



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2019 – 10:25 PM EST

PDB ID : 6HQB
Title : Monomeric cyanobacterial photosystem I
Authors : Netzer-El, S.Y.; Nelson, N.; Caspy, I.
Deposited on : 2018-09-24
Resolution : 4.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

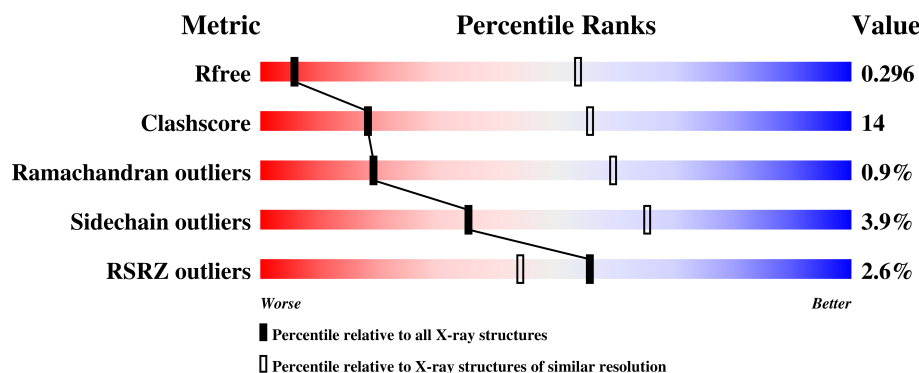
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	111664	1008 (4.38-3.62)
Clashscore	122126	1012 (4.34-3.66)
Ramachandran outliers	120053	1000 (4.36-3.64)
Sidechain outliers	120020	1023 (4.38-3.62)
RSRZ outliers	108989	1107 (4.40-3.60)

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	751	
2	B	731	
3	C	80	
4	D	141	
5	E	69	

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Mol	Chain	Length	Quality of chain
6	F	143	
7	I	40	
8	J	40	
9	K	70	
10	L	137	
11	M	31	

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
12	CLA	A	1011	X	-	-	-
12	CLA	A	1012	X	-	-	-
12	CLA	A	1013	X	-	-	-
12	CLA	A	1101	X	-	-	-
12	CLA	A	1102	X	-	-	-
12	CLA	A	1103	X	-	-	-
12	CLA	A	1104	X	-	-	-
12	CLA	A	1105	X	-	-	-
12	CLA	A	1106	X	-	-	-
12	CLA	A	1107	X	-	-	-
12	CLA	A	1108	X	-	-	-
12	CLA	A	1109	X	-	-	-
12	CLA	A	1110	X	-	-	-
12	CLA	A	1111	X	-	-	-
12	CLA	A	1112	X	-	-	-
12	CLA	A	1113	X	-	-	-
12	CLA	A	1114	X	-	-	-
12	CLA	A	1115	X	-	-	-
12	CLA	A	1116	X	-	-	-
12	CLA	A	1117	X	-	-	-
12	CLA	A	1118	X	-	-	-
12	CLA	A	1119	X	-	-	-
12	CLA	A	1120	X	-	-	-
12	CLA	A	1121	X	-	-	-
12	CLA	A	1122	X	-	-	-
12	CLA	A	1123	X	-	-	-
12	CLA	A	1124	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	1125	X	-	-	-
12	CLA	A	1126	X	-	-	-
12	CLA	A	1127	X	-	-	-
12	CLA	A	1128	X	-	-	-
12	CLA	A	1129	X	-	-	-
12	CLA	A	1130	X	-	-	-
12	CLA	A	1131	X	-	-	-
12	CLA	A	1132	X	-	-	-
12	CLA	A	1133	X	-	-	-
12	CLA	A	1134	X	-	-	-
12	CLA	A	1135	X	-	-	-
12	CLA	A	1136	X	-	-	-
12	CLA	A	1137	X	-	-	-
12	CLA	A	1138	X	-	-	-
12	CLA	A	1139	X	-	-	-
12	CLA	A	1140	X	-	-	-
12	CLA	A	1141	X	-	-	-
12	CLA	B	1021	X	-	-	-
12	CLA	B	1022	X	-	-	-
12	CLA	B	1023	X	-	-	-
12	CLA	B	1201	X	-	-	-
12	CLA	B	1202	X	-	-	-
12	CLA	B	1203	X	-	-	-
12	CLA	B	1204	X	-	-	-
12	CLA	B	1205	X	-	-	-
12	CLA	B	1206	X	-	-	-
12	CLA	B	1207	X	-	-	-
12	CLA	B	1208	X	-	-	-
12	CLA	B	1209	X	-	-	-
12	CLA	B	1210	X	-	-	-
12	CLA	B	1211	X	-	-	-
12	CLA	B	1212	X	-	-	-
12	CLA	B	1213	X	-	-	-
12	CLA	B	1214	X	-	-	-
12	CLA	B	1215	X	-	-	-
12	CLA	B	1216	X	-	-	-
12	CLA	B	1217	X	-	-	-
12	CLA	B	1218	X	-	-	-
12	CLA	B	1219	X	-	-	-
12	CLA	B	1220	X	-	-	-
12	CLA	B	1221	X	-	-	-
12	CLA	B	1222	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	B	1223	X	-	-	-
12	CLA	B	1224	X	-	-	-
12	CLA	B	1225	X	-	-	-
12	CLA	B	1226	X	-	-	-
12	CLA	B	1227	X	-	-	-
12	CLA	B	1228	X	-	-	-
12	CLA	B	1229	X	-	-	-
12	CLA	B	1230	X	-	-	-
12	CLA	B	1231	X	-	-	-
12	CLA	B	1232	X	-	-	-
12	CLA	B	1234	X	-	-	-
12	CLA	B	1235	X	-	-	-
12	CLA	B	1236	X	-	-	-
12	CLA	B	1237	X	-	-	-
12	CLA	B	1238	X	-	-	-
12	CLA	B	1239	X	-	-	-
12	CLA	B	1240	X	-	-	-
12	CLA	F	1301	X	-	-	-
12	CLA	F	1302	X	-	-	-
12	CLA	J	1302	X	-	-	-
12	CLA	J	1303	X	-	-	-
12	CLA	K	1401	X	-	-	-
12	CLA	K	1402	X	-	-	-
12	CLA	L	1502	X	-	-	-
15	BCR	A	4003	-	-	-	X
15	BCR	I	4018	-	-	-	X
19	ECH	M	4021	-	-	-	X
20	LMG	B	5005	-	-	-	X
21	SQD	B	5008	-	-	-	X
21	SQD	F	5001	-	-	-	X
25	EQ3	I	4020	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 23566 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
1	A	751	Total	C	N	O	S	0	0	0
			5876	3846	999	1003	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5783	3806	969	992	16			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1102	697	190	211	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			543	340	96	107			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	143	Total	C	N	O	S	0	0	0
			1113	718	185	205	5			

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	40	Total	C	N	O	S	0	0	0
			311	209	44	55	3			

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	70	Total	C	N	O	S	0	0	0
			510	337	81	87	5			

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	137	Total	C	N	O	S	0	0	0
			1030	674	167	187	2			

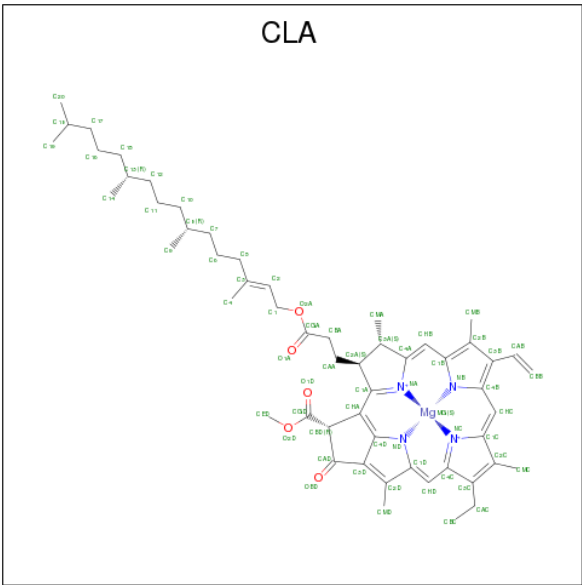
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	158	HIS	-	insertion	UNP P37277

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
12	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
12	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
12	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
12	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0

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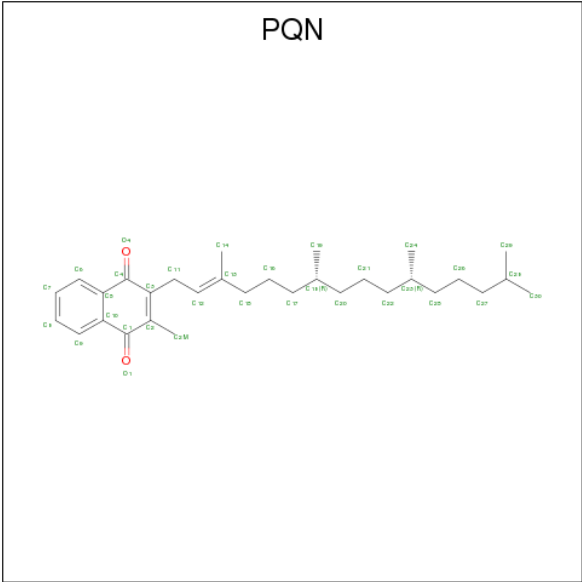
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12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0

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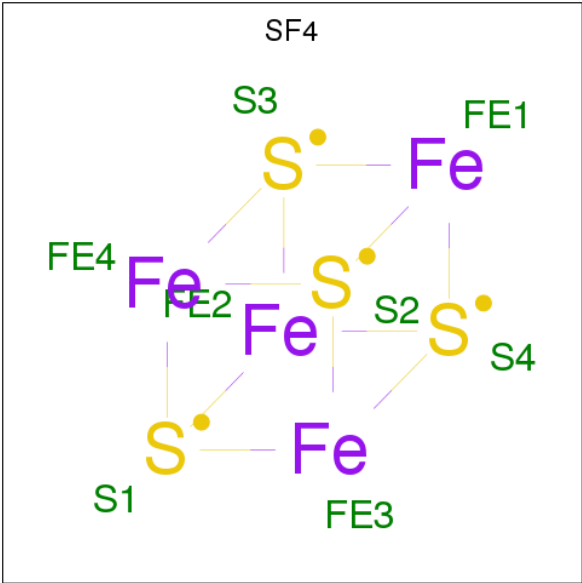
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
12	K	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	L	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

- Molecule 13 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



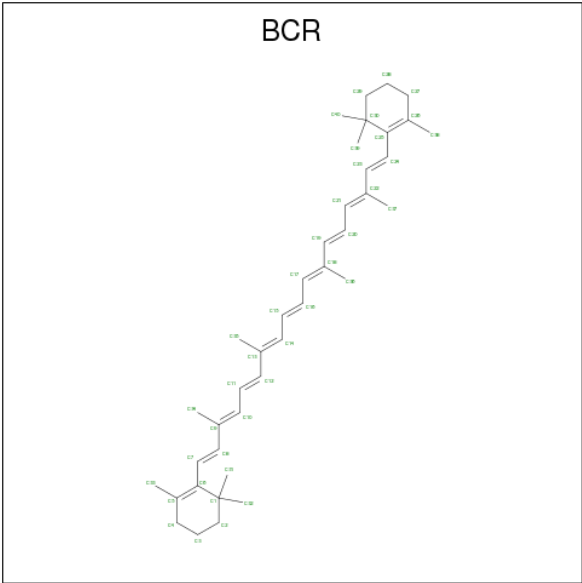
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	Fe	S	0	0
			8	4	4		
14	C	1	Total	Fe	S	0	0
			8	4	4		

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

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



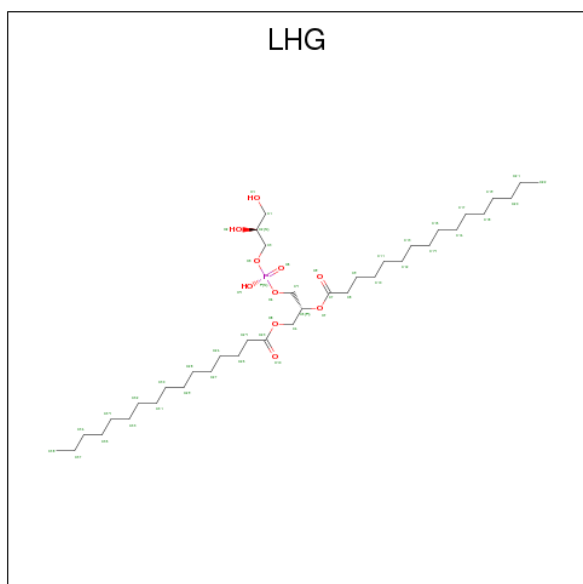
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	C	0	0
			40	40		
15	A	1	Total	C	0	0
			40	40		
15	A	1	Total	C	0	0
			40	40		
15	A	1	Total	C	0	0
			40	40		
15	A	1	Total	C	0	0
			40	40		
15	B	1	Total	C	0	0
			40	40		
15	B	1	Total	C	0	0
			40	40		
15	B	1	Total	C	0	0
			40	40		
15	B	1	Total	C	0	0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

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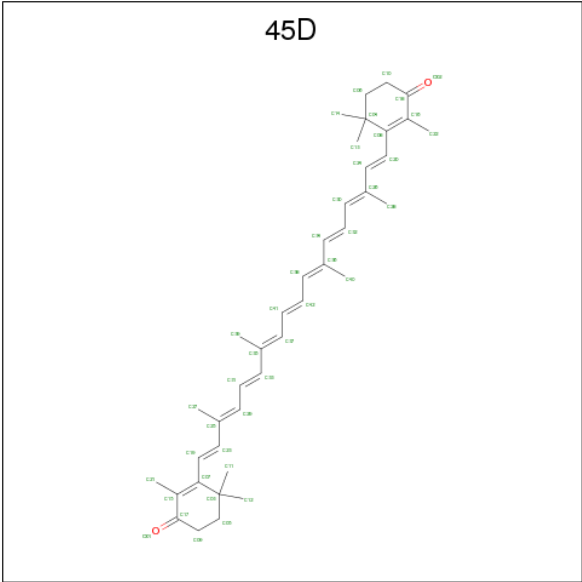
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	K	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 49 38 10 1	0	0
16	B	1	Total C O P 49 38 10 1	0	0
16	B	1	Total C O P 21 10 10 1	0	0

- Molecule 17 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).

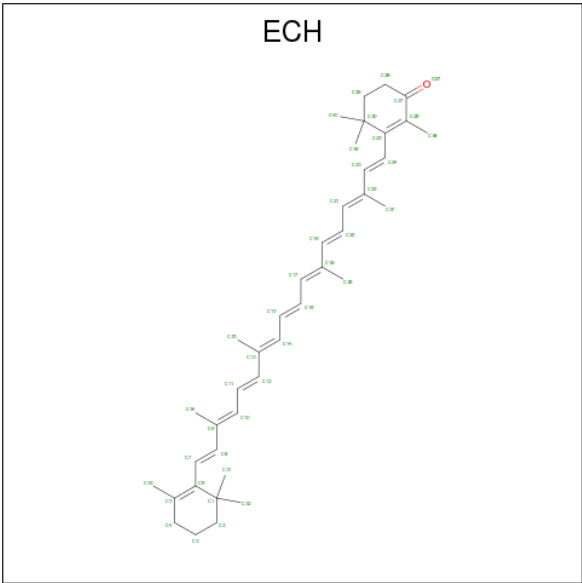


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	C	O	0
			42	40	2	

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

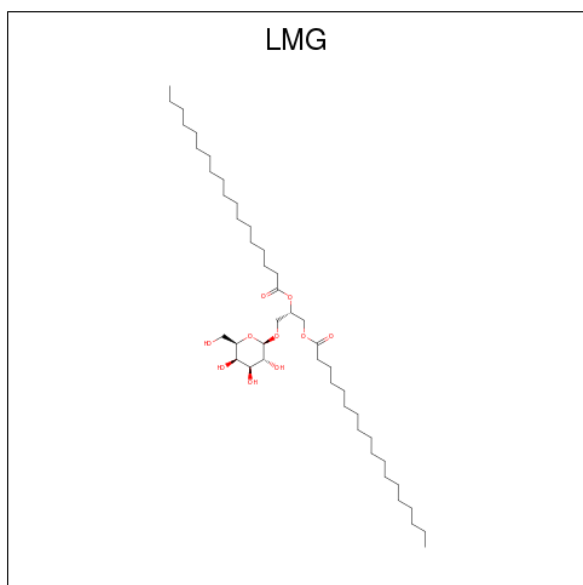
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	1	Total	Cl	0	0
			1	1		

- Molecule 19 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C₄₀H₅₄O).



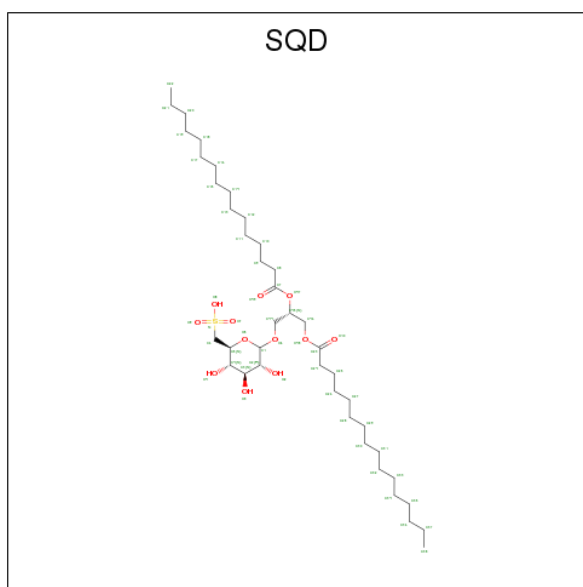
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			41	40	1		
19	M	1	Total	C	O	0	0
			41	40	1		

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			55	45	10		
20	B	1	Total	C	O	0	0
			55	45	10		

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

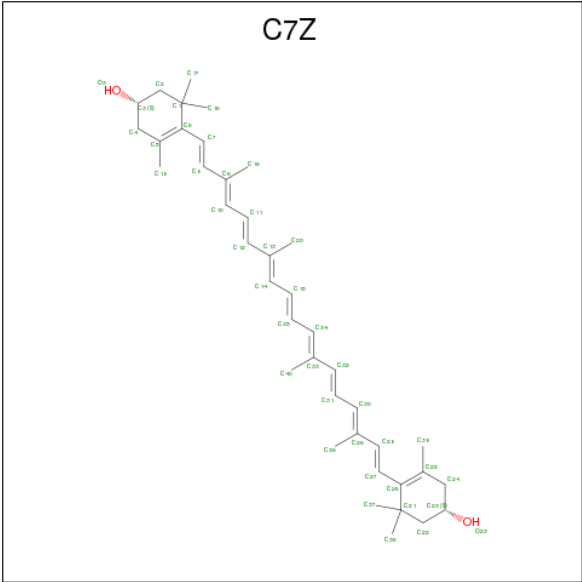


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	B	1	Total	C	O	S	0	0
			54	41	12	1		
21	F	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca).

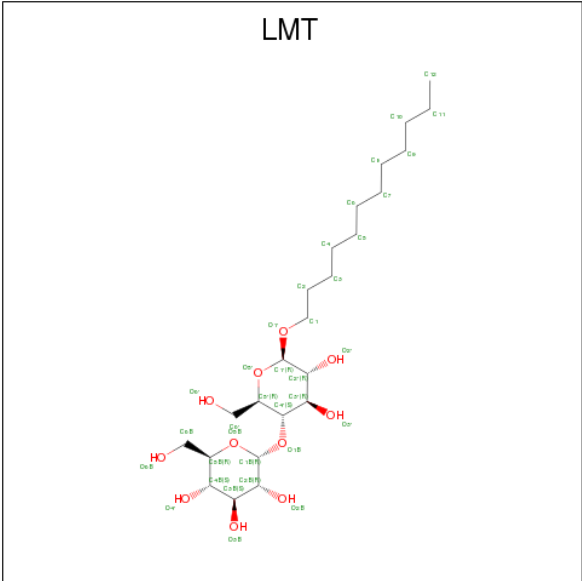
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Ca	0	0
			1	1		
22	L	1	Total	Ca	0	0
			1	1		

- Molecule 23 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C₄₀H₅₆O₂).



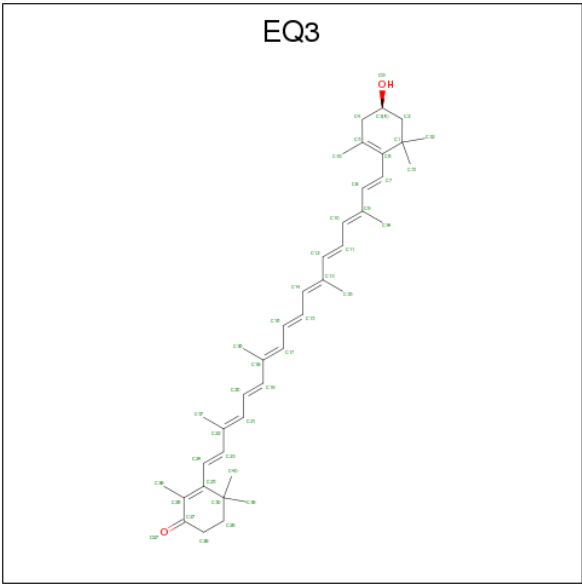
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	F	1	Total	C	O	0	0
			42	40	2		
23	J	1	Total	C	O	0	0
			42	40	2		

- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 25 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: C₄₀H₅₄O₂).

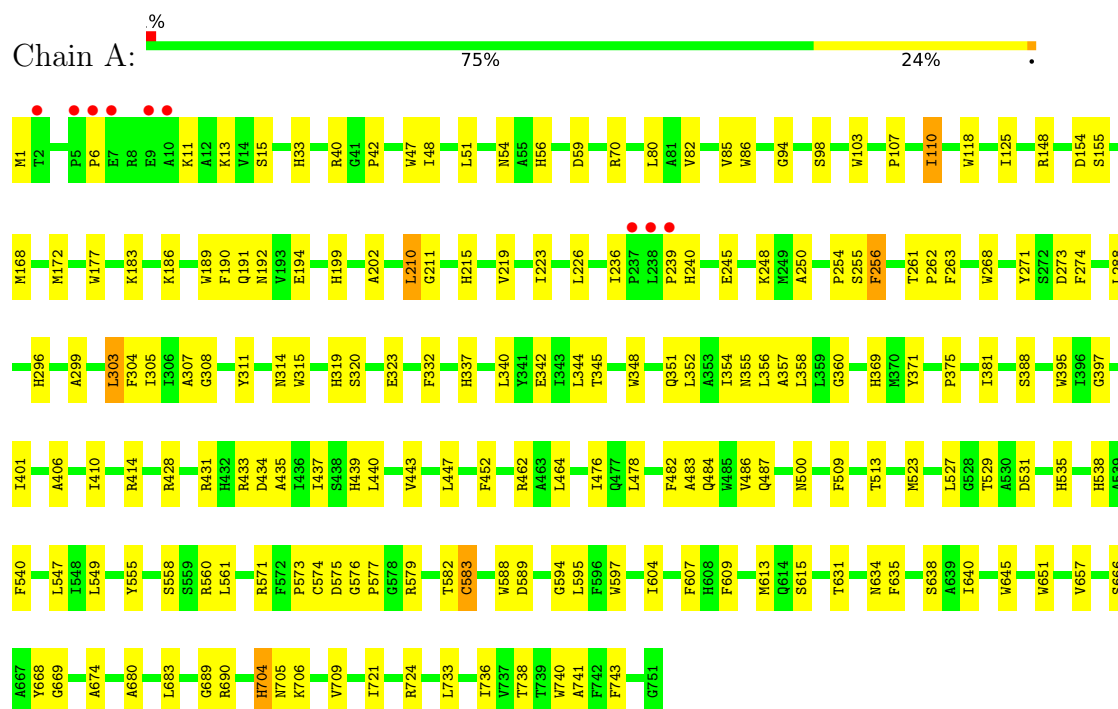


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
25	I	1	42	40	2	0	0

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 the various outlier classes 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



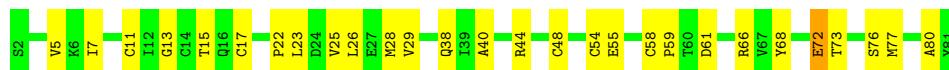
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





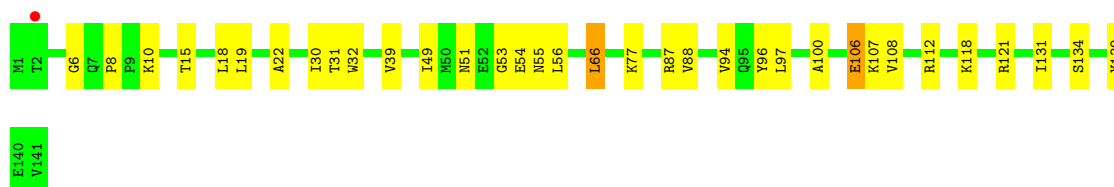
- Molecule 3: Photosystem I iron-sulfur center

Chain C: 65% 34% .



- Molecule 4: Photosystem I reaction center subunit II

Chain D: 76% 23% .



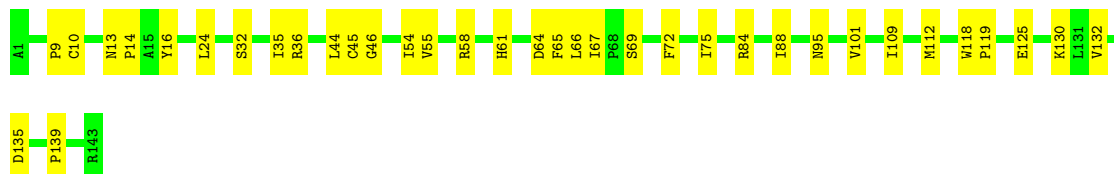
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 81% 16% .



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 75% 25% .



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 35% 45% 43% 13% .

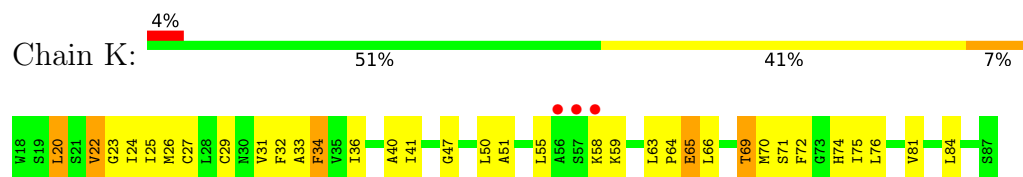


- Molecule 8: Photosystem I reaction center subunit IX

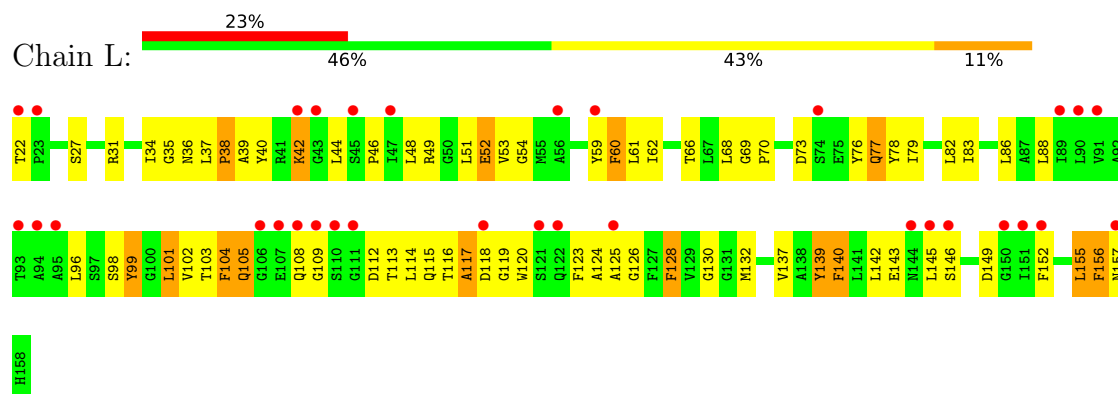
Chain J: 68% 30% .



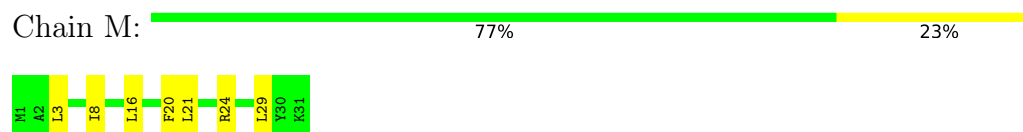
- Molecule 9: Photosystem I reaction center subunit PsaK 2



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.32Å 178.66Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 4.00 49.29 – 4.00	Depositor EDS
% Data completeness (in resolution range)	88.7 (49.29-4.00) 88.7 (49.29-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.14_3228: ???)	Depositor
R, R_{free}	0.255 , 0.295 0.256 , 0.296	Depositor DCC
R_{free} test set	584 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	23566	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, C7Z, CL, SF4, LMT, CLA, PQN, ECH, BCR, LMG, 45D, EQ3, CA, SQD

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	0.25	0/6075	0.39	0/8278
2	B	0.25	0/5994	0.40	0/8195
3	C	0.24	0/610	0.43	0/826
4	D	0.25	0/1126	0.44	0/1517
5	E	0.25	0/552	0.41	0/745
6	F	0.25	0/1143	0.40	0/1553
7	I	0.28	0/322	0.50	0/438
8	J	0.26	0/328	0.40	0/443
9	K	0.26	0/520	0.46	0/700
10	L	0.27	0/1057	0.47	0/1434
11	M	0.24	0/241	0.39	0/326
All	All	0.25	0/17968	0.41	0/24455

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5876	0	5739	157	0
2	B	5783	0	5565	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	600	0	589	18	0
4	D	1102	0	1101	17	0
5	E	543	0	525	11	0
6	F	1113	0	1110	23	0
7	I	311	0	304	19	0
8	J	319	0	328	14	0
9	K	510	0	534	27	0
10	L	1030	0	1011	60	0
11	M	238	0	260	7	0
12	A	2326	0	2027	171	0
12	B	2152	0	1801	145	0
12	F	98	0	76	3	0
12	J	98	0	76	2	0
12	K	94	0	71	0	0
12	L	49	0	38	4	0
13	A	33	0	46	2	0
13	B	33	0	46	3	0
14	A	8	0	0	1	0
14	C	16	0	0	1	0
15	A	200	0	265	21	0
15	B	200	0	264	9	0
15	F	40	0	53	9	0
15	I	40	0	52	5	0
15	J	40	0	53	9	0
15	K	40	0	53	6	0
16	A	98	0	148	5	0
16	B	70	0	83	9	0
17	B	42	0	52	5	0
18	B	1	0	0	0	0
19	B	41	0	54	4	0
19	M	41	0	54	5	0
20	B	110	0	172	7	0
21	B	54	0	77	1	0
21	F	54	0	77	3	0
22	B	1	0	0	0	0
22	L	1	0	0	0	0
23	F	42	0	0	1	0
23	J	42	0	0	0	0
24	F	35	0	45	1	0
25	I	42	0	0	1	0
All	All	23566	0	22749	666	0

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 14.

