	61	PHE	3.2
9	D	72	PRO	3.2
2	B	430	GLY	3.2
7	L	115	VAL	3.2
12	K	121	ASP	3.2
16	3	134	LEU	3.2
16	3	146	GLY	3.2
7	L	170	LYS	3.2
1	A	280	PHE	3.2
2	B	475	ASP	3.1
2	B	232	LEU	3.1
14	4	68	GLY	3.1
13	2	251	PHE	3.1
6	G	144	ASN	3.1
2	B	229	GLN	3.1
1	A	25	ASP	3.1
7	L	208	ASP	3.1
9	D	199	ILE	3.1
1	A	17	GLU	3.0
12	K	78	LEU	3.0
15	1	50	TYR	3.0
16	3	263	PRO	3.0
7	L	210	PRO	3.0
12	K	89	ALA	3.0
13	2	186	ASN	3.0
7	L	54	TYR	2.9
14	4	131	LYS	2.9
13	2	80	SER	2.9
14	4	53	LYS	2.9
7	L	121	ARG	2.9
13	2	145	TYR	2.9
15	1	59	PHE	2.9
15	1	151	MET	2.9
10	E	128	VAL	2.9
2	B	157	LEU	2.9
9	D	210	ASP	2.9
12	K	79	PHE	2.9
13	2	59	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
16	3	189	GLY	2.8
16	3	86	PRO	2.8
12	K	76	LEU	2.8
15	1	110	GLU	2.8
7	L	169	ARG	2.8
14	4	237	ILE	2.7
11	H	77	PRO	2.7
9	D	204	THR	2.7
11	H	73	ASP	2.7
10	E	92	THR	2.7
13	2	204	LEU	2.7
15	1	51	LEU	2.7
15	1	178	HIS	2.7
5	F	109	TYR	2.7
14	4	115	PHE	2.7
1	A	107	GLU	2.7
15	1	134	ILE	2.7
7	L	92	ALA	2.7
1	A	140	PHE	2.7
1	A	251	ASN	2.7
13	2	248	ASP	2.7
1	A	366	GLY	2.7
2	B	486	LEU	2.6
13	2	128	LYS	2.6
16	3	118	ALA	2.6
9	D	201	VAL	2.6
14	4	199	GLU	2.6
2	B	70	TRP	2.6
2	B	160	LYS	2.6
11	H	78	TYR	2.6
16	3	61	SER	2.6
1	A	26	PRO	2.6
2	B	374	HIS	2.6
16	3	94	GLU	2.5
12	K	83	PHE	2.5
16	3	58	TRP	2.5
1	A	520	LEU	2.5
14	4	188	ILE	2.5
13	2	126	LEU	2.5
6	G	88	ALA	2.5
6	G	111	TYR	2.5
8	C	35	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
16	3	185	GLN	2.5
4	J	3	ASP	2.5
15	1	165	PHE	2.5
8	C	34	CYS	2.5
13	2	79	GLY	2.5
2	B	277	HIS	2.5
15	1	47	ARG	2.5
15	1	152	GLU	2.5
2	B	294	ASN	2.5
1	A	138	GLY	2.5
1	A	241	GLU	2.4
9	D	156	TYR	2.4
10	E	106	ARG	2.4
6	G	145	GLY	2.4
12	K	75	THR	2.4
1	A	142	GLY	2.4
9	D	195	ASN	2.4
1	A	108	ALA	2.4
13	2	142	GLU	2.4
15	1	115	PRO	2.4
1	A	165	TYR	2.4
5	F	225	GLU	2.4
15	1	57	GLY	2.4
12	K	80	ALA	2.4
1	A	456	HIS	2.4
16	3	149	ASN	2.4
7	L	62	GLY	2.3
2	B	349	ALA	2.3
13	2	265	ALA	2.3
1	A	247	GLU	2.3
2	B	276	HIS	2.3
9	D	100	PHE	2.3
12	K	133	GLY	2.3
15	1	158	LYS	2.3
13	2	65	PRO	2.3
13	2	123	PRO	2.3
1	A	258	LEU	2.3
7	L	156	GLY	2.3
6	G	146	TYR	2.3
14	4	197	THR	2.3
13	2	125	PHE	2.3
10	E	129	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
14	4	82	ALA	2.3
2	B	219	PRO	2.3
16	3	99	ALA	2.3
2	B	211	ASN	2.3
2	B	220	GLN	2.3
16	3	147	THR	2.3
14	4	192	LEU	2.3
2	B	244	PHE	2.3
14	4	122	ASN	2.3
16	3	260	VAL	2.3
2	B	549	ASP	2.3
13	2	138	TYR	2.3
11	H	89	PHE	2.3
13	2	183	PHE	2.3
12	K	137	VAL	2.2
2	B	83	HIS	2.2
13	2	72	THR	2.2
9	D	209	TYR	2.2
