



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 07:48 AM EST

PDB ID : 1JB0
Title : Crystal Structure of Photosystem I: a Photosynthetic Reaction Center and Core Antenna System from Cyanobacteria
Authors : Jordan, P.; Fromme, P.; Witt, H.T.; Klukas, O.; Saenger, W.; Krauss, N.
Deposited on : 2001-06-01
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

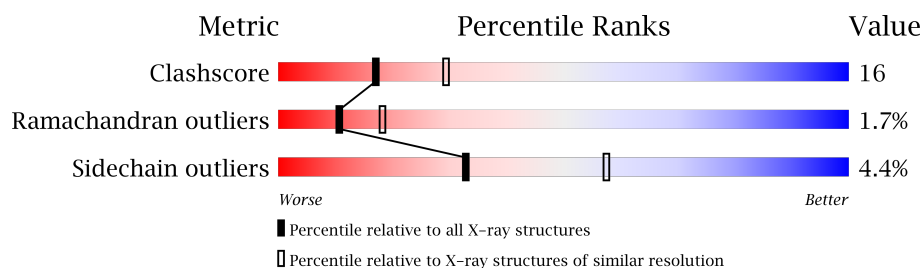
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

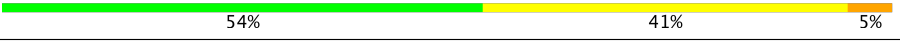
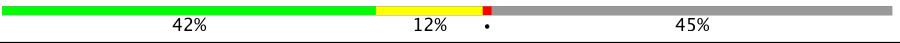



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	755	
2	B	740	
3	C	80	
4	D	138	
5	E	75	
6	F	164	
7	I	38	

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Mol	Chain	Length	Quality of chain
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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
13	CLA	A	1011	X	-	-	-
13	CLA	A	1013	X	-	-	-
13	CLA	A	1022	X	-	-	-
13	CLA	A	1101	X	-	-	-
13	CLA	A	1102	X	-	-	-
13	CLA	A	1103	X	-	-	-
13	CLA	A	1104	X	-	-	-
13	CLA	A	1105	X	-	-	-
13	CLA	A	1106	X	-	-	-
13	CLA	A	1107	X	-	-	-
13	CLA	A	1109	X	-	-	-
13	CLA	A	1110	X	-	-	-
13	CLA	A	1111	X	-	-	-
13	CLA	A	1112	X	-	-	-
13	CLA	A	1113	X	-	-	-
13	CLA	A	1114	X	-	-	-
13	CLA	A	1115	X	-	-	-
13	CLA	A	1116	X	-	-	-
13	CLA	A	1117	X	-	-	-
13	CLA	A	1118	X	-	-	-
13	CLA	A	1119	X	-	-	-
13	CLA	A	1120	X	-	-	-
13	CLA	A	1121	X	-	-	-
13	CLA	A	1122	X	-	-	-
13	CLA	A	1123	X	-	-	-
13	CLA	A	1124	X	-	-	-
13	CLA	A	1125	X	-	-	-
13	CLA	A	1126	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1127	X	-	-	-
13	CLA	A	1128	X	-	-	-
13	CLA	A	1129	X	-	-	-
13	CLA	A	1130	X	-	-	-
13	CLA	A	1132	X	-	-	-
13	CLA	A	1133	X	-	-	-
13	CLA	A	1134	X	-	-	-
13	CLA	A	1135	X	-	-	-
13	CLA	A	1136	X	-	-	-
13	CLA	A	1137	X	-	-	-
13	CLA	A	1138	X	-	-	-
13	CLA	A	1139	X	-	-	-
13	CLA	A	1140	X	-	-	-
13	CLA	A	1237	X	-	-	-
13	CLA	A	1402	X	-	-	-
13	CLA	A	1801	X	-	-	-
13	CLA	B	1012	X	-	-	-
13	CLA	B	1021	X	-	-	-
13	CLA	B	1023	X	-	-	-
13	CLA	B	1201	X	-	-	-
13	CLA	B	1202	X	-	-	-
13	CLA	B	1203	X	-	-	-
13	CLA	B	1204	X	-	-	-
13	CLA	B	1205	X	-	-	-
13	CLA	B	1206	X	-	-	-
13	CLA	B	1207	X	-	-	-
13	CLA	B	1208	X	-	-	-
13	CLA	B	1209	X	-	-	-
13	CLA	B	1210	X	-	-	-
13	CLA	B	1211	X	-	-	-
13	CLA	B	1212	X	-	-	-
13	CLA	B	1213	X	-	-	-
13	CLA	B	1214	X	-	-	-
13	CLA	B	1215	X	-	-	-
13	CLA	B	1216	X	-	-	-
13	CLA	B	1217	X	-	-	-
13	CLA	B	1218	X	-	-	-
13	CLA	B	1219	X	-	-	-
13	CLA	B	1220	X	-	-	-
13	CLA	B	1221	X	-	-	-
13	CLA	B	1222	X	-	-	-
13	CLA	B	1223	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	1224	X	-	-	-
13	CLA	B	1225	X	-	-	-
13	CLA	B	1226	X	-	-	-
13	CLA	B	1227	X	-	-	-
13	CLA	B	1228	X	-	-	-
13	CLA	B	1229	X	-	-	-
13	CLA	B	1230	X	-	-	-
13	CLA	B	1231	X	-	-	-
13	CLA	B	1232	X	-	-	-
13	CLA	B	1233	X	-	-	-
13	CLA	B	1234	X	-	-	-
13	CLA	B	1235	X	-	-	-
13	CLA	B	1238	X	-	-	-
13	CLA	B	1239	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	J	1302	X	-	-	-
13	CLA	J	1303	X	-	-	-
13	CLA	K	1401	X	-	-	-
13	CLA	L	1501	X	-	-	-
13	CLA	L	1502	X	-	-	-
13	CLA	L	1503	X	-	-	-
13	CLA	M	1601	X	-	-	-
13	CLA	X	1701	X	-	-	-
17	LHG	A	5003	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 24198 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	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

- Molecule 2 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

- 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
			598	367	103	117	11			

- Molecule 4 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

- Molecule 5 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			539	342	93	104			

- Molecule 6 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

- Molecule 8 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

- Molecule 9 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	S	0	0	0
			222	130	46	46				

- Molecule 10 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ARG	PRO	CONFLICT	UNP P25902
L	144	VAL	-	SEE REMARK 999	UNP P25902
L	145	VAL	-	SEE REMARK 999	UNP P25902
L	146	ASP	-	SEE REMARK 999	UNP P25902
L	147	GLY	-	SEE REMARK 999	UNP P25902
L	148	ILE	-	SEE REMARK 999	UNP P25902
L	149	MET	-	SEE REMARK 999	UNP P25902
L	150	THR	-	SEE REMARK 999	UNP P25902
L	151	GLY	-	SEE REMARK 999	UNP P25902
L	152	LEU	-	SEE REMARK 999	UNP P25902
L	153	PHE	-	SEE REMARK 999	UNP P25902
L	154	ASN	-	SEE REMARK 999	UNP P25902

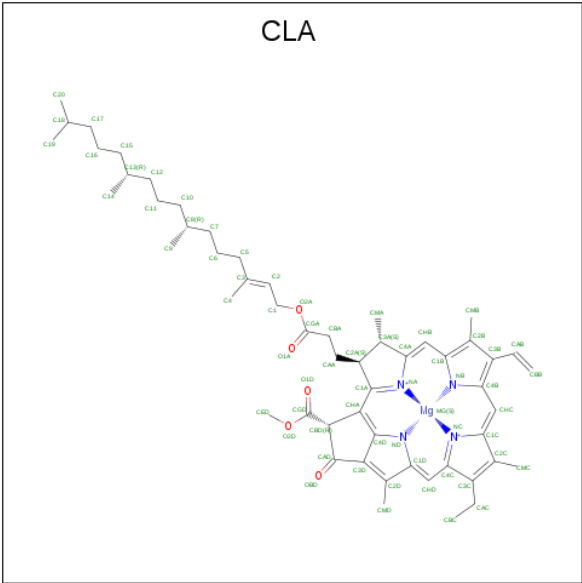
- Molecule 11 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	M	31	241	161	36	43	1	0	0	0

- Molecule 12 is a protein called PHOTOSYSTEM I SUBUNIT PSAX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	X	29	233	164	34	35	0	0	0

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	59	49	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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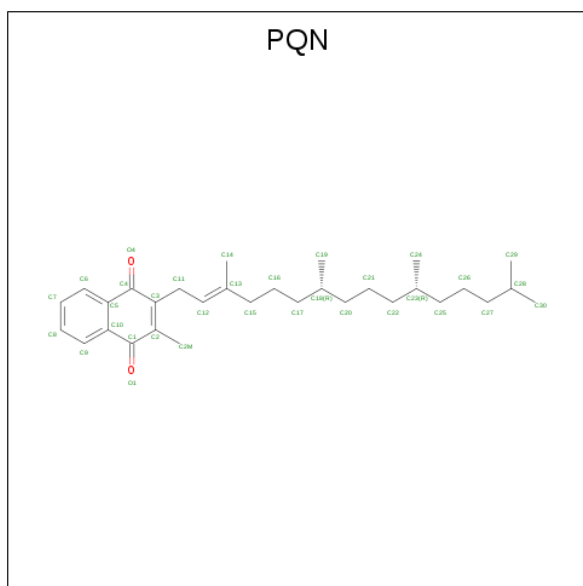
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	J	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	J	1	Total 37	C 31	Mg 1	N 4	O 1	0	0
13	K	1	Total 45	C 35	Mg 1	N 4	O 5	0	0