All (666) 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)
1:A:210:LEU:HD11	15:A:4001:BCR:H10C	1.42	1.01
12:B:1207:CLA:HBC3	15:I:4018:BCR:H21C	1.44	0.96
10:L:35:GLY:HA2	10:L:40:TYR:HB3	1.52	0.92
12:B:1220:CLA:HAB	12:B:1227:CLA:HMD2	1.55	0.87
12:A:1125:CLA:HED1	12:A:1133:CLA:HAB	1.58	0.86
1:A:395:TRP:CD1	12:A:1126:CLA:HAB	2.11	0.85
12:A:1118:CLA:HBB1	15:K:4001:BCR:H10C	1.61	0.83
15:B:4010:BCR:H24C	15:B:4018:BCR:H392	1.60	0.82
12:A:1132:CLA:HMA2	10:L:68:LEU:HB3	1.62	0.82
1:A:250:ALA:HA	1:A:256:PHE:HB3	1.62	0.79
1:A:1:MET:C	1:A:1:MET:CB	2.51	0.78
9:K:47:GLY:HA3	9:K:64:PRO:HG2	1.66	0.78
2:B:220:ALA:HB1	2:B:224:PRO:HG2	1.65	0.78
12:A:1138:CLA:HED2	2:B:422:TRP:HB2	1.65	0.77
2:B:556:CYS:SG	2:B:557:ASP:N	2.59	0.75
9:K:55:LEU:HD23	9:K:58:LYS:HE2	1.67	0.74
1:A:433:ARG:NH2	1:A:558:SER:O	2.21	0.74
12:B:1234:CLA:HMB2	12:B:1236:CLA:HED1	1.68	0.74
1:A:500:ASN:HB3	12:A:1115:CLA:HED2	1.70	0.73
1:A:388:SER:HB3	12:A:1126:CLA:HMA1	1.70	0.73
2:B:413:LYS:HA	2:B:416:LEU:HD12	1.72	0.72
2:B:691:LYS:HD3	7:I:37:GLU:HG3	1.72	0.71
12:B:1211:CLA:HHB	19:B:4006:ECH:H24	1.72	0.71
15:A:4012:BCR:HC7	8:J:26:LEU:HD23	1.73	0.71
2:B:687:LEU:HD22	10:L:39:ALA:HB3	1.73	0.70
1:A:357:ALA:HB1	15:A:4008:BCR:H10C	1.72	0.70
12:A:1011:CLA:HBB1	12:A:1011:CLA:HMB1	1.73	0.70
12:A:1107:CLA:CAB	12:B:1230:CLA:HMD2	2.21	0.70
12:A:1129:CLA:HMA2	10:L:22:THR:HG21	1.74	0.70
13:A:2001:PQN:H142	15:F:4014:BCR:H271	1.74	0.70
12:A:1011:CLA:HED2	12:A:1011:CLA:H2A	1.74	0.69
12:A:1013:CLA:H51	12:A:1013:CLA:HMA1	1.73	0.69
12:B:1236:CLA:HBA2	16:B:5004:LHG:H381	1.74	0.69
2:B:718:TYR:HB2	12:B:1021:CLA:HED3	1.75	0.69
12:A:1012:CLA:HED2	12:B:1021:CLA:H71	1.74	0.69
12:A:1101:CLA:HBB1	15:J:4013:BCR:H292	1.74	0.69
2:B:420:LEU:HD13	2:B:529:LEU:HA	1.75	0.69
10:L:52:GLU:HB3	12:L:1502:CLA:HED3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1125:CLA:HBB1	12:A:1125:CLA:HMB1	1.75	0.68
1:A:40:ARG:NH2	5:E:54:SER:OG	2.26	0.68
4:D:39:VAL:HG22	4:D:49:ILE:HG12	1.77	0.67
12:A:1123:CLA:HBB1	12:A:1123:CLA:HMB1	1.77	0.67
12:B:1234:CLA:HMB1	12:B:1234:CLA:HBB1	1.76	0.67
9:K:51:ALA:HA	9:K:59:LYS:HD2	1.76	0.67
9:K:55:LEU:HD11	15:K:4001:BCR:H271	1.75	0.67
12:B:1220:CLA:HBB1	16:B:5004:LHG:H111	1.76	0.67
10:L:49:ARG:NH2	10:L:112:ASP:OD2	2.28	0.67
12:A:1105:CLA:H8	15:J:4013:BCR:H19C	1.77	0.66
1:A:579:ARG:HH21	1:A:582:THR:HG21	1.60	0.66
12:A:1130:CLA:H12	10:L:34:ILE:HD11	1.77	0.66
8:J:27:ILE:HG21	15:J:4013:BCR:H10C	1.77	0.66
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.76	0.66
1:A:736:ILE:HG21	12:A:1126:CLA:HMC2	1.77	0.66
12:L:1502:CLA:HBA2	12:L:1502:CLA:HED2	1.77	0.66
12:B:1204:CLA:HMA1	12:B:1205:CLA:HMB3	1.78	0.66
12:B:1218:CLA:HMB1	12:B:1218:CLA:HBB1	1.77	0.65
1:A:574:CYS:SG	1:A:575:ASP:N	2.69	0.65
2:B:174:ARG:HE	12:B:1221:CLA:HMD1	1.61	0.65
1:A:219:VAL:HG22	1:A:239:PRO:HB3	1.78	0.65
11:M:16:LEU:HD22	19:M:4021:ECH:H8	1.79	0.65
1:A:666:SER:HB2	2:B:443:ALA:HB1	1.78	0.65
12:A:1131:CLA:HBB1	12:A:1131:CLA:HHC	1.76	0.65
2:B:460:TRP:HE1	2:B:474:VAL:HG21	1.62	0.65
2:B:654:TRP:HB2	2:B:713:GLY:HA3	1.79	0.65
2:B:587:LEU:HD12	12:B:1234:CLA:HAB	1.80	0.64
1:A:82:VAL:HG22	12:A:1109:CLA:H202	1.79	0.64
6:F:75:ILE:HG23	12:F:1301:CLA:HAA1	1.80	0.64
2:B:626:ALA:O	2:B:630:ASN:ND2	2.22	0.64
2:B:580:MET:HG3	12:B:1222:CLA:HBC1	1.80	0.64
12:B:1212:CLA:HBB1	15:B:4004:BCR:H323	1.80	0.63
2:B:276:HIS:HB2	12:B:1214:CLA:C1B	2.28	0.63
2:B:684:LEU:HA	2:B:687:LEU:HD21	1.81	0.63
3:C:15:THR:HG22	3:C:28:MET:HG3	1.80	0.63
1:A:571:ARG:HD2	1:A:721:ILE:HG21	1.81	0.63
1:A:70:ARG:HH21	1:A:186:LYS:HA	1.63	0.63
2:B:378:GLY:HA3	2:B:584:LEU:HD11	1.81	0.62
9:K:55:LEU:HD13	9:K:59:LYS:HB2	1.81	0.62
9:K:71:SER:HB2	15:K:4001:BCR:H341	1.81	0.62
2:B:5:PHE:HB2	7:I:33:HIS:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:GLN:HG3	20:B:5002:LMG:H142	1.82	0.62
1:A:500:ASN:HB2	12:A:1134:CLA:HED3	1.81	0.61
2:B:341:VAL:HG11	12:B:1223:CLA:H2	1.81	0.61
12:A:1138:CLA:H11	12:B:1229:CLA:HAA2	1.82	0.61
1:A:680:ALA:HB3	12:A:1013:CLA:HBB2	1.82	0.61
2:B:110:SER:O	7:I:1:MET:N	2.33	0.61
2:B:117:TYR:HA	2:B:365:THR:HG22	1.82	0.61
12:A:1122:CLA:H43	15:A:4007:BCR:H19C	1.83	0.61
9:K:22:VAL:HA	9:K:26:MET:HB2	1.83	0.61
12:B:1232:CLA:H41	20:B:5005:LMG:H182	1.82	0.61
2:B:385:PHE:HZ	12:B:1222:CLA:HAB	1.65	0.61
2:B:408:ARG:O	2:B:412:HIS:ND1	2.34	0.61
6:F:125:GLU:O	6:F:130:LYS:N	2.31	0.60
12:A:1101:CLA:HBA2	12:A:1101:CLA:HBD	1.83	0.60
12:A:1105:CLA:HMA1	12:A:1106:CLA:HMB3	1.83	0.60
12:B:1021:CLA:HMB3	12:B:1022:CLA:CAD	2.32	0.60
2:B:20:ARG:NH2	2:B:692:ASP:OD1	2.34	0.60
2:B:653:VAL:HG22	12:B:1239:CLA:HMB3	1.84	0.60
12:B:1216:CLA:HMB2	12:B:1221:CLA:HMA3	1.83	0.60
2:B:339:LEU:HD12	2:B:342:ILE:HD11	1.84	0.60
12:B:1223:CLA:HBB1	12:B:1231:CLA:HAA2	1.84	0.60
1:A:447:LEU:HB3	1:A:540:PHE:HB2	1.82	0.59
2:B:174:ARG:HH11	12:B:1210:CLA:HMD2	1.67	0.59
1:A:355:ASN:ND2	12:A:1103:CLA:OBD	2.35	0.59
12:A:1107:CLA:HAB	12:B:1230:CLA:HMD2	1.83	0.59
1:A:478:LEU:HB2	1:A:529:THR:HG23	1.84	0.59
2:B:375:TYR:HA	2:B:584:LEU:HD13	1.84	0.59
12:A:1132:CLA:HAA1	10:L:69:GLY:HA2	1.84	0.59
2:B:407:ALA:HB1	21:F:5001:SQD:H372	1.83	0.59
1:A:595:LEU:HD21	12:A:1128:CLA:HBC1	1.85	0.59
2:B:185:VAL:HG11	15:B:4005:BCR:H341	1.84	0.59
12:A:1134:CLA:HMB1	15:A:4008:BCR:H281	1.85	0.59
12:A:1011:CLA:HBB1	12:B:1021:CLA:HAA1	1.83	0.58
1:A:589:ASP:OD1	1:A:724:ARG:NH1	2.36	0.58
12:B:1234:CLA:H111	16:B:5004:LHG:H341	1.86	0.58
12:B:1203:CLA:H43	20:B:5002:LMG:H321	1.85	0.58
2:B:473:ASP:HB3	2:B:478:ASN:HD22	1.68	0.58
1:A:709:VAL:HG11	12:A:1138:CLA:HMB3	1.86	0.58
10:L:128:PHE:O	10:L:130:GLY:N	2.37	0.58
12:A:1128:CLA:HBB1	12:A:1128:CLA:HMB1	1.86	0.58
2:B:683:PRO:HB3	10:L:34:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:46:PRO:HG3	10:L:113:THR:HB	1.86	0.57
1:A:103:TRP:HA	1:A:110:ILE:HG21	1.85	0.57
3:C:7:ILE:HG12	3:C:40:ALA:HB3	1.86	0.57
12:A:1138:CLA:HHD	15:F:4014:BCR:H383	1.85	0.57
12:A:1138:CLA:HMB1	12:A:1138:CLA:HBB1	1.87	0.57
4:D:10:LYS:HB2	4:D:49:ILE:HB	1.84	0.57
1:A:226:LEU:HD12	1:A:236:ILE:HG23	1.86	0.57
1:A:690:ARG:HD3	2:B:563:GLY:HA3	1.87	0.57
10:L:66:THR:O	10:L:77:GLN:NE2	2.37	0.57
1:A:202:ALA:HA	1:A:305:ILE:HA	1.86	0.57
1:A:484:GLN:NE2	1:A:527:LEU:O	2.32	0.56
6:F:109:ILE:HA	6:F:112:MET:HE2	1.86	0.56
2:B:368:ALA:HB1	12:B:1224:CLA:HMA1	1.86	0.56
4:D:118:LYS:NZ	4:D:139:TYR:O	2.38	0.56
1:A:183:LYS:HD3	12:A:1108:CLA:HED3	1.87	0.56
6:F:13:ASN:ND2	6:F:46:GLY:O	2.37	0.56
1:A:738:THR:HB	12:A:1011:CLA:HED1	1.88	0.56
3:C:73:THR:H	3:C:76:SER:HG	1.52	0.56
10:L:76:TYR:HB3	10:L:79:ILE:HB	1.88	0.56
12:A:1102:CLA:H52	12:A:1109:CLA:H13	1.87	0.56
1:A:223:ILE:HG23	1:A:236:ILE:HG21	1.87	0.55
1:A:440:LEU:HB3	1:A:547:LEU:HD13	1.89	0.55
12:B:1214:CLA:HED3	12:B:1215:CLA:H12	1.87	0.55
2:B:689:ARG:HG3	10:L:103:THR:HG21	1.88	0.55
1:A:452:PHE:HE1	12:B:1022:CLA:HMA1	1.71	0.55
1:A:433:ARG:HH21	1:A:555:TYR:HA	1.72	0.55
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.88	0.55
2:B:304:ILE:HG12	12:B:1219:CLA:HED2	1.89	0.55
10:L:39:ALA:HA	10:L:49:ARG:NH2	2.22	0.55
12:A:1106:CLA:H8	15:A:4012:BCR:H372	1.88	0.55
1:A:428:ARG:HA	1:A:431:ARG:HG3	1.89	0.55
2:B:436:VAL:HG21	17:B:4011:45D:H311	1.88	0.55
4:D:121:ARG:NH1	5:E:15:GLU:OE1	2.40	0.55
12:A:1102:CLA:HBA2	12:A:1109:CLA:H51	1.88	0.55
2:B:349:HIS:HB3	12:B:1214:CLA:HED2	1.89	0.55
2:B:577:MET:HG3	2:B:707:LEU:HD21	1.88	0.55
12:A:1116:CLA:HMB1	12:A:1116:CLA:HBB1	1.89	0.54
1:A:464:LEU:HG	12:B:1206:CLA:HMC3	1.87	0.54
12:B:1218:CLA:HMD2	15:B:4004:BCR:H24C	1.89	0.54
1:A:560:ARG:HB3	3:C:80:ALA:HB3	1.89	0.54
12:B:1238:CLA:HAA2	7:I:31:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TRP:CE2	12:A:1108:CLA:HMA1	2.42	0.54
12:A:1107:CLA:HBB2	12:B:1230:CLA:CHD	2.37	0.54
1:A:254:PRO:HD2	1:A:273:ASP:HB3	1.90	0.54
12:B:1207:CLA:H43	10:L:83:ILE:HD12	1.89	0.54
12:A:1011:CLA:HAB	2:B:621:LEU:HD13	1.89	0.54
1:A:56:HIS:HB2	12:A:1128:CLA:HBA1	1.89	0.54
1:A:304:PHE:CE1	12:A:1119:CLA:HAB	2.43	0.54
12:B:1224:CLA:H3A	12:B:1224:CLA:CGA	2.37	0.54
6:F:24:LEU:O	6:F:36:ARG:NH2	2.41	0.54
12:A:1122:CLA:HMA1	12:A:1141:CLA:HAB	1.89	0.54
1:A:42:PRO:HB3	1:A:47:TRP:CE3	2.43	0.54
4:D:19:LEU:H	4:D:22:ALA:HB3	1.73	0.54
1:A:437:ILE:HG13	1:A:555:TYR:HE2	1.71	0.54
12:A:1132:CLA:H8	10:L:60:PHE:HE2	1.73	0.54
1:A:255:SER:HG	1:A:274:PHE:HD2	1.55	0.53
3:C:25:VAL:HG11	3:C:48:CYS:HB2	1.90	0.53
7:I:7:ALA:HB1	7:I:10:LEU:HD13	1.89	0.53
9:K:23:GLY:HA2	9:K:27:CYS:HB3	1.89	0.53
11:M:20:PHE:CZ	11:M:24:ARG:HD2	2.43	0.53
1:A:342:GLU:HA	1:A:345:THR:HG22	1.89	0.53
2:B:20:ARG:HH22	7:I:34:ILE:HG12	1.73	0.53
12:A:1105:CLA:H72	8:J:20:THR:HG21	1.90	0.53
1:A:263:PHE:HE1	12:A:1115:CLA:HBB1	1.74	0.53
1:A:434:ASP:OD1	1:A:555:TYR:OH	2.24	0.53
12:A:1011:CLA:CAB	12:A:1012:CLA:HED1	2.38	0.53
1:A:482:PHE:HB3	12:A:1135:CLA:H11	1.90	0.53
1:A:304:PHE:HE1	12:A:1119:CLA:HAB	1.74	0.53
12:A:1107:CLA:HBA1	12:A:1107:CLA:HBD	1.91	0.52
2:B:655:ALA:HB3	12:B:1023:CLA:HBB2	1.90	0.52
12:A:1012:CLA:HAB	2:B:579:TRP:CH2	2.44	0.52
12:A:1130:CLA:HMB1	12:B:1237:CLA:HAA2	1.90	0.52
2:B:313:THR:HG21	16:B:5004:LHG:HC11	1.91	0.52
2:B:48:ALA:HB3	11:M:29:LEU:HD21	1.89	0.52
12:A:1107:CLA:HMA1	8:J:27:ILE:HD13	1.92	0.52
1:A:263:PHE:CE1	12:A:1115:CLA:HBB1	2.44	0.52
12:A:1129:CLA:H12	16:A:5003:LHG:HC91	1.91	0.52
1:A:107:PRO:HG3	1:A:148:ARG:HH12	1.73	0.52
12:B:1235:CLA:H203	6:F:69:SER:HB2	1.91	0.52
1:A:634:ASN:O	1:A:638:SER:N	2.42	0.52
1:A:705:ASN:HD21	5:E:43:ARG:HH12	1.57	0.52
3:C:54:CYS:SG	3:C:55:GLU:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:CYS:SG	6:F:45:CYS:HB2	2.50	0.52
9:K:33:ALA:HA	9:K:36:ILE:HG12	1.91	0.52
1:A:560:ARG:NH2	4:D:15:THR:O	2.43	0.52
1:A:706:LYS:NZ	6:F:135:ASP:OD1	2.34	0.52
9:K:65:GLU:O	9:K:69:THR:HG23	2.10	0.52
1:A:583:CYS:HB2	2:B:664:TRP:HB3	1.92	0.52
3:C:72:GLU:HG2	3:C:77:MET:SD	2.50	0.52
9:K:36:ILE:O	9:K:40:ALA:HB3	2.10	0.52
12:A:1116:CLA:HBC3	12:A:1117:CLA:HBB2	1.92	0.52
1:A:369:HIS:ND1	12:A:1116:CLA:OBD	2.43	0.52
10:L:104:PHE:HD2	10:L:117:ALA:HA	1.74	0.52
1:A:190:PHE:O	1:A:192:ASN:N	2.41	0.51
12:A:1107:CLA:C2	15:A:4012:BCR:H19C	2.40	0.51
1:A:740:TRP:NE1	12:A:1126:CLA:O1A	2.43	0.51
12:B:1213:CLA:HBD	12:B:1213:CLA:HBA1	1.92	0.51
4:D:6:GLY:HA2	4:D:54:GLU:HG3	1.92	0.51
1:A:125:ILE:HG21	2:B:444:PHE:HA	1.92	0.51
2:B:375:TYR:CD2	12:B:1224:CLA:HAB	2.46	0.51
12:A:1132:CLA:HED2	12:A:1132:CLA:H2A	1.91	0.51
1:A:215:HIS:O	1:A:219:VAL:N	2.44	0.51
1:A:486:VAL:HG21	12:A:1135:CLA:H12	1.93	0.51
2:B:461:ILE:HD11	12:B:1234:CLA:H2	1.91	0.51
9:K:34:PHE:HE1	9:K:66:LEU:HA	1.75	0.51
7:I:12:TRP:O	7:I:16:PRO:HD2	2.10	0.51
1:A:319:HIS:NE2	12:A:1121:CLA:OBD	2.44	0.51
15:A:4001:BCR:H24C	9:K:72:PHE:HB2	1.92	0.51
1:A:704:HIS:NE2	12:A:1139:CLA:HAC1	2.26	0.51
2:B:490:TRP:HE1	12:B:1231:CLA:HED1	1.76	0.51
4:D:31:THR:HG22	4:D:56:LEU:HD13	1.92	0.51
2:B:5:PHE:HD1	2:B:6:PRO:HA	1.75	0.51
4:D:131:ILE:O	4:D:134:SER:OG	2.23	0.51
9:K:20:LEU:HD13	9:K:24:ILE:HD12	1.92	0.50
6:F:10:CYS:HB3	6:F:16:TYR:CE2	2.46	0.50
2:B:570:TRP:CD1	12:B:1226:CLA:HMD1	2.46	0.50
9:K:34:PHE:CZ	9:K:58:LYS:HA	2.47	0.50
2:B:371:THR:HG23	2:B:588:THR:HG21	1.92	0.50
12:A:1107:CLA:H12	15:A:4012:BCR:H17C	1.92	0.50
2:B:356:TYR:CE2	12:B:1225:CLA:HED2	2.46	0.50
12:A:1012:CLA:HMB3	12:B:1021:CLA:H18	1.93	0.50
6:F:67:ILE:HD12	8:J:39:HIS:CG	2.47	0.50
10:L:137:VAL:HA	10:L:140:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1102:CLA:HBD	12:A:1109:CLA:H2	1.93	0.50
1:A:733:LEU:HD22	12:A:1140:CLA:HMA1	1.93	0.50
1:A:597:TRP:CH2	12:B:1022:CLA:HAB	2.47	0.50
12:A:1140:CLA:H161	8:J:23:ALA:HB2	1.93	0.50
6:F:55:VAL:HG12	6:F:65:PHE:HB2	1.94	0.50
24:F:6001:LMT:H42	8:J:9:SER:HB3	1.94	0.49
1:A:168:MET:O	1:A:172:MET:HG2	2.12	0.49
1:A:211:GLY:C	12:A:1112:CLA:HAB	2.32	0.49
5:E:13:ARG:O	5:E:15:GLU:N	2.44	0.49
5:E:20:GLY:HA3	6:F:139:PRO:HA	1.95	0.49
12:A:1012:CLA:HMA2	2:B:613:LEU:HD13	1.93	0.49
12:B:1216:CLA:HBA1	12:B:1221:CLA:C3B	2.41	0.49
16:B:5004:LHG:H121	16:B:5004:LHG:H271	1.93	0.49
10:L:109:GLY:H	10:L:116:THR:HG22	1.77	0.49
1:A:154:ASP:OD1	1:A:155:SER:N	2.45	0.49
1:A:607:PHE:HB3	1:A:645:TRP:HZ3	1.77	0.49
10:L:113:THR:O	10:L:116:THR:OG1	2.30	0.49
1:A:54:ASN:OD1	1:A:571:ARG:NH2	2.45	0.49
3:C:17:CYS:HB2	3:C:54:CYS:HB2	1.94	0.49
10:L:98:SER:O	10:L:102:VAL:HG13	2.12	0.49
12:A:1138:CLA:HAB	12:A:1138:CLA:H111	1.93	0.49
1:A:33:HIS:HE2	12:A:1109:CLA:CGA	2.26	0.49
2:B:324:ILE:HD12	12:B:1221:CLA:HMC2	1.94	0.49
1:A:296:HIS:HB2	12:A:1116:CLA:C1B	2.43	0.49
15:I:4018:BCR:H24C	25:I:4020:EQ3:C19	2.43	0.49
2:B:385:PHE:CZ	12:B:1222:CLA:HAB	2.47	0.49
10:L:104:PHE:CD2	10:L:117:ALA:HA	2.48	0.49
1:A:177:TRP:HB2	12:A:1109:CLA:HMC3	1.94	0.49
10:L:116:THR:OG1	10:L:119:GLY:HA3	2.13	0.49
12:A:1140:CLA:H61	12:A:1140:CLA:H41	1.57	0.49
1:A:513:THR:HG23	1:A:523:MET:HB3	1.95	0.49
2:B:659:MET:HB2	12:B:1023:CLA:C1C	2.42	0.49
6:F:118:TRP:CG	6:F:119:PRO:HD3	2.47	0.49
1:A:245:GLU:HG3	1:A:248:LYS:HE2	1.95	0.48
2:B:426:PHE:O	2:B:430:HIS:ND1	2.41	0.48
2:B:504:SER:HA	2:B:507:LEU:HD21	1.95	0.48
1:A:189:TRP:CD1	12:A:1110:CLA:HED2	2.48	0.48
17:B:4011:45D:H092	15:F:4014:BCR:H14C	1.96	0.48
12:A:1124:CLA:HAB	15:A:4008:BCR:H311	1.94	0.48
1:A:538:HIS:HE1	1:A:604:ILE:HG22	1.78	0.48
9:K:34:PHE:HE2	9:K:58:LYS:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1140:CLA:H101	15:J:4013:BCR:H362	1.95	0.48
1:A:674:ALA:HB1	17:B:4011:45D:C42	2.44	0.48
2:B:177:HIS:CG	12:B:1210:CLA:HMC2	2.48	0.48
2:B:413:LYS:HB2	2:B:536:LEU:HD13	1.95	0.48
12:A:1112:CLA:HBA2	12:A:1112:CLA:H3A	1.54	0.48
1:A:348:TRP:HB3	12:A:1103:CLA:HAC1	1.95	0.48
10:L:124:ALA:O	10:L:126:GLY:N	2.46	0.48
12:A:1132:CLA:H61	12:A:1132:CLA:H41	1.47	0.48
2:B:456:VAL:H	12:B:1235:CLA:HMD1	1.78	0.48
2:B:99:GLY:HA3	2:B:637:VAL:HB	1.95	0.48
1:A:538:HIS:CD2	12:A:1135:CLA:HAB	2.49	0.48
1:A:531:ASP:O	1:A:535:HIS:ND1	2.38	0.48
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.95	0.48
2:B:210:ASP:OD1	2:B:210:ASP:N	2.46	0.48
2:B:711:THR:HB	20:B:5002:LMG:H411	1.95	0.48
10:L:38:PRO:HB3	10:L:44:LEU:HD22	1.95	0.48
12:A:1132:CLA:HBD	10:L:70:PRO:HD3	1.95	0.48
2:B:167:TRP:CZ2	12:B:1208:CLA:HMA1	2.48	0.48
12:A:1109:CLA:H72	12:A:1109:CLA:H112	1.74	0.48
2:B:679:HIS:CD2	2:B:690:TRP:HZ3	2.32	0.48
9:K:31:VAL:HA	9:K:34:PHE:HB2	1.96	0.48
1:A:299:ALA:HA	12:A:1115:CLA:HMC3	1.95	0.47
12:A:1119:CLA:HMB2	12:A:1123:CLA:HMA3	1.95	0.47
1:A:573:PRO:HG3	1:A:721:ILE:HG12	1.96	0.47
2:B:147:SER:HB3	11:M:21:LEU:HD12	1.97	0.47
2:B:190:TRP:HD1	2:B:277:HIS:CD2	2.31	0.47
1:A:576:GLY:HA2	2:B:559:PRO:HD3	1.96	0.47
12:A:1132:CLA:H8	10:L:60:PHE:CE2	2.49	0.47
1:A:255:SER:HB2	1:A:271:TYR:HA	1.96	0.47
13:B:2002:PQN:H142	15:B:4017:BCR:H271	1.96	0.47
15:J:4013:BCR:H15C	15:J:4013:BCR:H351	1.68	0.47
3:C:61:ASP:OD2	5:E:16:SER:OG	2.20	0.47
15:A:4001:BCR:H391	9:K:41:ILE:HG12	1.96	0.47
12:B:1235:CLA:H62	12:B:1235:CLA:H41	1.47	0.47
2:B:182:LEU:HD13	12:B:1210:CLA:HHB	1.95	0.47
6:F:58:ARG:HD2	6:F:61:HIS:HD1	1.80	0.47
15:K:4001:BCR:H351	15:K:4001:BCR:H15C	1.64	0.47
2:B:90:ALA:HA	2:B:113:VAL:HG23	1.97	0.47
12:B:1205:CLA:CAD	12:B:1224:CLA:HBA1	2.45	0.47
12:B:1234:CLA:H12	12:B:1235:CLA:CGA	2.45	0.47
2:B:322:ASP:O	2:B:326:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1122:CLA:HMA1	12:A:1141:CLA:CAB	2.44	0.47
1:A:574:CYS:SG	1:A:576:GLY:N	2.80	0.47
2:B:586:TRP:CE2	12:B:1021:CLA:H152	2.50	0.47
2:B:371:THR:HG22	12:B:1224:CLA:CAB	2.45	0.47
12:B:1202:CLA:H61	12:B:1202:CLA:H2	1.73	0.47
9:K:59:LYS:HZ3	9:K:63:LEU:HB2	1.80	0.47
1:A:577:PRO:HD3	2:B:558:GLY:HA2	1.96	0.47
12:B:1207:CLA:O1D	12:B:1207:CLA:H2	2.15	0.47
10:L:73:ASP:N	10:L:73:ASP:OD1	2.47	0.47
15:A:4001:BCR:H351	15:A:4001:BCR:H15C	1.56	0.46
12:B:1201:CLA:HMA2	11:M:29:LEU:HB3	1.97	0.46
12:B:1204:CLA:H12	7:I:14:LEU:HG	1.96	0.46
12:A:1112:CLA:NC	12:A:1114:CLA:HAB	2.29	0.46
12:B:1211:CLA:CHB	19:B:4006:ECH:H24	2.43	0.46
1:A:668:TYR:O	1:A:741:ALA:HB1	2.16	0.46
12:B:1239:CLA:HBA2	12:B:1239:CLA:H3A	1.82	0.46
2:B:167:TRP:CZ2	12:B:1210:CLA:HAC2	2.50	0.46
2:B:289:HIS:CE1	15:B:4004:BCR:H363	2.51	0.46
1:A:683:LEU:HB2	12:A:1013:CLA:HMC3	1.98	0.46
12:B:1203:CLA:HAB	12:B:1225:CLA:HBB1	1.97	0.46
12:B:1235:CLA:H162	12:B:1235:CLA:H141	1.80	0.46
2:B:232:VAL:O	2:B:235:ALA:HB2	2.16	0.46
2:B:203:ARG:NH2	2:B:253:ALA:O	2.47	0.46
2:B:676:VAL:HG13	2:B:690:TRP:CZ2	2.51	0.46
7:I:1:MET:O	7:I:3:GLY:N	2.48	0.46
1:A:320:SER:HB3	1:A:323:GLU:HG3	1.98	0.46
12:A:1103:CLA:H41	15:A:4003:BCR:H292	1.98	0.46
12:A:1109:CLA:H202	12:A:1109:CLA:H161	1.73	0.46
1:A:344:LEU:HB2	12:A:1123:CLA:HBC3	1.98	0.46
2:B:305:LEU:HD11	12:B:1221:CLA:HMC1	1.97	0.46
12:A:1011:CLA:HMB3	12:A:1012:CLA:OBD	2.15	0.46
12:A:1111:CLA:H3A	12:A:1111:CLA:HBA1	1.47	0.46
12:B:1211:CLA:HBB1	12:B:1211:CLA:HMB1	1.97	0.46
6:F:13:ASN:HB3	6:F:16:TYR:HB3	1.98	0.46
12:F:1301:CLA:C3B	15:F:4014:BCR:H10C	2.46	0.46
7:I:9:TYR:HD2	7:I:9:TYR:H	1.64	0.46
12:A:1013:CLA:HBB1	12:A:1013:CLA:HMB1	1.98	0.46
1:A:59:ASP:OD2	1:A:414:ARG:NH1	2.46	0.46
4:D:87:ARG:HH21	4:D:97:LEU:HD11	1.80	0.46
12:A:1109:CLA:H41	12:A:1109:CLA:H62	1.38	0.46
1:A:538:HIS:CE1	1:A:604:ILE:HG22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLY:O	1:A:98:SER:OG	2.34	0.45
2:B:372:HIS:HB2	12:B:1224:CLA:C1B	2.46	0.45
2:B:440:VAL:HG21	12:B:1230:CLA:HAC2	1.98	0.45
12:B:1214:CLA:H101	12:B:1232:CLA:HMA2	1.96	0.45
19:M:4021:ECH:H37	19:M:4021:ECH:H24	1.51	0.45
12:A:1106:CLA:H143	16:A:5001:LHG:H223	1.98	0.45
1:A:597:TRP:HE1	12:B:1023:CLA:C1D	2.29	0.45
10:L:139:TYR:HE1	10:L:142:LEU:HD12	1.80	0.45
10:L:96:LEU:HG	10:L:120:TRP:HE1	1.82	0.45
12:A:1102:CLA:H2A	12:A:1102:CLA:HED2	1.99	0.45
12:A:1138:CLA:H43	12:B:1229:CLA:HAA2	1.99	0.45
1:A:435:ALA:O	1:A:439:HIS:ND1	2.32	0.45
1:A:689:GLY:HA3	2:B:565:CYS:HB2	1.98	0.45
12:B:1214:CLA:H102	12:B:1214:CLA:H61	1.37	0.45
7:I:10:LEU:N	7:I:11:PRO:HD2	2.31	0.45
8:J:31:ARG:HD3	15:J:4013:BCR:H312	1.98	0.45
10:L:99:TYR:O	10:L:102:VAL:HG22	2.16	0.45
3:C:13:GLY:HA3	3:C:38:GLN:HG3	1.99	0.45
6:F:64:ASP:HA	8:J:38:PHE:HB2	1.98	0.45
12:A:1102:CLA:HMA2	12:A:1109:CLA:HMD2	1.99	0.45
15:A:4008:BCR:H351	15:A:4008:BCR:H15C	1.68	0.45
12:B:1202:CLA:H101	12:B:1210:CLA:HBA1	1.99	0.45
2:B:279:ALA:HA	12:B:1213:CLA:HMC3	1.98	0.45
2:B:51:PHE:HE1	12:B:1208:CLA:HBB1	1.80	0.45
1:A:406:ALA:O	1:A:410:ILE:HG13	2.16	0.45
1:A:48:ILE:O	1:A:51:LEU:HB3	2.17	0.45
10:L:155:LEU:HD12	10:L:156:PHE:H	1.80	0.45
10:L:44:LEU:HD21	10:L:48:LEU:O	2.17	0.45
12:B:1228:CLA:H3A	12:B:1228:CLA:HBA2	1.50	0.45
2:B:497:ALA:O	2:B:503:ASN:ND2	2.41	0.45
6:F:9:PRO:HA	6:F:44:LEU:HA	1.99	0.45
19:M:4021:ECH:H20	19:M:4021:ECH:H36	1.57	0.45
1:A:358:LEU:HD21	12:A:1123:CLA:HMB2	1.99	0.45
19:B:4006:ECH:H36	19:B:4006:ECH:H20	1.53	0.45
2:B:56:ILE:HD11	19:M:4021:ECH:H39B	1.99	0.45
7:I:15:ILE:HB	7:I:16:PRO:HD2	1.99	0.45
1:A:202:ALA:HB2	1:A:308:GLY:HA3	1.99	0.45
1:A:332:PHE:HB2	16:A:5003:LHG:HC41	1.97	0.45
2:B:422:TRP:CZ2	12:B:1228:CLA:HAB	2.51	0.45
12:B:1222:CLA:HMB2	12:B:1236:CLA:HBA1	1.99	0.45
12:B:1237:CLA:HMC3	12:B:1238:CLA:ND	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:5002:LMG:H331	20:B:5002:LMG:H302	1.65	0.45
12:B:1209:CLA:HMD2	21:B:5008:SQD:H212	1.99	0.45
1:A:680:ALA:C	12:A:1013:CLA:HAB	2.37	0.45
1:A:315:TRP:HB3	9:K:64:PRO:HB3	1.99	0.45
1:A:609:PHE:O	1:A:613:MET:HG2	2.17	0.45
2:B:180:ALA:HA	2:B:285:ILE:HA	1.99	0.45
10:L:49:ARG:HB3	10:L:123:PHE:HA	1.98	0.45
15:A:4012:BCR:H15C	15:A:4012:BCR:H351	1.83	0.44
2:B:256:THR:OG1	2:B:271:THR:OG1	2.20	0.44
2:B:372:HIS:O	2:B:376:ILE:HG12	2.16	0.44
12:A:1012:CLA:HED2	12:B:1021:CLA:H52	2.00	0.44
12:A:1102:CLA:HMC3	12:A:1104:CLA:HED2	1.98	0.44
2:B:385:PHE:CG	2:B:531:LEU:HB3	2.53	0.44
7:I:18:VAL:HG21	15:I:4018:BCR:HC41	2.00	0.44
12:J:1302:CLA:HED2	12:J:1302:CLA:H2A	1.99	0.44
10:L:101:LEU:HD22	10:L:101:LEU:HA	1.85	0.44
12:A:1126:CLA:H3A	12:A:1126:CLA:HBA2	1.54	0.44
2:B:279:ALA:O	2:B:283:ILE:HG13	2.17	0.44
12:B:1204:CLA:HBA2	12:B:1204:CLA:H3A	1.61	0.44
2:B:474:VAL:HG12	2:B:475:LEU:HG	1.99	0.44
2:B:523:GLY:HA2	2:B:579:TRP:HZ3	1.82	0.44
2:B:649:PHE:O	2:B:653:VAL:HG23	2.17	0.44
4:D:8:PRO:O	4:D:51:ASN:ND2	2.46	0.44
12:A:1105:CLA:H161	12:A:1105:CLA:H141	1.71	0.44
12:A:1117:CLA:HBB1	12:A:1117:CLA:HMB1	2.00	0.44
12:A:1106:CLA:H93	12:A:1128:CLA:H203	1.98	0.44
12:A:1129:CLA:HAB	12:A:1137:CLA:CBB	2.47	0.44
1:A:199:HIS:CG	12:A:1111:CLA:HMC2	2.53	0.44
12:A:1107:CLA:H2	15:A:4012:BCR:H19C	1.99	0.44
1:A:680:ALA:O	12:A:1013:CLA:HAB	2.17	0.44
12:B:1238:CLA:CGD	10:L:99:TYR:CD1	3.00	0.44
1:A:588:TRP:NE1	12:A:1128:CLA:HMD1	2.33	0.44
12:B:1021:CLA:HMB3	12:B:1022:CLA:OBD	2.17	0.44
12:B:1206:CLA:H43	15:I:4018:BCR:C11	2.46	0.44
12:B:1222:CLA:C2B	15:B:4010:BCR:H363	2.48	0.44
12:A:1126:CLA:C4C	17:B:4011:45D:H061	2.48	0.44
9:K:22:VAL:O	9:K:27:CYS:N	2.25	0.44
1:A:13:LYS:HE2	1:A:314:ASN:OD1	2.17	0.44
1:A:303:LEU:HD22	12:A:1119:CLA:HMC1	1.98	0.44
2:B:310:GLY:HA3	16:B:5004:LHG:HC32	2.00	0.44
3:C:54:CYS:N	14:C:3002:SF4:S4	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:1301:CLA:C2B	15:F:4014:BCR:H10C	2.47	0.44
10:L:78:TYR:HB2	10:L:143:GLU:HG2	2.00	0.44
12:A:1102:CLA:H192	15:A:4012:BCR:H383	2.00	0.44
2:B:675:ILE:HD13	12:B:1237:CLA:HMD3	1.99	0.44
2:B:618:ARG:NE	2:B:619:ASP:OD1	2.50	0.44
1:A:651:TRP:HD1	12:B:1021:CLA:HAC2	1.83	0.44
2:B:655:ALA:O	12:B:1023:CLA:HAB	2.18	0.44
12:B:1204:CLA:HMB3	12:B:1205:CLA:HMA1	2.00	0.44
12:B:1227:CLA:HAA2	21:F:5001:SQD:O7	2.17	0.44
1:A:352:LEU:HD13	12:A:1103:CLA:C2D	2.48	0.43
12:A:1111:CLA:HMA2	12:A:1111:CLA:H2	2.00	0.43
12:A:1126:CLA:H62	12:A:1126:CLA:H92	1.79	0.43
12:B:1222:CLA:H43	12:B:1235:CLA:HBA1	2.00	0.43
2:B:676:VAL:HG13	2:B:690:TRP:HZ2	1.82	0.43
3:C:58:CYS:O	5:E:47:ASN:ND2	2.51	0.43
8:J:31:ARG:HD3	15:J:4013:BCR:C31	2.48	0.43
9:K:75:ILE:HD13	15:K:4001:BCR:H321	2.00	0.43
10:L:61:LEU:HD13	10:L:88:LEU:HD23	1.99	0.43
12:A:1106:CLA:HBA2	12:A:1106:CLA:H3A	1.31	0.43
1:A:395:TRP:NE1	12:A:1126:CLA:HAB	2.32	0.43
1:A:85:VAL:HG21	12:A:1109:CLA:H191	2.01	0.43
12:B:1207:CLA:HMC1	12:B:1207:CLA:HBC2	2.00	0.43
13:B:2002:PQN:H141	12:B:1238:CLA:HBB2	1.99	0.43
2:B:167:TRP:CE2	12:B:1208:CLA:HMA1	2.53	0.43
2:B:621:LEU:O	2:B:625:SER:OG	2.27	0.43
7:I:13:ILE:O	7:I:17:MET:HB2	2.17	0.43
9:K:70:MET:O	9:K:74:HIS:ND1	2.51	0.43
11:M:3:LEU:HD23	11:M:8:ILE:HD11	2.01	0.43
13:A:2001:PQN:H201	12:A:1101:CLA:H12	2.00	0.43
12:A:1116:CLA:H3A	12:A:1116:CLA:HBA2	1.47	0.43
12:A:1118:CLA:HBA2	12:A:1118:CLA:H3A	1.62	0.43
2:B:314:GLY:HA3	2:B:408:ARG:HH11	1.83	0.43
2:B:616:TRP:HB3	12:B:1021:CLA:H101	1.99	0.43
1:A:42:PRO:HG3	6:F:101:VAL:HG21	1.99	0.43
7:I:36:SER:O	10:L:105:GLN:NE2	2.52	0.43
1:A:263:PHE:HZ	15:A:4001:BCR:H343	1.83	0.43
2:B:167:TRP:CE2	12:B:1210:CLA:HAC2	2.53	0.43
12:B:1222:CLA:O1A	12:B:1234:CLA:HHB	2.18	0.43
2:B:690:TRP:HA	12:B:1238:CLA:O1D	2.18	0.43
3:C:66:ARG:HB3	3:C:68:TYR:CE2	2.54	0.43
6:F:32:SER:HA	6:F:35:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:10:LEU:H	7:I:11:PRO:HD2	1.83	0.43
10:L:39:ALA:HB2	10:L:114:LEU:HD23	2.00	0.43
12:A:1138:CLA:HMC3	12:A:1139:CLA:C4D	2.49	0.43
1:A:500:ASN:ND2	12:A:1115:CLA:OBD	2.43	0.43
1:A:375:PRO:HB3	12:A:1117:CLA:HMA2	2.00	0.43
12:A:1134:CLA:CHA	12:A:1134:CLA:HBA1	2.48	0.43
1:A:118:TRP:CE3	15:J:4013:BCR:H323	2.53	0.43
12:A:1102:CLA:H193	12:A:1106:CLA:H152	1.99	0.43
12:B:1205:CLA:H3A	12:B:1205:CLA:HBA2	1.74	0.43
12:B:1207:CLA:HBD	12:B:1207:CLA:HBA2	2.00	0.43
12:B:1222:CLA:HMA2	12:B:1223:CLA:HED2	2.00	0.43
5:E:14:THR:OG1	5:E:15:GLU:N	2.52	0.43
12:A:1106:CLA:HBB2	12:A:1126:CLA:H142	2.01	0.43
12:B:1021:CLA:H61	12:B:1021:CLA:H41	1.42	0.43
2:B:375:TYR:HB3	12:B:1224:CLA:HMC3	2.01	0.43
4:D:106:GLU:OE1	4:D:106:GLU:N	2.47	0.43
1:A:268:TRP:HZ2	15:K:4001:BCR:HC31	1.84	0.43
10:L:120:TRP:HZ2	12:L:1502:CLA:HBC1	1.83	0.43
10:L:27:SER:O	10:L:31:ARG:HB2	2.19	0.43
12:A:1128:CLA:H41	12:A:1128:CLA:H61	1.61	0.43
1:A:307:ALA:HB2	12:A:1119:CLA:HBC2	2.01	0.43
1:A:640:ILE:HG12	1:A:640:ILE:H	1.71	0.43
12:B:1225:CLA:H3A	12:B:1225:CLA:HBA2	1.42	0.43
15:F:4014:BCR:H15C	15:F:4014:BCR:H351	1.80	0.43
10:L:82:LEU:O	10:L:86:LEU:HG	2.19	0.43
12:A:1112:CLA:C1A	12:A:1114:CLA:HMB3	2.49	0.43
12:A:1124:CLA:HAA2	12:A:1125:CLA:OBD	2.19	0.43
12:A:1121:CLA:HMB3	12:A:1141:CLA:C2C	2.49	0.43
1:A:261:THR:N	1:A:262:PRO:HD2	2.34	0.43
1:A:571:ARG:NH1	12:A:1128:CLA:OBD	2.49	0.43
13:B:2002:PQN:H262	13:B:2002:PQN:H302	1.75	0.43
1:A:462:ARG:NH2	2:B:634:PRO:HG3	2.33	0.43
12:A:1103:CLA:H3A	12:A:1103:CLA:HBA1	1.52	0.42
12:A:1115:CLA:H51	12:A:1115:CLA:H11	1.76	0.42
12:A:1138:CLA:H203	12:A:1139:CLA:H51	2.01	0.42
1:A:549:LEU:HD21	1:A:594:GLY:HA3	2.00	0.42
1:A:597:TRP:HE1	12:B:1023:CLA:CHD	2.32	0.42
12:B:1202:CLA:HBD	12:B:1202:CLA:H122	2.00	0.42
19:B:4006:ECH:H8	19:B:4006:ECH:H11	1.63	0.42
2:B:461:ILE:O	2:B:464:THR:OG1	2.24	0.42
15:B:4018:BCR:HC31	20:B:5005:LMG:H222	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:GLY:HA2	2:B:579:TRP:CZ3	2.54	0.42
1:A:240:HIS:NE2	12:A:1114:CLA:O1D	2.48	0.42
12:B:1222:CLA:H3A	12:B:1222:CLA:HBA2	1.59	0.42
12:A:1013:CLA:HBA1	2:B:425:LEU:HD12	2.01	0.42
2:B:428:GLY:HA2	2:B:522:LEU:HD22	2.01	0.42
3:C:29:VAL:HG12	4:D:112:ARG:HB2	2.01	0.42
9:K:25:ILE:HG21	9:K:81:VAL:HG23	2.02	0.42
10:L:139:TYR:CE1	10:L:142:LEU:HD12	2.53	0.42
10:L:86:LEU:HD22	10:L:132:MET:SD	2.60	0.42
12:A:1011:CLA:HAA1	12:B:1021:CLA:HMB1	2.00	0.42
15:B:4010:BCR:H341	16:B:5004:LHG:H223	2.00	0.42
3:C:25:VAL:HG13	3:C:44:ARG:O	2.19	0.42
4:D:88:VAL:HG22	4:D:94:VAL:HG22	2.00	0.42
8:J:12:PRO:HA	8:J:15:ILE:HG22	2.01	0.42
10:L:82:LEU:HB2	10:L:139:TYR:HD2	1.84	0.42
10:L:99:TYR:CD1	10:L:99:TYR:C	2.92	0.42
12:B:1229:CLA:CBB	15:F:4014:BCR:HC21	2.49	0.42
2:B:361:GLN:N	2:B:361:GLN:OE1	2.52	0.42
12:B:1236:CLA:C3D	16:B:5004:LHG:H372	2.50	0.42
2:B:661:LEU:HG	2:B:706:GLY:HA3	2.01	0.42
6:F:125:GLU:HB3	6:F:130:LYS:HB3	2.02	0.42
10:L:109:GLY:N	10:L:116:THR:HG22	2.34	0.42
12:A:1111:CLA:HMA2	12:A:1111:CLA:C2	2.50	0.42
12:A:1119:CLA:HMA2	12:A:1123:CLA:C1C	2.50	0.42
12:A:1139:CLA:H61	12:A:1139:CLA:H41	1.37	0.42
1:A:482:PHE:O	1:A:486:VAL:HG23	2.20	0.42
12:B:1235:CLA:H152	23:F:4016:C7Z:C28	2.50	0.42
2:B:276:HIS:CE1	2:B:280:ILE:HD13	2.54	0.42
1:A:86:TRP:HE1	12:A:1106:CLA:HBA1	1.84	0.42
2:B:422:TRP:CD1	12:B:1229:CLA:HED2	2.55	0.42
20:B:5005:LMG:H331	20:B:5005:LMG:H302	1.85	0.42
2:B:628:LEU:HD12	2:B:721:PHE:HD1	1.85	0.42
12:A:1013:CLA:CGA	12:A:1013:CLA:H3A	2.49	0.42
1:A:583:CYS:HB3	14:A:3001:SF4:S4	2.60	0.42
1:A:344:LEU:HB3	1:A:351:GLN:NE2	2.35	0.42
2:B:152:ALA:HB2	12:B:1208:CLA:HBC2	2.02	0.42
12:A:1125:CLA:HMB3	12:A:1133:CLA:H2	2.02	0.42
12:B:1224:CLA:O1D	12:B:1225:CLA:HMA1	2.19	0.42
2:B:461:ILE:HG12	12:B:1231:CLA:HMC3	2.02	0.42
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.55	0.42
1:A:15:SER:HB2	1:A:186:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1012:CLA:HMA1	12:B:1021:CLA:H202	2.02	0.41
12:B:1220:CLA:HAB	12:B:1227:CLA:CMD	2.38	0.41
12:B:1234:CLA:H91	12:B:1234:CLA:H111	1.85	0.41
2:B:460:TRP:O	2:B:464:THR:HG23	2.20	0.41
2:B:679:HIS:NE2	2:B:685:ALA:O	2.53	0.41
7:I:35:GLU:HB2	10:L:102:VAL:HG12	2.02	0.41
10:L:112:ASP:HB3	10:L:115:GLN:HG2	2.02	0.41
12:B:1203:CLA:H3A	12:B:1203:CLA:HBA1	1.80	0.41
2:B:2:ALA:HA	2:B:14:GLN:HA	2.03	0.41
2:B:431:THR:HG22	12:B:1021:CLA:H192	2.01	0.41
9:K:34:PHE:HD1	9:K:34:PHE:HA	1.78	0.41
10:L:139:TYR:HD1	10:L:139:TYR:HA	1.68	0.41
12:B:1229:CLA:HBA2	12:B:1229:CLA:H3A	1.47	0.41
2:B:320:LEU:HD23	2:B:320:LEU:HA	1.87	0.41
21:F:5001:SQD:H182	21:F:5001:SQD:H152	1.88	0.41
15:I:4018:BCR:H351	15:I:4018:BCR:H15C	1.67	0.41
9:K:29:CYS:HB3	9:K:76:LEU:HB2	2.01	0.41
10:L:155:LEU:C	10:L:157:ASN:H	2.23	0.41
12:A:1126:CLA:H62	12:A:1126:CLA:H41	1.79	0.41
1:A:215:HIS:HB2	12:A:1112:CLA:CHC	2.51	0.41
1:A:576:GLY:O	1:A:582:THR:OG1	2.31	0.41
2:B:654:TRP:CD2	12:B:1021:CLA:HMA2	2.55	0.41
12:B:1202:CLA:H42	12:B:1203:CLA:HBB2	2.02	0.41
3:C:5:VAL:HG11	3:C:26:LEU:HD21	2.01	0.41
5:E:17:TYR:CE2	5:E:45:ASN:HA	2.55	0.41
12:A:1107:CLA:HBB1	15:A:4012:BCR:HC8	2.02	0.41
1:A:354:ILE:HD11	15:A:4007:BCR:HC7	2.01	0.41
10:L:114:LEU:HD11	10:L:123:PHE:CD2	2.56	0.41
1:A:33:HIS:NE2	12:A:1109:CLA:O1A	2.39	0.41
12:A:1116:CLA:O1D	12:A:1117:CLA:HHB	2.20	0.41
1:A:194:GLU:HB3	1:A:311:TYR:HB3	2.03	0.41
2:B:376:ILE:O	2:B:380:LEU:HG	2.20	0.41
8:J:20:THR:HG23	15:J:4013:BCR:H351	2.02	0.41
10:L:52:GLU:O	10:L:54:GLY:N	2.54	0.41
1:A:356:LEU:HD21	12:A:1128:CLA:HAB	2.02	0.41
2:B:405:VAL:O	2:B:409:MET:HG2	2.21	0.41
8:J:30:ASN:O	8:J:34:PRO:HB3	2.20	0.41
2:B:220:ALA:CB	2:B:224:PRO:HG2	2.44	0.41
2:B:429:PHE:HZ	15:F:4014:BCR:H372	1.86	0.41
1:A:736:ILE:HD13	12:A:1126:CLA:HMC2	2.03	0.41
12:A:1133:CLA:HMD2	12:A:1134:CLA:CAB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:5001:LHG:H151	16:A:5001:LHG:H182	1.86	0.41
1:A:615:SER:CB	1:A:635:PHE:HB2	2.51	0.41
12:B:1202:CLA:H61	12:B:1202:CLA:H102	1.76	0.41
12:B:1205:CLA:O1A	12:B:1224:CLA:HBD	2.21	0.41
2:B:315:ALA:HB3	2:B:404:ASN:HA	2.02	0.41
2:B:556:CYS:HB2	2:B:564:THR:O	2.21	0.41
10:L:49:ARG:HH21	10:L:114:LEU:H	1.69	0.41
1:A:288:LEU:HD12	1:A:375:PRO:HB3	2.03	0.41
2:B:346:VAL:O	2:B:350:MET:HG3	2.21	0.41
2:B:697:LEU:HD22	2:B:701:GLN:NE2	2.36	0.41
1:A:483:ALA:HA	12:A:1135:CLA:HBA1	2.03	0.41
1:A:487:GLN:HA	1:A:509:PHE:HB3	2.03	0.41
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.92	0.41
12:B:1204:CLA:HED2	7:I:11:PRO:HB3	2.03	0.41
1:A:674:ALA:HA	17:B:4011:45D:H371	2.03	0.41
2:B:88:ALA:HB2	2:B:116:ALA:HA	2.02	0.41
10:L:62:ILE:O	10:L:66:THR:OG1	2.30	0.41
1:A:337:HIS:CE1	16:A:5003:LHG:HC12	2.56	0.40
1:A:395:TRP:HB3	12:A:1126:CLA:HMC3	2.02	0.40
1:A:439:HIS:O	1:A:443:VAL:HG23	2.19	0.40
12:B:1226:CLA:HMB1	12:B:1226:CLA:HBB1	2.03	0.40
2:B:305:LEU:HD12	2:B:321:TYR:HB2	2.02	0.40
1:A:340:LEU:HD21	12:A:1122:CLA:HBC3	2.02	0.40
12:A:1126:CLA:O1D	12:A:1127:CLA:HMA1	2.21	0.40
2:B:374:GLN:NE2	2:B:587:LEU:HD11	2.36	0.40
2:B:691:LYS:HZ1	7:I:37:GLU:HA	1.87	0.40
8:J:28:GLU:HG3	12:J:1302:CLA:C1C	2.51	0.40
10:L:37:LEU:HD13	12:L:1502:CLA:O1D	2.22	0.40
12:B:1215:CLA:HBA2	12:B:1215:CLA:H3A	1.61	0.40
12:B:1226:CLA:H2A	12:B:1226:CLA:HED2	2.03	0.40
2:B:181:GLY:HA3	12:B:1210:CLA:HBB1	2.03	0.40
12:B:1222:CLA:H42	16:B:5004:LHG:H362	2.03	0.40
5:E:13:ARG:HB3	5:E:16:SER:HB2	2.03	0.40
10:L:49:ARG:HA	10:L:49:ARG:HD2	1.70	0.40
1:A:704:HIS:CD2	12:A:1139:CLA:HAC1	2.56	0.40
2:B:460:TRP:CZ2	2:B:474:VAL:HG11	2.56	0.40
12:A:1130:CLA:H2	2:B:683:PRO:HG2	2.04	0.40
3:C:23:LEU:HA	4:D:66:LEU:HD13	2.03	0.40
6:F:84:ARG:O	6:F:88:ILE:HG12	2.22	0.40
10:L:36:ASN:OD1	10:L:42:LYS:NZ	2.31	0.40
1:A:360:GLY:HA2	1:A:397:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ILE:HG23	15:A:4008:BCR:H343	2.03	0.40
1:A:657:VAL:HG12	1:A:669:GLY:HA2	2.03	0.40
12:B:1211:CLA:H2A	12:B:1211:CLA:HED2	2.04	0.40
12:B:1231:CLA:O1A	12:B:1232:CLA:HHB	2.21	0.40
12:B:1220:CLA:HMB2	12:B:1240:CLA:HBC3	2.02	0.40
2:B:223:MET:HB2	2:B:224:PRO:HD3	2.04	0.40
4:D:30:ILE:HG23	4:D:32:TRP:HZ3	1.85	0.40
4:D:53:GLY:O	4:D:55:ASN:ND2	2.54	0.40
5:E:18:TRP:CH2	5:E:45:ASN:HB3	2.57	0.40
6:F:72:PHE:CD1	15:F:4014:BCR:H343	2.57	0.40
6:F:54:ILE:HB	6:F:61:HIS:ND1	2.36	0.40
9:K:59:LYS:NZ	9:K:63:LEU:HB2	2.35	0.40
11:M:20:PHE:HB2	19:M:4021:ECH:H2A	2.02	0.40