14	4	224	VAL	2.2
7	L	108	PHE	2.2
13	2	73	PRO	2.2
7	L	111	VAL	2.2
2	B	345	THR	2.2
8	C	13	GLY	2.2
3	I	8	PHE	2.2
11	H	72	SER	2.2
1	A	633	VAL	2.2
15	1	97	PRO	2.2
16	3	272	LEU	2.2
1	A	116	ILE	2.2
2	B	426	SER	2.2
5	F	187	ASP	2.2
7	L	78	LEU	2.2
2	B	158	GLN	2.2
5	F	113	SER	2.2
5	F	188	GLU	2.2
15	1	101	GLY	2.1
14	4	59	GLY	2.1
9	D	73	PRO	2.1
13	2	239	HIS	2.1
14	4	117	SER	2.1
1	A	139	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	66	PHE	2.1
16	3	178	LYS	2.1
15	1	114	LEU	2.1
2	B	281	ALA	2.1
1	A	455	PHE	2.1
9	D	166	TYR	2.1
13	2	199	LEU	2.1
15	1	61	PHE	2.1
2	B	433	THR	2.1
2	B	688	ALA	2.1
2	B	84	VAL	2.1
16	3	250	VAL	2.1
2	B	434	LEU	2.0
2	B	154	TRP	2.0
15	1	52	ASP	2.0
13	2	187	LYS	2.0
2	B	605	ASN	2.0
6	G	62	LEU	2.0
7	L	209	LEU	2.0
1	A	141	ARG	2.0
1	A	628	ILE	2.0
1	A	282	THR	2.0
1	A	273	ASN	2.0
1	A	513	LEU	2.0
13	2	63	ASP	2.0
1	A	278	ALA	2.0
14	4	179	ALA	2.0
4	J	2	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	LUT	3	3501	42/42	0.68	0.63	5.74	202,209,216,218	0
29	ZEX	4	4505	42/42	0.89	0.25	4.93	85,96,107,114	0
22	BCR	B	6005	40/40	0.72	0.41	3.92	87,103,182,184	0
27	LUT	2	2502	42/42	0.85	0.36	3.79	102,115,124,131	0
22	BCR	J	6012	40/40	0.83	0.31	3.70	67,80,89,91	0
22	BCR	A	6007	40/40	0.86	0.30	3.29	77,90,147,151	0
22	BCR	L	6019	40/40	0.81	0.40	3.19	88,105,132,135	0
18	CLA	A	1117	65/65	0.93	0.36	3.16	85,98,110,114	0
22	BCR	A	6003	40/40	0.85	0.34	2.97	79,94,139,140	0
27	LUT	3	3502	42/42	0.74	0.34	2.89	133,142,164,166	0
27	LUT	4	4503	42/42	0.84	0.37	2.71	110,135,158,160	0
22	BCR	J	6013	40/40	0.75	0.34	2.66	74,94,112,116	0
18	CLA	3	3008	48/65	0.84	0.46	2.45	180,199,214,217	0
18	CLA	B	1222	65/65	0.86	0.30	2.37	58,74,103,110	0
28	CHL	3	3011	56/66	0.80	0.34	2.35	144,156,197,200	0
22	BCR	B	6004	40/40	0.77	0.36	2.30	105,112,138,144	0
18	CLA	A	1140	65/65	0.90	0.28	2.27	58,66,78,106	0
18	CLA	2	2012	55/65	0.90	0.29	2.22	86,104,149,153	0
22	BCR	B	6009	40/40	0.85	0.28	2.19	63,78,94,95	0
18	CLA	J	1302	50/65	0.84	0.35	2.13	137,152,189,196	0
22	BCR	L	6020	40/40	0.89	0.37	2.05	98,131,157,164	0
18	CLA	2	2005	55/65	0.91	0.25	1.98	93,103,129,135	0
18	CLA	A	1106	65/65	0.90	0.28	1.96	59,74,90,106	0
22	BCR	B	6010	40/40	0.85	0.28	1.93	64,73,96,100	0
21	LHG	A	7001	49/49	0.91	0.23	1.91	56,72,84,92	0
18	CLA	B	1227	65/65	0.89	0.23	1.90	60,74,99,105	0
22	BCR	A	6002	40/40	0.91	0.28	1.89	82,115,168,169	0
27	LUT	2	2501	42/42	0.70	0.36	1.88	121,137,141,143	0
18	CLA	B	1220	65/65	0.92	0.23	1.88	61,76,114,118	0