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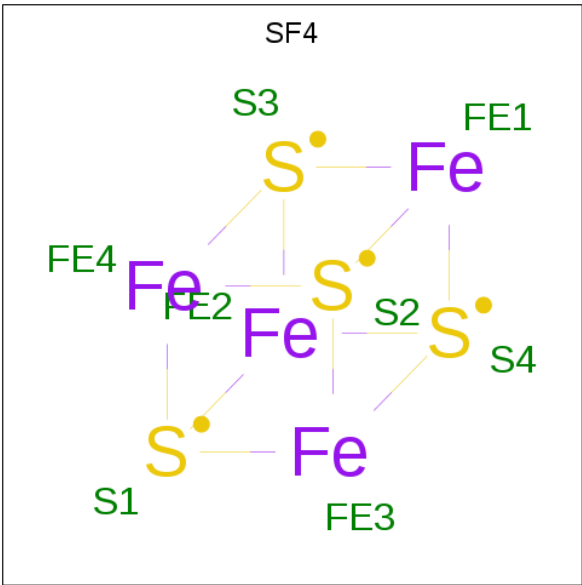
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



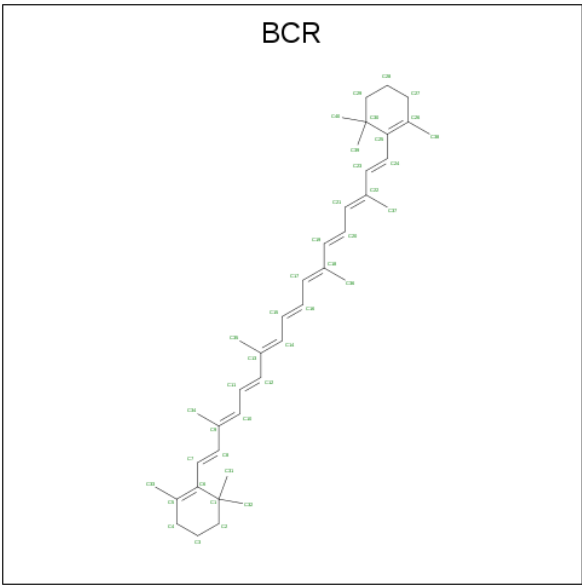
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			33	31	2		
14	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



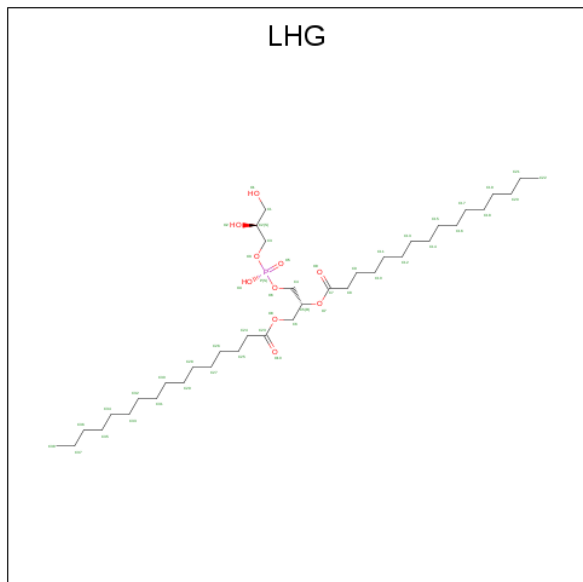
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	C	0	0
			40	40		

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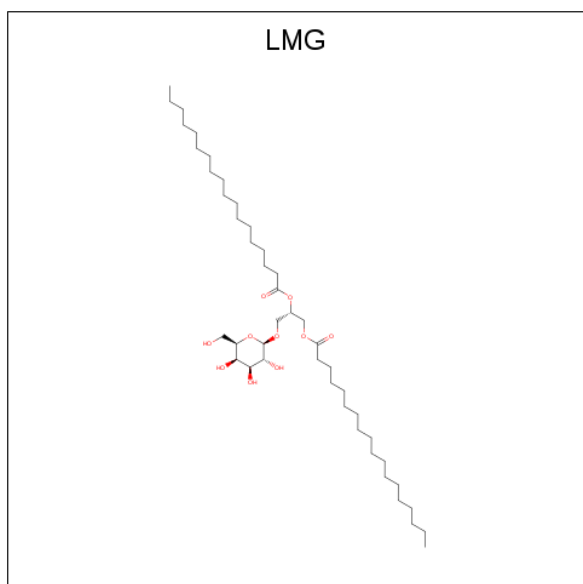
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 25 25	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	F	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	M	1	Total C 40 40	0	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			49	38	10	1		
17	A	1	Total	C	O	P	0	0
			27	16	10	1		
17	B	1	Total	C	O	P	0	0
			23	12	10	1		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

- Molecule 20 is water.

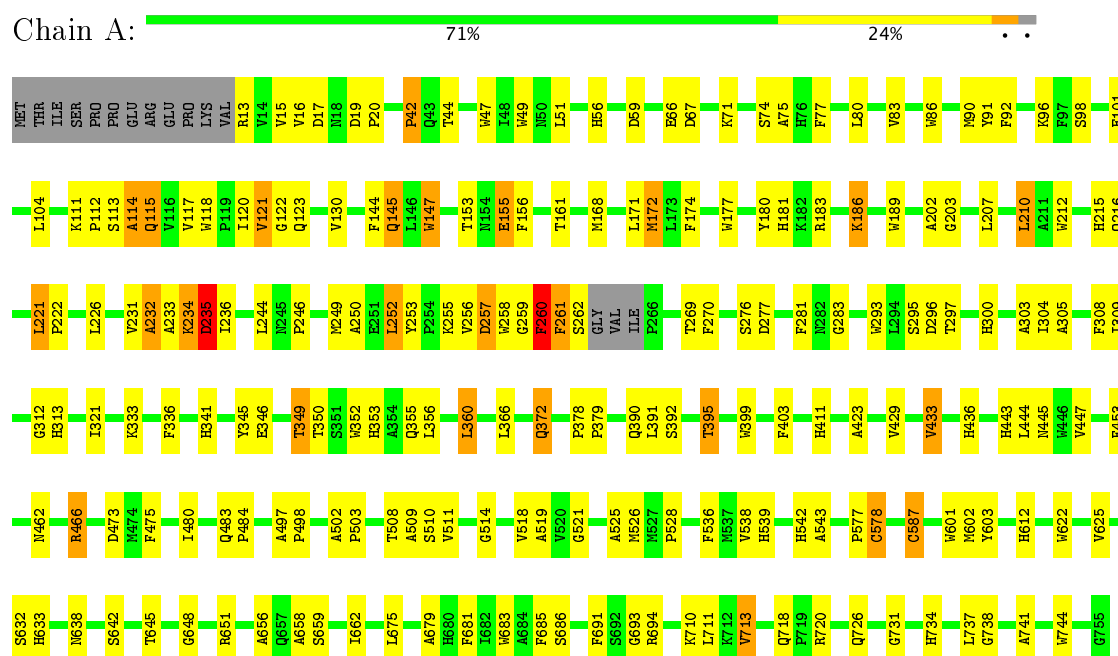
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	53	Total	O	0	0
			53	53		
20	B	65	Total	O	0	0
			65	65		
20	C	21	Total	O	0	0
			21	21		
20	D	17	Total	O	0	0
			17	17		
20	E	5	Total	O	0	0
			5	5		
20	F	6	Total	O	0	0
			6	6		
20	I	3	Total	O	0	0
			3	3		
20	J	1	Total	O	0	0
			1	1		
20	L	27	Total	O	0	0
			27	27		
20	M	3	Total	O	0	0
			3	3		

3 Residue-property plots

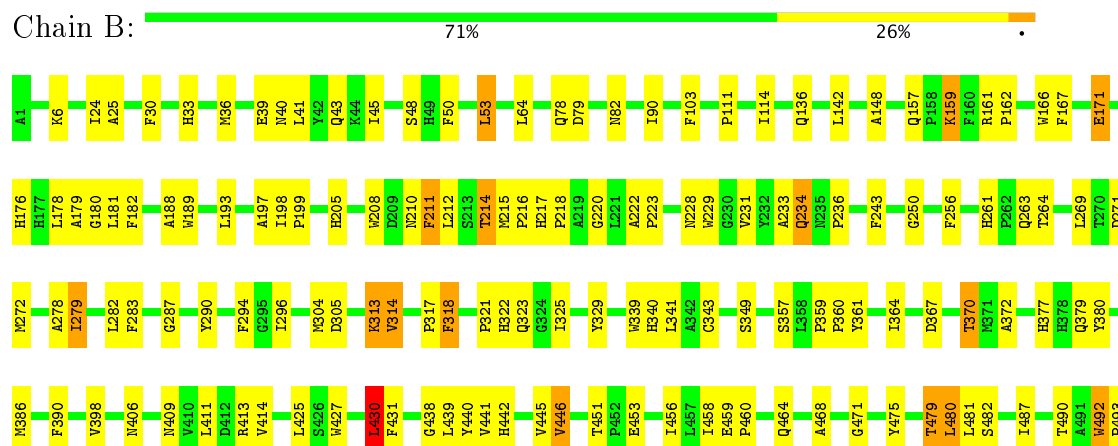
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

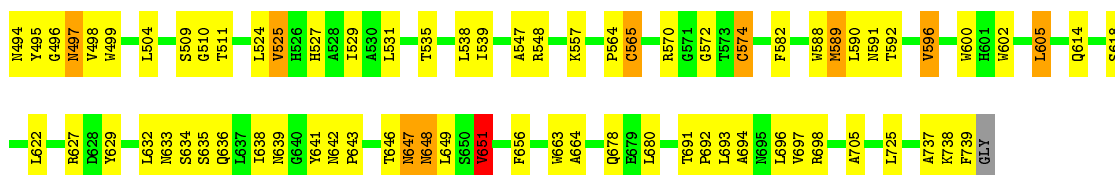
Note EDS was not executed.