There are no symmetry-related clashes.

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	749/751 (100%)	694 (93%)	52 (7%)	3 (0%)	36	76
2	B	729/731 (100%)	685 (94%)	43 (6%)	1 (0%)	53	87
3	C	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	13	53
4	D	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	12	51
5	E	67/69 (97%)	59 (88%)	6 (9%)	2 (3%)	5	37
6	F	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	12	51
7	I	38/40 (95%)	29 (76%)	6 (16%)	3 (8%)	1	16
8	J	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
9	K	68/70 (97%)	61 (90%)	6 (9%)	1 (2%)	11	51
10	L	135/137 (98%)	104 (77%)	25 (18%)	6 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
All	All	2211/2233 (99%)	2022 (92%)	168 (8%)	21 (1%)	19	60

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
10	L	105	GLN
1	A	191	GLN
5	E	14	THR
2	B	556	CYS
5	E	54	SER
7	I	2	ASP
10	L	38	PRO
10	L	117	ALA
4	D	106	GLU
9	K	84	LEU
10	L	125	ALA
10	L	146	SER
4	D	100	ALA
7	I	12	TRP
10	L	53	VAL
6	F	14	PRO
6	F	95	ASN
7	I	38	GLY
3	C	59	PRO
1	A	476	ILE

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	602/603 (100%)	590 (98%)	12 (2%)	58	80
2	B	583/583 (100%)	569 (98%)	14 (2%)	52	76
3	C	68/68 (100%)	66 (97%)	2 (3%)	45	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	116/116 (100%)	110 (95%)	6 (5%)	25	59
5	E	58/58 (100%)	56 (97%)	2 (3%)	40	69
6	F	119/119 (100%)	117 (98%)	2 (2%)	63	83
7	I	32/32 (100%)	27 (84%)	5 (16%)	3	20
8	J	35/35 (100%)	34 (97%)	1 (3%)	45	71
9	K	53/54 (98%)	46 (87%)	7 (13%)	4	25
10	L	102/102 (100%)	83 (81%)	19 (19%)	2	13
11	M	25/25 (100%)	25 (100%)	0	100	100
All	All	1793/1795 (100%)	1723 (96%)	70 (4%)	35	65

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	110	ILE
1	A	210	LEU
1	A	256	PHE
1	A	303	LEU
1	A	371	TYR
1	A	381	ILE
1	A	561	LEU
1	A	583	CYS
1	A	631	THR
1	A	704	HIS
1	A	743	PHE
2	B	5	PHE
2	B	47	PHE
2	B	145	LEU
2	B	257	PHE
2	B	406	LEU
2	B	418	SER
2	B	543	LEU
2	B	565	CYS
2	B	567	ILE
2	B	573	PHE
2	B	628	LEU
2	B	686	ASN
2	B	687	LEU
2	B	729	LYS

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Mol	Chain	Res	Type
3	C	11	CYS
3	C	72	GLU
4	D	18	LEU
4	D	66	LEU
4	D	77	LYS
4	D	96	TYR
4	D	107	LYS
4	D	108	VAL
5	E	30	LYS
5	E	66	LEU
6	F	66	LEU
6	F	132	VAL
7	I	1	MET
7	I	9	TYR
7	I	13	ILE
7	I	14	LEU
7	I	20	TRP
8	J	26	LEU
9	K	20	LEU
9	K	22	VAL
9	K	32	PHE
9	K	34	PHE
9	K	50	LEU
9	K	65	GLU
9	K	69	THR
10	L	42	LYS
10	L	51	LEU
10	L	52	GLU
10	L	59	TYR
10	L	60	PHE
10	L	77	GLN
10	L	99	TYR
10	L	101	LEU
10	L	104	PHE
10	L	108	GLN
10	L	118	ASP
10	L	128	PHE
10	L	139	TYR
10	L	140	PHE
10	L	145	LEU
10	L	149	ASP
10	L	152	PHE