18	CLA	A	1127	65/65	0.92	0.33	1.87	69,83,95,99	0
18	CLA	3	3001	50/65	0.87	0.31	1.80	147,169,201,206	0
22	BCR	A	6011	40/40	0.92	0.36	1.75	61,73,88,96	0
18	CLA	A	1122	65/65	0.92	0.23	1.73	76,96,122,139	0
22	BCR	A	6008	40/40	0.83	0.31	1.69	76,97,137,139	0
18	CLA	B	1234	60/65	0.85	0.29	1.62	64,77,106,108	0
27	LUT	1	1501	42/42	0.79	0.31	1.58	115,142,189,197	0
18	CLA	2	2001	60/65	0.89	0.29	1.54	114,134,167,169	0
22	BCR	G	2011	40/40	0.68	0.28	1.50	112,132,172,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CLA	A	1126	65/65	0.92	0.28	1.48	65,79,87,97	0
25	DGD	B	7101	61/66	0.87	0.24	1.47	62,79,104,113	0
18	CLA	A	1104	65/65	0.89	0.28	1.44	55,73,81,85	0
18	CLA	A	1110	55/65	0.87	0.27	1.41	97,114,138,143	0
18	CLA	B	1210	65/65	0.92	0.28	1.30	81,94,107,113	0
18	CLA	A	1107	65/65	0.86	0.29	1.30	60,77,94,105	0
22	BCR	B	6006	40/40	0.78	0.35	1.28	94,115,164,164	0
18	CLA	3	3003	60/65	0.80	0.25	1.27	137,170,188,190	0
18	CLA	3	3010	60/65	0.82	0.29	1.26	122,158,181,196	0
18	CLA	A	1123	65/65	0.87	0.31	1.25	70,88,93,96	0
21	LHG	A	5003	40/49	0.92	0.21	1.23	101,117,132,134	0
18	CLA	A	1135	51/65	0.91	0.28	1.18	72,92,114,117	0
18	CLA	H	1000	46/65	0.85	0.31	1.18	119,150,170,176	0
22	BCR	K	2011	40/40	0.79	0.37	1.18	125,136,144,147	0
20	PQN	B	5002	33/33	0.94	0.23	1.13	54,72,91,93	0
18	CLA	B	1214	59/65	0.85	0.30	1.12	71,91,100,108	0
18	CLA	1	1013	46/65	0.77	0.34	1.12	127,154,181,185	0
18	CLA	B	1216	65/65	0.90	0.25	1.11	73,86,105,108	0
20	PQN	A	5001	33/33	0.92	0.23	1.10	53,63,76,85	0
18	CLA	A	1237	60/65	0.94	0.29	1.07	75,94,113,116	0
27	LUT	1	1502	42/42	0.85	0.26	1.02	85,116,128,129	0
18	CLA	A	1129	50/65	0.92	0.24	1.01	71,93,115,126	0
23	LMG	B	5005	38/55	0.60	0.31	1.00	76,120,141,143	0
18	CLA	A	1022	65/65	0.90	0.24	0.99	58,76,88,99	0
18	CLA	A	1013	65/65	0.93	0.32	0.97	49,62,74,90	0
18	CLA	1	1003	55/65	0.91	0.19	0.96	100,122,134,142	0
18	CLA	4	4016	46/65	0.79	0.30	0.96	126,166,177,183	0
18	CLA	A	1116	60/65	0.91	0.25	0.95	89,119,137,142	0
18	CLA	A	1139	65/65	0.91	0.25	0.93	56,70,98,104	0
17	CL0	A	1011	65/65	0.94	0.24	0.93	52,70,82,84	0
28	CHL	2	2011	48/66	0.88	0.24	0.92	108,124,129,136	0
22	BCR	F	6016	40/40	0.90	0.21	0.90	66,75,91,94	0
18	CLA	B	1226	65/65	0.93	0.23	0.89	65,76,97,103	0
22	BCR	F	6014	40/40	0.87	0.27	0.86	54,64,73,74	0
18	CLA	B	1224	65/65	0.92	0.30	0.85	65,83,100,107	0
18	CLA	B	1239	65/65	0.92	0.24	0.84	69,82,111,116	0
18	CLA	B	1207	65/65	0.92	0.23	0.80	78,102,122,129	0