• Molecule 1: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



• Molecule 2: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2





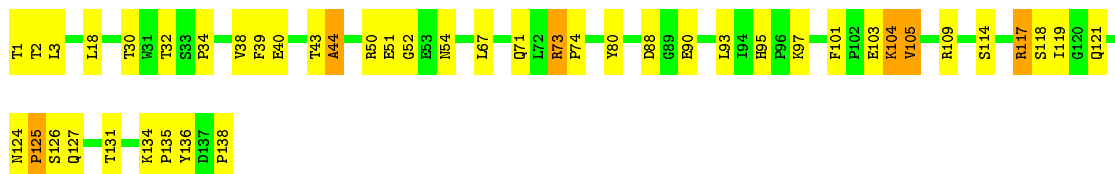
• Molecule 3: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C: 74% 25%



• Molecule 4: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II

Chain D: 67% 28%



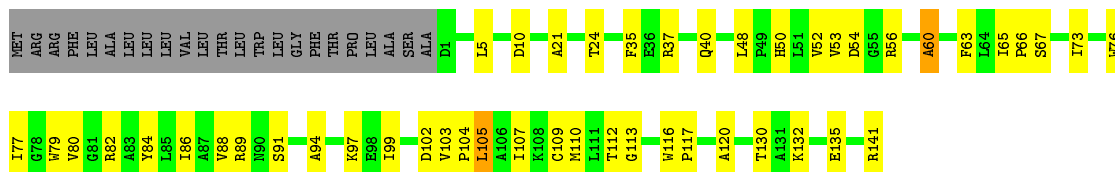
• Molecule 5: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV

Chain E: 72% 16% 8%



• Molecule 6: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III

Chain F: 57% 28% 14%



• Molecule 7: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII

Chain I: 74% 21% 5%

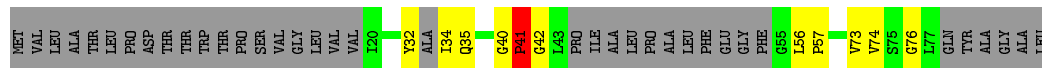


• Molecule 8: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX

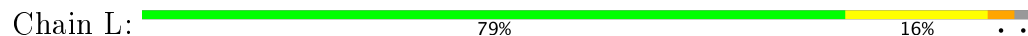
Chain J: 54% 41% 5%



- Molecule 9: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X



- Molecule 10: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI



- Molecule 11: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII



- Molecule 12: PHOTOSYSTEM I SUBUNIT PSAX



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00 Å 281.00 Å 165.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (30.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.199 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24198	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/5983	0.66	2/8158 (0.0%)
2	B	0.56	0/6096	0.67	2/8332 (0.0%)
3	C	0.74	0/608	0.96	4/824 (0.5%)
4	D	0.57	0/1101	0.81	1/1492 (0.1%)
5	E	0.57	0/551	0.84	2/750 (0.3%)
6	F	0.47	0/1087	0.66	0/1476
7	I	0.66	0/312	0.75	0/425
8	J	0.45	0/350	0.65	0/477
9	K	0.52	0/219	0.86	3/297 (1.0%)
10	L	0.67	0/1148	0.75	0/1558
11	M	0.63	0/244	0.85	1/332 (0.3%)
12	X	0.55	0/242	0.67	0/332
All	All	0.55	0/17941	0.70	15/24453 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	TYR	CA-C-O	9.95	140.99	120.10
11	M	30	TYR	N-CA-C	7.84	132.18	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.52	131.91	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	GLY	N-CA-C	-6.39	97.13	113.10
3	C	60	ASP	CA-C-N	-6.29	103.37	117.20
9	K	57	PRO	N-CA-CB	6.14	110.67	103.30
3	C	60	ASP	C-N-CA	5.89	136.41	121.70
1	A	114	ALA	N-CA-C	-5.87	95.16	111.00
3	C	61	PHE	N-CA-CB	5.85	121.14	110.60
9	K	41	PRO	N-CA-CB	5.78	110.24	103.30
9	K	35	GLN	N-CA-C	5.35	125.45	111.00
2	B	430	LEU	CA-CB-CG	5.12	127.08	115.30
2	B	651	VAL	CB-CA-C	-5.10	101.72	111.40
5	E	55	VAL	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	215	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	40	0
5	E	539	0	528	10	0
6	F	1065	0	1079	42	0
7	I	301	0	306	7	0
8	J	338	0	347	23	0
9	K	222	0	110	4	0
10	L	1119	0	1125	22	0
11	M	241	0	264	13	0
12	X	233	0	231	6	0
13	A	2687	0	2675	143	0
13	B	2349	0	2304	152	0
13	F	45	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	11	0
13	M	45	0	33	1	0
13	X	45	0	33	1	0
14	A	33	0	46	1	0
14	B	33	0	46	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
16	A	240	0	336	22	0
16	B	265	0	369	17	0
16	F	40	0	56	2	0
16	I	80	0	112	3	0
16	J	120	0	168	16	0
16	L	80	0	112	1	0
16	M	40	0	56	2	0
17	A	76	0	98	6	0
17	B	23	0	16	1	0
18	B	55	0	86	5	0
19	L	1	0	0	0	0
20	A	53	0	0	5	0
20	B	65	0	0	3	0
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	1
20	M	3	0	0	1	0
All	All	24198	0	23804	743	1

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 16.