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Mol	Chain	Res	Type
10	L	155	LEU
10	L	156	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	HIS
2	B	299	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 3 are monoatomic - leaving 127 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	$\# Z > 2$
12	CLA	A	1011	-	48,63,73	1.29	4 (8%)	54,101,113	1.48	9 (16%)
12	CLA	A	1012	-	42,57,73	1.36	5 (11%)	47,93,113	1.61	7 (14%)
12	CLA	A	1013	-	58,73,73	1.12	5 (8%)	66,113,113	1.28	7 (10%)
12	CLA	A	1101	-	42,57,73	1.36	4 (9%)	47,93,113	1.79	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	1102	12	58,73,73	1.13	4 (6%)	66,113,113	1.37	8 (12%)
12	CLA	A	1103	-	42,57,73	1.34	4 (9%)	47,93,113	1.61	7 (14%)
12	CLA	A	1104	-	42,57,73	1.37	4 (9%)	47,93,113	1.57	6 (12%)
12	CLA	A	1105	-	58,73,73	1.17	4 (6%)	66,113,113	1.32	6 (9%)
12	CLA	A	1106	-	58,73,73	1.14	4 (6%)	66,113,113	1.35	8 (12%)
12	CLA	A	1107	1	43,58,73	1.55	6 (13%)	48,95,113	1.32	7 (14%)
12	CLA	A	1108	-	42,57,73	1.36	4 (9%)	47,93,113	1.60	7 (14%)
12	CLA	A	1109	12	58,73,73	1.14	4 (6%)	66,113,113	1.29	7 (10%)
12	CLA	A	1110	-	42,57,73	1.36	4 (9%)	47,93,113	1.56	7 (14%)
12	CLA	A	1111	-	42,57,73	1.34	4 (9%)	47,93,113	1.55	7 (14%)
12	CLA	A	1112	-	42,57,73	1.35	4 (9%)	47,93,113	1.66	9 (19%)
12	CLA	A	1113	-	42,57,73	1.35	4 (9%)	47,93,113	1.58	7 (14%)
12	CLA	A	1114	-	42,57,73	1.37	4 (9%)	47,93,113	1.58	7 (14%)
12	CLA	A	1115	-	49,64,73	1.24	4 (8%)	55,102,113	1.41	8 (14%)
12	CLA	A	1116	-	42,57,73	1.35	4 (9%)	47,93,113	1.66	9 (19%)
12	CLA	A	1117	-	42,57,73	1.32	4 (9%)	47,93,113	1.63	9 (19%)
12	CLA	A	1118	-	43,58,73	1.33	4 (9%)	48,95,113	1.44	7 (14%)
12	CLA	A	1119	-	39,54,73	1.43	4 (10%)	44,90,113	1.30	4 (9%)
12	CLA	A	1120	-	42,57,73	1.33	4 (9%)	47,93,113	1.66	7 (14%)
12	CLA	A	1121	-	42,57,73	1.35	4 (9%)	47,93,113	1.69	8 (17%)
12	CLA	A	1122	-	42,57,73	1.35	4 (9%)	47,93,113	1.59	9 (19%)
12	CLA	A	1123	-	53,68,73	1.21	4 (7%)	60,107,113	1.45	9 (15%)
12	CLA	A	1124	-	42,57,73	1.35	4 (9%)	47,93,113	1.62	8 (17%)
12	CLA	A	1125	-	42,57,73	1.35	4 (9%)	47,93,113	1.72	10 (21%)
12	CLA	A	1126	-	53,68,73	1.19	4 (7%)	60,107,113	1.32	8 (13%)
12	CLA	A	1127	-	42,57,73	1.36	4 (9%)	47,93,113	1.61	7 (14%)
12	CLA	A	1128	-	58,73,73	1.13	4 (6%)	66,113,113	1.39	9 (13%)
12	CLA	A	1129	-	42,57,73	1.33	4 (9%)	47,93,113	1.64	8 (17%)
12	CLA	A	1130	-	42,57,73	1.34	4 (9%)	47,93,113	1.62	8 (17%)
12	CLA	A	1131	-	42,57,73	1.36	4 (9%)	47,93,113	1.53	7 (14%)
12	CLA	A	1132	10	48,63,73	1.27	4 (8%)	54,101,113	1.36	6 (11%)
12	CLA	A	1133	-	42,57,73	1.36	4 (9%)	47,93,113	1.56	8 (17%)
12	CLA	A	1134	1	42,57,73	1.35	4 (9%)	47,93,113	1.62	7 (14%)
12	CLA	A	1135	-	42,57,73	1.36	4 (9%)	47,93,113	1.71	9 (19%)
12	CLA	A	1136	-	42,57,73	1.36	4 (9%)	47,93,113	1.61	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	1137	-	42,57,73	1.36	4 (9%)	47,93,113	1.60	7 (14%)
12	CLA	A	1138	-	58,73,73	1.14	4 (6%)	66,113,113	1.33	7 (10%)
12	CLA	A	1139	-	48,63,73	1.27	4 (8%)	54,101,113	1.41	5 (9%)
12	CLA	A	1140	-	58,73,73	1.16	4 (6%)	66,113,113	1.27	6 (9%)
12	CLA	A	1141	-	35,53,73	1.46	4 (11%)	38,89,113	1.41	4 (10%)
13	PQN	A	2001	-	34,34,34	0.41	0	42,45,45	1.04	2 (4%)
14	SF4	A	3001	-	0,12,12	0.00	-	0,24,24	0.00	-
15	BCR	A	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.37	18 (32%)
15	BCR	A	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.30	16 (28%)
15	BCR	A	4007	-	41,41,41	1.83	4 (9%)	56,56,56	4.40	16 (28%)
15	BCR	A	4008	-	41,41,41	1.84	4 (9%)	56,56,56	4.40	17 (30%)
15	BCR	A	4012	-	41,41,41	1.84	4 (9%)	56,56,56	4.31	14 (25%)
16	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.06	4 (7%)
16	LHG	A	5003	-	48,48,48	0.38	0	51,54,54	1.09	3 (5%)
12	CLA	B	1021	-	58,73,73	1.18	4 (6%)	66,113,113	1.28	7 (10%)
12	CLA	B	1022	-	53,68,73	1.23	4 (7%)	60,107,113	1.39	8 (13%)
12	CLA	B	1023	-	42,57,73	1.34	4 (9%)	47,93,113	1.58	6 (12%)
12	CLA	B	1201	-	42,57,73	1.34	4 (9%)	47,93,113	1.63	7 (14%)
12	CLA	B	1202	-	58,73,73	1.15	4 (6%)	66,113,113	1.36	7 (10%)
12	CLA	B	1203	-	42,57,73	1.34	4 (9%)	47,93,113	1.48	7 (14%)
12	CLA	B	1204	-	42,57,73	1.38	4 (9%)	47,93,113	1.56	8 (17%)
12	CLA	B	1205	-	42,57,73	1.39	4 (9%)	47,93,113	1.69	8 (17%)
12	CLA	B	1206	-	42,57,73	1.35	4 (9%)	47,93,113	1.63	9 (19%)
12	CLA	B	1207	-	42,57,73	1.37	4 (9%)	47,93,113	1.67	8 (17%)
12	CLA	B	1208	-	42,57,73	1.38	4 (9%)	47,93,113	1.56	6 (12%)
12	CLA	B	1209	-	42,57,73	1.36	4 (9%)	47,93,113	1.63	7 (14%)
12	CLA	B	1210	-	42,57,73	1.35	4 (9%)	47,93,113	1.66	9 (19%)
12	CLA	B	1211	-	42,57,73	1.37	4 (9%)	47,93,113	1.66	8 (17%)
12	CLA	B	1212	-	42,57,73	1.36	4 (9%)	47,93,113	1.60	7 (14%)
12	CLA	B	1213	-	42,57,73	1.34	4 (9%)	47,93,113	1.76	9 (19%)
12	CLA	B	1214	-	53,68,73	1.21	4 (7%)	60,107,113	1.30	8 (13%)
12	CLA	B	1215	-	42,57,73	1.35	4 (9%)	47,93,113	1.62	8 (17%)
12	CLA	B	1216	-	42,57,73	1.36	4 (9%)	47,93,113	1.60	8 (17%)
12	CLA	B	1217	-	42,57,73	1.37	4 (9%)	47,93,113	1.65	9 (19%)
12	CLA	B	1218	-	42,57,73	1.33	4 (9%)	47,93,113	1.64	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	1219	-	42,57,73	1.37	4 (9%)	47,93,113	1.59	7 (14%)
12	CLA	B	1220	-	42,57,73	1.36	4 (9%)	47,93,113	1.74	9 (19%)
12	CLA	B	1221	-	42,57,73	1.35	5 (11%)	47,93,113	1.68	8 (17%)
12	CLA	B	1222	-	43,58,73	1.36	4 (9%)	48,95,113	1.53	5 (10%)
12	CLA	B	1223	-	42,57,73	1.45	5 (11%)	47,93,113	1.64	8 (17%)
12	CLA	B	1224	-	48,63,73	1.28	4 (8%)	54,101,113	1.42	6 (11%)
12	CLA	B	1225	-	42,57,73	1.36	4 (9%)	47,93,113	1.50	5 (10%)
12	CLA	B	1226	-	42,57,73	1.33	4 (9%)	47,93,113	1.72	9 (19%)
12	CLA	B	1227	-	42,57,73	1.37	4 (9%)	47,93,113	1.67	6 (12%)
12	CLA	B	1228	-	42,57,73	1.35	4 (9%)	47,93,113	1.61	8 (17%)
12	CLA	B	1229	-	48,63,73	1.28	5 (10%)	54,101,113	1.41	7 (12%)
12	CLA	B	1230	-	42,57,73	1.38	4 (9%)	47,93,113	1.66	7 (14%)
12	CLA	B	1231	-	42,57,73	1.37	4 (9%)	47,93,113	1.59	6 (12%)
12	CLA	B	1232	-	42,57,73	1.39	4 (9%)	47,93,113	1.61	8 (17%)
12	CLA	B	1234	-	53,68,73	1.22	4 (7%)	60,107,113	1.39	8 (13%)
12	CLA	B	1235	-	58,73,73	1.16	4 (6%)	66,113,113	1.34	9 (13%)
12	CLA	B	1236	-	42,57,73	1.38	4 (9%)	47,93,113	1.60	7 (14%)
12	CLA	B	1237	-	42,57,73	1.35	4 (9%)	47,93,113	1.62	8 (17%)
12	CLA	B	1238	-	42,57,73	1.37	4 (9%)	47,93,113	1.58	6 (12%)
12	CLA	B	1239	-	42,57,73	1.37	4 (9%)	47,93,113	1.56	6 (12%)
12	CLA	B	1240	-	42,57,73	1.37	4 (9%)	47,93,113	1.67	7 (14%)
13	PQN	B	2002	-	34,34,34	0.38	0	42,45,45	1.04	2 (4%)
15	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.49	15 (26%)
15	BCR	B	4005	-	41,41,41	1.85	4 (9%)	56,56,56	4.44	14 (25%)
19	ECH	B	4006	-	42,42,42	0.84	1 (2%)	55,58,58	2.47	13 (23%)
15	BCR	B	4010	-	41,41,41	1.91	4 (9%)	56,56,56	4.51	18 (32%)
17	45D	B	4011	-	43,43,43	3.55	16 (37%)	54,60,60	2.15	17 (31%)
15	BCR	B	4017	-	41,41,41	1.85	4 (9%)	56,56,56	4.46	15 (26%)
15	BCR	B	4018	-	41,41,41	1.85	4 (9%)	56,56,56	4.20	16 (28%)
20	LMG	B	5002	-	55,55,55	1.12	6 (10%)	63,63,63	1.02	3 (4%)
16	LHG	B	5004	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
20	LMG	B	5005	-	55,55,55	1.13	6 (10%)	63,63,63	1.07	3 (4%)
16	LHG	B	5006	2	20,20,48	0.58	0	23,26,54	1.46	2 (8%)
21	SQD	B	5008	-	53,54,54	0.78	0	63,65,65	0.90	2 (3%)
14	SF4	C	3002	-	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	SF4	C	3003	-	0,12,12	0.00	-	0,24,24	0.00	-
12	CLA	F	1301	-	42,57,73	1.34	4 (9%)	47,93,113	1.60	8 (17%)
12	CLA	F	1302	10	42,57,73	1.37	4 (9%)	47,93,113	1.66	8 (17%)
15	BCR	F	4014	-	41,41,41	1.86	4 (9%)	56,56,56	4.33	14 (25%)
23	C7Z	F	4016	-	43,43,43	5.36	18 (41%)	56,60,60	5.33	32 (57%)
21	SQD	F	5001	-	53,54,54	0.79	0	63,65,65	0.91	2 (3%)
24	LMT	F	6001	-	36,36,36	1.11	4 (11%)	47,47,47	1.01	2 (4%)
15	BCR	I	4018	-	41,41,41	1.85	4 (9%)	56,56,56	4.38	20 (35%)
25	EQ3	I	4020	-	43,43,43	4.18	25 (58%)	55,60,60	2.38	20 (36%)
12	CLA	J	1302	8	42,57,73	1.35	4 (9%)	47,93,113	1.61	7 (14%)
12	CLA	J	1303	10	42,57,73	1.34	4 (9%)	47,93,113	1.64	8 (17%)
15	BCR	J	4013	-	41,41,41	1.87	4 (9%)	56,56,56	4.36	15 (26%)
23	C7Z	J	4015	-	43,43,43	5.33	18 (41%)	56,60,60	5.29	31 (55%)
12	CLA	K	1401	-	35,53,73	1.48	4 (11%)	38,89,113	1.48	5 (13%)
12	CLA	K	1402	-	42,57,73	1.36	4 (9%)	47,93,113	1.68	10 (21%)
15	BCR	K	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.41	15 (26%)
12	CLA	L	1502	-	42,57,73	1.37	5 (11%)	47,93,113	1.70	9 (19%)
19	ECH	M	4021	-	42,42,42	0.84	2 (4%)	55,58,58	2.63	15 (27%)

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
12	CLA	A	1011	-	3/3/18/25	0/25/123/135	0/0/9/9
12	CLA	A	1012	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1013	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	A	1101	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1102	12	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	A	1103	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1104	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1105	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	A	1106	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	A	1107	1	3/3/17/25	0/19/117/135	0/0/9/9
12	CLA	A	1108	-	3/3/16/25	0/18/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	1109	12	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	A	1110	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1111	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1112	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1113	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1114	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1115	-	3/3/18/25	0/27/125/135	0/0/9/9
12	CLA	A	1116	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1117	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1118	-	3/3/17/25	0/19/117/135	0/0/9/9
12	CLA	A	1119	-	3/3/16/25	0/15/113/135	0/0/9/9
12	CLA	A	1120	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1121	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1122	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1123	-	3/3/19/25	0/31/129/135	0/0/9/9
12	CLA	A	1124	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1125	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1126	-	3/3/19/25	0/31/129/135	0/0/9/9
12	CLA	A	1127	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	A	1129	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1130	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1131	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1132	10	3/3/18/25	0/25/123/135	0/0/9/9
12	CLA	A	1133	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1134	1	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1135	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1136	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1137	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	A	1138	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	A	1139	-	3/3/18/25	0/25/123/135	0/0/9/9
12	CLA	A	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	A	1141	-	3/3/16/25	0/11/111/135	0/0/9/9
13	PQN	A	2001	-	-	0/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	A	3001	-	-	0/0/48/48	0/6/5/5
15	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
15	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
15	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
15	BCR	A	4008	-	-	0/29/63/63	0/2/2/2
15	BCR	A	4012	-	-	0/29/63/63	0/2/2/2
16	LHG	A	5001	-	-	0/53/53/53	0/0/0/0
16	LHG	A	5003	-	-	0/53/53/53	0/0/0/0
12	CLA	B	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	B	1022	-	3/3/19/25	0/31/129/135	0/0/9/9
12	CLA	B	1023	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1201	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1202	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	B	1203	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1204	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1205	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1206	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1207	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1208	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1209	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1210	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1211	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1212	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1213	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1214	-	3/3/19/25	0/31/129/135	0/0/9/9
12	CLA	B	1215	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1216	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1217	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1218	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1219	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1220	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1221	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1222	-	3/3/17/25	0/19/117/135	0/0/9/9
12	CLA	B	1223	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1224	-	3/3/18/25	0/25/123/135	0/0/9/9
12	CLA	B	1225	-	3/3/16/25	0/18/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	1226	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1227	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1228	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1229	-	3/3/18/25	0/25/123/135	0/0/9/9
12	CLA	B	1230	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1231	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1232	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1234	-	3/3/19/25	0/31/129/135	0/0/9/9
12	CLA	B	1235	-	3/3/20/25	0/37/135/135	0/0/9/9
12	CLA	B	1236	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1237	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1238	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1239	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	B	1240	-	3/3/16/25	0/18/116/135	0/0/9/9
13	PQN	B	2002	-	-	0/23/43/43	0/2/2/2
15	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
15	BCR	B	4005	-	-	0/29/63/63	0/2/2/2
19	ECH	B	4006	-	-	0/29/66/66	0/2/2/2
15	BCR	B	4010	-	-	0/29/63/63	0/2/2/2
17	45D	B	4011	-	-	0/29/69/69	0/2/2/2
15	BCR	B	4017	-	-	0/29/63/63	0/2/2/2
15	BCR	B	4018	-	-	0/29/63/63	0/2/2/2
20	LMG	B	5002	-	-	0/50/70/70	0/1/1/1
16	LHG	B	5004	-	-	0/53/53/53	0/0/0/0
20	LMG	B	5005	-	-	0/50/70/70	0/1/1/1
16	LHG	B	5006	2	-	0/23/23/53	0/0/0/0
21	SQD	B	5008	-	-	0/49/69/69	0/1/1/1
14	SF4	C	3002	-	-	0/0/48/48	0/6/5/5
14	SF4	C	3003	-	-	0/0/48/48	0/6/5/5
12	CLA	F	1301	-	3/3/16/25	0/18/116/135	0/0/9/9
12	CLA	F	1302	10	3/3/16/25	0/18/116/135	0/0/9/9
15	BCR	F	4014	-	-	2/29/63/63	0/2/2/2
23	C7Z	F	4016	-	-	2/29/67/67	0/2/2/2
21	SQD	F	5001	-	-	0/49/69/69	0/1/1/1
24	LMT	F	6001	-	-	0/21/61/61	0/2/2/2
15	BCR	I	4018	-	-	1/29/63/63	0/2/2/2
25	EQ3	I	4020	-	-	0/29/68/68	0/2/2/2
12	CLA	J	1302	8	3/3/16/25	0/18/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	J	1303	10	3/3/16/25	0/18/116/135	0/0/9/9
15	BCR	J	4013	-	-	0/29/63/63	0/2/2/2
23	C7Z	J	4015	-	-	1/29/67/67	0/2/2/2
12	CLA	K	1401	-	3/3/16/25	0/11/111/135	0/0/9/9
12	CLA	K	1402	-	3/3/16/25	0/18/116/135	0/0/9/9
15	BCR	K	4001	-	-	2/29/63/63	0/2/2/2
12	CLA	L	1502	-	3/3/16/25	0/18/116/135	0/0/9/9
19	ECH	M	4021	-	-	0/29/66/66	0/2/2/2

All (532) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	I	4020	EQ3	C2-C3	-6.16	1.43	1.52
15	B	4010	BCR	C11-C12	-5.23	1.21	1.34
15	A	4007	BCR	C11-C12	-5.22	1.21	1.34
15	A	4008	BCR	C11-C12	-5.21	1.21	1.34
15	F	4014	BCR	C11-C12	-5.17	1.21	1.34
15	B	4004	BCR	C11-C12	-5.16	1.21	1.34
15	A	4012	BCR	C11-C12	-5.15	1.21	1.34
15	A	4003	BCR	C11-C12	-5.13	1.21	1.34
15	J	4013	BCR	C11-C12	-5.12	1.21	1.34
15	I	4018	BCR	C11-C12	-5.06	1.21	1.34
15	B	4017	BCR	C11-C12	-5.05	1.21	1.34
15	B	4018	BCR	C11-C12	-5.05	1.21	1.34
15	B	4005	BCR	C11-C12	-5.02	1.21	1.34
15	K	4001	BCR	C11-C12	-5.00	1.21	1.34
15	A	4001	BCR	C11-C12	-4.92	1.22	1.34
25	I	4020	EQ3	C1-C6	-4.80	1.47	1.53
15	I	4018	BCR	C16-C17	-4.46	1.30	1.43
25	I	4020	EQ3	C4-C5	-4.35	1.44	1.51
15	A	4007	BCR	C16-C17	-4.34	1.30	1.43
15	A	4008	BCR	C16-C17	-4.33	1.30	1.43
15	A	4012	BCR	C16-C17	-4.33	1.30	1.43
15	A	4001	BCR	C16-C17	-4.32	1.30	1.43
15	B	4017	BCR	C16-C17	-4.31	1.30	1.43
15	B	4004	BCR	C16-C17	-4.29	1.30	1.43
15	A	4003	BCR	C16-C17	-4.29	1.30	1.43
15	B	4010	BCR	C16-C17	-4.28	1.30	1.43
15	J	4013	BCR	C16-C17	-4.26	1.30	1.43
15	B	4005	BCR	C16-C17	-4.25	1.30	1.43
15	F	4014	BCR	C16-C17	-4.23	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	4018	BCR	C16-C17	-4.21	1.30	1.43
15	K	4001	BCR	C16-C17	-4.20	1.30	1.43
12	A	1107	CLA	C4A-NA	-3.36	1.33	1.38
20	B	5005	LMG	C19-C18	-3.20	1.33	1.51
20	B	5002	LMG	C19-C18	-3.19	1.33	1.51
20	B	5005	LMG	C22-C21	-3.19	1.33	1.51
20	B	5005	LMG	C25-C24	-3.18	1.33	1.51
20	B	5002	LMG	C22-C21	-3.17	1.33	1.51
20	B	5005	LMG	C43-C42	-3.17	1.33	1.51
20	B	5005	LMG	C37-C36	-3.16	1.33	1.51
20	B	5002	LMG	C40-C39	-3.16	1.33	1.51
20	B	5002	LMG	C25-C24	-3.16	1.33	1.51
20	B	5002	LMG	C43-C42	-3.16	1.33	1.51
20	B	5002	LMG	C37-C36	-3.15	1.33	1.51
20	B	5005	LMG	C40-C39	-3.15	1.33	1.51
25	I	4020	EQ3	O3-C3	-3.12	1.34	1.43
12	B	1223	CLA	OBD-CAD	-3.04	1.18	1.22
12	B	1022	CLA	C3B-C2B	-2.99	1.36	1.40
12	B	1229	CLA	C3B-C2B	-2.99	1.36	1.40
12	B	1219	CLA	C3B-C2B	-2.93	1.36	1.40
12	B	1232	CLA	C3B-C2B	-2.91	1.36	1.40
12	B	1216	CLA	C3B-C2B	-2.90	1.36	1.40
12	B	1238	CLA	C3B-C2B	-2.90	1.36	1.40
12	B	1208	CLA	C3B-C2B	-2.88	1.36	1.40
12	B	1225	CLA	C3B-C2B	-2.87	1.36	1.40
12	B	1224	CLA	C3B-C2B	-2.85	1.36	1.40
12	A	1137	CLA	C3B-C2B	-2.84	1.36	1.40
12	B	1209	CLA	C3B-C2B	-2.84	1.36	1.40
12	B	1207	CLA	C3B-C2B	-2.83	1.36	1.40
12	A	1114	CLA	C3B-C2B	-2.83	1.36	1.40
12	B	1227	CLA	C3B-C2B	-2.83	1.36	1.40
12	A	1012	CLA	C3B-C2B	-2.82	1.36	1.40
12	A	1140	CLA	C3B-C2B	-2.82	1.36	1.40
12	B	1239	CLA	C3B-C2B	-2.80	1.36	1.40
12	A	1139	CLA	C3B-C2B	-2.79	1.36	1.40
12	A	1110	CLA	C3B-C2B	-2.79	1.36	1.40
12	B	1220	CLA	C3B-C2B	-2.79	1.36	1.40
12	B	1217	CLA	C3B-C2B	-2.78	1.36	1.40
12	B	1230	CLA	C3B-C2B	-2.78	1.36	1.40
12	K	1401	CLA	C3B-C2B	-2.77	1.36	1.40
12	A	1133	CLA	C3B-C2B	-2.76	1.36	1.40
12	A	1105	CLA	C3B-C2B	-2.76	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1131	CLA	C3B-C2B	-2.76	1.36	1.40
12	B	1236	CLA	C3B-C2B	-2.75	1.36	1.40
12	A	1132	CLA	C3B-C2B	-2.75	1.36	1.40
12	F	1302	CLA	C3B-C2B	-2.74	1.36	1.40
12	A	1113	CLA	C3B-C2B	-2.74	1.36	1.40
12	A	1136	CLA	C3B-C2B	-2.73	1.36	1.40
12	B	1204	CLA	C3B-C2B	-2.71	1.36	1.40
12	A	1101	CLA	C3B-C2B	-2.70	1.36	1.40
12	B	1212	CLA	C3B-C2B	-2.70	1.36	1.40
12	J	1302	CLA	C3B-C2B	-2.69	1.36	1.40
12	B	1240	CLA	C3B-C2B	-2.69	1.36	1.40
12	B	1214	CLA	C3B-C2B	-2.67	1.36	1.40
12	A	1134	CLA	C3B-C2B	-2.66	1.36	1.40
12	L	1502	CLA	C3B-C2B	-2.65	1.36	1.40
12	B	1222	CLA	C3B-C2B	-2.65	1.36	1.40
12	B	1205	CLA	C3B-C2B	-2.64	1.36	1.40
12	A	1126	CLA	C3B-C2B	-2.64	1.36	1.40
12	B	1223	CLA	C3B-C2B	-2.62	1.36	1.40
12	A	1119	CLA	C3B-C2B	-2.60	1.36	1.40
12	A	1122	CLA	C3B-C2B	-2.60	1.36	1.40
12	B	1021	CLA	C3B-C2B	-2.60	1.36	1.40
12	A	1111	CLA	C3B-C2B	-2.60	1.36	1.40
12	B	1231	CLA	C3B-C2B	-2.58	1.36	1.40
12	A	1124	CLA	C3B-C2B	-2.55	1.36	1.40
12	A	1104	CLA	C3B-C2B	-2.54	1.36	1.40
12	K	1402	CLA	C3B-C2B	-2.53	1.36	1.40
24	F	6001	LMT	O3'-C3'	-2.51	1.36	1.43
12	A	1128	CLA	C3B-C2B	-2.48	1.36	1.40
12	A	1109	CLA	C3B-C2B	-2.48	1.36	1.40
12	B	1203	CLA	C3B-C2B	-2.47	1.36	1.40
12	A	1135	CLA	C3B-C2B	-2.46	1.37	1.40
12	B	1226	CLA	C3B-C2B	-2.45	1.37	1.40
12	A	1118	CLA	C3B-C2B	-2.45	1.37	1.40
12	A	1121	CLA	C3B-C2B	-2.45	1.37	1.40
12	B	1215	CLA	C3B-C2B	-2.45	1.37	1.40
12	B	1206	CLA	C3B-C2B	-2.45	1.37	1.40
12	B	1221	CLA	C3B-C2B	-2.45	1.37	1.40
12	F	1301	CLA	C3B-C2B	-2.42	1.37	1.40
12	A	1129	CLA	C3B-C2B	-2.41	1.37	1.40
12	A	1103	CLA	C3B-C2B	-2.41	1.37	1.40
12	B	1202	CLA	C3B-C2B	-2.41	1.37	1.40
12	B	1023	CLA	C3B-C2B	-2.39	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1235	CLA	C3B-C2B	-2.38	1.37	1.40
12	A	1141	CLA	C3B-C2B	-2.38	1.37	1.40
12	A	1112	CLA	C3B-C2B	-2.38	1.37	1.40
12	A	1106	CLA	C3B-C2B	-2.38	1.37	1.40
12	A	1013	CLA	C3B-C2B	-2.37	1.37	1.40
12	B	1237	CLA	C3B-C2B	-2.35	1.37	1.40
12	A	1127	CLA	C3B-C2B	-2.35	1.37	1.40
12	B	1213	CLA	C3B-C2B	-2.34	1.37	1.40
12	B	1228	CLA	C3B-C2B	-2.34	1.37	1.40
17	B	4011	45D	O02-C18	-2.33	1.18	1.23
12	B	1210	CLA	C3B-C2B	-2.32	1.37	1.40
12	A	1130	CLA	C3B-C2B	-2.31	1.37	1.40
12	A	1102	CLA	C3B-C2B	-2.31	1.37	1.40
19	B	4006	ECH	C1-C6	-2.31	1.50	1.53
12	A	1115	CLA	C3B-C2B	-2.30	1.37	1.40
12	A	1120	CLA	C3B-C2B	-2.30	1.37	1.40
19	M	4021	ECH	C25-C26	-2.27	1.32	1.35
12	A	1011	CLA	C3B-C2B	-2.26	1.37	1.40
12	A	1117	CLA	C3B-C2B	-2.25	1.37	1.40
12	B	1201	CLA	C3B-C2B	-2.24	1.37	1.40
24	F	6001	LMT	O2'-C2'	-2.23	1.37	1.43
12	A	1108	CLA	C3B-C2B	-2.23	1.37	1.40
12	A	1138	CLA	C3B-C2B	-2.23	1.37	1.40
12	B	1234	CLA	C3B-C2B	-2.20	1.37	1.40
12	A	1116	CLA	C3B-C2B	-2.19	1.37	1.40
24	F	6001	LMT	O3B-C3B	-2.16	1.37	1.43
24	F	6001	LMT	O2B-C2B	-2.15	1.37	1.43
12	A	1125	CLA	C3B-C2B	-2.15	1.37	1.40
12	J	1303	CLA	C3B-C2B	-2.14	1.37	1.40
12	B	1218	CLA	C3B-C2B	-2.14	1.37	1.40
12	B	1211	CLA	C3B-C2B	-2.13	1.37	1.40
12	A	1123	CLA	C3B-C2B	-2.09	1.37	1.40
12	A	1107	CLA	C3B-C2B	-2.04	1.37	1.40
19	M	4021	ECH	C30-C25	-2.01	1.51	1.53
23	F	4016	C7Z	C38-C25	2.01	1.54	1.51
23	J	4015	C7Z	C38-C25	2.01	1.54	1.51
12	B	1221	CLA	C1A-CHA	2.02	1.51	1.43
12	A	1012	CLA	C1A-CHA	2.03	1.51	1.43
12	L	1502	CLA	C1A-CHA	2.03	1.51	1.43
12	B	1229	CLA	CHC-C1C	2.03	1.41	1.35
12	A	1013	CLA	CHC-C1C	2.07	1.41	1.35
12	A	1128	CLA	C1C-C2C	2.10	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1107	CLA	CHC-C1C	2.15	1.41	1.35
17	B	4011	45D	C23-C19	2.15	1.39	1.33
12	A	1111	CLA	C1C-C2C	2.17	1.48	1.44
17	B	4011	45D	C18-C16	2.20	1.52	1.47
12	B	1023	CLA	C1C-C2C	2.23	1.48	1.44
12	A	1112	CLA	C1C-C2C	2.25	1.48	1.44
12	A	1011	CLA	C1C-C2C	2.26	1.48	1.44
12	K	1401	CLA	C1C-C2C	2.26	1.48	1.44
12	B	1216	CLA	C1C-C2C	2.27	1.48	1.44
12	B	1222	CLA	C1C-C2C	2.28	1.48	1.44
12	A	1109	CLA	C1C-C2C	2.28	1.48	1.44
23	F	4016	C7Z	C18-C5	2.28	1.54	1.51
12	B	1237	CLA	C1C-C2C	2.29	1.49	1.44
25	I	4020	EQ3	C40-C30	2.29	1.58	1.53
12	B	1226	CLA	C1C-C2C	2.30	1.49	1.44
12	A	1122	CLA	C1C-C2C	2.30	1.49	1.44
12	B	1203	CLA	C1C-C2C	2.33	1.49	1.44
12	B	1206	CLA	C1C-C2C	2.33	1.49	1.44
12	A	1133	CLA	C1C-C2C	2.33	1.49	1.44
12	L	1502	CLA	C1C-C2C	2.33	1.49	1.44
12	B	1220	CLA	C1C-C2C	2.33	1.49	1.44
12	B	1021	CLA	C1C-C2C	2.33	1.49	1.44
12	B	1236	CLA	C1C-C2C	2.34	1.49	1.44
12	A	1131	CLA	C1C-C2C	2.34	1.49	1.44
12	B	1205	CLA	C1C-C2C	2.35	1.49	1.44
12	F	1301	CLA	C1C-C2C	2.35	1.49	1.44
12	B	1211	CLA	C1C-C2C	2.37	1.49	1.44
12	A	1118	CLA	C1C-C2C	2.37	1.49	1.44
12	A	1117	CLA	C1C-C2C	2.37	1.49	1.44
12	A	1121	CLA	C1C-C2C	2.37	1.49	1.44
12	A	1129	CLA	C1C-C2C	2.37	1.49	1.44
12	A	1138	CLA	C1C-C2C	2.38	1.49	1.44
12	B	1214	CLA	C1C-C2C	2.39	1.49	1.44
12	B	1221	CLA	C1C-C2C	2.39	1.49	1.44
12	A	1115	CLA	C1C-C2C	2.39	1.49	1.44
12	A	1126	CLA	C1C-C2C	2.40	1.49	1.44
12	A	1123	CLA	C1C-C2C	2.40	1.49	1.44
12	B	1225	CLA	C1C-C2C	2.41	1.49	1.44
12	A	1137	CLA	C1C-C2C	2.41	1.49	1.44
12	B	1240	CLA	C1C-C2C	2.41	1.49	1.44
12	B	1231	CLA	C1C-C2C	2.41	1.49	1.44
12	B	1213	CLA	C1C-C2C	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1012	CLA	C1C-C2C	2.41	1.49	1.44
12	J	1302	CLA	C1C-C2C	2.42	1.49	1.44
12	B	1239	CLA	C1C-C2C	2.42	1.49	1.44
12	A	1103	CLA	C1C-C2C	2.42	1.49	1.44
12	A	1132	CLA	C1C-C2C	2.43	1.49	1.44
12	B	1234	CLA	C1C-C2C	2.43	1.49	1.44
12	A	1120	CLA	C1C-C2C	2.43	1.49	1.44
12	B	1224	CLA	C1C-C2C	2.43	1.49	1.44
12	A	1136	CLA	C1C-C2C	2.43	1.49	1.44
12	B	1210	CLA	C1C-C2C	2.43	1.49	1.44
12	B	1212	CLA	C1C-C2C	2.44	1.49	1.44
12	A	1106	CLA	C1C-C2C	2.44	1.49	1.44
12	B	1218	CLA	C1C-C2C	2.44	1.49	1.44
12	A	1104	CLA	C1C-C2C	2.45	1.49	1.44
12	B	1235	CLA	C1C-C2C	2.45	1.49	1.44
12	A	1108	CLA	C1C-C2C	2.45	1.49	1.44
12	F	1302	CLA	C1C-C2C	2.45	1.49	1.44
12	A	1125	CLA	C1C-C2C	2.45	1.49	1.44
12	B	1232	CLA	C1C-C2C	2.46	1.49	1.44
12	B	1209	CLA	C1C-C2C	2.46	1.49	1.44
12	A	1102	CLA	C1C-C2C	2.47	1.49	1.44
12	B	1219	CLA	C1C-C2C	2.47	1.49	1.44
12	B	1215	CLA	C1C-C2C	2.47	1.49	1.44
12	B	1227	CLA	C1C-C2C	2.48	1.49	1.44
12	B	1223	CLA	C1C-C2C	2.48	1.49	1.44
12	B	1229	CLA	C1C-C2C	2.48	1.49	1.44
12	B	1202	CLA	C1C-C2C	2.48	1.49	1.44
12	A	1134	CLA	C1C-C2C	2.49	1.49	1.44
12	A	1119	CLA	C1C-C2C	2.49	1.49	1.44
12	A	1124	CLA	C1C-C2C	2.49	1.49	1.44
12	B	1204	CLA	C1C-C2C	2.49	1.49	1.44
12	A	1127	CLA	C1C-C2C	2.50	1.49	1.44
12	A	1110	CLA	C1C-C2C	2.50	1.49	1.44
12	B	1230	CLA	C1C-C2C	2.50	1.49	1.44
12	A	1140	CLA	C1C-C2C	2.50	1.49	1.44
12	B	1217	CLA	C1C-C2C	2.50	1.49	1.44
12	B	1022	CLA	C1C-C2C	2.50	1.49	1.44
12	A	1114	CLA	C1C-C2C	2.50	1.49	1.44
12	K	1402	CLA	C1C-C2C	2.51	1.49	1.44
12	A	1116	CLA	C1C-C2C	2.51	1.49	1.44
12	A	1139	CLA	C1C-C2C	2.51	1.49	1.44
12	B	1201	CLA	C1C-C2C	2.51	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1135	CLA	C1C-C2C	2.51	1.49	1.44
12	A	1141	CLA	C1C-C2C	2.52	1.49	1.44
23	J	4015	C7Z	C18-C5	2.52	1.55	1.51
12	A	1013	CLA	C1C-C2C	2.52	1.49	1.44
12	B	1208	CLA	C1C-C2C	2.52	1.49	1.44
12	J	1303	CLA	C1C-C2C	2.52	1.49	1.44
12	A	1113	CLA	C1C-C2C	2.53	1.49	1.44
12	A	1130	CLA	C1C-C2C	2.53	1.49	1.44
25	I	4020	EQ3	C8-C9	2.55	1.51	1.45
12	B	1207	CLA	C1C-C2C	2.55	1.49	1.44
17	B	4011	45D	C17-C15	2.56	1.53	1.47
12	A	1101	CLA	C1C-C2C	2.58	1.49	1.44
25	I	4020	EQ3	C28-C27	2.60	1.54	1.50
12	A	1105	CLA	C1C-C2C	2.60	1.49	1.44
12	B	1238	CLA	C1C-C2C	2.61	1.49	1.44
12	B	1228	CLA	C1C-C2C	2.61	1.49	1.44
25	I	4020	EQ3	C33-C5	2.62	1.55	1.51
12	A	1107	CLA	C1C-C2C	2.63	1.49	1.44
25	I	4020	EQ3	C27-C26	2.66	1.53	1.47
23	F	4016	C7Z	C8-C9	2.80	1.52	1.45
23	F	4016	C7Z	C27-C26	2.82	1.55	1.45
23	J	4015	C7Z	C8-C9	2.83	1.52	1.45
23	F	4016	C7Z	C7-C6	2.85	1.55	1.45
25	I	4020	EQ3	C24-C25	2.86	1.55	1.45
23	J	4015	C7Z	C7-C6	2.87	1.55	1.45
25	I	4020	EQ3	C17-C18	2.87	1.39	1.35
25	I	4020	EQ3	C35-C13	2.89	1.57	1.50
23	F	4016	C7Z	C32-C33	2.94	1.52	1.45
25	I	4020	EQ3	C38-C26	2.94	1.57	1.50
23	J	4015	C7Z	C32-C33	2.95	1.52	1.45
17	B	4011	45D	C19-C07	2.95	1.56	1.45
17	B	4011	45D	C20-C08	2.97	1.56	1.45
23	F	4016	C7Z	C28-C29	3.05	1.52	1.45
25	I	4020	EQ3	C20-C21	3.09	1.53	1.43
23	J	4015	C7Z	C28-C29	3.23	1.52	1.45
12	A	1115	CLA	CBB-CAB	3.23	1.51	1.29
12	B	1229	CLA	CBB-CAB	3.23	1.51	1.29
23	J	4015	C7Z	C27-C26	3.24	1.57	1.45
25	I	4020	EQ3	C16-C17	3.24	1.53	1.43
12	B	1238	CLA	CBB-CAB	3.26	1.51	1.29
12	B	1203	CLA	CBB-CAB	3.26	1.51	1.29
12	B	1225	CLA	CBB-CAB	3.26	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1107	CLA	CBB-CAB	3.27	1.51	1.29
12	B	1237	CLA	CBB-CAB	3.27	1.51	1.29
12	B	1022	CLA	CBB-CAB	3.27	1.51	1.29
12	A	1140	CLA	CBB-CAB	3.28	1.51	1.29
12	A	1101	CLA	CBB-CAB	3.28	1.51	1.29
12	A	1129	CLA	CBB-CAB	3.28	1.51	1.29
12	B	1219	CLA	CBB-CAB	3.28	1.51	1.29
12	A	1125	CLA	CBB-CAB	3.29	1.51	1.29
12	A	1138	CLA	CBB-CAB	3.29	1.51	1.29
12	A	1108	CLA	CBB-CAB	3.29	1.51	1.29
12	B	1220	CLA	CBB-CAB	3.29	1.51	1.29
12	B	1216	CLA	CBB-CAB	3.29	1.51	1.29
12	B	1235	CLA	CBB-CAB	3.29	1.51	1.29
12	A	1130	CLA	CBB-CAB	3.29	1.51	1.29
12	A	1113	CLA	CBB-CAB	3.29	1.51	1.29
12	A	1118	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1114	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1111	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1208	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1119	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1127	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1207	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1210	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1106	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1139	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1137	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1136	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1232	CLA	CBB-CAB	3.30	1.51	1.29
12	F	1302	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1122	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1228	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1217	CLA	CBB-CAB	3.30	1.51	1.29
12	A	1124	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1227	CLA	CBB-CAB	3.30	1.51	1.29
12	B	1214	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1204	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1226	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1110	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1231	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1224	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1134	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1221	CLA	CBB-CAB	3.31	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1239	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1104	CLA	CBB-CAB	3.31	1.51	1.29
12	F	1301	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1234	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1205	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1023	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1133	CLA	CBB-CAB	3.31	1.51	1.29
12	J	1303	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1213	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1218	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1212	CLA	CBB-CAB	3.31	1.51	1.29
12	K	1402	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1230	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1121	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1223	CLA	CBB-CAB	3.31	1.51	1.29
12	J	1302	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1126	CLA	CBB-CAB	3.31	1.51	1.29
12	L	1502	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1135	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1120	CLA	CBB-CAB	3.31	1.51	1.29
12	A	1105	CLA	CBB-CAB	3.31	1.51	1.29
12	B	1222	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1132	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1209	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1240	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1211	CLA	CBB-CAB	3.32	1.51	1.29
12	K	1401	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1128	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1021	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1102	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1206	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1116	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1012	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1123	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1103	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1112	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1202	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1011	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1109	CLA	CBB-CAB	3.32	1.51	1.29
12	B	1215	CLA	CBB-CAB	3.32	1.51	1.29
12	A	1131	CLA	CBB-CAB	3.33	1.51	1.29
12	A	1141	CLA	CBB-CAB	3.33	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1117	CLA	CBB-CAB	3.33	1.51	1.29
12	B	1201	CLA	CBB-CAB	3.34	1.51	1.29
12	B	1236	CLA	CBB-CAB	3.34	1.51	1.29
12	A	1013	CLA	CBB-CAB	3.34	1.51	1.29
23	F	4016	C7Z	C31-C30	3.47	1.54	1.43
23	J	4015	C7Z	C11-C10	3.47	1.54	1.43
25	I	4020	EQ3	C2-C1	3.54	1.65	1.54
23	J	4015	C7Z	C31-C30	3.55	1.54	1.43
23	F	4016	C7Z	C11-C10	3.55	1.54	1.43
17	B	4011	45D	C32-C30	3.62	1.54	1.43
23	J	4015	C7Z	C12-C13	3.62	1.53	1.45
17	B	4011	45D	C31-C29	3.63	1.54	1.43
23	F	4016	C7Z	C12-C13	3.64	1.53	1.45
23	J	4015	C7Z	C15-C14	3.65	1.54	1.43
23	F	4016	C7Z	C15-C14	3.69	1.54	1.43
23	J	4015	C7Z	C35-C34	3.73	1.55	1.43
23	F	4016	C7Z	C35-C34	3.75	1.55	1.43
17	B	4011	45D	C41-C37	3.78	1.55	1.43
17	B	4011	45D	C42-C38	3.85	1.55	1.43
25	I	4020	EQ3	C7-C6	3.95	1.59	1.45
25	I	4020	EQ3	C19-C18	4.14	1.54	1.45
25	I	4020	EQ3	C12-C13	4.23	1.55	1.45
17	B	4011	45D	C34-C36	4.33	1.55	1.45
17	B	4011	45D	C33-C35	4.69	1.56	1.45
25	I	4020	EQ3	C11-C10	4.70	1.57	1.43
17	B	4011	45D	C24-C26	4.72	1.56	1.45
25	I	4020	EQ3	C23-C22	4.85	1.56	1.45
25	I	4020	EQ3	C15-C14	4.95	1.58	1.43
12	A	1013	CLA	CHB-C4A	5.01	1.39	1.33
17	B	4011	45D	C23-C25	5.08	1.57	1.45
12	A	1139	CLA	CHB-C4A	5.40	1.39	1.33
12	B	1238	CLA	CHB-C4A	5.43	1.39	1.33
12	A	1132	CLA	CHB-C4A	5.43	1.39	1.33
12	A	1117	CLA	CHB-C4A	5.45	1.39	1.33
12	A	1128	CLA	CHB-C4A	5.49	1.39	1.33
12	A	1126	CLA	CHB-C4A	5.50	1.39	1.33
12	B	1226	CLA	CHB-C4A	5.50	1.39	1.33
12	A	1102	CLA	CHB-C4A	5.51	1.39	1.33
12	A	1109	CLA	CHB-C4A	5.51	1.39	1.33
12	B	1224	CLA	CHB-C4A	5.51	1.39	1.33
12	A	1119	CLA	CHB-C4A	5.52	1.39	1.33
15	I	4018	BCR	C24-C23	5.53	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1229	CLA	CHB-C4A	5.54	1.39	1.33
12	A	1140	CLA	CHB-C4A	5.54	1.39	1.33
12	A	1012	CLA	CHB-C4A	5.56	1.39	1.33
12	A	1138	CLA	CHB-C4A	5.57	1.39	1.33
12	A	1103	CLA	CHB-C4A	5.59	1.40	1.33
12	B	1201	CLA	CHB-C4A	5.59	1.40	1.33
15	B	4004	BCR	C24-C23	5.60	1.50	1.33
15	B	4005	BCR	C24-C23	5.60	1.50	1.33
12	J	1302	CLA	CHB-C4A	5.61	1.40	1.33
12	A	1141	CLA	CHB-C4A	5.61	1.40	1.33
12	B	1225	CLA	CHB-C4A	5.61	1.40	1.33
12	A	1137	CLA	CHB-C4A	5.61	1.40	1.33
12	B	1235	CLA	CHB-C4A	5.61	1.40	1.33
12	A	1101	CLA	CHB-C4A	5.62	1.40	1.33
12	A	1106	CLA	CHB-C4A	5.62	1.40	1.33
12	A	1120	CLA	CHB-C4A	5.62	1.40	1.33
15	A	4001	BCR	C24-C23	5.62	1.50	1.33
15	B	4010	BCR	C24-C23	5.63	1.50	1.33
12	B	1236	CLA	CHB-C4A	5.63	1.40	1.33
12	A	1134	CLA	CHB-C4A	5.63	1.40	1.33
12	B	1023	CLA	CHB-C4A	5.63	1.40	1.33
12	A	1129	CLA	CHB-C4A	5.64	1.40	1.33
15	B	4017	BCR	C24-C23	5.64	1.50	1.33
12	A	1111	CLA	CHB-C4A	5.64	1.40	1.33
12	B	1209	CLA	CHB-C4A	5.65	1.40	1.33
15	A	4008	BCR	C24-C23	5.65	1.50	1.33
12	A	1130	CLA	CHB-C4A	5.65	1.40	1.33
12	B	1212	CLA	CHB-C4A	5.65	1.40	1.33
12	A	1118	CLA	CHB-C4A	5.65	1.40	1.33
12	A	1113	CLA	CHB-C4A	5.65	1.40	1.33
15	A	4012	BCR	C24-C23	5.66	1.50	1.33
15	A	4007	BCR	C24-C23	5.66	1.50	1.33
12	A	1116	CLA	CHB-C4A	5.67	1.40	1.33
12	B	1219	CLA	CHB-C4A	5.67	1.40	1.33
12	A	1124	CLA	CHB-C4A	5.67	1.40	1.33
15	J	4013	BCR	C24-C23	5.67	1.50	1.33
12	B	1227	CLA	CHB-C4A	5.67	1.40	1.33
12	A	1131	CLA	CHB-C4A	5.68	1.40	1.33
12	B	1221	CLA	CHB-C4A	5.68	1.40	1.33
12	B	1228	CLA	CHB-C4A	5.68	1.40	1.33
12	A	1125	CLA	CHB-C4A	5.68	1.40	1.33
12	B	1218	CLA	CHB-C4A	5.69	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1207	CLA	CHB-C4A	5.69	1.40	1.33
12	B	1216	CLA	CHB-C4A	5.69	1.40	1.33
15	A	4003	BCR	C24-C23	5.69	1.50	1.33
12	B	1203	CLA	CHB-C4A	5.70	1.40	1.33
12	J	1303	CLA	CHB-C4A	5.70	1.40	1.33
12	B	1220	CLA	CHB-C4A	5.70	1.40	1.33
12	K	1402	CLA	CHB-C4A	5.71	1.40	1.33
12	A	1110	CLA	CHB-C4A	5.71	1.40	1.33
12	B	1022	CLA	CHB-C4A	5.71	1.40	1.33
12	A	1136	CLA	CHB-C4A	5.72	1.40	1.33
12	K	1401	CLA	CHB-C4A	5.72	1.40	1.33
15	F	4014	BCR	C24-C23	5.72	1.50	1.33
12	F	1301	CLA	CHB-C4A	5.73	1.40	1.33
12	B	1215	CLA	CHB-C4A	5.73	1.40	1.33
12	F	1302	CLA	CHB-C4A	5.74	1.40	1.33
12	A	1121	CLA	CHB-C4A	5.74	1.40	1.33
15	B	4018	BCR	C24-C23	5.74	1.50	1.33
12	A	1135	CLA	CHB-C4A	5.74	1.40	1.33
12	A	1122	CLA	CHB-C4A	5.74	1.40	1.33
12	A	1105	CLA	CHB-C4A	5.74	1.40	1.33
12	B	1208	CLA	CHB-C4A	5.75	1.40	1.33
12	B	1202	CLA	CHB-C4A	5.75	1.40	1.33
12	B	1213	CLA	CHB-C4A	5.75	1.40	1.33
12	B	1210	CLA	CHB-C4A	5.76	1.40	1.33
15	K	4001	BCR	C24-C23	5.76	1.50	1.33
12	B	1239	CLA	CHB-C4A	5.76	1.40	1.33
12	B	1217	CLA	CHB-C4A	5.76	1.40	1.33
12	A	1114	CLA	CHB-C4A	5.76	1.40	1.33
12	A	1104	CLA	CHB-C4A	5.77	1.40	1.33
12	A	1115	CLA	CHB-C4A	5.77	1.40	1.33
12	B	1214	CLA	CHB-C4A	5.77	1.40	1.33
12	B	1231	CLA	CHB-C4A	5.77	1.40	1.33
12	A	1133	CLA	CHB-C4A	5.77	1.40	1.33
12	B	1223	CLA	CHB-C4A	5.79	1.40	1.33
12	B	1230	CLA	CHB-C4A	5.80	1.40	1.33
12	A	1112	CLA	CHB-C4A	5.80	1.40	1.33
12	B	1237	CLA	CHB-C4A	5.81	1.40	1.33
12	B	1240	CLA	CHB-C4A	5.82	1.40	1.33
12	B	1206	CLA	CHB-C4A	5.82	1.40	1.33
12	B	1204	CLA	CHB-C4A	5.83	1.40	1.33
12	B	1234	CLA	CHB-C4A	5.83	1.40	1.33
12	B	1211	CLA	CHB-C4A	5.83	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1232	CLA	CHB-C4A	5.83	1.40	1.33
12	A	1011	CLA	CHB-C4A	5.84	1.40	1.33
12	B	1021	CLA	CHB-C4A	5.85	1.40	1.33
12	A	1127	CLA	CHB-C4A	5.86	1.40	1.33
12	L	1502	CLA	CHB-C4A	5.86	1.40	1.33
12	B	1222	CLA	CHB-C4A	5.88	1.40	1.33
12	A	1108	CLA	CHB-C4A	5.91	1.40	1.33
12	A	1123	CLA	CHB-C4A	5.99	1.40	1.33
12	B	1205	CLA	CHB-C4A	6.02	1.40	1.33
12	A	1107	CLA	CHB-C4A	6.91	1.41	1.33
15	A	4007	BCR	C10-C9	7.00	1.45	1.35
15	A	4008	BCR	C10-C9	7.07	1.45	1.35
15	A	4012	BCR	C10-C9	7.20	1.45	1.35
15	A	4003	BCR	C10-C9	7.22	1.45	1.35
15	I	4018	BCR	C10-C9	7.26	1.45	1.35
15	B	4018	BCR	C10-C9	7.30	1.45	1.35
15	B	4004	BCR	C10-C9	7.35	1.45	1.35
15	F	4014	BCR	C10-C9	7.35	1.45	1.35
15	B	4017	BCR	C10-C9	7.39	1.45	1.35
15	K	4001	BCR	C10-C9	7.41	1.45	1.35
15	B	4005	BCR	C10-C9	7.49	1.45	1.35
15	J	4013	BCR	C10-C9	7.55	1.45	1.35
15	A	4001	BCR	C10-C9	7.63	1.45	1.35
15	B	4010	BCR	C10-C9	7.83	1.46	1.35
25	I	4020	EQ3	C5-C6	10.76	1.53	1.34
25	I	4020	EQ3	C4-C3	11.15	1.72	1.52
23	J	4015	C7Z	C5-C6	11.56	1.54	1.34
23	F	4016	C7Z	C5-C6	11.75	1.54	1.34
23	F	4016	C7Z	C25-C26	11.89	1.55	1.34
23	J	4015	C7Z	C25-C26	12.12	1.55	1.34
17	B	4011	45D	C08-C16	12.74	1.53	1.35
17	B	4011	45D	C07-C15	13.01	1.53	1.35
25	I	4020	EQ3	C25-C26	13.59	1.54	1.35
23	J	4015	C7Z	C10-C9	13.82	1.54	1.35
23	F	4016	C7Z	C10-C9	14.18	1.54	1.35
23	J	4015	C7Z	C14-C13	14.20	1.54	1.35
23	J	4015	C7Z	C34-C33	14.29	1.54	1.35
23	J	4015	C7Z	C30-C29	14.32	1.54	1.35
23	F	4016	C7Z	C34-C33	14.37	1.54	1.35
23	F	4016	C7Z	C14-C13	14.40	1.54	1.35
23	F	4016	C7Z	C30-C29	14.43	1.54	1.35