18	CLA	A	1138	65/65	0.92	0.26	0.79	55,65,75,82	0
18	CLA	A	1130	50/65	0.90	0.23	0.79	83,100,123,127	0
18	CLA	K	1001	46/65	0.79	0.35	0.78	147,173,200,209	0
18	CLA	3	3013	46/65	0.86	0.19	0.77	127,157,166,176	0
18	CLA	B	1215	60/65	0.93	0.30	0.73	82,91,102,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CLA	B	1225	65/65	0.92	0.30	0.73	66,81,98,105	0
18	CLA	B	1205	65/65	0.94	0.26	0.73	90,103,116,152	0
18	CLA	B	1240	65/65	0.93	0.19	0.69	66,84,103,108	0
18	CLA	A	1132	65/65	0.92	0.28	0.69	79,94,120,129	0
18	CLA	3	3002	46/65	0.89	0.24	0.68	173,188,195,222	0
23	LMG	G	2021	41/55	0.75	0.28	0.68	138,156,175,176	0
18	CLA	B	1229	65/65	0.91	0.26	0.65	60,72,82,84	0
22	BCR	3	3503	40/40	0.76	0.31	0.63	119,136,175,177	0
27	LUT	4	4502	42/42	0.86	0.26	0.63	88,106,117,121	0
18	CLA	A	1112	65/65	0.86	0.25	0.62	101,118,138,140	0
18	CLA	A	1108	46/65	0.91	0.29	0.61	85,101,121,126	0
18	CLA	B	1012	65/65	0.91	0.27	0.61	51,69,85,92	0
18	CLA	3	3004	60/65	0.81	0.26	0.59	125,139,154,155	0
18	CLA	A	1133	55/65	0.91	0.23	0.58	83,109,120,126	0
18	CLA	A	1111	60/65	0.90	0.24	0.58	75,91,112,118	0
18	CLA	2	2007	60/65	0.83	0.30	0.57	116,142,189,195	0
18	CLA	3	3005	55/65	0.87	0.25	0.56	107,131,144,157	0
18	CLA	B	1218	65/65	0.89	0.25	0.56	86,100,155,160	0
28	CHL	4	4010	47/66	0.83	0.28	0.54	105,125,180,187	0
18	CLA	A	1109	65/65	0.88	0.22	0.53	71,85,94,101	0
18	CLA	3	3012	50/65	0.85	0.22	0.51	117,135,142,144	0
18	CLA	F	1301	45/65	0.89	0.23	0.48	61,73,86,101	0
18	CLA	B	1206	65/65	0.94	0.21	0.47	86,104,112,127	0
21	LHG	1	1801	49/49	0.87	0.26	0.47	94,113,164,170	0
22	BCR	I	6020	40/40	0.92	0.25	0.44	85,97,110,111	0
27	LUT	4	4501	42/42	0.82	0.25	0.44	107,121,142,149	0
18	CLA	L	1502	60/65	0.89	0.23	0.43	86,116,125,130	0
18	CLA	A	1103	65/65	0.89	0.25	0.42	66,83,104,107	0
18	CLA	B	1238	65/65	0.93	0.22	0.42	70,85,96,116	0
18	CLA	3	3007	50/65	0.81	0.23	0.41	175,193,239,246	0
18	CLA	B	1221	65/65	0.94	0.24	0.41	66,78,115,122	0
18	CLA	A	1119	65/65	0.92	0.23	0.40	78,95,107,115	0
18	CLA	A	1118	46/65	0.89	0.22	0.38	99,108,127,131	0
18	CLA	B	1217	46/65	0.92	0.27	0.34	96,109,124,127	0
18	CLA	B	1201	50/65	0.94	0.18	0.34	80,93,131,134	0
28	CHL	4	4011	51/66	0.91	0.23	0.32	117,131,149,154	0
22	BCR	A	6017	40/40	0.92	0.25	0.31	71,86,105,122	0
18	CLA	4	4001	60/65	0.84	0.28	0.28	113,129,158,160	0
23	LMG	4	4801	35/55	0.87	0.25	0.28	104,117,128,132	0
18	CLA	A	1131	65/65	0.93	0.30	0.28	79,93,103,112	0
18	CLA	4	4005	60/65	0.91	0.21	0.26	84,97,106,120	0