All (743) 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)
8:J:31:ARG:HD3	16:J:4013:BCR:H312	1.25	1.17
2:B:622:LEU:HD12	13:B:1012:CLA:H11	1.29	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.05
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01
2:B:243:PHE:H	2:B:263:GLN:HE22	1.07	1.01
2:B:231:VAL:O	2:B:234:GLN:HG2	1.63	0.99
2:B:406:ASN:HD22	2:B:409:ASN:HD21	0.98	0.96
1:A:536:PHE:HA	13:A:1136:CLA:HED1	1.45	0.96
2:B:494:ASN:HD22	2:B:496:GLY:H	1.13	0.93
11:M:31:LYS:O	11:M:31:LYS:HG2	1.70	0.92
1:A:353:HIS:HD2	1:A:411:HIS:HD1	1.21	0.88
4:D:117:ARG:HG3	4:D:121:GLN:HB2	1.54	0.88
16:A:4011:BCR:H362	13:B:1012:CLA:H42	1.55	0.87
1:A:117:VAL:HG13	1:A:123:GLN:HE21	1.42	0.84
2:B:406:ASN:ND2	2:B:409:ASN:HD21	1.76	0.83
8:J:24:GLY:HA3	13:J:1302:CLA:HBB1	1.60	0.83
4:D:101:PHE:HB2	4:D:104:LYS:HE2	1.59	0.83
8:J:31:ARG:HD3	16:J:4013:BCR:C31	2.08	0.83
1:A:333:LYS:O	13:A:1801:CLA:HBC3	1.81	0.81
2:B:509:SER:O	2:B:511:THR:N	2.12	0.81
1:A:203:GLY:HA2	13:A:1118:CLA:HBC1	1.63	0.80
1:A:391:LEU:O	1:A:395:THR:HG23	1.81	0.80
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.12	0.80
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.63	0.79
6:F:88:VAL:HG11	6:F:97:LYS:HB2	1.64	0.79
1:A:345:TYR:O	1:A:349:THR:HB	1.84	0.78
2:B:494:ASN:ND2	2:B:496:GLY:H	1.80	0.78
2:B:459:GLU:HG3	6:F:5:LEU:HD11	1.63	0.78
2:B:243:PHE:H	2:B:263:GLN:NE2	1.82	0.78
1:A:508:THR:HG22	1:A:510:SER:N	1.96	0.77
2:B:313:LYS:O	2:B:314:VAL:HG22	1.85	0.77
3:C:37:GLN:NE2	4:D:105:VAL:HG22	1.99	0.77
2:B:278:ALA:HB2	13:B:1214:CLA:HBB1	1.66	0.77
2:B:339:TRP:HE1	13:B:1221:CLA:C2B	1.99	0.76
2:B:25:ALA:HB2	18:B:5002:LMG:H121	1.67	0.76
13:A:1011:CLA:HBB1	13:B:1012:CLA:HED1	1.67	0.75
1:A:231:VAL:O	1:A:232:ALA:HB3	1.87	0.75
13:A:1126:CLA:H192	16:J:4012:BCR:H14C	1.69	0.75
2:B:367:ASP:CG	2:B:370:THR:HG23	2.07	0.75
2:B:647:ASN:HD22	2:B:649:LEU:H	1.35	0.75
13:B:1215:CLA:HMB1	13:B:1215:CLA:HBB1	1.68	0.75
13:A:1126:CLA:H93	16:J:4012:BCR:H361	1.69	0.74
1:A:453:PHE:O	13:A:1132:CLA:HBB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1222:CLA:HAA2	13:B:1223:CLA:OBD	1.87	0.74
2:B:639:ASN:HD22	2:B:642:ASN:HD22	1.36	0.74
2:B:229:TRP:HB2	13:B:1213:CLA:H12	1.70	0.73
2:B:497:ASN:O	2:B:498:VAL:HB	1.87	0.73
4:D:50:ARG:N	4:D:54:ASN:HD21	1.84	0.73
2:B:159:LYS:H	2:B:159:LYS:CD	1.92	0.73
2:B:494:ASN:HD22	2:B:496:GLY:N	1.84	0.72
2:B:181:LEU:HG	13:B:1210:CLA:H43	1.71	0.72
2:B:425:LEU:HG	13:B:1236:CLA:CBB	2.20	0.72
2:B:622:LEU:HD12	13:B:1012:CLA:C1	2.15	0.72
2:B:725:LEU:HD11	13:B:1226:CLA:H203	1.69	0.72
11:M:31:LYS:O	11:M:31:LYS:CG	2.34	0.72
2:B:329:TYR:OH	2:B:340:HIS:HE1	1.71	0.72
3:C:39:ALA:O	20:C:3012:HOH:O	2.07	0.72
2:B:343:CYS:HB3	13:B:1221:CLA:H42	1.72	0.71
13:B:1216:CLA:HAA2	13:B:1221:CLA:HBB1	1.72	0.71
2:B:36:MET:HE3	2:B:40:ASN:HB2	1.72	0.71
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.71	0.71
1:A:221:LEU:HB2	1:A:222:PRO:HD3	1.73	0.71
1:A:341:HIS:HE1	17:A:5003:LHG:HC11	1.56	0.70
5:E:68:VAL:HG23	5:E:69:ALA:H	1.56	0.70
1:A:255:LYS:HB2	1:A:277:ASP:OD2	1.92	0.69
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.74	0.69
2:B:589:MET:HE1	2:B:590:LEU:HA	1.75	0.69
1:A:13:ARG:HE	1:A:15:VAL:CG2	2.05	0.68
2:B:602:TRP:HE1	2:B:614:GLN:HE21	1.40	0.68
13:A:1136:CLA:H101	13:L:1502:CLA:H191	1.75	0.68
1:A:221:LEU:HD11	1:A:295:SER:HA	1.76	0.68
1:A:399:TRP:CD1	13:A:1126:CLA:HAB	2.29	0.68
6:F:52:VAL:HG12	6:F:54:ASP:HB2	1.76	0.67
1:A:117:VAL:HG13	1:A:123:GLN:NE2	2.08	0.67
2:B:25:ALA:HA	13:B:1226:CLA:H42	1.76	0.67
1:A:101:GLU:OE2	1:A:155:GLU:HG2	1.95	0.66
6:F:102:ASP:OD2	6:F:105:LEU:HB2	1.95	0.66
9:K:73:VAL:HA	13:K:1401:CLA:HBB1	1.77	0.66
1:A:336:PHE:HB2	17:A:5003:LHG:HC41	1.78	0.66
2:B:339:TRP:HZ2	13:B:1221:CLA:HAB	1.58	0.66
3:C:65:ARG:HG2	3:C:67:TYR:CZ	2.31	0.66
14:A:2001:PQN:H172	16:B:4014:BCR:H382	1.77	0.66
4:D:50:ARG:H	4:D:54:ASN:ND2	1.89	0.66
2:B:188:ALA:HA	13:B:1212:CLA:CBB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:TRP:HB3	13:A:1103:CLA:HAC1	1.77	0.65
2:B:210:ASN:O	2:B:214:THR:HG23	1.96	0.65
2:B:318:PHE:HB2	13:B:1220:CLA:HMA1	1.78	0.65
2:B:318:PHE:CD1	13:B:1219:CLA:HAB	2.32	0.65
2:B:41:LEU:O	2:B:45:ILE:HG12	1.97	0.65
6:F:63:PHE:C	6:F:66:PRO:HD2	2.17	0.65
1:A:249:MET:O	1:A:252:LEU:O	2.15	0.65
1:A:257:ASP:OD1	1:A:262:SER:HB3	1.96	0.65
2:B:492:TRP:CE3	2:B:493:PRO:HD3	2.32	0.65
1:A:269:THR:O	1:A:270:PHE:HB2	1.96	0.65
2:B:313:LYS:O	2:B:314:VAL:HG13	1.97	0.65
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.78	0.65
10:L:6:LYS:HB2	10:L:7:PRO:HD2	1.79	0.65
13:A:1237:CLA:H191	13:L:1502:CLA:HBB1	1.78	0.65
6:F:54:ASP:OD2	12:X:30:TYR:CE2	2.50	0.64
13:B:1226:CLA:HMB1	13:B:1226:CLA:HBB1	1.78	0.64
2:B:304:MET:HG3	2:B:322:HIS:O	1.97	0.64
2:B:647:ASN:ND2	2:B:649:LEU:H	1.95	0.64
10:L:61:PRO:HB3	13:L:1503:CLA:HBB1	1.78	0.64
1:A:473:ASP:OD1	10:L:69:ARG:NH2	2.31	0.64
2:B:641:TYR:HB2	2:B:646:THR:HG22	1.79	0.64
8:J:12:PRO:HB2	16:J:4013:BCR:H391	1.78	0.64
13:B:1203:CLA:H162	13:B:1225:CLA:HBB2	1.80	0.64
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.79	0.63
3:C:23:ASP:OD2	4:D:95:HIS:HD2	1.81	0.63
13:B:1023:CLA:H111	16:B:4017:BCR:H362	1.79	0.63
6:F:63:PHE:O	6:F:66:PRO:HD2	1.98	0.63
13:A:1011:CLA:HAB	13:B:1021:CLA:NA	2.14	0.63
2:B:318:PHE:HA	13:B:1219:CLA:CAB	2.28	0.63
4:D:117:ARG:HG2	4:D:118:SER:O	1.98	0.63