All (1073) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	4016	C7Z	C18-C5-C6	-14.88	107.85	124.51
23	J	4015	C7Z	C18-C5-C6	-13.15	109.79	124.51
23	F	4016	C7Z	C38-C25-C26	-11.66	111.45	124.51
23	F	4016	C7Z	C15-C14-C13	-10.95	111.69	127.31
23	J	4015	C7Z	C38-C25-C26	-10.75	112.47	124.51
23	J	4015	C7Z	C11-C10-C9	-10.64	112.12	127.31
23	F	4016	C7Z	C35-C34-C33	-10.61	112.17	127.31
23	J	4015	C7Z	C15-C14-C13	-10.53	112.28	127.31
23	F	4016	C7Z	C31-C30-C29	-9.91	113.17	127.31
23	J	4015	C7Z	C35-C34-C33	-9.87	113.22	127.31
23	J	4015	C7Z	C31-C30-C29	-9.86	113.24	127.31
23	J	4015	C7Z	C19-C9-C10	-9.83	109.16	122.92
23	J	4015	C7Z	C39-C29-C30	-9.65	109.40	122.92
23	F	4016	C7Z	C40-C33-C34	-9.64	109.42	122.92
23	F	4016	C7Z	C11-C10-C9	-9.62	113.58	127.31
23	J	4015	C7Z	C20-C13-C14	-9.61	109.46	122.92
23	F	4016	C7Z	C39-C29-C30	-9.47	109.66	122.92
23	F	4016	C7Z	C19-C9-C10	-9.26	109.95	122.92
23	J	4015	C7Z	C40-C33-C34	-9.23	109.99	122.92
19	M	4021	ECH	C16-C17-C18	-9.20	114.18	127.31
25	I	4020	EQ3	C16-C17-C18	-9.18	114.21	127.31
19	M	4021	ECH	C20-C21-C22	-9.15	114.25	127.31
23	F	4016	C7Z	C20-C13-C14	-9.07	110.22	122.92
19	B	4006	ECH	C16-C17-C18	-8.28	115.49	127.31
23	J	4015	C7Z	C21-C26-C25	-7.80	111.63	122.59
17	B	4011	45D	C20-C24-C26	-7.09	115.56	126.21
23	F	4016	C7Z	C28-C29-C30	-6.88	108.38	118.94
19	B	4006	ECH	C11-C10-C9	-6.85	117.53	127.31
23	J	4015	C7Z	C32-C33-C34	-6.57	108.86	118.94
23	F	4016	C7Z	C8-C9-C10	-6.31	109.25	118.94
23	J	4015	C7Z	C8-C9-C10	-6.23	109.38	118.94
19	M	4021	ECH	C24-C23-C22	-6.13	117.00	126.21
23	J	4015	C7Z	C12-C13-C14	-6.09	109.60	118.94
23	J	4015	C7Z	C28-C29-C30	-5.97	109.77	118.94
19	B	4006	ECH	C20-C21-C22	-5.97	118.79	127.31
23	F	4016	C7Z	C12-C13-C14	-5.93	109.85	118.94
23	J	4015	C7Z	C1-C6-C5	-5.82	114.42	122.59
17	B	4011	45D	C31-C29-C25	-5.76	119.09	127.31
23	F	4016	C7Z	C40-C33-C32	-5.61	109.17	118.10
23	F	4016	C7Z	C19-C9-C8	-5.53	109.29	118.10
25	I	4020	EQ3	C7-C8-C9	-5.50	117.95	126.21
19	B	4006	ECH	C24-C23-C22	-5.42	118.07	126.21
23	F	4016	C7Z	C32-C33-C34	-5.27	110.85	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	4016	C7Z	C20-C13-C12	-5.25	109.73	118.10
23	F	4016	C7Z	C7-C6-C5	-5.22	109.09	121.54
23	J	4015	C7Z	C39-C29-C28	-5.15	109.89	118.10
23	J	4015	C7Z	C20-C13-C12	-5.09	109.99	118.10
23	J	4015	C7Z	C19-C9-C8	-5.06	110.03	118.10
23	J	4015	C7Z	C40-C33-C32	-5.00	110.13	118.10
23	F	4016	C7Z	C39-C29-C28	-4.99	110.16	118.10
23	F	4016	C7Z	C27-C26-C25	-4.97	109.70	121.54
17	B	4011	45D	C41-C37-C35	-4.71	120.58	127.31
19	B	4006	ECH	C28-C27-C26	-4.69	114.71	118.79
25	I	4020	EQ3	C33-C5-C6	-4.63	119.32	124.51
23	F	4016	C7Z	C18-C5-C4	-4.61	105.86	114.34
19	M	4021	ECH	C20-C19-C18	-4.56	113.59	126.42
19	B	4006	ECH	C33-C5-C6	-4.54	119.42	124.51
25	I	4020	EQ3	C16-C15-C14	-4.47	113.92	123.46
23	J	4015	C7Z	C27-C28-C29	-4.38	119.64	126.21
23	F	4016	C7Z	C21-C26-C25	-4.35	116.48	122.59
19	B	4006	ECH	C16-C15-C14	-4.31	114.26	123.46
15	B	4004	BCR	C33-C5-C6	-4.23	119.77	124.51
23	J	4015	C7Z	C18-C5-C4	-4.23	106.56	114.34
15	A	4001	BCR	C15-C14-C13	-4.22	121.29	127.31
23	J	4015	C7Z	C7-C6-C5	-4.19	111.56	121.54
15	J	4013	BCR	C33-C5-C6	-4.15	119.86	124.51
12	B	1222	CLA	C1-C2-C3	-4.15	120.03	126.77
19	M	4021	ECH	C28-C27-C26	-4.13	115.20	118.79
19	M	4021	ECH	C16-C15-C14	-4.13	114.65	123.46
12	A	1101	CLA	CAA-C2A-C3A	-4.09	101.59	112.81
19	M	4021	ECH	C33-C5-C6	-4.04	119.98	124.51
15	B	4010	BCR	C15-C14-C13	-4.04	121.54	127.31
15	B	4004	BCR	C15-C14-C13	-4.00	121.60	127.31
23	F	4016	C7Z	C1-C6-C5	-3.98	117.00	122.59
19	M	4021	ECH	C11-C10-C9	-3.94	121.68	127.31
15	B	4005	BCR	C33-C5-C6	-3.93	120.11	124.51
15	A	4003	BCR	C33-C5-C6	-3.89	120.15	124.51
15	B	4018	BCR	C36-C18-C17	-3.87	117.50	122.92
23	J	4015	C7Z	C7-C8-C9	-3.87	120.40	126.21
15	A	4012	BCR	C33-C5-C6	-3.80	120.25	124.51
19	M	4021	ECH	C7-C8-C9	-3.79	120.52	126.21
12	B	1021	CLA	C1-C2-C3	-3.79	118.98	125.96
21	F	5001	SQD	O7-S-C6	-3.77	102.45	106.94
12	B	1235	CLA	C1-C2-C3	-3.73	119.09	125.96
23	F	4016	C7Z	C7-C8-C9	-3.72	120.62	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	4018	BCR	C27-C26-C25	-3.66	117.37	122.74
12	A	1118	CLA	C1-C2-C3	-3.62	120.90	126.77
15	I	4018	BCR	C4-C5-C6	-3.60	117.45	122.74
17	B	4011	45D	C42-C38-C36	-3.59	122.18	127.31
25	I	4020	EQ3	C21-C20-C19	-3.58	112.35	123.26
25	I	4020	EQ3	C36-C18-C17	-3.55	117.96	122.92
15	B	4017	BCR	C33-C5-C6	-3.53	120.56	124.51
17	B	4011	45D	C22-C16-C08	-3.52	118.45	124.11
15	A	4007	BCR	C33-C5-C6	-3.50	120.59	124.51
21	B	5008	SQD	O7-S-C6	-3.50	102.78	106.94
12	A	1105	CLA	C1-C2-C3	-3.47	119.57	125.96
15	B	4018	BCR	C30-C25-C26	-3.45	117.74	122.59
15	A	4012	BCR	C36-C18-C17	-3.45	118.09	122.92
15	B	4010	BCR	C28-C27-C26	-3.43	107.98	113.99
12	A	1139	CLA	C1-C2-C3	-3.43	119.65	125.96
19	B	4006	ECH	C11-C12-C13	-3.39	116.90	126.42
17	B	4011	45D	C28-C26-C30	-3.38	118.19	122.92
15	J	4013	BCR	C15-C14-C13	-3.36	122.52	127.31
15	F	4014	BCR	C36-C18-C17	-3.36	118.22	122.92
15	K	4001	BCR	C36-C18-C17	-3.35	118.22	122.92
12	B	1224	CLA	C1-C2-C3	-3.35	119.78	125.96
23	J	4015	C7Z	C24-C25-C26	-3.35	113.22	120.86
23	F	4016	C7Z	C28-C27-C26	-3.34	117.90	127.25
25	I	4020	EQ3	C2-C3-C4	-3.27	105.81	110.28
23	J	4015	C7Z	C4-C5-C6	-3.23	113.50	120.86
12	B	1202	CLA	C1-C2-C3	-3.22	120.02	125.96
19	B	4006	ECH	C20-C19-C18	-3.20	117.44	126.42
15	B	4005	BCR	C23-C24-C25	-3.19	118.32	127.25
15	B	4017	BCR	C15-C14-C13	-3.19	122.76	127.31
15	I	4018	BCR	C1-C6-C5	-3.19	118.11	122.59
15	K	4001	BCR	C33-C5-C6	-3.14	121.00	124.51
15	B	4010	BCR	C37-C22-C21	-3.11	118.57	122.92
12	A	1138	CLA	C1-C2-C3	-3.10	120.25	125.96
15	B	4010	BCR	C33-C5-C6	-3.09	121.05	124.51
17	B	4011	45D	C19-C23-C25	-3.07	121.60	126.21
15	K	4001	BCR	C37-C22-C21	-3.07	118.62	122.92
13	B	2002	PQN	C11-C12-C13	-3.06	121.61	126.79
15	K	4001	BCR	C15-C14-C13	-3.06	122.95	127.31
12	B	1229	CLA	C1-C2-C3	-3.05	120.33	125.96
17	B	4011	45D	C23-C19-C07	-3.03	118.76	127.25
15	A	4003	BCR	C36-C18-C17	-3.01	118.70	122.92
15	A	4001	BCR	C33-C5-C6	-3.01	121.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	4017	BCR	C36-C18-C17	-3.01	118.71	122.92
12	B	1234	CLA	C1-C2-C3	-3.00	120.42	125.96
15	B	4018	BCR	C4-C5-C6	-2.99	118.36	122.74
12	A	1132	CLA	C1-C2-C3	-2.99	120.46	125.96
15	B	4005	BCR	C27-C26-C25	-2.98	118.36	122.74
25	I	4020	EQ3	C34-C9-C10	-2.98	118.75	122.92
16	B	5006	LHG	C5-O7-C7	-2.97	112.30	117.91
12	A	1109	CLA	C1-C2-C3	-2.95	120.52	125.96
12	A	1106	CLA	C1-C2-C3	-2.94	120.54	125.96
12	B	1202	CLA	O2D-CGD-O1D	-2.94	117.98	123.82
19	B	4006	ECH	C8-C7-C6	-2.93	119.05	127.25
23	F	4016	C7Z	C24-C25-C26	-2.93	114.19	120.86
15	B	4010	BCR	C27-C26-C25	-2.92	118.45	122.74
15	I	4018	BCR	C23-C24-C25	-2.92	119.08	127.25
15	A	4008	BCR	C15-C14-C13	-2.92	123.15	127.31
15	F	4014	BCR	C33-C5-C6	-2.92	121.24	124.51
12	A	1125	CLA	OBD-CAD-C3D	-2.90	122.81	128.09
12	A	1123	CLA	C1-C2-C3	-2.90	120.61	125.96
15	B	4017	BCR	C23-C24-C25	-2.90	119.14	127.25
12	B	1022	CLA	C1-C2-C3	-2.89	120.64	125.96
15	A	4008	BCR	C36-C18-C17	-2.86	118.91	122.92
12	A	1115	CLA	C1-C2-C3	-2.86	120.68	125.96
19	B	4006	ECH	C7-C8-C9	-2.86	121.92	126.21
12	A	1012	CLA	OBD-CAD-C3D	-2.85	122.90	128.09
12	A	1011	CLA	C1-C2-C3	-2.85	120.70	125.96
12	B	1230	CLA	O2D-CGD-O1D	-2.84	118.17	123.82
12	A	1102	CLA	C1-C2-C3	-2.84	120.72	125.96
12	B	1226	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
12	L	1502	CLA	O2D-CGD-O1D	-2.82	118.22	123.82
15	A	4008	BCR	C34-C9-C10	-2.81	118.98	122.92
12	B	1022	CLA	OBD-CAD-C3D	-2.80	123.00	128.09
12	B	1238	CLA	O1D-CGD-CBD	-2.79	119.40	124.58
15	I	4018	BCR	C38-C26-C25	-2.79	121.39	124.51
15	A	4001	BCR	C37-C22-C21	-2.76	119.05	122.92
15	A	4008	BCR	C33-C5-C6	-2.76	121.42	124.51
12	A	1140	CLA	C1-C2-C3	-2.76	120.87	125.96
19	M	4021	ECH	C11-C12-C13	-2.75	118.69	126.42
15	A	4007	BCR	C36-C18-C17	-2.73	119.09	122.92
17	B	4011	45D	C41-C42-C38	-2.73	117.64	123.46
12	B	1227	CLA	O2D-CGD-O1D	-2.72	118.42	123.82
15	A	4008	BCR	C37-C22-C21	-2.72	119.11	122.92
15	I	4018	BCR	C34-C9-C10	-2.72	119.12	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1123	CLA	C1C-NC-C4C	-2.71	105.52	107.05
17	B	4011	45D	C30-C32-C34	-2.71	115.00	123.26
12	B	1240	CLA	O2D-CGD-O1D	-2.70	118.47	123.82
12	A	1011	CLA	O1D-CGD-CBD	-2.69	119.59	124.58
23	F	4016	C7Z	C38-C25-C24	-2.69	109.40	114.34
24	F	6001	LMT	C3'-C4'-C5'	-2.68	104.70	110.93
12	A	1101	CLA	O2D-CGD-O1D	-2.68	118.50	123.82
20	B	5005	LMG	C8-O7-C10	-2.67	111.56	117.88
15	J	4013	BCR	C36-C18-C17	-2.67	119.18	122.92
12	B	1220	CLA	C1C-NC-C4C	-2.67	105.55	107.05
12	B	1234	CLA	O2D-CGD-O1D	-2.67	118.53	123.82
12	F	1302	CLA	O2D-CGD-O1D	-2.66	118.54	123.82
15	A	4007	BCR	C27-C26-C25	-2.66	118.84	122.74
15	F	4014	BCR	C37-C22-C21	-2.66	119.20	122.92
15	F	4014	BCR	C34-C9-C10	-2.66	119.20	122.92
12	A	1128	CLA	O2D-CGD-O1D	-2.65	118.55	123.82
12	A	1120	CLA	O2D-CGD-O1D	-2.64	118.59	123.82
13	A	2001	PQN	C11-C12-C13	-2.63	122.33	126.79
12	B	1209	CLA	O2D-CGD-O1D	-2.63	118.60	123.82
25	I	4020	EQ3	C38-C26-C25	-2.62	119.89	124.11
19	M	4021	ECH	C15-C14-C13	-2.62	123.56	127.31
19	B	4006	ECH	C23-C24-C25	-2.61	119.93	127.25
12	K	1401	CLA	O2D-CGD-O1D	-2.61	118.63	123.82
12	A	1104	CLA	O2D-CGD-O1D	-2.61	118.64	123.82
12	B	1236	CLA	O2D-CGD-O1D	-2.61	118.64	123.82
12	A	1103	CLA	O2D-CGD-O1D	-2.61	118.64	123.82
17	B	4011	45D	C21-C15-C07	-2.61	119.92	124.11
15	B	4018	BCR	C28-C27-C26	-2.61	109.42	113.99
12	A	1012	CLA	O2D-CGD-O1D	-2.60	118.66	123.82
15	A	4007	BCR	C23-C24-C25	-2.60	119.98	127.25
12	B	1213	CLA	O2D-CGD-O1D	-2.59	118.67	123.82
12	B	1205	CLA	O1D-CGD-CBD	-2.59	119.77	124.58
12	A	1135	CLA	O2D-CGD-O1D	-2.59	118.68	123.82
12	J	1303	CLA	O2D-CGD-O1D	-2.58	118.69	123.82
12	B	1205	CLA	O2D-CGD-O1D	-2.58	118.71	123.82
15	A	4001	BCR	C27-C26-C25	-2.57	118.96	122.74
12	A	1126	CLA	C1-C2-C3	-2.57	121.22	125.96
15	B	4017	BCR	C27-C26-C25	-2.56	118.98	122.74
15	A	4001	BCR	C36-C18-C17	-2.56	119.33	122.92
15	B	4018	BCR	C34-C9-C10	-2.56	119.34	122.92
16	A	5001	LHG	C5-O7-C7	-2.56	111.84	117.88
12	B	1213	CLA	O1D-CGD-CBD	-2.55	119.85	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	F	6001	LMT	C1'-O5'-C5'	-2.55	108.68	113.71
12	K	1402	CLA	CAA-C2A-C3A	-2.55	105.82	112.81
12	A	1113	CLA	O2D-CGD-O1D	-2.55	118.76	123.82
12	A	1112	CLA	O2D-CGD-O1D	-2.55	118.76	123.82
12	B	1222	CLA	O2D-CGD-O1D	-2.54	118.78	123.82
12	B	1207	CLA	O2D-CGD-O1D	-2.54	118.78	123.82
12	A	1128	CLA	C1-C2-C3	-2.54	121.28	125.96
12	B	1214	CLA	C1-C2-C3	-2.54	121.28	125.96
12	A	1106	CLA	O2D-CGD-O1D	-2.53	118.79	123.82
15	B	4004	BCR	C37-C22-C21	-2.53	119.38	122.92
12	J	1302	CLA	O2D-CGD-O1D	-2.53	118.80	123.82
12	B	1227	CLA	O1D-CGD-CBD	-2.53	119.89	124.58
12	A	1141	CLA	O2D-CGD-O1D	-2.53	118.81	123.82
12	A	1110	CLA	O2D-CGD-O1D	-2.53	118.81	123.82
12	A	1116	CLA	O2D-CGD-O1D	-2.52	118.81	123.82
12	B	1022	CLA	C1C-NC-C4C	-2.52	105.63	107.05
12	B	1205	CLA	C1C-NC-C4C	-2.52	105.63	107.05
15	B	4010	BCR	C4-C5-C6	-2.52	119.04	122.74
12	B	1229	CLA	O1D-CGD-CBD	-2.51	119.92	124.58
12	B	1208	CLA	O2D-CGD-O1D	-2.50	118.85	123.82
12	B	1220	CLA	O2D-CGD-O1D	-2.50	118.85	123.82
12	A	1106	CLA	O1D-CGD-CBD	-2.50	119.95	124.58
12	B	1201	CLA	O2D-CGD-O1D	-2.50	118.87	123.82
12	B	1219	CLA	O2D-CGD-O1D	-2.50	118.87	123.82
12	B	1229	CLA	O2D-CGD-O1D	-2.49	118.88	123.82
12	A	1128	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
15	J	4013	BCR	C34-C9-C10	-2.49	119.44	122.92
15	B	4005	BCR	C15-C14-C13	-2.49	123.76	127.31
12	B	1221	CLA	O1D-CGD-CBD	-2.48	119.97	124.58
12	B	1226	CLA	O1D-CGD-CBD	-2.48	119.98	124.58
12	B	1210	CLA	O2D-CGD-O1D	-2.48	118.89	123.82
12	B	1221	CLA	O2D-CGD-O1D	-2.48	118.90	123.82
12	B	1239	CLA	C1C-NC-C4C	-2.48	105.65	107.05
12	B	1234	CLA	C1C-NC-C4C	-2.48	105.65	107.05
25	I	4020	EQ3	C10-C11-C12	-2.48	115.72	123.26
12	A	1134	CLA	O2D-CGD-O1D	-2.48	118.91	123.82
12	B	1224	CLA	O1D-CGD-CBD	-2.47	120.00	124.58
23	J	4015	C7Z	C1-C6-C7	-2.47	108.80	115.73
12	A	1140	CLA	O2D-CGD-O1D	-2.47	118.92	123.82
12	B	1206	CLA	C1C-NC-C4C	-2.46	105.66	107.05
12	A	1136	CLA	O2D-CGD-O1D	-2.46	118.94	123.82
12	A	1139	CLA	O2D-CGD-O1D	-2.46	118.94	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	4011	45D	C31-C33-C35	-2.45	119.53	126.42
16	A	5003	LHG	C5-O7-C7	-2.44	112.10	117.88
15	A	4001	BCR	C4-C5-C6	-2.44	119.16	122.74
12	A	1111	CLA	O2D-CGD-O1D	-2.44	118.97	123.82
15	A	4012	BCR	C37-C22-C21	-2.44	119.50	122.92
15	A	4007	BCR	C15-C14-C13	-2.43	123.84	127.31
12	B	1239	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
12	A	1121	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
12	A	1108	CLA	O2D-CGD-O1D	-2.42	119.01	123.82
12	B	1212	CLA	O2D-CGD-O1D	-2.42	119.01	123.82
16	B	5004	LHG	C5-O7-C7	-2.42	112.15	117.88
12	A	1105	CLA	O2D-CGD-O1D	-2.42	119.01	123.82
25	I	4020	EQ3	C7-C6-C5	-2.42	115.78	121.54
12	A	1102	CLA	O2D-CGD-O1D	-2.42	119.03	123.82
15	B	4018	BCR	C1-C6-C5	-2.41	119.20	122.59
12	B	1235	CLA	O2D-CGD-O1D	-2.41	119.04	123.82
15	B	4004	BCR	C34-C9-C10	-2.41	119.55	122.92
12	A	1124	CLA	O2D-CGD-O1D	-2.40	119.05	123.82
15	A	4001	BCR	C34-C9-C10	-2.40	119.56	122.92
12	B	1240	CLA	O1D-CGD-CBD	-2.39	120.14	124.58
12	B	1022	CLA	O2D-CGD-O1D	-2.39	119.07	123.82
23	F	4016	C7Z	C31-C32-C33	-2.39	119.70	126.42
19	M	4021	ECH	C8-C7-C6	-2.39	120.56	127.25
12	A	1127	CLA	O2D-CGD-O1D	-2.39	119.08	123.82
12	A	1123	CLA	O1D-CGD-CBD	-2.39	120.15	124.58
15	I	4018	BCR	C15-C14-C13	-2.39	123.90	127.31
15	A	4003	BCR	C34-C9-C10	-2.39	119.58	122.92
12	B	1218	CLA	O2D-CGD-O1D	-2.37	119.11	123.82
12	B	1209	CLA	O1D-CGD-CBD	-2.37	120.18	124.58
12	A	1102	CLA	O1D-CGD-CBD	-2.37	120.18	124.58
15	J	4013	BCR	C37-C22-C21	-2.37	119.60	122.92
12	A	1130	CLA	O2D-CGD-O1D	-2.37	119.11	123.82
12	B	1232	CLA	O2D-CGD-O1D	-2.37	119.11	123.82
12	A	1125	CLA	O2D-CGD-O1D	-2.37	119.12	123.82
12	B	1217	CLA	O2D-CGD-O1D	-2.37	119.13	123.82
12	A	1118	CLA	O2D-CGD-O1D	-2.36	119.13	123.82
12	F	1301	CLA	O2D-CGD-O1D	-2.36	119.13	123.82
12	B	1207	CLA	C1C-NC-C4C	-2.36	105.72	107.05
12	B	1211	CLA	O2D-CGD-O1D	-2.36	119.14	123.82
12	B	1216	CLA	O2D-CGD-O1D	-2.36	119.14	123.82
12	A	1128	CLA	O1D-CGD-CBD	-2.36	120.21	124.58
12	B	1228	CLA	O1D-CGD-CBD	-2.35	120.22	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1215	CLA	C1C-NC-C4C	-2.35	105.72	107.05
12	A	1129	CLA	O2D-CGD-O1D	-2.35	119.15	123.82
12	A	1105	CLA	O1D-CGD-CBD	-2.35	120.22	124.58
12	A	1012	CLA	C1C-NC-C4C	-2.35	105.72	107.05
12	B	1223	CLA	O2D-CGD-O1D	-2.35	119.16	123.82
12	B	1213	CLA	C1C-NC-C4C	-2.34	105.73	107.05
12	A	1134	CLA	O1D-CGD-CBD	-2.33	120.27	124.58
12	A	1131	CLA	O2D-CGD-O1D	-2.32	119.21	123.82
23	J	4015	C7Z	C27-C26-C25	-2.32	116.00	121.54
12	B	1236	CLA	C1C-NC-C4C	-2.32	105.74	107.05
12	B	1226	CLA	O2D-CGD-O1D	-2.32	119.22	123.82
12	A	1134	CLA	C1C-NC-C4C	-2.32	105.74	107.05
12	B	1217	CLA	C1C-NC-C4C	-2.31	105.75	107.05
12	B	1023	CLA	O2D-CGD-O1D	-2.30	119.25	123.82
12	B	1214	CLA	C1C-NC-C4C	-2.30	105.75	107.05
12	A	1112	CLA	O1D-CGD-CBD	-2.30	120.32	124.58
12	A	1117	CLA	O1D-CGD-CBD	-2.30	120.32	124.58
12	A	1109	CLA	O2D-CGD-O1D	-2.29	119.27	123.82
12	A	1137	CLA	O2D-CGD-O1D	-2.29	119.27	123.82
12	B	1221	CLA	C1C-NC-C4C	-2.29	105.76	107.05
12	A	1113	CLA	C1C-NC-C4C	-2.29	105.76	107.05
12	A	1123	CLA	O2D-CGD-O1D	-2.29	119.27	123.82
15	A	4008	BCR	C38-C26-C25	-2.29	121.95	124.51
12	A	1119	CLA	O2D-CGD-O1D	-2.29	119.28	123.82
12	B	1240	CLA	C1C-NC-C4C	-2.29	105.76	107.05
12	B	1204	CLA	O2D-CGD-O1D	-2.29	119.28	123.82
12	A	1115	CLA	O2D-CGD-O1D	-2.28	119.29	123.82
21	B	5008	SQD	O3-C3-C2	-2.28	105.01	110.34
12	A	1126	CLA	OBD-CAD-C3D	-2.28	123.94	128.09
12	B	1211	CLA	O1D-CGD-CBD	-2.28	120.35	124.58
23	F	4016	C7Z	C1-C6-C7	-2.28	109.33	115.73
12	A	1115	CLA	O1D-CGD-CBD	-2.28	120.35	124.58
12	B	1215	CLA	O2D-CGD-O1D	-2.28	119.30	123.82
12	B	1230	CLA	O1D-CGD-CBD	-2.28	120.35	124.58
12	A	1109	CLA	CAA-C2A-C3A	-2.28	106.56	112.81
12	A	1135	CLA	O1D-CGD-CBD	-2.28	120.36	124.58
12	F	1302	CLA	O1D-CGD-CBD	-2.28	120.36	124.58
12	B	1223	CLA	C1C-NC-C4C	-2.28	105.77	107.05
12	B	1232	CLA	C1C-NC-C4C	-2.27	105.77	107.05
12	A	1135	CLA	C1C-NC-C4C	-2.27	105.77	107.05
12	A	1013	CLA	O2D-CGD-O1D	-2.27	119.32	123.82
12	A	1111	CLA	C1C-NC-C4C	-2.27	105.77	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1126	CLA	O2D-CGD-O1D	-2.26	119.33	123.82
12	B	1204	CLA	C1C-NC-C4C	-2.26	105.78	107.05
12	F	1301	CLA	C1C-NC-C4C	-2.26	105.78	107.05
12	L	1502	CLA	C1C-NC-C4C	-2.25	105.78	107.05
12	B	1228	CLA	O2D-CGD-O1D	-2.25	119.36	123.82
12	A	1125	CLA	O1D-CGD-CBD	-2.25	120.41	124.58
15	A	4012	BCR	C23-C24-C25	-2.24	120.97	127.25
15	A	4001	BCR	C8-C7-C6	-2.24	120.97	127.25
15	J	4013	BCR	C23-C24-C25	-2.24	120.97	127.25
12	K	1402	CLA	O2D-CGD-O1D	-2.24	119.37	123.82
12	A	1116	CLA	O1D-CGD-CBD	-2.24	120.42	124.58
15	K	4001	BCR	C38-C26-C25	-2.24	122.00	124.51
15	I	4018	BCR	C23-C22-C21	-2.24	115.51	118.94
12	A	1114	CLA	O2D-CGD-O1D	-2.23	119.39	123.82
12	A	1112	CLA	C1C-NC-C4C	-2.23	105.79	107.05
12	B	1231	CLA	C1C-NC-C4C	-2.23	105.79	107.05
12	B	1237	CLA	O2D-CGD-O1D	-2.23	119.40	123.82
12	B	1217	CLA	O1D-CGD-CBD	-2.23	120.45	124.58
21	F	5001	SQD	O3-C3-C2	-2.23	105.14	110.34
15	B	4004	BCR	C38-C26-C25	-2.23	122.02	124.51
12	B	1230	CLA	C1C-NC-C4C	-2.23	105.80	107.05
19	M	4021	ECH	C23-C24-C25	-2.23	121.02	127.25
12	A	1116	CLA	OBD-CAD-C3D	-2.22	124.05	128.09
12	J	1303	CLA	O1D-CGD-CBD	-2.22	120.46	124.58
17	B	4011	45D	C27-C25-C29	-2.22	119.81	122.92
15	A	4003	BCR	C23-C24-C25	-2.22	121.04	127.25
12	A	1133	CLA	O1D-CGD-CBD	-2.22	120.47	124.58
12	B	1213	CLA	CAA-C2A-C3A	-2.22	106.73	112.81
12	B	1021	CLA	O1D-CGD-CBD	-2.22	120.47	124.58
12	A	1107	CLA	CAA-C2A-C3A	-2.22	106.73	112.81
12	A	1133	CLA	O2D-CGD-O1D	-2.22	119.42	123.82
12	J	1302	CLA	O1D-CGD-CBD	-2.21	120.47	124.58
12	B	1212	CLA	C1C-NC-C4C	-2.21	105.80	107.05
12	B	1210	CLA	C1C-NC-C4C	-2.21	105.80	107.05
12	B	1215	CLA	O1D-CGD-CBD	-2.21	120.48	124.58
12	B	1214	CLA	O1D-CGD-CBD	-2.20	120.49	124.58
12	A	1132	CLA	O1D-CGD-CBD	-2.20	120.49	124.58
15	B	4005	BCR	C34-C9-C10	-2.20	119.84	122.92
12	A	1131	CLA	C1C-NC-C4C	-2.20	105.81	107.05
12	A	1122	CLA	O2D-CGD-O1D	-2.19	119.47	123.82
12	B	1225	CLA	O2D-CGD-O1D	-2.19	119.47	123.82
12	A	1124	CLA	O1D-CGD-CBD	-2.19	120.52	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1136	CLA	O1D-CGD-CBD	-2.19	120.53	124.58
12	A	1130	CLA	C1C-NC-C4C	-2.18	105.82	107.05
15	J	4013	BCR	C38-C26-C25	-2.18	122.06	124.51
12	B	1236	CLA	O1D-CGD-CBD	-2.18	120.53	124.58
12	A	1011	CLA	OBD-CAD-C3D	-2.18	124.12	128.09
23	F	4016	C7Z	C4-C5-C6	-2.18	115.88	120.86
12	A	1013	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
12	B	1209	CLA	C1C-NC-C4C	-2.18	105.82	107.05
15	A	4007	BCR	C31-C1-C6	-2.18	106.78	110.31
12	K	1402	CLA	OBD-CAD-C3D	-2.18	124.13	128.09
12	A	1126	CLA	O1D-CGD-CBD	-2.18	120.54	124.58
12	A	1102	CLA	CAA-CBA-CGA	-2.18	106.85	113.35
12	B	1232	CLA	CAA-C2A-C3A	-2.18	106.85	112.81
12	J	1302	CLA	C1C-NC-C4C	-2.17	105.82	107.05
12	A	1133	CLA	C1C-NC-C4C	-2.17	105.83	107.05
12	A	1108	CLA	C1C-NC-C4C	-2.17	105.83	107.05
12	A	1125	CLA	C1C-NC-C4C	-2.17	105.83	107.05
12	B	1211	CLA	C1C-NC-C4C	-2.17	105.83	107.05
12	A	1011	CLA	O2D-CGD-O1D	-2.17	119.52	123.82
12	B	1219	CLA	C1C-NC-C4C	-2.16	105.83	107.05
12	B	1237	CLA	O1D-CGD-CBD	-2.16	120.57	124.58
12	B	1207	CLA	CAA-C2A-C3A	-2.16	106.89	112.81
15	B	4004	BCR	C23-C24-C25	-2.16	121.21	127.25
12	B	1238	CLA	O2D-CGD-O1D	-2.15	119.55	123.82
12	A	1114	CLA	O1D-CGD-CBD	-2.15	120.59	124.58
12	A	1013	CLA	CAA-C2A-C3A	-2.15	106.92	112.81
12	B	1235	CLA	O1D-CGD-CBD	-2.15	120.60	124.58
12	A	1130	CLA	O1D-CGD-CBD	-2.15	120.60	124.58
12	B	1237	CLA	C1C-NC-C4C	-2.14	105.84	107.05
12	B	1206	CLA	OBD-CAD-C3D	-2.14	124.20	128.09
15	A	4007	BCR	C37-C22-C21	-2.14	119.93	122.92
12	B	1235	CLA	C1C-NC-C4C	-2.14	105.84	107.05
12	B	1214	CLA	OBD-CAD-C3D	-2.14	124.21	128.09
12	A	1137	CLA	C1C-NC-C4C	-2.13	105.85	107.05
12	B	1212	CLA	O1D-CGD-CBD	-2.13	120.63	124.58
12	A	1131	CLA	O1D-CGD-CBD	-2.13	120.63	124.58
12	F	1302	CLA	C1C-NC-C4C	-2.13	105.85	107.05
12	A	1135	CLA	OBD-CAD-C3D	-2.13	124.22	128.09
12	K	1401	CLA	O1D-CGD-CBD	-2.12	120.64	124.58
12	A	1138	CLA	C1C-NC-C4C	-2.12	105.85	107.05
12	B	1223	CLA	OBD-CAD-C3D	-2.12	124.23	128.09
15	A	4012	BCR	C38-C26-C25	-2.12	122.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1122	CLA	C1C-NC-C4C	-2.12	105.86	107.05
15	A	4003	BCR	C27-C26-C25	-2.11	119.64	122.74
12	B	1219	CLA	O1D-CGD-CBD	-2.11	120.66	124.58
12	A	1132	CLA	CAA-C2A-C3A	-2.11	107.02	112.81
12	A	1140	CLA	CAA-C2A-C3A	-2.11	107.03	112.81
12	A	1118	CLA	O1D-CGD-CBD	-2.11	120.67	124.58
12	B	1022	CLA	O1D-CGD-CBD	-2.11	120.67	124.58
12	B	1202	CLA	C1C-NC-C4C	-2.11	105.86	107.05
12	B	1204	CLA	O1D-CGD-CBD	-2.11	120.67	124.58
12	A	1122	CLA	OBD-CAD-C3D	-2.10	124.27	128.09
15	B	4005	BCR	C30-C25-C26	-2.10	119.64	122.59
15	A	4003	BCR	C38-C26-C25	-2.10	122.16	124.51
23	J	4015	C7Z	C38-C25-C24	-2.10	110.48	114.34
25	I	4020	EQ3	C1-C6-C5	-2.10	119.65	122.59
15	F	4014	BCR	C31-C1-C6	-2.09	106.91	110.31
12	A	1125	CLA	CAA-C2A-C3A	-2.09	107.07	112.81
15	B	4010	BCR	C36-C18-C17	-2.09	119.99	122.92
12	B	1223	CLA	O1D-CGD-CBD	-2.09	120.71	124.58
12	A	1121	CLA	O1D-CGD-CBD	-2.09	120.71	124.58
12	A	1129	CLA	C1C-NC-C4C	-2.09	105.87	107.05
23	F	4016	C7Z	C11-C12-C13	-2.09	120.55	126.42
12	B	1218	CLA	O1D-CGD-CBD	-2.09	120.71	124.58
12	B	1203	CLA	O2D-CGD-O1D	-2.09	119.68	123.82
15	A	4007	BCR	C30-C25-C26	-2.09	119.66	122.59
12	A	1136	CLA	C1C-NC-C4C	-2.09	105.87	107.05
12	A	1110	CLA	C1C-NC-C4C	-2.09	105.87	107.05
12	L	1502	CLA	O1D-CGD-CBD	-2.08	120.72	124.58
23	J	4015	C7Z	C11-C12-C13	-2.08	120.57	126.42
12	B	1021	CLA	O2D-CGD-O1D	-2.08	119.70	123.82
15	B	4010	BCR	C34-C9-C10	-2.08	120.01	122.92
12	B	1207	CLA	O1D-CGD-CBD	-2.08	120.73	124.58
23	F	4016	C7Z	C27-C28-C29	-2.08	123.09	126.21
25	I	4020	EQ3	C15-C14-C13	-2.08	124.35	127.31
12	A	1113	CLA	O1D-CGD-CBD	-2.08	120.73	124.58
12	B	1203	CLA	C1C-NC-C4C	-2.07	105.88	107.05
12	A	1117	CLA	O2D-CGD-O1D	-2.07	119.71	123.82
12	F	1301	CLA	O1D-CGD-CBD	-2.06	120.75	124.58
12	A	1138	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
20	B	5002	LMG	O8-C28-O10	-2.06	118.55	123.58
12	B	1216	CLA	C1C-NC-C4C	-2.06	105.89	107.05
12	A	1122	CLA	O1D-CGD-CBD	-2.06	120.76	124.58
12	B	1215	CLA	OBD-CAD-C3D	-2.06	124.34	128.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1220	CLA	O1D-CGD-CBD	-2.06	120.76	124.58
25	I	4020	EQ3	C11-C10-C9	-2.06	124.37	127.31
12	A	1124	CLA	C1C-NC-C4C	-2.06	105.89	107.05
12	K	1402	CLA	CAA-CBA-CGA	-2.05	107.22	113.35
12	B	1210	CLA	O1D-CGD-CBD	-2.05	120.78	124.58
12	A	1120	CLA	C1C-NC-C4C	-2.05	105.90	107.05
15	B	4017	BCR	C34-C9-C10	-2.05	120.06	122.92
12	B	1214	CLA	O2D-CGD-O1D	-2.05	119.76	123.82
12	A	1114	CLA	C1C-NC-C4C	-2.04	105.90	107.05
12	J	1303	CLA	C1C-NC-C4C	-2.04	105.90	107.05
12	A	1101	CLA	O1D-CGD-CBD	-2.04	120.79	124.58
15	I	4018	BCR	C33-C5-C6	-2.04	122.22	124.51
12	B	1229	CLA	CAA-C2A-C1A	-2.04	105.29	111.97
16	A	5001	LHG	C37-C36-C35	-2.04	95.66	115.39
12	B	1201	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
12	A	1137	CLA	O1D-CGD-CBD	-2.04	120.80	124.58
12	B	1218	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
12	B	1228	CLA	C1C-NC-C4C	-2.03	105.91	107.05
12	B	1206	CLA	O2D-CGD-O1D	-2.03	119.80	123.82
12	A	1107	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
15	F	4014	BCR	C4-C5-C6	-2.02	119.77	122.74
12	B	1206	CLA	O1D-CGD-CBD	-2.02	120.83	124.58
12	A	1118	CLA	C1C-NC-C4C	-2.02	105.91	107.05
12	K	1401	CLA	C1C-NC-C4C	-2.02	105.91	107.05
12	A	1101	CLA	C1C-NC-C4C	-2.02	105.91	107.05
12	A	1104	CLA	C1C-NC-C4C	-2.02	105.91	107.05
12	L	1502	CLA	OBD-CAD-C3D	-2.02	124.42	128.09
12	A	1116	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
12	B	1208	CLA	C1C-NC-C4C	-2.02	105.91	107.05
15	A	4001	BCR	C35-C13-C14	-2.01	120.11	122.92
15	B	4004	BCR	C27-C26-C25	-2.01	119.79	122.74
19	M	4021	ECH	C7-C6-C5	-2.01	116.76	121.54
12	A	1110	CLA	OBD-CAD-C3D	-2.01	124.44	128.09
12	B	1220	CLA	CAA-CBA-CGA	-2.01	107.36	113.35
15	A	4008	BCR	C4-C5-C6	-2.00	119.80	122.74
12	A	1117	CLA	CMB-C2B-C1B	-2.00	125.38	128.46
12	B	1216	CLA	O1D-CGD-CBD	-2.00	120.87	124.58
12	B	1226	CLA	CAA-C2A-C3A	-2.00	107.32	112.81
12	A	1103	CLA	C4A-NA-C1A	2.00	108.91	106.32
12	B	1021	CLA	C4A-NA-C1A	2.01	108.91	106.32
19	B	4006	ECH	O27-C27-C26	2.01	122.68	120.92
12	A	1124	CLA	CMB-C2B-C3B	2.01	128.54	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	I	4020	EQ3	C35-C13-C12	2.01	121.30	118.10
12	A	1118	CLA	CMB-C2B-C3B	2.03	128.57	124.88
12	B	1021	CLA	CMB-C2B-C3B	2.03	128.57	124.88
12	B	1235	CLA	C1-O2A-CGA	2.03	121.44	116.77
12	A	1133	CLA	C1-O2A-CGA	2.03	121.46	116.77
12	B	1203	CLA	CMB-C2B-C3B	2.04	128.59	124.88
12	B	1210	CLA	CAC-C3C-C4C	2.04	127.63	124.82
12	A	1126	CLA	CMB-C2B-C3B	2.04	128.60	124.88
12	B	1216	CLA	C1-O2A-CGA	2.05	121.49	116.77
17	B	4011	45D	C22-C16-C18	2.05	118.62	115.49
12	B	1217	CLA	C1-O2A-CGA	2.05	121.49	116.77
12	A	1112	CLA	C1-O2A-CGA	2.05	121.49	116.77
12	B	1224	CLA	CMB-C2B-C3B	2.05	128.62	124.88
12	B	1217	CLA	CAC-C3C-C4C	2.06	127.65	124.82
12	A	1011	CLA	C4A-NA-C1A	2.06	108.97	106.32
12	B	1206	CLA	CMB-C2B-C3B	2.07	128.65	124.88
23	J	4015	C7Z	C22-C23-C24	2.07	113.11	110.28
12	K	1402	CLA	CMB-C2B-C3B	2.07	128.65	124.88
12	B	1205	CLA	C4A-NA-C1A	2.07	109.00	106.32
15	K	4001	BCR	C33-C5-C4	2.07	117.49	113.56
12	A	1135	CLA	C1-O2A-CGA	2.08	121.55	116.77
12	A	1117	CLA	C1-O2A-CGA	2.08	121.56	116.77
12	B	1235	CLA	CMB-C2B-C3B	2.08	128.67	124.88
12	A	1121	CLA	CMB-C2B-C3B	2.08	128.67	124.88
12	A	1119	CLA	CMB-C2B-C3B	2.08	128.68	124.88
12	A	1129	CLA	C1-O2A-CGA	2.09	121.58	116.77