18	CLA	4	4007	60/65	0.85	0.29	0.25	110,130,179,183	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CLA	A	1134	55/65	0.86	0.27	0.25	112,124,168,172	0
18	CLA	A	1151	50/65	0.86	0.24	0.24	99,113,187,189	0
18	CLA	1	1008	46/65	0.80	0.25	0.24	112,129,142,150	0
18	CLA	B	1023	65/65	0.88	0.24	0.23	57,70,94,105	0
18	CLA	A	1105	51/65	0.88	0.25	0.23	66,88,97,100	0
18	CLA	2	2016	50/65	0.66	0.30	0.22	114,164,207,211	0
18	CLA	2	2008	50/65	0.91	0.20	0.21	109,138,148,156	0
23	LMG	F	5001	23/55	0.87	0.27	0.21	86,94,106,109	0
18	CLA	B	1021	65/65	0.91	0.25	0.20	61,72,80,83	0
18	CLA	B	1202	65/65	0.95	0.22	0.20	71,82,91,104	0
18	CLA	B	1228	60/65	0.87	0.26	0.17	63,73,111,114	0
18	CLA	L	1501	50/65	0.86	0.22	0.17	106,129,153,159	0
18	CLA	1	1014	46/65	0.88	0.17	0.16	83,110,123,143	0
18	CLA	B	1213	60/65	0.86	0.23	0.14	85,105,118,126	0
18	CLA	B	1231	60/65	0.86	0.23	0.13	65,81,101,104	0
18	CLA	B	1211	65/65	0.91	0.23	0.11	93,107,131,136	0
18	CLA	4	4004	60/65	0.87	0.25	0.11	76,99,112,118	0
18	CLA	B	1235	65/65	0.92	0.22	0.10	54,68,78,92	0
18	CLA	A	1101	65/65	0.90	0.23	0.10	58,72,90,113	0
18	CLA	2	2004	65/65	0.91	0.22	0.10	84,105,117,125	0
23	LMG	J	5001	55/55	0.85	0.22	0.09	62,96,110,122	0
18	CLA	A	1102	50/65	0.92	0.20	0.08	58,69,95,104	0
18	CLA	1	1007	46/65	0.91	0.19	0.08	112,131,162,181	0
18	CLA	B	1212	55/65	0.84	0.26	0.08	109,129,146,154	0
18	CLA	4	4012	65/65	0.92	0.21	0.07	92,104,117,120	0
28	CHL	1	1009	56/66	0.87	0.25	0.05	92,105,113,130	0
18	CLA	4	4003	65/65	0.90	0.23	0.05	84,106,135,143	0
18	CLA	4	4008	46/65	0.85	0.25	0.02	93,112,129,137	0
18	CLA	3	3018	50/65	0.81	0.31	0.01	173,190,207,213	0
18	CLA	A	1128	65/65	0.92	0.21	-0.06	56,66,74,85	0
18	CLA	3	3006	50/65	0.81	0.26	-0.06	125,157,167,170	0
18	CLA	1	1011	50/65	0.85	0.28	-0.07	126,153,175,185	0
28	CHL	2	2010	47/66	0.84	0.25	-0.08	111,134,142,143	0
18	CLA	4	4009	50/65	0.93	0.20	-0.09	85,94,116,131	0
18	CLA	B	1219	60/65	0.92	0.20	-0.09	82,97,134,135	0
18	CLA	L	1503	50/65	0.83	0.38	-0.10	106,114,143,149	0
28	CHL	2	2013	46/66	0.90	0.22	-0.11	110,125,130,135	0
21	LHG	B	5004	21/49	0.92	0.16	-0.13	86,102,116,119	0
18	CLA	A	1125	60/65	0.92	0.22	-0.14	79,94,102,114	0
18	CLA	A	1124	55/65	0.92	0.23	-0.15	59,77,104,116	0
18	CLA	2	2006	55/65	0.86	0.23	-0.17	105,132,173,174	0
18	CLA	G	1002	46/65	0.94	0.19	-0.19	142,160,173,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CLA	G	1001	55/65	0.88	0.17	-0.19	119,145,181,184	0