2:B:622:LEU:CD1	13:B:1012:CLA:H11	2.16	0.63
6:F:60:ALA:O	6:F:65:ILE:HG12	1.98	0.62
1:A:177:TRP:HB2	13:A:1109:CLA:HMC3	1.80	0.62
2:B:166:TRP:CZ2	13:B:1208:CLA:HMA1	2.33	0.62
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.80	0.62
11:M:29:LEU:O	11:M:30:TYR:HB2	1.99	0.62
1:A:104:LEU:HD11	1:A:153:THR:HA	1.81	0.62
1:A:651:ARG:HB2	2:B:638:ILE:HG23	1.81	0.62
1:A:86:TRP:HA	13:A:1105:CLA:HBB2	1.82	0.62
2:B:136:GLN:HE22	2:B:208:TRP:HE1	1.46	0.62
2:B:228:ASN:O	2:B:231:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:MET:HG2	13:A:1124:CLA:HBC1	1.80	0.62
2:B:647:ASN:HD21	2:B:649:LEU:HB2	1.64	0.62
2:B:480:LEU:C	2:B:482:SER:H	2.02	0.62
1:A:356:LEU:O	1:A:360:LEU:HB2	2.00	0.62
1:A:353:HIS:CD2	1:A:411:HIS:HD1	2.11	0.61
2:B:278:ALA:CB	13:B:1214:CLA:HBB1	2.29	0.61
13:A:1237:CLA:HMA1	2:B:694:ALA:CB	2.29	0.61
13:A:1124:CLA:HAA2	13:A:1125:CLA:OBD	2.00	0.61
1:A:543:ALA:HB1	13:A:1136:CLA:HMB3	1.83	0.61
1:A:429:VAL:O	1:A:433:VAL:HG13	1.99	0.61
2:B:438:GLY:HA3	13:B:1230:CLA:CBB	2.31	0.61
1:A:42:PRO:HG2	6:F:99:ILE:HD13	1.83	0.61
11:M:24:ARG:HG3	11:M:24:ARG:HH11	1.64	0.61
1:A:90:MET:HE3	13:A:1106:CLA:HED2	1.82	0.61
13:B:1234:CLA:HMB2	13:B:1236:CLA:HED1	1.81	0.61
13:A:1801:CLA:HBD	13:A:1801:CLA:H61	1.83	0.61
1:A:453:PHE:O	13:A:1132:CLA:CBB	2.48	0.61
1:A:726:GLN:HG3	17:A:5001:LHG:O9	2.01	0.61
1:A:601:TRP:HH2	13:A:1022:CLA:HBB1	1.66	0.60
1:A:518:VAL:HG22	1:A:525:ALA:HB3	1.82	0.60
10:L:153:PHE:O	10:L:154:ASN:HB2	1.99	0.60
13:B:1203:CLA:H151	13:B:1203:CLA:H102	1.84	0.60
3:C:30:TRP:O	3:C:36:GLY:HA2	2.00	0.60
1:A:303:ALA:HB2	13:A:1116:CLA:HBB1	1.83	0.60
9:K:32:TYR:O	9:K:34:ILE:N	2.34	0.60
1:A:484:PRO:HB3	13:A:1136:CLA:HED3	1.83	0.60
13:A:1011:CLA:HBB1	13:B:1012:CLA:CED	2.31	0.60
1:A:168:MET:CE	1:A:171:LEU:HD23	2.31	0.60
13:A:1013:CLA:H71	13:A:1140:CLA:HMC3	1.83	0.59
1:A:210:LEU:HD21	16:A:4001:BCR:H342	1.84	0.59
1:A:300:HIS:O	1:A:304:ILE:HG12	2.03	0.59
1:A:19:ASP:HA	1:A:181:HIS:O	2.02	0.59
1:A:231:VAL:O	1:A:232:ALA:CB	2.50	0.59
13:B:1227:CLA:HBC1	16:B:4009:BCR:H23C	1.83	0.59
1:A:259:GLY:O	1:A:261:PHE:N	2.35	0.59
2:B:181:LEU:HD21	13:B:1210:CLA:H12	1.85	0.59
13:A:1138:CLA:H43	13:B:1229:CLA:HAA2	1.84	0.59
2:B:36:MET:CE	2:B:41:LEU:N	2.66	0.59
2:B:642:ASN:HB2	2:B:643:PRO:HD2	1.84	0.59
4:D:40:GLU:H	4:D:71:GLN:NE2	2.01	0.59
1:A:257:ASP:CG	1:A:258:TRP:N	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.83	0.59
2:B:591:ASN:HB2	13:B:1012:CLA:HBC2	1.83	0.58
7:I:37:GLU:C	7:I:38:ALA:OXT	2.41	0.58
1:A:16:VAL:HG12	1:A:17:ASP:N	2.17	0.58
1:A:207:LEU:HD22	16:A:4002:BCR:H361	1.84	0.58
2:B:438:GLY:HA3	13:B:1230:CLA:HBB1	1.85	0.58
10:L:36:ALA:HB2	13:L:1502:CLA:HMD1	1.84	0.58
1:A:86:TRP:HA	13:A:1105:CLA:CBB	2.33	0.58
13:A:1121:CLA:HMA1	13:A:1801:CLA:HAC2	1.85	0.58
2:B:589:MET:HE2	2:B:589:MET:O	2.02	0.58
13:B:1230:CLA:O1D	8:J:35:ASP:HA	2.02	0.58
2:B:243:PHE:N	2:B:263:GLN:HE22	1.90	0.58
13:A:1106:CLA:HMC2	13:A:1126:CLA:H142	1.84	0.58
1:A:145:GLN:NE2	1:A:145:GLN:H	2.02	0.58
1:A:744:TRP:HB2	13:A:1126:CLA:HBB1	1.86	0.58
2:B:367:ASP:OD1	2:B:370:THR:HG23	2.03	0.58
2:B:648:ASN:HD22	2:B:648:ASN:N	2.02	0.58
16:A:4011:BCR:H321	16:A:4011:BCR:HC8	1.83	0.58
2:B:380:TYR:CD1	13:B:1224:CLA:HBB1	2.39	0.57
1:A:91:TYR:CZ	1:A:147:TRP:CZ3	2.91	0.57
1:A:392:SER:HB3	13:A:1126:CLA:HMA1	1.87	0.57
2:B:414:VAL:HG11	16:B:4009:BCR:H401	1.85	0.57
6:F:82:ARG:O	6:F:86:ILE:HG12	2.04	0.57
13:A:1013:CLA:H12	2:B:430:LEU:HD12	1.85	0.57
1:A:542:HIS:HB3	13:A:1135:CLA:HBB1	1.87	0.57
2:B:557:LYS:HD2	4:D:124:ASN:OD1	2.04	0.57
2:B:279:ILE:HD11	13:B:1214:CLA:CBC	2.35	0.57
5:E:24:ALA:O	5:E:25:SER:HB3	2.05	0.57
13:A:1106:CLA:H112	13:A:1128:CLA:H203	1.87	0.56
1:A:355:GLN:HG3	13:A:1123:CLA:H152	1.87	0.56
1:A:349:THR:HG22	1:A:350:THR:HG23	1.87	0.56
1:A:694:ARG:HD3	2:B:572:GLY:HA3	1.86	0.56
2:B:678:GLN:NE2	2:B:705:ALA:H	2.03	0.56
6:F:37:ARG:O	6:F:40:GLN:HG2	2.04	0.56
1:A:189:TRP:CZ2	13:A:1108:CLA:HMA1	2.40	0.56
1:A:67:ASP:O	1:A:71:LYS:HG3	2.05	0.56
2:B:282:LEU:HD12	13:B:1216:CLA:HMC1	1.87	0.56
8:J:15:ALA:O	8:J:19:MET:HB2	2.06	0.56
1:A:233:ALA:O	1:A:235:ASP:N	2.36	0.56
2:B:234:GLN:OE1	2:B:234:GLN:HA	2.06	0.56
2:B:339:TRP:CH2	16:B:4009:BCR:H372	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:20:LEU:HD11	12:X:24:PHE:HE1	1.71	0.56
2:B:279:ILE:HG23	2:B:283:PHE:CE2	2.41	0.56
2:B:339:TRP:CZ2	13:B:1221:CLA:HAB	2.39	0.56
2:B:480:LEU:O	2:B:482:SER:N	2.38	0.56
6:F:76:TRP:CE2	6:F:113:GLY:HA3	2.40	0.56
1:A:66:GLU:OE2	1:A:186:LYS:HG3	2.05	0.56
13:A:1011:CLA:HAB	13:B:1021:CLA:C1A	2.36	0.56
12:X:9:TYR:O	12:X:10:ALA:HB2	2.05	0.56
1:A:366:LEU:HD11	13:A:1117:CLA:H71	1.87	0.56
1:A:297:THR:O	1:A:300:HIS:HB3	2.06	0.56
1:A:741:ALA:HB2	16:A:4011:BCR:H323	1.88	0.56
13:A:1102:CLA:HMC3	13:A:1104:CLA:HED2	1.86	0.55
13:A:1130:CLA:H12	13:L:1502:CLA:H93	1.86	0.55
4:D:117:ARG:CG	4:D:121:GLN:HB2	2.33	0.55
2:B:588:TRP:HH2	13:B:1012:CLA:CBB	2.19	0.55
2:B:589:MET:HE1	2:B:590:LEU:CA	2.36	0.55
9:K:40:GLY:O	9:K:41:PRO:C	2.44	0.55
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.41	0.55
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.36	0.55
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.89	0.55
1:A:681:PHE:CD2	16:A:4011:BCR:H363	2.42	0.55
13:B:1225:CLA:H51	16:B:4006:BCR:H392	1.88	0.55
13:B:1224:CLA:HBC3	18:B:5002:LMG:H421	1.88	0.55
2:B:261:HIS:CD2	2:B:264:THR:H	2.25	0.55