12	B	1231	CLA	CMA-C3A-C4A	2.09	117.38	111.77
12	A	1106	CLA	O2A-CGA-CBA	2.09	117.97	111.92
12	L	1502	CLA	C4A-NA-C1A	2.11	109.04	106.32
12	A	1123	CLA	C4A-NA-C1A	2.11	109.04	106.32
12	A	1140	CLA	O2A-CGA-CBA	2.11	118.02	111.92
12	B	1210	CLA	CMB-C2B-C3B	2.12	128.73	124.88
12	A	1112	CLA	CMB-C2B-C3B	2.12	128.74	124.88
12	A	1119	CLA	CMA-C3A-C4A	2.12	117.47	111.77
12	F	1302	CLA	O2A-CGA-CBA	2.13	118.07	111.92
12	B	1203	CLA	CMA-C3A-C4A	2.13	117.50	111.77
12	A	1108	CLA	CMB-C2B-C3B	2.13	128.76	124.88
12	A	1139	CLA	C1-O2A-CGA	2.14	121.69	116.77
12	A	1122	CLA	O2A-CGA-CBA	2.14	118.11	111.92
15	A	4003	BCR	C35-C13-C12	2.15	121.52	118.10
12	A	1115	CLA	O2A-CGA-CBA	2.16	118.15	111.92
12	A	1127	CLA	C1-O2A-CGA	2.16	121.74	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1234	CLA	C1-O2A-CGA	2.16	121.74	116.77
12	B	1023	CLA	CAC-C3C-C4C	2.16	127.79	124.82
12	B	1234	CLA	O2A-CGA-CBA	2.16	118.16	111.92
12	B	1237	CLA	CMB-C2B-C3B	2.16	128.81	124.88
12	A	1101	CLA	CBA-CAA-C2A	2.16	120.23	113.82
12	B	1235	CLA	O2A-CGA-CBA	2.17	118.19	111.92
15	A	4001	BCR	C19-C18-C17	2.17	122.27	118.94
15	K	4001	BCR	C38-C26-C27	2.17	117.67	113.56
25	I	4020	EQ3	C8-C9-C10	2.18	122.29	118.94
15	A	4008	BCR	C29-C28-C27	2.19	116.38	111.36
12	B	1213	CLA	CMB-C2B-C3B	2.19	128.87	124.88
12	A	1111	CLA	CAC-C3C-C4C	2.19	127.84	124.82
19	M	4021	ECH	C19-C18-C17	2.20	122.31	118.94
12	A	1122	CLA	C1-O2A-CGA	2.20	121.83	116.77
12	F	1301	CLA	CMB-C2B-C3B	2.20	128.89	124.88
12	F	1301	CLA	O2A-CGA-CBA	2.20	118.29	111.92
15	A	4001	BCR	C38-C26-C27	2.20	117.73	113.56
12	A	1106	CLA	CMB-C2B-C3B	2.21	128.90	124.88
15	J	4013	BCR	C38-C26-C27	2.21	117.74	113.56
12	A	1128	CLA	C1-O2A-CGA	2.21	121.86	116.77
12	A	1123	CLA	O2A-CGA-CBA	2.23	118.36	111.92
12	B	1228	CLA	O2A-CGA-CBA	2.23	118.37	111.92
15	I	4018	BCR	C30-C25-C24	2.23	122.00	115.73
12	A	1109	CLA	CMB-C2B-C3B	2.23	128.95	124.88
12	A	1107	CLA	C1-O2A-CGA	2.23	121.92	116.77
12	B	1204	CLA	C1-O2A-CGA	2.24	121.92	116.77
12	B	1202	CLA	CMB-C2B-C3B	2.24	128.96	124.88
12	A	1115	CLA	C1-O2A-CGA	2.24	121.93	116.77
15	I	4018	BCR	C35-C13-C12	2.24	121.67	118.10
12	B	1216	CLA	O2A-CGA-CBA	2.24	118.40	111.92
12	A	1111	CLA	O2A-CGA-CBA	2.25	118.41	111.92
12	B	1232	CLA	O2A-CGA-CBA	2.25	118.42	111.92
15	B	4010	BCR	C30-C25-C24	2.25	122.06	115.73
12	B	1219	CLA	O2A-CGA-CBA	2.26	118.45	111.92
12	B	1227	CLA	O2A-CGA-CBA	2.26	118.45	111.92
12	A	1133	CLA	O2A-CGA-CBA	2.26	118.46	111.92
12	A	1011	CLA	CMB-C2B-C3B	2.26	129.00	124.88
12	B	1212	CLA	O2A-CGA-CBA	2.26	118.46	111.92
12	B	1211	CLA	O2A-CGA-CBA	2.26	118.47	111.92
12	A	1103	CLA	O2A-CGA-CBA	2.27	118.48	111.92
12	A	1106	CLA	C1-O2A-CGA	2.28	122.01	116.77
12	A	1129	CLA	CMB-C2B-C3B	2.28	129.03	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1127	CLA	CMB-C2B-C3B	2.28	129.03	124.88
12	B	1021	CLA	O2A-CGA-CBA	2.28	118.52	111.92
12	K	1402	CLA	C1-O2A-CGA	2.29	122.03	116.77
12	B	1221	CLA	CMB-C2B-C3B	2.29	129.04	124.88
12	B	1204	CLA	O2A-CGA-CBA	2.29	118.55	111.92
12	A	1109	CLA	O2A-CGA-CBA	2.30	118.56	111.92
12	B	1226	CLA	O2A-CGA-CBA	2.30	118.57	111.92
12	A	1104	CLA	O2A-CGA-CBA	2.30	118.57	111.92
15	A	4008	BCR	C38-C26-C27	2.30	117.92	113.56
12	A	1129	CLA	O2A-CGA-CBA	2.30	118.58	111.92
12	A	1141	CLA	CMB-C2B-C3B	2.31	129.09	124.88
12	A	1112	CLA	O2A-CGA-CBA	2.31	118.60	111.92
15	A	4003	BCR	C19-C18-C17	2.31	122.49	118.94
12	A	1113	CLA	O2A-CGA-CBA	2.31	118.61	111.92
12	A	1103	CLA	CMB-C2B-C3B	2.32	129.10	124.88
12	A	1134	CLA	O2A-CGA-CBA	2.32	118.62	111.92
12	A	1130	CLA	CMB-C2B-C3B	2.32	129.11	124.88
12	A	1123	CLA	CMB-C2B-C3B	2.32	129.11	124.88
12	B	1221	CLA	CMA-C3A-C4A	2.33	118.03	111.77
12	B	1232	CLA	C1-O2A-CGA	2.33	122.13	116.77
12	A	1133	CLA	CMA-C3A-C4A	2.34	118.06	111.77
12	A	1110	CLA	O2A-CGA-CBA	2.35	118.71	111.92
12	A	1115	CLA	CMB-C2B-C3B	2.35	129.16	124.88
12	A	1130	CLA	O2A-CGA-CBA	2.35	118.72	111.92
12	B	1236	CLA	O2A-CGA-CBA	2.35	118.73	111.92
12	B	1210	CLA	O2A-CGA-CBA	2.35	118.73	111.92
12	A	1117	CLA	O2A-CGA-CBA	2.36	118.73	111.92
12	A	1127	CLA	O2A-CGA-CBA	2.36	118.73	111.92
12	A	1120	CLA	O2A-CGA-CBA	2.36	118.74	111.92
15	A	4008	BCR	C19-C18-C17	2.37	122.57	118.94
12	A	1135	CLA	O2A-CGA-CBA	2.38	118.80	111.92
12	B	1239	CLA	O2A-CGA-CBA	2.38	118.81	111.92
12	A	1131	CLA	O2A-CGA-CBA	2.39	118.82	111.92
12	B	1213	CLA	C1-O2A-CGA	2.39	122.27	116.77
12	A	1103	CLA	CMA-C3A-C4A	2.39	118.20	111.77
12	A	1120	CLA	CMB-C2B-C3B	2.39	129.24	124.88
12	A	1102	CLA	CMB-C2B-C3B	2.39	129.24	124.88
12	L	1502	CLA	O2A-CGA-CBA	2.40	118.84	111.92
12	A	1121	CLA	C1-O2A-CGA	2.40	122.29	116.77
12	A	1112	CLA	CMA-C3A-C4A	2.40	118.22	111.77
12	B	1215	CLA	O2A-CGA-CBA	2.40	118.86	111.92
12	B	1208	CLA	O2A-CGA-CBA	2.40	118.86	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1228	CLA	CMB-C2B-C3B	2.41	129.26	124.88
12	B	1230	CLA	CMA-C3A-C4A	2.41	118.24	111.77
12	B	1237	CLA	O2A-CGA-CBA	2.41	118.88	111.92
15	I	4018	BCR	C36-C18-C19	2.41	121.94	118.10
12	A	1105	CLA	O2A-CGA-CBA	2.41	118.89	111.92
12	B	1023	CLA	CMB-C2B-C3B	2.42	129.28	124.88
12	B	1238	CLA	O2A-CGA-CBA	2.42	118.91	111.92
12	A	1132	CLA	O2A-CGA-CBA	2.42	118.91	111.92
12	B	1225	CLA	O2A-CGA-CBA	2.42	118.91	111.92
12	B	1217	CLA	O2A-CGA-CBA	2.42	118.92	111.92
12	A	1012	CLA	O2A-CGA-CBA	2.43	118.93	111.92
15	A	4012	BCR	C35-C13-C12	2.43	121.97	118.10
15	B	4017	BCR	C38-C26-C27	2.43	118.16	113.56
12	A	1111	CLA	CMA-C3A-C4A	2.44	118.34	111.77
12	B	1220	CLA	C1-O2A-CGA	2.44	122.40	116.77
15	B	4004	BCR	C38-C26-C27	2.45	118.19	113.56
12	A	1104	CLA	CMA-C3A-C4A	2.45	118.35	111.77
12	B	1209	CLA	O2A-CGA-CBA	2.45	119.00	111.92
12	B	1211	CLA	CMB-C2B-C3B	2.45	129.34	124.88
15	A	4003	BCR	C38-C26-C27	2.45	118.20	113.56
12	B	1205	CLA	O2A-CGA-CBA	2.45	119.01	111.92
12	A	1114	CLA	O2A-CGA-CBA	2.45	119.01	111.92
12	B	1240	CLA	O2A-CGA-CBA	2.46	119.03	111.92
12	A	1012	CLA	CMA-C3A-C4A	2.46	118.38	111.77
15	A	4007	BCR	C33-C5-C4	2.46	118.22	113.56
12	B	1222	CLA	O2A-CGA-CBA	2.46	119.05	111.92
12	B	1201	CLA	O2A-CGA-CBA	2.47	119.05	111.92
12	K	1402	CLA	O2A-CGA-CBA	2.47	119.06	111.92
15	B	4010	BCR	C23-C22-C21	2.47	122.73	118.94
15	B	4018	BCR	C38-C26-C27	2.47	118.24	113.56
12	A	1126	CLA	O2A-CGA-CBA	2.48	119.08	111.92
12	B	1231	CLA	C1-O2A-CGA	2.48	122.47	116.77
12	J	1303	CLA	O2A-CGA-CBA	2.48	119.09	111.92
12	B	1234	CLA	CMB-C2B-C3B	2.48	129.40	124.88
12	A	1106	CLA	CMA-C3A-C4A	2.49	118.45	111.77
12	B	1236	CLA	CMA-C3A-C4A	2.49	118.45	111.77
12	A	1011	CLA	O2A-CGA-CBA	2.49	119.11	111.92
12	B	1231	CLA	O2A-CGA-CBA	2.49	119.13	111.92
17	B	4011	45D	C21-C15-C17	2.49	119.30	115.49
12	B	1223	CLA	O2A-CGA-CBA	2.50	119.14	111.92
12	A	1107	CLA	O2A-CGA-CBA	2.50	119.15	111.92
12	A	1137	CLA	O2A-CGA-CBA	2.50	119.16	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1022	CLA	O2A-CGA-CBA	2.51	119.16	111.92
12	A	1101	CLA	C1-O2A-CGA	2.51	122.54	116.77
15	B	4005	BCR	C33-C5-C4	2.51	118.31	113.56
12	J	1302	CLA	O2A-CGA-CBA	2.51	119.17	111.92
12	A	1124	CLA	O2A-CGA-CBA	2.51	119.19	111.92
12	A	1118	CLA	O2A-CGA-CBA	2.52	119.20	111.92
15	B	4017	BCR	C19-C18-C17	2.52	122.81	118.94
12	B	1202	CLA	CMA-C3A-C4A	2.52	118.56	111.77
12	B	1230	CLA	O2A-CGA-CBA	2.53	119.22	111.92
12	F	1302	CLA	C1-O2A-CGA	2.53	122.59	116.77
12	J	1303	CLA	CMB-C2B-C3B	2.53	129.49	124.88
12	B	1229	CLA	O2A-CGA-CBA	2.54	119.25	111.92
17	B	4011	45D	C05-C03-C07	2.54	114.45	110.48
15	K	4001	BCR	C23-C22-C21	2.54	122.85	118.94
12	B	1229	CLA	CMA-C3A-C4A	2.55	118.62	111.77
12	A	1108	CLA	O2A-CGA-CBA	2.55	119.28	111.92
12	A	1136	CLA	O2A-CGA-CBA	2.55	119.30	111.92
12	A	1125	CLA	O2A-CGA-CBA	2.56	119.31	111.92
12	A	1131	CLA	CMA-C3A-C4A	2.56	118.65	111.77
12	A	1101	CLA	CMA-C3A-C4A	2.56	118.67	111.77
12	B	1214	CLA	O2A-CGA-CBA	2.56	119.33	111.92
12	B	1203	CLA	O2A-CGA-CBA	2.57	119.35	111.92
12	A	1138	CLA	O2A-CGA-CBA	2.58	119.37	111.92
12	B	1218	CLA	O2A-CGA-CBA	2.58	119.39	111.92
12	A	1116	CLA	O2A-CGA-CBA	2.59	119.40	111.92
12	A	1011	CLA	CMA-C3A-C4A	2.59	118.73	111.77
12	A	1117	CLA	CMB-C2B-C3B	2.59	129.60	124.88
12	B	1220	CLA	O2A-CGA-CBA	2.59	119.42	111.92
12	F	1301	CLA	CMA-C3A-C4A	2.60	118.77	111.77
25	I	4020	EQ3	C38-C26-C27	2.60	119.47	115.49
15	I	4018	BCR	C37-C22-C23	2.61	122.25	118.10
12	A	1132	CLA	CMA-C3A-C4A	2.62	118.80	111.77
12	B	1238	CLA	CMA-C3A-C4A	2.62	118.82	111.77
12	A	1013	CLA	O2A-CGA-CBA	2.64	119.54	111.92
15	I	4018	BCR	C38-C26-C27	2.64	118.56	113.56
12	B	1239	CLA	CMA-C3A-C4A	2.64	118.88	111.77
15	B	4005	BCR	C38-C26-C27	2.65	118.57	113.56
12	A	1125	CLA	CMB-C2B-C3B	2.65	129.71	124.88
12	B	1201	CLA	CMA-C3A-C4A	2.65	118.91	111.77
12	A	1102	CLA	CMA-C3A-C4A	2.66	118.92	111.77
15	A	4007	BCR	C38-C26-C27	2.66	118.60	113.56
12	A	1141	CLA	CMA-C3A-C4A	2.66	118.93	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	I	4020	EQ3	C33-C5-C4	2.67	119.25	114.34
12	B	1204	CLA	CMA-C3A-C4A	2.67	118.95	111.77
12	B	1224	CLA	CMA-C3A-C4A	2.68	118.98	111.77
12	B	1023	CLA	O2A-CGA-CBA	2.69	119.70	111.92
12	A	1116	CLA	CMB-C2B-C3B	2.70	129.79	124.88
12	A	1128	CLA	CMB-C2B-C3B	2.70	129.80	124.88
12	A	1121	CLA	O2A-CGA-CBA	2.70	119.74	111.92
12	B	1206	CLA	O2A-CGA-CBA	2.71	119.75	111.92
12	B	1221	CLA	O2A-CGA-CBA	2.71	119.75	111.92
12	B	1210	CLA	CMA-C3A-C4A	2.71	119.06	111.77
12	B	1201	CLA	CMB-C2B-C3B	2.71	129.82	124.88
12	B	1218	CLA	CMB-C2B-C3B	2.72	129.83	124.88
12	B	1226	CLA	CMA-C3A-C4A	2.72	119.08	111.77
12	A	1128	CLA	O2A-CGA-CBA	2.72	119.79	111.92
12	A	1107	CLA	CMA-C3A-C4A	2.73	119.11	111.77
12	A	1101	CLA	O2A-CGA-CBA	2.74	119.83	111.92
16	A	5001	LHG	O8-C23-C24	2.74	119.84	111.92
15	A	4008	BCR	C33-C5-C4	2.76	118.78	113.56
12	B	1215	CLA	CMA-C3A-C4A	2.77	119.21	111.77
12	A	1128	CLA	CMA-C3A-C4A	2.77	119.21	111.77
12	A	1138	CLA	CMB-C2B-C3B	2.77	129.93	124.88
12	A	1116	CLA	CMA-C3A-C4A	2.78	119.23	111.77
15	B	4010	BCR	C38-C26-C27	2.78	118.82	113.56
15	J	4013	BCR	C33-C5-C4	2.78	118.83	113.56
12	A	1013	CLA	C1-O2A-CGA	2.78	123.18	116.77
16	B	5004	LHG	O8-C23-C24	2.78	119.97	111.92
16	A	5003	LHG	O8-C23-C24	2.80	120.03	111.92
13	A	2001	PQN	C14-C13-C15	2.80	120.12	115.29
12	B	1216	CLA	CMA-C3A-C4A	2.81	119.31	111.77
12	A	1140	CLA	CMA-C3A-C4A	2.81	119.32	111.77
12	A	1129	CLA	CMA-C3A-C4A	2.81	119.32	111.77
12	B	1225	CLA	CMA-C3A-C4A	2.83	119.37	111.77
12	B	1206	CLA	CMA-C3A-C4A	2.83	119.39	111.77
12	B	1234	CLA	CMA-C3A-C4A	2.84	119.41	111.77
12	B	1205	CLA	CMA-C3A-C4A	2.85	119.42	111.77
12	B	1222	CLA	CMA-C3A-C4A	2.85	119.43	111.77
12	B	1228	CLA	CMA-C3A-C4A	2.85	119.44	111.77
15	F	4014	BCR	C33-C5-C4	2.86	118.98	113.56
12	B	1226	CLA	CMB-C2B-C3B	2.87	130.10	124.88
12	B	1227	CLA	CMA-C3A-C4A	2.88	119.50	111.77
12	A	1138	CLA	CMA-C3A-C4A	2.89	119.53	111.77
12	B	1224	CLA	O2A-CGA-CBA	2.91	120.33	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1127	CLA	CMA-C3A-C4A	2.91	119.59	111.77
12	B	1211	CLA	CMA-C3A-C4A	2.92	119.62	111.77
12	A	1124	CLA	CMA-C3A-C4A	2.92	119.62	111.77
12	A	1108	CLA	CMA-C3A-C4A	2.93	119.64	111.77
12	B	1212	CLA	CMA-C3A-C4A	2.93	119.64	111.77
12	B	1207	CLA	CMA-C3A-C4A	2.93	119.64	111.77
12	A	1013	CLA	CMB-C2B-C3B	2.93	130.22	124.88
12	A	1137	CLA	CMA-C3A-C4A	2.94	119.67	111.77
17	B	4011	45D	C24-C26-C30	2.94	123.45	118.94
12	J	1302	CLA	CMA-C3A-C4A	2.95	119.70	111.77
20	B	5005	LMG	O8-C28-C29	2.95	120.46	111.92
12	A	1114	CLA	CMA-C3A-C4A	2.96	119.72	111.77
12	B	1219	CLA	CMA-C3A-C4A	2.96	119.72	111.77
12	A	1126	CLA	CMA-C3A-C4A	2.97	119.75	111.77
12	A	1134	CLA	CMA-C3A-C4A	2.97	119.75	111.77
12	B	1217	CLA	CMA-C3A-C4A	2.97	119.76	111.77
12	K	1402	CLA	CMA-C3A-C4A	2.98	119.78	111.77
12	B	1223	CLA	CMA-C3A-C4A	2.98	119.79	111.77
12	B	1235	CLA	CMA-C3A-C4A	2.99	119.82	111.77
12	B	1218	CLA	CMA-C3A-C4A	3.00	119.83	111.77
12	B	1232	CLA	CMA-C3A-C4A	3.00	119.83	111.77
13	B	2002	PQN	C14-C13-C15	3.00	120.47	115.29
12	K	1401	CLA	CMA-C3A-C4A	3.00	119.85	111.77
15	B	4018	BCR	C33-C5-C4	3.00	119.25	113.56
12	A	1110	CLA	CMA-C3A-C4A	3.01	119.87	111.77
12	A	1136	CLA	CMA-C3A-C4A	3.01	119.87	111.77
12	A	1105	CLA	CMA-C3A-C4A	3.02	119.88	111.77
25	I	4020	EQ3	C37-C22-C23	3.02	122.91	118.10
12	B	1214	CLA	CMA-C3A-C4A	3.03	119.91	111.77
12	B	1202	CLA	O2A-CGA-CBA	3.03	120.69	111.92
12	B	1213	CLA	CMA-C3A-C4A	3.03	119.92	111.77
15	B	4004	BCR	C33-C5-C4	3.03	119.30	113.56
12	A	1102	CLA	O2A-CGA-CBA	3.03	120.69	111.92
20	B	5002	LMG	O8-C28-C29	3.04	120.70	111.92
12	B	1237	CLA	CMA-C3A-C4A	3.05	119.96	111.77
12	A	1109	CLA	CMA-C3A-C4A	3.05	119.97	111.77
12	B	1208	CLA	CMA-C3A-C4A	3.05	119.97	111.77
12	B	1022	CLA	CMA-C3A-C4A	3.06	119.98	111.77
12	A	1125	CLA	CMA-C3A-C4A	3.06	119.99	111.77
12	B	1207	CLA	O2A-CGA-CBA	3.06	120.77	111.92
12	F	1302	CLA	CMA-C3A-C4A	3.06	120.01	111.77
12	A	1120	CLA	CMA-C3A-C4A	3.07	120.01	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	4017	BCR	C33-C5-C4	3.07	119.36	113.56
12	A	1121	CLA	CMA-C3A-C4A	3.07	120.02	111.77
12	B	1209	CLA	CMA-C3A-C4A	3.07	120.02	111.77
12	A	1115	CLA	CMA-C3A-C4A	3.07	120.03	111.77
12	A	1113	CLA	CMA-C3A-C4A	3.08	120.05	111.77
12	A	1122	CLA	CMA-C3A-C4A	3.08	120.05	111.77
12	J	1303	CLA	CMA-C3A-C4A	3.08	120.06	111.77
15	A	4012	BCR	C33-C5-C4	3.09	119.41	113.56
12	A	1135	CLA	CMA-C3A-C4A	3.11	120.14	111.77
12	A	1130	CLA	CMA-C3A-C4A	3.12	120.15	111.77
12	B	1220	CLA	CMA-C3A-C4A	3.13	120.19	111.77
12	A	1117	CLA	CMA-C3A-C4A	3.14	120.22	111.77
12	L	1502	CLA	CMA-C3A-C4A	3.21	120.40	111.77
12	A	1139	CLA	CMA-C3A-C4A	3.21	120.40	111.77
15	A	4001	BCR	C33-C5-C4	3.25	119.70	113.56
12	A	1123	CLA	CMA-C3A-C4A	3.26	120.52	111.77
15	A	4012	BCR	C19-C18-C17	3.33	124.05	118.94
15	B	4010	BCR	C33-C5-C4	3.35	119.90	113.56
15	F	4014	BCR	C19-C18-C17	3.38	124.12	118.94
15	A	4003	BCR	C33-C5-C4	3.40	120.00	113.56
12	A	1107	CLA	O2D-CGD-CBD	3.48	117.46	111.28
15	K	4001	BCR	C19-C18-C17	3.50	124.31	118.94
15	I	4018	BCR	C33-C5-C4	3.58	120.33	113.56
12	B	1240	CLA	CMA-C3A-C4A	3.58	121.39	111.77
12	A	1107	CLA	C4A-NA-C1A	3.86	111.30	106.32
20	B	5002	LMG	O7-C10-C11	3.87	119.71	111.55
16	A	5001	LHG	O7-C7-C8	3.90	119.76	111.55
20	B	5005	LMG	O7-C10-C11	3.97	119.93	111.55
16	B	5004	LHG	O7-C7-C8	4.04	120.06	111.55
25	I	4020	EQ3	C19-C18-C17	4.04	125.14	118.94
16	A	5003	LHG	O7-C7-C8	4.15	120.30	111.55
15	B	4018	BCR	C19-C18-C17	4.21	125.40	118.94
12	B	1203	CLA	O2D-CGD-CBD	4.30	118.90	111.28
12	B	1231	CLA	O2D-CGD-CBD	4.33	118.96	111.28
12	A	1138	CLA	O2D-CGD-CBD	4.36	119.02	111.28
12	B	1023	CLA	O2D-CGD-CBD	4.42	119.12	111.28
12	A	1013	CLA	O2D-CGD-CBD	4.45	119.17	111.28
12	B	1225	CLA	O2D-CGD-CBD	4.56	119.37	111.28
12	B	1206	CLA	O2D-CGD-CBD	4.56	119.37	111.28
12	A	1139	CLA	O2D-CGD-CBD	4.61	119.45	111.28
12	A	1012	CLA	O2D-CGD-CBD	4.61	119.46	111.28
12	A	1109	CLA	O2D-CGD-CBD	4.62	119.47	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1132	CLA	O2D-CGD-CBD	4.62	119.47	111.28
12	K	1402	CLA	O2D-CGD-CBD	4.69	119.59	111.28
12	A	1119	CLA	O2D-CGD-CBD	4.71	119.63	111.28
12	A	1141	CLA	O2D-CGD-CBD	4.76	119.72	111.28
12	B	1214	CLA	O2D-CGD-CBD	4.77	119.74	111.28
12	A	1122	CLA	O2D-CGD-CBD	4.79	119.77	111.28
12	B	1224	CLA	O2D-CGD-CBD	4.82	119.82	111.28
12	B	1232	CLA	O2D-CGD-CBD	4.82	119.82	111.28
12	B	1021	CLA	O2D-CGD-CBD	4.82	119.83	111.28
12	A	1111	CLA	O2D-CGD-CBD	4.84	119.86	111.28
16	B	5006	LHG	O7-C7-C8	4.85	120.16	111.10
12	A	1127	CLA	O2D-CGD-CBD	4.86	119.90	111.28
12	A	1137	CLA	O2D-CGD-CBD	4.88	119.92	111.28
12	A	1117	CLA	O2D-CGD-CBD	4.90	119.96	111.28
12	A	1129	CLA	O2D-CGD-CBD	4.90	119.97	111.28
12	B	1216	CLA	O2D-CGD-CBD	4.91	119.99	111.28
12	A	1114	CLA	O2D-CGD-CBD	4.93	120.02	111.28
12	B	1201	CLA	O2D-CGD-CBD	4.93	120.03	111.28
12	B	1237	CLA	O2D-CGD-CBD	4.93	120.03	111.28
12	B	1204	CLA	O2D-CGD-CBD	4.94	120.04	111.28
12	A	1108	CLA	O2D-CGD-CBD	4.95	120.05	111.28
12	A	1110	CLA	O2D-CGD-CBD	4.96	120.08	111.28
12	B	1239	CLA	O2D-CGD-CBD	4.97	120.10	111.28
12	A	1133	CLA	O2D-CGD-CBD	4.98	120.11	111.28
12	F	1301	CLA	O2D-CGD-CBD	4.98	120.11	111.28
12	A	1126	CLA	O2D-CGD-CBD	4.99	120.13	111.28
12	B	1223	CLA	O2D-CGD-CBD	5.00	120.14	111.28
12	A	1140	CLA	O2D-CGD-CBD	5.00	120.14	111.28
12	A	1131	CLA	O2D-CGD-CBD	5.01	120.16	111.28
12	B	1208	CLA	O2D-CGD-CBD	5.02	120.18	111.28
12	B	1218	CLA	O2D-CGD-CBD	5.02	120.18	111.28
12	A	1104	CLA	O2D-CGD-CBD	5.03	120.19	111.28
12	A	1118	CLA	O2D-CGD-CBD	5.03	120.20	111.28
12	B	1215	CLA	O2D-CGD-CBD	5.04	120.22	111.28
12	A	1113	CLA	O2A-C1-C2	5.05	120.90	109.00
12	B	1222	CLA	O2D-CGD-CBD	5.06	120.25	111.28
12	B	1022	CLA	O2D-CGD-CBD	5.06	120.25	111.28
12	B	1240	CLA	O2A-C1-C2	5.06	120.94	109.00
12	A	1110	CLA	O2A-C1-C2	5.07	120.96	109.00
12	J	1303	CLA	O2A-C1-C2	5.07	120.96	109.00
12	A	1130	CLA	O2D-CGD-CBD	5.08	120.28	111.28
12	A	1121	CLA	O2D-CGD-CBD	5.08	120.29	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1207	CLA	O2A-C1-C2	5.09	121.01	109.00
12	A	1134	CLA	O2A-C1-C2	5.10	121.03	109.00
12	B	1203	CLA	O2A-C1-C2	5.10	121.03	109.00
12	B	1210	CLA	O2D-CGD-CBD	5.10	120.33	111.28
12	B	1208	CLA	O2A-C1-C2	5.12	121.06	109.00
12	A	1115	CLA	O2D-CGD-CBD	5.12	120.35	111.28
12	B	1212	CLA	O2D-CGD-CBD	5.12	120.36	111.28
12	B	1235	CLA	O2D-CGD-CBD	5.12	120.36	111.28
12	A	1103	CLA	O2D-CGD-CBD	5.13	120.37	111.28
12	B	1234	CLA	O2D-CGD-CBD	5.14	120.39	111.28
12	B	1220	CLA	O2D-CGD-CBD	5.14	120.39	111.28
12	B	1228	CLA	O2D-CGD-CBD	5.15	120.42	111.28
12	B	1217	CLA	O2D-CGD-CBD	5.16	120.43	111.28
12	A	1124	CLA	O2D-CGD-CBD	5.16	120.43	111.28
12	B	1206	CLA	O2A-C1-C2	5.17	121.19	109.00
12	B	1209	CLA	O2A-C1-C2	5.18	121.21	109.00
12	A	1125	CLA	O2D-CGD-CBD	5.18	120.47	111.28
12	B	1219	CLA	O2D-CGD-CBD	5.18	120.47	111.28
12	B	1207	CLA	O2D-CGD-CBD	5.19	120.49	111.28
12	A	1113	CLA	O2D-CGD-CBD	5.20	120.50	111.28
12	A	1114	CLA	O2A-C1-C2	5.20	121.27	109.00
12	B	1211	CLA	O2D-CGD-CBD	5.20	120.51	111.28
12	A	1111	CLA	O2A-C1-C2	5.21	121.28	109.00
12	A	1120	CLA	O2D-CGD-CBD	5.21	120.52	111.28
12	A	1131	CLA	O2A-C1-C2	5.21	121.30	109.00
12	A	1136	CLA	O2D-CGD-CBD	5.22	120.53	111.28
12	J	1302	CLA	O2A-C1-C2	5.23	121.34	109.00
12	A	1123	CLA	O2D-CGD-CBD	5.24	120.56	111.28
12	A	1116	CLA	O2A-C1-C2	5.24	121.36	109.00
12	A	1136	CLA	O2A-C1-C2	5.24	121.36	109.00
12	B	1218	CLA	O2A-C1-C2	5.26	121.40	109.00
12	A	1124	CLA	O2A-C1-C2	5.26	121.41	109.00
12	A	1133	CLA	O2A-C1-C2	5.26	121.41	109.00
12	B	1211	CLA	O2A-C1-C2	5.27	121.42	109.00
12	B	1238	CLA	O2A-C1-C2	5.27	121.42	109.00
12	B	1204	CLA	O2A-C1-C2	5.29	121.46	109.00
12	B	1223	CLA	O2A-C1-C2	5.29	121.48	109.00
12	A	1104	CLA	O2A-C1-C2	5.30	121.50	109.00
12	F	1302	CLA	O2A-C1-C2	5.30	121.51	109.00
12	A	1120	CLA	O2A-C1-C2	5.31	121.51	109.00
12	B	1236	CLA	O2A-C1-C2	5.31	121.52	109.00
12	B	1227	CLA	O2A-C1-C2	5.31	121.53	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1101	CLA	O2D-CGD-CBD	5.31	120.70	111.28
12	A	1130	CLA	O2A-C1-C2	5.32	121.54	109.00
12	J	1302	CLA	O2D-CGD-CBD	5.32	120.72	111.28
12	K	1401	CLA	O2D-CGD-CBD	5.33	120.72	111.28
12	A	1108	CLA	O2A-C1-C2	5.34	121.59	109.00
12	A	1127	CLA	O2A-C1-C2	5.34	121.60	109.00
12	A	1012	CLA	O2A-C1-C2	5.34	121.60	109.00
12	A	1116	CLA	O2D-CGD-CBD	5.35	120.76	111.28
12	A	1105	CLA	O2D-CGD-CBD	5.35	120.77	111.28
12	B	1219	CLA	O2A-C1-C2	5.35	121.63	109.00
12	A	1125	CLA	O2A-C1-C2	5.36	121.64	109.00
12	A	1122	CLA	O2A-C1-C2	5.36	121.64	109.00
12	A	1102	CLA	O2D-CGD-CBD	5.37	120.79	111.28
12	A	1117	CLA	O2A-C1-C2	5.37	121.67	109.00
12	L	1502	CLA	O2A-C1-C2	5.37	121.67	109.00
12	B	1226	CLA	O2D-CGD-CBD	5.37	120.81	111.28
12	A	1134	CLA	O2D-CGD-CBD	5.38	120.82	111.28
12	B	1236	CLA	O2D-CGD-CBD	5.39	120.83	111.28
12	J	1303	CLA	O2D-CGD-CBD	5.40	120.85	111.28
12	B	1023	CLA	O2A-C1-C2	5.40	121.74	109.00
12	B	1239	CLA	O2A-C1-C2	5.40	121.75	109.00
12	B	1212	CLA	O2A-C1-C2	5.41	121.75	109.00
12	B	1228	CLA	O2A-C1-C2	5.41	121.75	109.00
12	A	1103	CLA	O2A-C1-C2	5.41	121.76	109.00
12	A	1011	CLA	O2D-CGD-CBD	5.42	120.88	111.28
12	B	1201	CLA	O2A-C1-C2	5.42	121.79	109.00
12	B	1213	CLA	O2A-C1-C2	5.42	121.79	109.00
12	A	1112	CLA	O2D-CGD-CBD	5.44	120.92	111.28
12	B	1237	CLA	O2A-C1-C2	5.44	121.82	109.00
12	F	1301	CLA	O2A-C1-C2	5.44	121.83	109.00
12	B	1225	CLA	O2A-C1-C2	5.46	121.87	109.00
12	A	1135	CLA	O2D-CGD-CBD	5.46	120.96	111.28
12	B	1202	CLA	O2D-CGD-CBD	5.47	120.98	111.28
12	B	1232	CLA	O2A-C1-C2	5.47	121.91	109.00
12	B	1221	CLA	O2A-C1-C2	5.50	121.97	109.00
12	B	1238	CLA	O2D-CGD-CBD	5.51	121.05	111.28
12	L	1502	CLA	O2D-CGD-CBD	5.52	121.06	111.28
12	B	1226	CLA	O2A-C1-C2	5.52	122.01	109.00
12	A	1112	CLA	O2A-C1-C2	5.52	122.02	109.00
12	F	1302	CLA	O2D-CGD-CBD	5.54	121.10	111.28
12	B	1205	CLA	O2A-C1-C2	5.54	122.08	109.00
12	B	1221	CLA	O2D-CGD-CBD	5.55	121.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1217	CLA	O2A-C1-C2	5.57	122.13	109.00
12	A	1137	CLA	O2A-C1-C2	5.60	122.20	109.00
12	B	1230	CLA	O2A-C1-C2	5.60	122.20	109.00
12	B	1210	CLA	O2A-C1-C2	5.60	122.20	109.00
12	B	1229	CLA	O2D-CGD-CBD	5.60	121.21	111.28
12	B	1209	CLA	O2D-CGD-CBD	5.61	121.22	111.28
12	B	1215	CLA	O2A-C1-C2	5.61	122.22	109.00
12	A	1128	CLA	O2D-CGD-CBD	5.62	121.24	111.28
12	A	1106	CLA	O2D-CGD-CBD	5.63	121.26	111.28
12	B	1240	CLA	O2D-CGD-CBD	5.70	121.39	111.28
12	A	1135	CLA	O2A-C1-C2	5.71	122.46	109.00
12	B	1230	CLA	O2D-CGD-CBD	5.75	121.47	111.28
12	B	1213	CLA	O2D-CGD-CBD	5.75	121.48	111.28
12	A	1101	CLA	O2A-C1-C2	5.76	122.58	109.00
12	A	1129	CLA	O2A-C1-C2	5.76	122.59	109.00
12	B	1205	CLA	O2D-CGD-CBD	5.78	121.52	111.28
12	B	1216	CLA	O2A-C1-C2	5.78	122.63	109.00
12	K	1402	CLA	O2A-C1-C2	5.79	122.65	109.00
15	B	4018	BCR	C20-C19-C18	5.81	142.73	126.42
12	B	1231	CLA	O2A-C1-C2	5.81	122.70	109.00
12	B	1227	CLA	O2D-CGD-CBD	5.87	121.69	111.28
12	A	1121	CLA	O2A-C1-C2	5.89	122.88	109.00
12	B	1220	CLA	O2A-C1-C2	6.06	123.30	109.00
15	K	4001	BCR	C20-C19-C18	6.22	143.90	126.42
15	A	4001	BCR	C20-C19-C18	7.06	146.26	126.42
15	A	4012	BCR	C20-C19-C18	7.12	146.42	126.42
15	A	4008	BCR	C20-C19-C18	7.15	146.51	126.42
15	B	4004	BCR	C20-C19-C18	7.15	146.52	126.42
15	A	4003	BCR	C20-C19-C18	7.21	146.66	126.42
15	F	4014	BCR	C20-C19-C18	7.22	146.70	126.42
15	B	4017	BCR	C20-C19-C18	7.70	148.05	126.42
15	J	4013	BCR	C20-C19-C18	7.97	148.81	126.42
15	B	4010	BCR	C20-C19-C18	8.07	149.10	126.42
15	A	4007	BCR	C20-C19-C18	8.11	149.21	126.42
15	I	4018	BCR	C11-C12-C13	8.74	150.97	126.42
15	B	4005	BCR	C20-C19-C18	9.29	152.52	126.42
15	I	4018	BCR	C20-C19-C18	9.48	153.06	126.42
15	A	4001	BCR	C11-C12-C13	9.51	153.14	126.42
15	J	4013	BCR	C11-C12-C13	9.68	153.61	126.42
15	B	4005	BCR	C11-C12-C13	9.69	153.65	126.42
15	K	4001	BCR	C11-C12-C13	9.78	153.88	126.42
15	A	4007	BCR	C11-C12-C13	9.86	154.11	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	4004	BCR	C11-C12-C13	9.93	154.31	126.42
15	B	4018	BCR	C21-C20-C19	10.05	153.87	123.26
15	B	4017	BCR	C11-C12-C13	10.15	154.93	126.42
15	A	4003	BCR	C11-C12-C13	10.37	155.55	126.42
15	A	4008	BCR	C11-C12-C13	10.41	155.67	126.42
15	B	4010	BCR	C11-C12-C13	10.55	156.05	126.42
15	I	4018	BCR	C21-C20-C19	10.61	155.58	123.26
15	F	4014	BCR	C11-C12-C13	10.67	156.40	126.42
15	B	4018	BCR	C11-C12-C13	10.70	156.47	126.42
15	A	4012	BCR	C11-C12-C13	10.83	156.85	126.42
15	A	4012	BCR	C16-C15-C14	10.88	146.69	123.46
15	A	4003	BCR	C21-C20-C19	10.94	156.58	123.26
15	B	4005	BCR	C21-C20-C19	11.06	156.96	123.26
15	F	4014	BCR	C16-C15-C14	11.18	147.32	123.46
15	A	4001	BCR	C11-C10-C9	11.29	143.43	127.31
15	B	4018	BCR	C16-C15-C14	11.72	148.48	123.46
15	B	4018	BCR	C11-C10-C9	11.82	144.18	127.31
15	J	4013	BCR	C21-C20-C19	12.17	160.36	123.26
15	A	4007	BCR	C21-C20-C19	12.18	160.38	123.26
15	B	4010	BCR	C21-C20-C19	12.20	160.44	123.26
15	A	4003	BCR	C16-C15-C14	12.22	149.54	123.46
15	B	4010	BCR	C11-C10-C9	12.25	144.79	127.31
15	B	4017	BCR	C21-C20-C19	12.25	160.58	123.26
15	K	4001	BCR	C16-C15-C14	12.38	149.89	123.46
15	B	4017	BCR	C11-C10-C9	12.39	144.99	127.31
15	A	4008	BCR	C16-C15-C14	12.45	150.04	123.46
15	A	4012	BCR	C21-C20-C19	12.74	162.06	123.26
15	J	4013	BCR	C11-C10-C9	12.77	145.53	127.31
15	A	4007	BCR	C11-C10-C9	12.79	145.57	127.31
15	A	4008	BCR	C21-C20-C19	12.84	162.40	123.26
15	F	4014	BCR	C21-C20-C19	12.89	162.53	123.26
15	B	4004	BCR	C11-C10-C9	12.95	145.80	127.31
15	B	4004	BCR	C21-C20-C19	13.00	162.87	123.26
15	F	4014	BCR	C11-C10-C9	13.02	145.89	127.31
15	A	4008	BCR	C11-C10-C9	13.02	145.90	127.31
15	J	4013	BCR	C16-C15-C14	13.21	151.65	123.46
15	K	4001	BCR	C11-C10-C9	13.23	146.19	127.31
15	A	4001	BCR	C21-C20-C19	13.24	163.59	123.26
15	A	4003	BCR	C11-C10-C9	13.31	146.30	127.31
15	B	4005	BCR	C11-C10-C9	13.42	146.46	127.31
15	B	4010	BCR	C16-C15-C14	13.44	152.16	123.46
15	I	4018	BCR	C16-C15-C14	13.47	152.22	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4012	BCR	C11-C10-C9	13.53	146.62	127.31
15	A	4007	BCR	C16-C15-C14	13.63	152.55	123.46
15	K	4001	BCR	C21-C20-C19	13.81	165.35	123.26
15	A	4001	BCR	C16-C15-C14	13.81	152.95	123.46
15	B	4004	BCR	C16-C15-C14	13.91	153.16	123.46
15	I	4018	BCR	C11-C10-C9	14.04	147.35	127.31
15	B	4005	BCR	C16-C15-C14	14.18	153.73	123.46
15	B	4017	BCR	C16-C15-C14	14.18	153.73	123.46
15	I	4018	BCR	C10-C11-C12	16.63	173.94	123.26
15	A	4012	BCR	C10-C11-C12	17.13	175.47	123.26
15	A	4001	BCR	C10-C11-C12	17.59	176.86	123.26
15	J	4013	BCR	C10-C11-C12	17.61	176.91	123.26
15	A	4003	BCR	C10-C11-C12	17.64	177.00	123.26
15	B	4005	BCR	C10-C11-C12	17.77	177.41	123.26
15	A	4007	BCR	C10-C11-C12	17.84	177.61	123.26
15	A	4008	BCR	C10-C11-C12	17.90	177.79	123.26
15	F	4014	BCR	C10-C11-C12	17.90	177.81	123.26
15	B	4018	BCR	C10-C11-C12	17.98	178.04	123.26
15	B	4004	BCR	C10-C11-C12	17.99	178.06	123.26
15	K	4001	BCR	C10-C11-C12	18.08	178.35	123.26
15	B	4017	BCR	C10-C11-C12	18.29	178.98	123.26
15	B	4010	BCR	C10-C11-C12	18.60	179.93	123.26