18	CLA	2	2003	55/65	0.89	0.16	-0.20	103,127,135,158	0
18	CLA	A	1114	46/65	0.89	0.29	-0.20	107,117,124,136	0
18	CLA	G	1003	60/65	0.84	0.24	-0.21	97,121,149,153	0
18	CLA	1	1004	65/65	0.89	0.23	-0.26	98,114,122,125	0
18	CLA	B	1203	65/65	0.96	0.22	-0.26	68,82,97,104	0
18	CLA	B	1230	58/65	0.91	0.20	-0.26	58,74,83,86	0
18	CLA	4	4006	50/65	0.80	0.24	-0.28	110,127,148,156	0
18	CLA	B	1236	55/65	0.91	0.24	-0.31	56,69,117,124	0
18	CLA	B	1208	55/65	0.91	0.19	-0.31	82,114,133,137	0
18	CLA	1	1006	50/65	0.83	0.24	-0.35	125,138,144,148	0
18	CLA	A	1113	46/65	0.85	0.27	-0.36	119,135,172,187	0
18	CLA	A	1115	46/65	0.88	0.24	-0.39	107,141,170,178	0
18	CLA	A	1120	60/65	0.90	0.18	-0.40	95,118,178,182	0
18	CLA	B	1223	65/65	0.91	0.22	-0.42	59,78,90,96	0
26	LMU	B	8002	35/35	0.84	0.23	-0.44	162,173,189,191	0
18	CLA	1	1012	50/65	0.94	0.16	-0.56	103,125,130,132	0
18	CLA	A	1121	55/65	0.92	0.17	-0.56	104,123,209,211	0
28	CHL	1	1010	47/66	0.86	0.17	-0.58	125,137,152,155	0
18	CLA	B	1232	55/65	0.90	0.22	-0.61	80,97,118,122	0
21	LHG	2	2801	24/49	0.81	0.25	-0.62	109,123,148,152	0
28	CHL	4	4013	47/66	0.91	0.20	-0.62	98,118,130,134	0
18	CLA	1	1001	60/65	0.84	0.20	-0.63	122,151,165,171	0
18	CLA	2	2009	50/65	0.90	0.18	-0.63	100,117,138,139	0
18	CLA	A	1137	55/65	0.93	0.22	-0.66	71,85,125,126	0
18	CLA	B	1204	55/65	0.91	0.20	-0.70	80,103,118,124	0
18	CLA	B	1209	46/65	0.93	0.22	-0.71	100,109,118,145	0
18	CLA	A	1136	56/65	0.92	0.17	-0.91	84,98,115,119	0
18	CLA	F	1302	50/65	0.94	0.16	-1.13	67,84,114,124	0
19	SF4	C	3002	8/8	0.95	0.12	-1.47	73,103,107,107	0
19	SF4	C	3003	8/8	0.97	0.07	-2.30	89,106,119,126	0
19	SF4	A	3001	8/8	0.97	0.10	-2.79	69,95,97,99	0
24	CA	B	6000	1/1	0.89	0.06	-4.01	100,100,100,100	0
18	CLA	3	3019	27/65	0.29	0.59	-	158,174,188,189	1
23	LMG	2	2802	35/55	0.81	0.41	-	108,127,149,152	0
18	CLA	4	4002	50/65	0.81	0.24	-	107,141,171,211	0
18	CLA	2	2002	46/65	0.81	0.21	-	137,154,171,183	0
18	CLA	3	3017	46/65	0.88	0.24	-	101,119,134,145	0
18	CLA	4	4017	65/65	0.89	0.27	-	93,103,120,121	0
18	CLA	1	1002	46/65	0.88	0.19	-	120,155,171,194	0
18	CLA	1	1005	55/65	0.87	0.20	-	84,113,122,124	0
23	LMG	F	5002	37/55	0.85	0.39	-	84,107,120,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CLA	2	2019	27/65	0.78	0.18	-	148,159,174,174	1
27	LUT	I	6018	42/42	0.87	0.28	-	101,109,116,121	0
26	LMU	B	8001	35/35	0.79	0.28	-	104,158,168,172	0

6.5 Other polymers [i](#)

There are no such residues in this entry.