1:A:372:GLN:HG3	13:A:1124:CLA:CED	2.37	0.55
2:B:233:ALA:O	2:B:234:GLN:O	2.25	0.55
13:A:1116:CLA:H41	13:A:1133:CLA:HAA2	1.88	0.54
1:A:244:LEU:O	1:A:246:PRO:HD3	2.06	0.54
1:A:681:PHE:CG	16:A:4011:BCR:H363	2.43	0.54
13:B:1238:CLA:H18	16:I:4018:BCR:H362	1.89	0.54
13:A:1237:CLA:HMA1	2:B:694:ALA:HB1	1.88	0.54
16:A:4007:BCR:H333	16:A:4008:BCR:H333	1.89	0.54
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.89	0.54
2:B:525:VAL:HG13	13:B:1021:CLA:H141	1.89	0.54
1:A:390:GLN:HA	1:A:390:GLN:HE21	1.71	0.54
1:A:403:PHE:HB3	13:A:1104:CLA:H112	1.90	0.54
2:B:205:HIS:ND1	20:B:5051:HOH:O	2.24	0.54
4:D:43:THR:O	4:D:44:ALA:HB3	2.07	0.54
10:L:35:PRO:HG3	13:L:1502:CLA:HED2	1.88	0.54
2:B:413:ARG:HD3	13:B:1227:CLA:OBD	2.07	0.54
13:B:1216:CLA:HMB2	13:B:1221:CLA:HMA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:GLN:O	2:B:161:ARG:HG3	2.08	0.54
2:B:318:PHE:HA	13:B:1219:CLA:HAB	1.88	0.54
2:B:592:THR:O	2:B:596:VAL:HG13	2.08	0.54
1:A:308:PHE:HE2	13:A:1119:CLA:HAB	1.72	0.54
2:B:171:GLU:HB3	2:B:290:TYR:HB3	1.90	0.54
12:X:25:LEU:O	12:X:29:TYR:HD1	1.89	0.54
1:A:42:PRO:HG3	1:A:47:TRP:CE3	2.42	0.54
2:B:589:MET:HE2	2:B:589:MET:C	2.29	0.54
2:B:103:PHE:CZ	2:B:651:VAL:HG22	2.42	0.54
2:B:614:GLN:O	2:B:618:SER:HB2	2.08	0.54
5:E:6:LYS:HD3	5:E:22:THR:HG22	1.89	0.54
13:A:1022:CLA:OBD	13:B:1021:CLA:HMB3	2.08	0.53
2:B:212:LEU:HD21	16:B:4006:BCR:H341	1.90	0.53
1:A:305:ALA:O	1:A:309:ILE:HG12	2.08	0.53
6:F:52:VAL:CG1	6:F:54:ASP:HB2	2.37	0.53
11:M:24:ARG:HH11	11:M:24:ARG:CG	2.20	0.53
13:A:1125:CLA:HBB1	13:A:1133:CLA:HMA2	1.89	0.53
13:A:1011:CLA:HMB3	13:B:1012:CLA:OBD	2.09	0.53
13:A:1013:CLA:H142	16:A:4011:BCR:H402	1.90	0.53
13:A:1101:CLA:HED1	8:J:12:PRO:HA	1.90	0.53
1:A:466:ARG:O	2:B:646:THR:HG21	2.09	0.53
2:B:479:THR:O	2:B:480:LEU:O	2.27	0.53
13:B:1226:CLA:H143	18:B:5002:LMG:H231	1.89	0.53
6:F:53:VAL:HG12	6:F:63:PHE:HB2	1.90	0.53
6:F:88:VAL:HG11	6:F:97:LYS:CB	2.37	0.53
13:A:1124:CLA:H162	16:A:4007:BCR:H272	1.91	0.53
13:A:1128:CLA:H111	17:A:5001:LHG:H202	1.90	0.53
1:A:622:TRP:O	1:A:633:HIS:HD2	1.92	0.53
8:J:19:MET:CE	8:J:19:MET:HA	2.38	0.53
10:L:16:HIS:CD2	10:L:17:LEU:H	2.27	0.53
1:A:13:ARG:HE	1:A:15:VAL:HG22	1.72	0.53
1:A:168:MET:HE1	1:A:171:LEU:HD23	1.91	0.53
13:A:1013:CLA:O1A	2:B:531:LEU:HD11	2.10	0.52
13:A:1119:CLA:HMB2	13:A:1123:CLA:HMA3	1.92	0.52
1:A:221:LEU:HD11	1:A:295:SER:CA	2.39	0.52
1:A:59:ASP:OD2	1:A:353:HIS:HE1	1.91	0.52
2:B:406:ASN:HD22	2:B:409:ASN:ND2	1.84	0.52
1:A:296:ASP:HB3	13:A:1116:CLA:HMA1	1.90	0.52
1:A:244:LEU:C	1:A:246:PRO:HD3	2.30	0.52
2:B:430:LEU:HB3	13:B:1229:CLA:HED3	1.90	0.52
6:F:40:GLN:OE1	8:J:40:PRO:O	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MET:CE	13:A:1106:CLA:HED2	2.39	0.52
2:B:78:GLN:OE1	2:B:78:GLN:HA	2.10	0.52
1:A:356:LEU:HG	1:A:360:LEU:HD22	1.91	0.52
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.91	0.52
6:F:79:TRP:CH2	6:F:120:ALA:HA	2.44	0.52
2:B:217:HIS:CG	2:B:218:PRO:HD2	2.44	0.52
2:B:36:MET:HE2	2:B:41:LEU:N	2.25	0.52
1:A:744:TRP:CZ2	13:A:1126:CLA:H43	2.44	0.52
13:A:1133:CLA:HMD2	13:A:1134:CLA:HBB1	1.92	0.52
1:A:578:CYS:HB3	1:A:587:CYS:HA	1.91	0.52
8:J:28:GLU:OE1	8:J:28:GLU:HA	2.09	0.52
2:B:634:SER:O	2:B:638:ILE:HB	2.10	0.52
1:A:77:PHE:CE2	13:A:1108:CLA:HBB1	2.45	0.52
1:A:718:GLN:NE2	5:E:42:LYS:HD3	2.25	0.52
2:B:294:PHE:HE1	13:B:1209:CLA:HMA1	1.75	0.52
1:A:83:VAL:HG11	13:A:1103:CLA:H72	1.92	0.51
1:A:16:VAL:HG11	1:A:183:ARG:HB3	1.92	0.51
2:B:279:ILE:HD11	13:B:1214:CLA:HBC2	1.92	0.51
1:A:226:LEU:HD22	1:A:231:VAL:HG21	1.93	0.51
1:A:259:GLY:C	1:A:261:PHE:H	2.14	0.51
2:B:398:VAL:HG23	2:B:547:ALA:HB1	1.93	0.51
10:L:31:ILE:HA	10:L:34:LEU:HD22	1.92	0.51
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.09	0.51
1:A:71:LYS:NZ	20:A:5034:HOH:O	2.43	0.51
13:A:1125:CLA:HMB3	13:A:1133:CLA:H12	1.93	0.51
1:A:257:ASP:O	1:A:258:TRP:HB2	2.11	0.51
2:B:456:ILE:HG22	2:B:458:ILE:CD1	2.40	0.51
2:B:159:LYS:HD2	2:B:159:LYS:N	2.03	0.51
1:A:303:ALA:CB	13:A:1116:CLA:HBB1	2.40	0.51
1:A:444:LEU:HB2	13:A:1137:CLA:CBB	2.40	0.51
1:A:453:PHE:C	13:A:1132:CLA:HBB2	2.31	0.51
13:B:1238:CLA:HBB2	14:B:2002:PQN:H141	1.91	0.51
2:B:379:GLN:HA	2:B:379:GLN:OE1	2.11	0.51
2:B:453:GLU:HA	6:F:48:LEU:HD22	1.93	0.51
1:A:118:TRP:CB	16:J:4013:BCR:H323	2.41	0.51
13:B:1216:CLA:HMD1	13:B:1218:CLA:HBB1	1.93	0.50
4:D:117:ARG:HG2	4:D:118:SER:N	2.26	0.50
7:I:30:LEU:O	7:I:34:ILE:HG12	2.11	0.50
1:A:16:VAL:CG1	1:A:17:ASP:N	2.74	0.50
3:C:14:THR:HG22	3:C:27:MET:HG3	1.93	0.50
2:B:638:ILE:HD11	2:B:656:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:GLN:HG2	2:B:475:TYR:CE2	2.47	0.50
11:M:30:TYR:O	11:M:31:LYS:OXT	2.29	0.50
2:B:339:TRP:HE1	13:B:1221:CLA:C3B	2.23	0.50
13:B:1220:CLA:HBB1	13:B:1227:CLA:HMD2	1.94	0.50
2:B:588:TRP:HH2	13:B:1012:CLA:HBB1	1.77	0.50
4:D:32:THR:HA	4:D:52:GLY:O	2.12	0.50
13:A:1013:CLA:HBB1	13:B:1012:CLA:NB	2.27	0.50
13:B:1221:CLA:H61	13:B:1223:CLA:H42	1.94	0.50
13:B:1226:CLA:H8	18:B:5002:LMG:H242	1.94	0.50
2:B:431:PHE:CZ	16:J:4015:BCR:HC41	2.46	0.50
5:E:68:VAL:O	5:E:69:ALA:O	2.30	0.49
7:I:9:PHE:CE1	7:I:10:LEU:HD13	2.46	0.49
1:A:691:PHE:HB2	13:A:1013:CLA:HBC2	1.95	0.49
2:B:340:HIS:HD2	13:B:1202:CLA:OBD	1.95	0.49
4:D:101:PHE:HB3	4:D:103:GLU:OE2	2.11	0.49
2:B:459:GLU:OE2	6:F:50:HIS:ND1	2.40	0.49
2:B:548:ARG:HH22	4:D:124:ASN:ND2	2.10	0.49
2:B:548:ARG:HH22	4:D:124:ASN:CG	2.15	0.49