All (279) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1112	CLA	NC
12	A	1112	CLA	ND
12	A	1112	CLA	NA
12	A	1118	CLA	NC
12	A	1118	CLA	ND
12	A	1118	CLA	NA
12	A	1139	CLA	NC
12	A	1139	CLA	ND
12	A	1139	CLA	NA
12	A	1106	CLA	NC
12	A	1106	CLA	ND
12	A	1106	CLA	NA
12	A	1130	CLA	NC
12	A	1130	CLA	ND
12	A	1130	CLA	NA
12	A	1103	CLA	NC

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Mol	Chain	Res	Type	Atom
12	A	1103	CLA	ND
12	A	1103	CLA	NA
12	B	1221	CLA	NC
12	B	1221	CLA	ND
12	B	1221	CLA	NA
12	A	1116	CLA	NC
12	A	1116	CLA	ND
12	A	1116	CLA	NA
12	B	1239	CLA	NC
12	B	1239	CLA	ND
12	B	1239	CLA	NA
12	J	1303	CLA	NC
12	J	1303	CLA	ND
12	J	1303	CLA	NA
12	A	1105	CLA	NC
12	A	1105	CLA	ND
12	A	1105	CLA	NA
12	A	1123	CLA	NC
12	A	1123	CLA	ND
12	A	1123	CLA	NA
12	A	1115	CLA	NC
12	A	1115	CLA	ND
12	A	1115	CLA	NA
12	A	1129	CLA	NC
12	A	1129	CLA	ND
12	A	1129	CLA	NA
12	F	1301	CLA	NC
12	F	1301	CLA	ND
12	F	1301	CLA	NA
12	L	1502	CLA	NC
12	L	1502	CLA	ND
12	L	1502	CLA	NA
12	A	1101	CLA	NC
12	A	1101	CLA	ND
12	A	1101	CLA	NA
12	B	1223	CLA	NC
12	B	1223	CLA	ND
12	B	1223	CLA	NA
12	A	1133	CLA	NC
12	A	1133	CLA	ND
12	A	1133	CLA	NA
12	B	1205	CLA	NC