2:B:664:ALA:C	13:B:1023:CLA:HBB1	2.31	0.49
6:F:80:VAL:HG22	6:F:109:CYS:O	2.13	0.49
13:A:1237:CLA:H52	13:B:1238:CLA:H43	1.93	0.49
10:L:105:GLY:O	10:L:106:SER:HB2	2.11	0.49
13:A:1117:CLA:HMB1	13:A:1117:CLA:HBB1	1.93	0.49
2:B:114:ILE:O	13:B:1205:CLA:HMD3	2.13	0.49
2:B:425:LEU:HG	13:B:1236:CLA:HBB1	1.94	0.49
2:B:458:ILE:HD12	2:B:458:ILE:N	2.28	0.49
4:D:30:THR:O	4:D:80:TYR:HA	2.13	0.49
2:B:162:PRO:HB2	2:B:167:PHE:CE1	2.48	0.49
13:B:1021:CLA:H72	13:B:1012:CLA:CED	2.41	0.49
13:B:1216:CLA:CMB	13:B:1221:CLA:HMA3	2.42	0.49
5:E:7:VAL:O	5:E:20:VAL:HA	2.13	0.49
6:F:84:TYR:O	6:F:88:VAL:HG23	2.13	0.49
1:A:293:TRP:O	1:A:296:ASP:HB2	2.13	0.49
1:A:662:ILE:HD12	2:B:627:ARG:HG3	1.95	0.49
2:B:261:HIS:CD2	2:B:263:GLN:H	2.31	0.49
2:B:487:ILE:HG12	13:B:1232:CLA:HMD3	1.94	0.49
10:L:143:LEU:HD12	10:L:143:LEU:HA	1.61	0.49
2:B:294:PHE:O	2:B:296:ILE:HG22	2.13	0.48
2:B:390:PHE:CE1	16:B:4010:BCR:H373	2.48	0.48
13:B:1203:CLA:H143	13:B:1225:CLA:HBB2	1.95	0.48
2:B:182:PHE:CE2	13:B:1210:CLA:H61	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:VAL:HG13	2:B:451:THR:O	2.13	0.48
13:A:1013:CLA:H71	13:A:1140:CLA:CMC	2.42	0.48
1:A:399:TRP:NE1	13:A:1126:CLA:HAB	2.27	0.48
1:A:120:ILE:C	1:A:122:GLY:H	2.16	0.48
1:A:444:LEU:HB2	13:A:1137:CLA:HBB1	1.96	0.48
2:B:261:HIS:HD2	2:B:263:GLN:H	1.62	0.48
13:B:1221:CLA:H61	13:B:1221:CLA:H41	1.68	0.48
1:A:651:ARG:HG3	2:B:638:ILE:CG2	2.43	0.48
8:J:33:TYR:N	8:J:34:PRO:HD3	2.28	0.48
1:A:118:TRP:HB3	16:J:4013:BCR:H323	1.94	0.48
1:A:658:ALA:O	1:A:662:ILE:HG12	2.14	0.48
13:B:1203:CLA:H91	18:B:5002:LMG:H401	1.96	0.48
2:B:271:ASP:HB3	13:B:1214:CLA:HMA1	1.96	0.48
6:F:109:CYS:O	6:F:112:THR:HB	2.12	0.48
6:F:73:ILE:O	6:F:76:TRP:HB3	2.14	0.48
13:A:1107:CLA:HMA1	8:J:27:ILE:HD13	1.95	0.48
1:A:283:GLY:O	1:A:508:THR:O	2.32	0.48
6:F:88:VAL:HG13	6:F:97:LYS:HD2	1.95	0.48
8:J:31:ARG:CD	16:J:4013:BCR:H312	2.19	0.48
1:A:360:LEU:CD1	13:A:1128:CLA:HBB1	2.44	0.48
1:A:497:ALA:N	1:A:498:PRO:CD	2.76	0.48
1:A:693:GLY:HA3	2:B:574:CYS:HB2	1.95	0.48
2:B:180:GLY:HA3	13:B:1210:CLA:HBB1	1.96	0.48
9:K:74:VAL:C	9:K:76:GLY:H	2.16	0.48
1:A:203:GLY:O	1:A:207:LEU:HB2	2.14	0.47
1:A:577:PRO:O	1:A:578:CYS:HB3	2.14	0.47
11:M:24:ARG:NH1	20:M:155:HOH:O	2.46	0.47
1:A:686:SER:HB3	1:A:734:HIS:HB2	1.95	0.47
6:F:10:ASP:HB3	20:F:4022:HOH:O	2.14	0.47
1:A:168:MET:O	1:A:172:MET:HB2	2.14	0.47
1:A:74:SER:OG	1:A:180:TYR:HB2	2.15	0.47
1:A:691:PHE:HB2	13:A:1013:CLA:CBC	2.44	0.47
13:B:1211:CLA:HAB	13:B:1225:CLA:H13	1.96	0.47
2:B:329:TYR:OH	2:B:340:HIS:CE1	2.61	0.47
13:A:1101:CLA:H8	8:J:16:ALA:HA	1.96	0.47
2:B:647:ASN:HD22	2:B:649:LEU:N	2.08	0.47
4:D:124:ASN:O	4:D:127:GLN:HB2	2.13	0.47
13:B:1205:CLA:HMB2	13:B:1205:CLA:H142	1.96	0.47
13:A:1112:CLA:HBA2	13:A:1114:CLA:HMB3	1.96	0.47
1:A:121:VAL:HB	13:B:1230:CLA:HMD1	1.96	0.47
1:A:399:TRP:HB3	13:A:1126:CLA:HMC3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:CG	13:A:1103:CLA:HAB	2.49	0.47
2:B:525:VAL:CG1	13:B:1021:CLA:H141	2.45	0.47
2:B:589:MET:CE	2:B:589:MET:C	2.83	0.47
2:B:693:LEU:HD12	13:L:1502:CLA:H11	1.97	0.47
1:A:174:PHE:HD2	13:A:1108:CLA:CBC	2.28	0.47
2:B:313:LYS:O	2:B:314:VAL:CG2	2.60	0.47
11:M:24:ARG:CG	11:M:24:ARG:NH1	2.78	0.47
13:A:1103:CLA:HMC3	13:A:1128:CLA:HMA1	1.97	0.47
8:J:40:PRO:O	8:J:41:LEU:HB2	2.14	0.47
1:A:447:VAL:HG21	13:A:1137:CLA:C2C	2.45	0.47
1:A:379:PRO:HB2	13:A:1117:CLA:HAA2	1.96	0.47
2:B:641:TYR:CB	2:B:646:THR:HG22	2.42	0.47
2:B:696:LEU:HD11	10:L:36:ALA:HB1	1.97	0.47
13:B:1217:CLA:HBB1	16:B:4004:BCR:H14C	1.97	0.46
2:B:198:ILE:HB	2:B:199:PRO:HD3	1.96	0.46
3:C:65:ARG:HG2	3:C:67:TYR:OH	2.15	0.46
6:F:88:VAL:CG1	6:F:97:LYS:HB2	2.41	0.46
13:A:1140:CLA:H172	8:J:19:MET:HG3	1.98	0.46
13:B:1207:CLA:H42	10:L:81:SER:HA	1.96	0.46
1:A:638:ASN:O	1:A:642:SER:HB2	2.16	0.46
13:A:1140:CLA:H2	13:A:1140:CLA:O1A	2.15	0.46
1:A:603:TYR:OH	13:A:1011:CLA:HED1	2.15	0.46
13:B:1225:CLA:H3A	13:B:1225:CLA:HBA2	1.64	0.46
2:B:39:GLU:O	2:B:43:GLN:HG3	2.15	0.46
3:C:57:CYS:HA	3:C:58:PRO:HD3	1.71	0.46
13:A:1119:CLA:CMB	13:A:1123:CLA:HMA3	2.46	0.46
4:D:34:PRO:O	4:D:51:GLU:HG3	2.16	0.46
13:B:1235:CLA:H203	6:F:67:SER:HB3	1.98	0.46
2:B:386:MET:HE1	16:B:4010:BCR:H361	1.98	0.46
10:L:33:ASN:HB3	13:L:1501:CLA:HAC1	1.97	0.46
13:A:1118:CLA:HBC2	13:A:1118:CLA:HMC1	1.97	0.46
1:A:656:ALA:O	1:A:659:SER:HB2	2.16	0.46
1:A:90:MET:HE1	13:A:1106:CLA:HAA2	1.98	0.46
13:B:1012:CLA:H41	13:B:1012:CLA:H61	1.56	0.46
2:B:361:TYR:O	2:B:364:ILE:HG22	2.15	0.46
3:C:61:PHE:HD2	4:D:119:ILE:HG21	1.81	0.46
11:M:17:LEU:HB3	11:M:18:PRO:CD	2.46	0.46
13:A:1011:CLA:HED1	20:A:5011:HOH:O	2.14	0.46
1:A:686:SER:HB3	1:A:734:HIS:CB	2.46	0.46
6:F:80:VAL:HG11	6:F:110:MET:HG2	1.97	0.46
1:A:19:ASP:N	1:A:20:PRO:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1207:CLA:HHC	13:B:1207:CLA:HBB1	1.97	0.46
2:B:479:THR:H	2:B:482:SER:HB3	1.79	0.46
1:A:744:TRP:CG	16:A:4011:BCR:HC22	2.51	0.46
1:A:445:ASN:ND2	13:B:1023:CLA:HED2	2.31	0.46
3:C:23:ASP:OD2	4:D:95:HIS:CD2	2.67	0.46
1:A:91:TYR:CZ	1:A:147:TRP:HZ3	2.33	0.46
2:B:189:TRP:CA	13:B:1211:CLA:HBB1	2.45	0.46
16:A:4011:BCR:H381	13:B:1229:CLA:HMA1	1.97	0.46
2:B:642:ASN:HB2	2:B:643:PRO:HD3	1.95	0.46
2:B:738:LYS:O	2:B:739:PHE:CB	2.64	0.46
13:B:1204:CLA:H102	16:I:4018:BCR:HC31	1.98	0.46
11:M:13:VAL:HG23	16:M:4021:BCR:H402	1.98	0.46
1:A:257:ASP:OD2	1:A:262:SER:C	2.55	0.45