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Mol	Chain	Res	Type	Atom
12	B	1205	CLA	ND
12	B	1205	CLA	NA
12	A	1012	CLA	NC
12	A	1012	CLA	ND
12	A	1012	CLA	NA
12	B	1023	CLA	NC
12	B	1023	CLA	ND
12	B	1023	CLA	NA
12	B	1229	CLA	NC
12	B	1229	CLA	ND
12	B	1229	CLA	NA
12	A	1135	CLA	NC
12	A	1135	CLA	ND
12	A	1135	CLA	NA
12	A	1127	CLA	NC
12	A	1127	CLA	ND
12	A	1127	CLA	NA
12	A	1141	CLA	NC
12	A	1141	CLA	ND
12	A	1141	CLA	NA
12	B	1201	CLA	NC
12	B	1201	CLA	ND
12	B	1201	CLA	NA
12	K	1401	CLA	NC
12	K	1401	CLA	ND
12	K	1401	CLA	NA
12	B	1227	CLA	NC
12	B	1227	CLA	ND
12	B	1227	CLA	NA
12	B	1240	CLA	NC
12	B	1240	CLA	ND
12	B	1240	CLA	NA
12	A	1120	CLA	NC
12	A	1120	CLA	ND
12	A	1120	CLA	NA
12	A	1125	CLA	NC
12	A	1125	CLA	ND
12	A	1125	CLA	NA
12	A	1117	CLA	NC
12	A	1117	CLA	ND
12	A	1117	CLA	NA
12	A	1136	CLA	NC

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Mol	Chain	Res	Type	Atom
12	A	1136	CLA	ND
12	A	1136	CLA	NA
12	A	1110	CLA	NC
12	A	1110	CLA	ND
12	A	1110	CLA	NA
12	B	1211	CLA	NC
12	B	1211	CLA	ND
12	B	1211	CLA	NA
12	B	1214	CLA	NC
12	B	1214	CLA	ND
12	B	1214	CLA	NA
12	A	1131	CLA	NC
12	A	1131	CLA	ND
12	A	1131	CLA	NA
12	K	1402	CLA	NC
12	K	1402	CLA	ND
12	K	1402	CLA	NA
12	B	1219	CLA	NC
12	B	1219	CLA	ND
12	B	1219	CLA	NA
12	B	1218	CLA	NC
12	B	1218	CLA	ND
12	B	1218	CLA	NA
12	A	1107	CLA	NC
12	A	1107	CLA	ND
12	A	1107	CLA	NA
12	B	1224	CLA	NC
12	B	1224	CLA	ND
12	B	1224	CLA	NA
12	F	1302	CLA	NC
12	F	1302	CLA	ND
12	F	1302	CLA	NA
12	A	1122	CLA	NC
12	A	1122	CLA	ND
12	A	1122	CLA	NA
12	B	1208	CLA	NC
12	B	1208	CLA	ND
12	B	1208	CLA	NA
12	B	1204	CLA	NC
12	B	1204	CLA	ND
12	B	1204	CLA	NA
12	A	1011	CLA	NC

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Mol	Chain	Res	Type	Atom
12	A	1011	CLA	ND
12	A	1011	CLA	NA
12	B	1216	CLA	NC
12	B	1216	CLA	ND
12	B	1216	CLA	NA
12	A	1124	CLA	NC
12	A	1124	CLA	ND
12	A	1124	CLA	NA
12	A	1113	CLA	NC
12	A	1113	CLA	ND
12	A	1113	CLA	NA
12	B	1213	CLA	NC
12	B	1213	CLA	ND
12	B	1213	CLA	NA
12	A	1134	CLA	NC
12	A	1134	CLA	ND
12	A	1134	CLA	NA
12	B	1237	CLA	NC
12	B	1237	CLA	ND
12	B	1237	CLA	NA
12	B	1215	CLA	NC
12	B	1215	CLA	ND
12	B	1215	CLA	NA
12	B	1238	CLA	NC
12	B	1238	CLA	ND
12	B	1238	CLA	NA
12	B	1232	CLA	NC
12	B	1232	CLA	ND
12	B	1232	CLA	NA
12	A	1128	CLA	NC
12	A	1128	CLA	ND
12	A	1128	CLA	NA
12	A	1119	CLA	NC
12	A	1119	CLA	ND
12	A	1119	CLA	NA
12	B	1217	CLA	NC
12	B	1217	CLA	ND
12	B	1217	CLA	NA
12	B	1212	CLA	NC
12	B	1212	CLA	ND
12	B	1212	CLA	NA
12	B	1210	CLA	NC

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Mol	Chain	Res	Type	Atom
12	B	1210	CLA	ND
12	B	1210	CLA	NA
12	A	1104	CLA	NC
12	A	1104	CLA	ND
12	A	1104	CLA	NA
12	B	1202	CLA	NC
12	B	1202	CLA	ND
12	B	1202	CLA	NA
12	B	1226	CLA	NC
12	B	1226	CLA	ND
12	B	1226	CLA	NA
12	A	1102	CLA	NC
12	A	1102	CLA	ND
12	A	1102	CLA	NA
12	A	1132	CLA	NC
12	A	1132	CLA	ND
12	A	1132	CLA	NA
12	B	1220	CLA	NC
12	B	1220	CLA	ND
12	B	1220	CLA	NA
12	B	1222	CLA	NC
12	B	1222	CLA	ND
12	B	1222	CLA	NA
12	B	1230	CLA	NC
12	B	1230	CLA	ND
12	B	1230	CLA	NA
12	A	1108	CLA	NC
12	A	1108	CLA	ND
12	A	1108	CLA	NA
12	B	1225	CLA	NC
12	B	1225	CLA	ND
12	B	1225	CLA	NA
12	B	1206	CLA	NC
12	B	1206	CLA	ND
12	B	1206	CLA	NA
12	A	1137	CLA	NC
12	A	1137	CLA	ND
12	A	1137	CLA	NA
12	B	1207	CLA	NC
12	B	1207	CLA	ND
12	B	1207	CLA	NA
12	A	1013	CLA	NC

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Mol	Chain	Res	Type	Atom
12	A	1013	CLA	ND
12	A	1013	CLA	NA
12	B	1235	CLA	NC
12	B	1235	CLA	ND
12	B	1235	CLA	NA
12	J	1302	CLA	NC
12	J	1302	CLA	ND
12	J	1302	CLA	NA
12	A	1126	CLA	NC
12	A	1126	CLA	ND
12	A	1126	CLA	NA
12	A	1140	CLA	NC
12	A	1140	CLA	ND
12	A	1140	CLA	NA
12	A	1111	CLA	NC
12	A	1111	CLA	ND
12	A	1111	CLA	NA
12	A	1114	CLA	NC
12	A	1114	CLA	ND
12	A	1114	CLA	NA
12	A	1138	CLA	NC
12	A	1138	CLA	ND
12	A	1138	CLA	NA
12	A	1121	CLA	NC
12	A	1121	CLA	ND
12	A	1121	CLA	NA
12	B	1231	CLA	NC
12	B	1231	CLA	ND
12	B	1231	CLA	NA
12	B	1021	CLA	NC
12	B	1021	CLA	ND
12	B	1021	CLA	NA
12	B	1234	CLA	NC
12	B	1234	CLA	ND
12	B	1234	CLA	NA
12	B	1209	CLA	NC
12	B	1209	CLA	ND
12	B	1209	CLA	NA
12	B	1236	CLA	NC
12	B	1236	CLA	ND
12	B	1236	CLA	NA
12	B	1022	CLA	NC

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Mol	Chain	Res	Type	Atom
12	B	1022	CLA	ND
12	B	1022	CLA	NA
12	B	1228	CLA	NC
12	B	1228	CLA	ND
12	B	1228	CLA	NA
12	A	1109	CLA	NC
12	A	1109	CLA	ND
12	A	1109	CLA	NA
12	B	1203	CLA	NC
12	B	1203	CLA	ND
12	B	1203	CLA	NA

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	F	4016	C7Z	C31-C30-C29-C39
15	K	4001	BCR	C11-C10-C9-C8
15	K	4001	BCR	C11-C10-C9-C34
23	J	4015	C7Z	C15-C14-C13-C20
23	F	4016	C7Z	C35-C34-C33-C32
15	F	4014	BCR	C11-C10-C9-C8
15	F	4014	BCR	C11-C10-C9-C34
15	I	4018	BCR	C10-C11-C12-C13

There are no ring outliers.

116 monomers are involved in 375 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1011	CLA	8	0
12	A	1012	CLA	8	0
12	A	1013	CLA	8	0
12	A	1101	CLA	3	0
12	A	1102	CLA	8	0
12	A	1103	CLA	5	0
12	A	1104	CLA	1	0
12	A	1105	CLA	4	0
12	A	1106	CLA	8	0
12	A	1107	CLA	9	0
12	A	1108	CLA	2	0
12	A	1109	CLA	12	0
12	A	1110	CLA	1	0
12	A	1111	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1112	CLA	5	0
12	A	1114	CLA	3	0
12	A	1115	CLA	6	0
12	A	1116	CLA	6	0
12	A	1117	CLA	4	0
12	A	1118	CLA	2	0
12	A	1119	CLA	6	0
12	A	1121	CLA	2	0
12	A	1122	CLA	4	0
12	A	1123	CLA	5	0
12	A	1124	CLA	2	0
12	A	1125	CLA	4	0
12	A	1126	CLA	13	0
12	A	1127	CLA	1	0
12	A	1128	CLA	8	0
12	A	1129	CLA	3	0
12	A	1130	CLA	3	0
12	A	1131	CLA	1	0
12	A	1132	CLA	7	0
12	A	1133	CLA	3	0
12	A	1134	CLA	4	0
12	A	1135	CLA	4	0
12	A	1137	CLA	1	0
12	A	1138	CLA	9	0
12	A	1139	CLA	5	0
12	A	1140	CLA	4	0
12	A	1141	CLA	3	0
13	A	2001	PQN	2	0
14	A	3001	SF4	1	0
15	A	4001	BCR	5	0
15	A	4003	BCR	1	0
15	A	4007	BCR	2	0
15	A	4008	BCR	5	0
15	A	4012	BCR	8	0
16	A	5001	LHG	2	0
16	A	5003	LHG	3	0
12	B	1021	CLA	15	0
12	B	1022	CLA	4	0
12	B	1023	CLA	5	0
12	B	1201	CLA	1	0
12	B	1202	CLA	5	0
12	B	1203	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1204	CLA	5	0
12	B	1205	CLA	5	0
12	B	1206	CLA	2	0
12	B	1207	CLA	5	0
12	B	1208	CLA	4	0
12	B	1209	CLA	1	0
12	B	1210	CLA	7	0
12	B	1211	CLA	4	0
12	B	1212	CLA	1	0
12	B	1213	CLA	2	0
12	B	1214	CLA	5	0
12	B	1215	CLA	2	0
12	B	1216	CLA	2	0
12	B	1218	CLA	2	0
12	B	1219	CLA	1	0
12	B	1220	CLA	4	0
12	B	1221	CLA	5	0
12	B	1222	CLA	10	0
12	B	1223	CLA	3	0
12	B	1224	CLA	9	0
12	B	1225	CLA	4	0
12	B	1226	CLA	3	0
12	B	1227	CLA	3	0
12	B	1228	CLA	2	0
12	B	1229	CLA	5	0
12	B	1230	CLA	4	0
12	B	1231	CLA	4	0
12	B	1232	CLA	3	0
12	B	1234	CLA	8	0
12	B	1235	CLA	7	0
12	B	1236	CLA	4	0
12	B	1237	CLA	3	0
12	B	1238	CLA	5	0
12	B	1239	CLA	2	0
12	B	1240	CLA	1	0
13	B	2002	PQN	3	0
15	B	4004	BCR	3	0
15	B	4005	BCR	1	0
19	B	4006	ECH	4	0
15	B	4010	BCR	3	0
17	B	4011	45D	5	0
15	B	4017	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	4018	BCR	2	0
20	B	5002	LMG	4	0
16	B	5004	LHG	9	0
20	B	5005	LMG	3	0
21	B	5008	SQD	1	0
14	C	3002	SF4	1	0
12	F	1301	CLA	3	0
15	F	4014	BCR	9	0
23	F	4016	C7Z	1	0
21	F	5001	SQD	3	0
24	F	6001	LMT	1	0
15	I	4018	BCR	5	0
25	I	4020	EQ3	1	0
12	J	1302	CLA	2	0
15	J	4013	BCR	9	0
15	K	4001	BCR	6	0
12	L	1502	CLA	4	0
19	M	4021	ECH	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	751/751 (100%)	-0.54	9 (1%) 79 69	27, 117, 229, 322	0
2	B	731/731 (100%)	-0.68	0 100 100	18, 95, 176, 428	0
3	C	80/80 (100%)	-0.56	0 100 100	31, 87, 122, 144	0
4	D	141/141 (100%)	-0.29	1 (0%) 87 81	67, 112, 187, 399	0
5	E	69/69 (100%)	-0.58	0 100 100	45, 81, 154, 170	0
6	F	143/143 (100%)	-0.75	0 100 100	28, 98, 148, 186	0
7	I	40/40 (100%)	1.25	14 (35%) 0 0	228, 290, 404, 432	0
8	J	40/40 (100%)	-0.77	0 100 100	73, 106, 144, 149	0
9	K	70/70 (100%)	-0.34	3 (4%) 35 26	150, 241, 380, 499	0
10	L	137/137 (100%)	0.96	32 (23%) 0 0	231, 373, 583, 606	0
11	M	31/31 (100%)	-0.48	0 100 100	123, 149, 199, 221	0
All	All	2233/2233 (100%)	-0.46	59 (2%) 56 44	18, 109, 335, 606	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	110	SER	6.3
10	L	23	PRO	5.6
10	L	74	SER	5.5
1	A	237	PRO	4.9
10	L	43	GLY	4.6
10	L	109	GLY	4.4
10	L	150	GLY	4.3
1	A	7	GLU	4.2
7	I	6	ALA	4.2
10	L	146	SER	4.2
9	K	57	SER	4.0
10	L	108	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	5	PRO	3.9
10	L	107	GLU	3.7
1	A	238	LEU	3.7
10	L	145	LEU	3.6
10	L	45	SER	3.6
1	A	9	GLU	3.6
10	L	89	ILE	3.6
9	K	56	ALA	3.6
7	I	1	MET	3.5
7	I	2	ASP	3.5
10	L	94	ALA	3.4
7	I	4	SER	3.4
7	I	28	GLY	3.4
7	I	3	GLY	3.3
1	A	6	PRO	3.3
10	L	47	ILE	3.3
10	L	91	VAL	3.3
4	D	2	THR	3.1
10	L	144	ASN	3.0
10	L	90	LEU	2.8
7	I	8	SER	2.7
7	I	7	ALA	2.7
7	I	26	THR	2.7
10	L	152	PHE	2.6
10	L	157	ASN	2.6
10	L	93	THR	2.6
10	L	111	GLY	2.6
7	I	29	LEU	2.5
10	L	121	SER	2.5
7	I	9	TYR	2.4
7	I	5	TYR	2.4
10	L	151	ILE	2.4
10	L	42	LYS	2.3
1	A	239	PRO	2.3
1	A	2	THR	2.3
10	L	122	GLN	2.3
10	L	22	THR	2.2
1	A	10	ALA	2.2
10	L	125	ALA	2.2
9	K	58	LYS	2.2
10	L	106	GLY	2.1
10	L	95	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
7	I	12	TRP	2.1
10	L	59	TYR	2.1
7	I	27	MET	2.1
10	L	118	ASP	2.1
10	L	56	ALA	2.1

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. 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	B-factors(\AA^2)	Q<0.9
12	CLA	L	1502	49/65	0.50	0.35	382,393,407,412	0
22	CA	L	1001	1/1	0.52	0.15	156,156,156,156	0
25	EQ3	I	4020	42/42	0.59	0.53	224,232,241,245	0
19	ECH	M	4021	41/41	0.63	0.44	148,166,189,200	0
21	SQD	B	5008	54/54	0.66	0.69	92,154,193,201	0
15	BCR	A	4003	40/40	0.66	0.63	124,164,188,189	0
15	BCR	I	4018	40/40	0.72	0.65	161,194,217,223	0
16	LHG	B	5006	21/49	0.76	0.30	154,179,195,201	0
20	LMG	B	5005	55/55	0.76	0.45	80,149,188,190	0
21	SQD	F	5001	54/54	0.79	0.58	149,164,176,178	0
15	BCR	A	4001	40/40	0.83	0.30	148,169,184,185	0
19	ECH	B	4006	41/41	0.83	0.34	111,135,146,150	0
12	CLA	B	1207	49/65	0.84	0.24	131,157,223,227	0
24	LMT	F	6001	35/35	0.84	0.39	78,142,171,178	0
15	BCR	K	4001	40/40	0.85	0.48	129,194,221,223	0
15	BCR	B	4004	40/40	0.87	0.67	105,125,134,138	0
12	CLA	B	1212	49/65	0.87	0.34	124,146,166,171	0
12	CLA	A	1118	50/65	0.87	0.24	120,151,195,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	CLA	J	1303	49/65	0.87	0.45	145,167,176,202	0
12	CLA	A	1112	49/65	0.88	0.41	138,146,155,164	0
16	LHG	A	5003	49/49	0.88	0.46	106,135,156,160	0
12	CLA	A	1113	49/65	0.88	0.49	135,160,184,192	0
12	CLA	A	1141	45/65	0.89	0.40	137,156,176,188	0
12	CLA	B	1204	49/65	0.89	0.28	94,111,127,139	0
12	CLA	K	1401	45/65	0.89	0.32	127,147,170,175	0
12	CLA	A	1114	49/65	0.89	0.23	142,154,173,178	0
12	CLA	K	1402	49/65	0.89	0.24	168,189,213,218	0
12	CLA	B	1240	49/65	0.90	0.49	76,105,156,163	0
12	CLA	A	1132	55/65	0.90	0.27	107,148,273,351	0
12	CLA	B	1211	49/65	0.90	0.18	100,120,130,134	0
12	CLA	F	1302	49/65	0.90	0.23	63,82,106,112	0
12	CLA	B	1217	49/65	0.90	0.33	72,85,95,103	0
12	CLA	A	1111	49/65	0.90	0.32	70,113,131,146	0
15	BCR	B	4018	40/40	0.90	0.55	61,121,136,140	0
12	CLA	A	1105	65/65	0.90	0.36	66,114,126,130	0
12	CLA	F	1301	49/65	0.91	0.31	80,98,136,138	0
12	CLA	A	1120	49/65	0.91	0.26	130,149,195,200	0
15	BCR	B	4017	40/40	0.91	0.47	50,68,88,91	0
12	CLA	J	1302	49/65	0.91	0.28	134,150,159,160	0
15	BCR	A	4007	40/40	0.91	0.54	66,82,134,137	0
15	BCR	F	4014	40/40	0.91	0.43	57,85,104,106	0
12	CLA	B	1209	49/65	0.91	0.33	107,131,139,144	0
12	CLA	A	1110	49/65	0.91	0.34	130,154,173,179	0
15	BCR	J	4013	40/40	0.91	0.37	88,110,132,133	0
12	CLA	B	1203	49/65	0.91	0.33	75,86,99,103	0
12	CLA	A	1119	46/65	0.92	0.32	106,126,144,154	0
12	CLA	B	1219	49/65	0.92	0.22	64,91,133,135	0
12	CLA	A	1130	49/65	0.92	0.18	77,95,130,133	0
12	CLA	A	1125	49/65	0.92	0.26	108,124,132,135	0
12	CLA	A	1116	49/65	0.92	0.21	96,126,142,150	0
12	CLA	B	1208	49/65	0.92	0.33	90,107,128,130	0
12	CLA	B	1201	49/65	0.92	0.25	77,89,106,110	0
12	CLA	A	1011	55/65	0.92	0.22	43,63,72,89	0
12	CLA	A	1108	49/65	0.92	0.28	89,101,135,142	0
12	CLA	A	1115	56/65	0.92	0.21	118,146,155,156	0
12	CLA	B	1216	49/65	0.92	0.41	58,113,119,124	0
20	LMG	B	5002	55/55	0.92	0.45	37,69,102,118	0
22	CA	B	6001	1/1	0.92	0.15	171,171,171,171	0
15	BCR	A	4008	40/40	0.92	0.50	43,110,125,125	0
16	LHG	B	5004	49/49	0.92	0.44	57,80,128,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	CLA	B	1213	49/65	0.92	0.29	105,121,132,141	0
15	BCR	A	4012	40/40	0.92	0.48	66,81,92,93	0
18	CL	B	6000	1/1	0.92	0.21	89,89,89,89	0
12	CLA	A	1135	49/65	0.92	0.39	110,119,124,128	0
15	BCR	B	4005	40/40	0.93	0.40	31,63,141,143	0
12	CLA	A	1137	49/65	0.93	0.33	92,112,121,126	0
12	CLA	B	1238	49/65	0.93	0.23	82,108,125,127	0
12	CLA	A	1129	49/65	0.93	0.32	96,116,153,160	0
13	PQN	B	2002	33/33	0.93	0.45	72,83,105,111	0
12	CLA	A	1131	49/65	0.93	0.25	111,130,156,163	0
12	CLA	B	1218	49/65	0.93	0.24	64,90,122,130	0
23	C7Z	F	4016	42/42	0.93	0.32	35,58,93,97	0
12	CLA	B	1234	60/65	0.93	0.25	55,77,106,112	0
12	CLA	A	1133	49/65	0.93	0.24	98,115,131,133	0
12	CLA	B	1236	49/65	0.93	0.24	49,63,76,77	0
12	CLA	A	1117	49/65	0.93	0.24	78,99,110,116	0
12	CLA	A	1109	65/65	0.93	0.22	64,113,123,126	0
12	CLA	A	1134	49/65	0.93	0.25	109,140,149,156	0
12	CLA	A	1122	49/65	0.93	0.29	90,108,122,124	0
12	CLA	B	1221	49/65	0.94	0.36	60,105,115,122	0
12	CLA	B	1225	49/65	0.94	0.24	36,61,78,80	0
12	CLA	B	1215	49/65	0.94	0.20	67,79,87,89	0
12	CLA	A	1136	49/65	0.94	0.42	128,139,145,149	0
12	CLA	A	1013	65/65	0.94	0.27	19,57,67,79	0
12	CLA	B	1235	65/65	0.94	0.22	37,60,72,74	0
12	CLA	B	1232	49/65	0.94	0.18	70,82,98,101	0
12	CLA	A	1103	49/65	0.94	0.21	75,90,108,114	0
12	CLA	A	1126	60/65	0.94	0.23	28,79,96,102	0
12	CLA	B	1223	49/65	0.94	0.30	81,96,110,113	0
12	CLA	A	1124	49/65	0.94	0.34	100,122,134,135	0
12	CLA	B	1227	49/65	0.94	0.34	80,91,140,146	0
12	CLA	A	1121	49/65	0.94	0.38	90,117,137,142	0
12	CLA	A	1123	60/65	0.94	0.22	67,85,100,104	0
12	CLA	A	1127	49/65	0.94	0.24	72,86,97,103	0
17	45D	B	4011	42/42	0.94	0.28	45,59,68,68	0
12	CLA	B	1205	49/65	0.94	0.36	57,73,97,106	0
12	CLA	B	1022	60/65	0.94	0.22	31,89,94,102	0
12	CLA	B	1220	49/65	0.94	0.31	77,91,96,98	0
12	CLA	A	1012	49/65	0.94	0.20	38,63,73,74	0
12	CLA	B	1222	50/65	0.94	0.22	69,81,93,97	0
12	CLA	B	1237	49/65	0.94	0.17	92,112,121,127	0
12	CLA	A	1140	65/65	0.95	0.32	16,65,78,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	CLA	A	1128	65/65	0.95	0.26	32,87,97,104	0
15	BCR	B	4010	40/40	0.95	0.41	43,57,71,73	0
23	C7Z	J	4015	42/42	0.95	0.33	60,87,96,101	0
12	CLA	A	1107	50/65	0.95	0.27	42,53,69,94	0
12	CLA	B	1231	49/65	0.95	0.21	49,85,97,109	0
12	CLA	B	1021	65/65	0.95	0.19	22,41,55,65	0
16	LHG	A	5001	49/49	0.95	0.32	38,59,91,113	0
12	CLA	B	1206	49/65	0.95	0.22	75,86,127,132	0
12	CLA	A	1104	49/65	0.95	0.20	60,85,96,101	0
12	CLA	B	1224	55/65	0.95	0.24	13,49,70,75	0
12	CLA	B	1226	49/65	0.95	0.23	29,59,81,85	0
12	CLA	A	1102	65/65	0.95	0.27	70,86,98,104	0
12	CLA	B	1228	49/65	0.95	0.39	56,67,96,97	0
12	CLA	B	1214	60/65	0.95	0.23	46,80,102,105	0
12	CLA	A	1106	65/65	0.95	0.27	72,95,117,130	0
12	CLA	A	1139	55/65	0.95	0.26	43,59,110,117	0
12	CLA	B	1230	49/65	0.96	0.21	66,77,81,86	0
13	PQN	A	2001	33/33	0.96	0.38	13,27,42,50	0
12	CLA	B	1023	49/65	0.96	0.15	65,80,89,93	0
12	CLA	B	1239	49/65	0.96	0.27	36,61,108,114	0
12	CLA	B	1202	65/65	0.96	0.26	12,70,77,79	0
12	CLA	B	1229	55/65	0.96	0.19	33,44,62,64	0
12	CLA	A	1101	49/65	0.96	0.23	52,74,79,86	0
12	CLA	A	1138	65/65	0.97	0.23	26,55,72,76	0
12	CLA	B	1210	49/65	0.97	0.24	42,72,80,82	0
14	SF4	C	3002	8/8	0.99	0.12	32,41,89,113	0
14	SF4	A	3001	8/8	0.99	0.13	36,63,86,101	0
14	SF4	C	3003	8/8	1.00	0.16	32,57,177,197	0

6.5 Other polymers ⓘ

There are no such residues in this entry.