1:A:539:HIS:CG	13:A:1136:CLA:HED2	2.51	0.45
4:D:124:ASN:HB2	4:D:127:GLN:NE2	2.31	0.45
1:A:44:THR:HB	1:A:720:ARG:HG2	1.98	0.45
1:A:475:PHE:HA	1:A:480:ILE:O	2.16	0.45
1:A:508:THR:HG21	20:A:5033:HOH:O	2.15	0.45
2:B:468:ALA:O	2:B:482:SER:HB2	2.16	0.45
13:B:1217:CLA:H3A	13:B:1217:CLA:HBA2	1.64	0.45
13:B:1225:CLA:H12	16:B:4005:BCR:H393	1.97	0.45
13:B:1227:CLA:HBA2	13:B:1227:CLA:H3A	1.49	0.45
2:B:339:TRP:CZ3	16:B:4009:BCR:H372	2.51	0.45
2:B:36:MET:CE	2:B:40:ASN:HB2	2.45	0.45
2:B:509:SER:O	2:B:509:SER:OG	2.25	0.45
2:B:589:MET:HE1	2:B:590:LEU:HD23	1.97	0.45
13:L:1501:CLA:C1B	13:L:1502:CLA:HED1	2.46	0.45
13:A:1120:CLA:H3A	13:A:1120:CLA:HBA2	1.44	0.45
1:A:91:TYR:CE2	1:A:161:THR:HG21	2.52	0.45
1:A:313:HIS:CE1	16:A:4001:BCR:H363	2.51	0.45
13:A:1123:CLA:HAB	16:A:4007:BCR:H341	1.98	0.45
2:B:64:LEU:HD11	16:B:4006:BCR:H271	1.98	0.45
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.47	0.45
8:J:22:THR:O	8:J:26:LEU:HD13	2.15	0.45
10:L:115:GLU:O	10:L:119:GLN:HG3	2.17	0.45
2:B:220:GLY:HA3	13:B:1212:CLA:HMD1	1.98	0.45
13:B:1215:CLA:H41	13:B:1215:CLA:H62	1.70	0.45
13:A:1118:CLA:H3A	13:A:1118:CLA:HBA2	1.83	0.45
1:A:112:PRO:HB3	1:A:144:PHE:CD1	2.51	0.45
13:B:1213:CLA:H41	13:B:1213:CLA:H62	1.71	0.45
2:B:570:ARG:HH11	2:B:570:ARG:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:PHE:HB2	4:D:71:GLN:HE21	1.81	0.45
1:A:168:MET:HE2	1:A:171:LEU:HD23	1.97	0.45
1:A:508:THR:HG22	1:A:509:ALA:N	2.31	0.45
13:B:1229:CLA:HBB1	13:B:1230:CLA:HMB2	1.98	0.45
2:B:50:PHE:HB3	2:B:148:ALA:O	2.17	0.45
11:M:17:LEU:HB3	11:M:18:PRO:HD3	1.98	0.45
1:A:321:ILE:HD11	13:A:1118:CLA:H2A	1.99	0.45
13:A:1011:CLA:NA	13:B:1021:CLA:HAB	2.31	0.45
2:B:445:VAL:HG21	13:B:1230:CLA:HAC2	1.97	0.45
1:A:445:ASN:ND2	2:B:680:LEU:HD21	2.32	0.45
1:A:90:MET:HE2	13:A:1126:CLA:HED1	1.99	0.45
4:D:134:LYS:HG2	4:D:136:TYR:CZ	2.52	0.45
1:A:711:LEU:HD23	6:F:130:THR:HG22	1.98	0.45
8:J:1:MET:O	8:J:1:MET:HE2	2.17	0.45
1:A:250:ALA:HA	1:A:258:TRP:CD1	2.52	0.45
1:A:737:LEU:HD22	13:A:1140:CLA:HMA1	1.99	0.45
1:A:86:TRP:HE1	13:A:1106:CLA:HBA1	1.82	0.45
2:B:497:ASN:O	2:B:499:TRP:CE3	2.70	0.45
4:D:114:SER:N	20:D:144:HOH:O	2.50	0.45
2:B:557:LYS:NZ	4:D:124:ASN:OD1	2.43	0.45
1:A:75:ALA:HB1	13:A:1103:CLA:HBB1	1.99	0.44
13:A:1104:CLA:H3A	13:A:1128:CLA:HAB	1.99	0.44
13:B:1224:CLA:CGA	13:B:1224:CLA:H3A	2.47	0.44
2:B:215:MET:HA	2:B:216:PRO:HD3	1.83	0.44
1:A:92:PHE:CZ	1:A:96:LYS:HG3	2.53	0.44
13:B:1207:CLA:H43	13:B:1207:CLA:CED	2.47	0.44
2:B:531:LEU:HD21	13:B:1012:CLA:HBB1	1.99	0.44
1:A:212:TRP:N	13:A:1112:CLA:HBB1	2.32	0.44
2:B:370:THR:HG21	20:B:5026:HOH:O	2.16	0.44
13:B:1211:CLA:HBA1	16:B:4006:BCR:H383	2.00	0.44
2:B:480:LEU:C	2:B:482:SER:N	2.70	0.44
3:C:6:ILE:HD12	3:C:6:ILE:N	2.33	0.44
5:E:6:LYS:CD	5:E:22:THR:HG22	2.47	0.44
13:B:1228:CLA:HBC3	16:F:4016:BCR:H362	1.99	0.44
13:B:1232:CLA:HMB1	16:B:4010:BCR:HC31	1.98	0.44
2:B:441:VAL:O	2:B:445:VAL:HG23	2.17	0.44
2:B:48:SER:HB3	13:B:1202:CLA:HBB1	1.98	0.44
2:B:79:ASP:OD2	2:B:82:ASN:HB2	2.18	0.44
13:M:1601:CLA:H3A	13:M:1601:CLA:HBA2	1.69	0.44
1:A:111:LYS:HB2	1:A:130:VAL:HB	2.00	0.44
1:A:484:PRO:HB3	13:A:1136:CLA:CED	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:125:PRO:HG3	4:D:135:PRO:HG3	2.00	0.44
13:A:1103:CLA:H71	16:A:4003:BCR:H402	2.00	0.44
3:C:65:ARG:HD2	4:D:119:ILE:CD1	2.48	0.44
6:F:132:LYS:HB2	6:F:135:GLU:HG3	1.99	0.44
10:L:56:TYR:OH	13:L:1503:CLA:HED2	2.18	0.44
13:A:1107:CLA:HBC2	13:A:1126:CLA:H141	1.99	0.44
1:A:98:SER:HB2	1:A:113:SER:O	2.18	0.44
16:A:4011:BCR:H23C	16:A:4011:BCR:H403	1.99	0.44
1:A:462:ASN:HB3	1:A:645:THR:HG22	1.99	0.44
1:A:642:SER:O	1:A:648:GLY:HA3	2.17	0.44
2:B:430:LEU:HB3	13:B:1229:CLA:CED	2.48	0.44
2:B:181:LEU:HD13	13:B:1210:CLA:HBB	2.00	0.44
5:E:17:TYR:O	5:E:18:ASN:HB2	2.18	0.44
13:A:1140:CLA:H41	13:A:1140:CLA:H62	1.73	0.43
13:B:1206:CLA:H102	13:B:1224:CLA:H193	1.99	0.43
2:B:427:TRP:CE2	13:B:1228:CLA:HBB1	2.53	0.43
2:B:211:PHE:CE2	2:B:212:LEU:HG	2.53	0.43
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.44	0.43
1:A:519:ALA:HB2	1:A:625:VAL:HG21	2.00	0.43
13:B:1232:CLA:HBA2	13:B:1233:CLA:HMB3	2.00	0.43
2:B:236:PRO:O	2:B:250:GLY:HA3	2.18	0.43
2:B:317:PRO:HB3	20:B:5053:HOH:O	2.18	0.43
2:B:529:ILE:HG21	13:B:1234:CLA:HAB	1.99	0.43
2:B:439:LEU:HD11	16:J:4015:BCR:H342	2.00	0.43
8:J:1:MET:HE2	8:J:5:LEU:HG	2.01	0.43
10:L:7:PRO:HB3	10:L:12:PRO:HA	2.00	0.43
2:B:531:LEU:HD21	13:B:1012:CLA:CBB	2.48	0.43
2:B:431:PHE:HD2	13:B:1235:CLA:HBB2	1.84	0.43
2:B:36:MET:HE1	2:B:41:LEU:N	2.33	0.43
13:B:1203:CLA:H41	13:B:1203:CLA:H61	1.60	0.43
2:B:305:ASP:OD1	2:B:323:GLN:HA	2.18	0.43
2:B:339:TRP:CE2	13:B:1223:CLA:H91	2.54	0.43
2:B:636:GLN:HG3	2:B:737:ALA:CB	2.49	0.43
1:A:212:TRP:CA	13:A:1112:CLA:HBB1	2.49	0.43
13:A:1117:CLA:HMB1	13:A:1117:CLA:CBB	2.48	0.43
1:A:91:TYR:CE2	1:A:147:TRP:CZ3	3.07	0.43
13:B:1215:CLA:H3A	13:B:1215:CLA:HBA2	1.92	0.43
2:B:234:GLN:O	2:B:236:PRO:HD3	2.19	0.43
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.54	0.43
1:A:215:HIS:HB2	13:A:1112:CLA:C1C	2.48	0.43
1:A:261:PHE:CD2	1:A:261:PHE:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:HIS:CD2	13:A:1129:CLA:HMB1	2.53	0.43
13:B:1236:CLA:HBC2	13:X:1701:CLA:HBC3	2.00	0.43
2:B:231:VAL:C	2:B:234:GLN:HG2	2.36	0.43
6:F:21:ALA:HB2	6:F:35:PHE:CD1	2.54	0.43
16:J:4015:BCR:H361	16:J:4015:BCR:H20C	1.89	0.43
1:A:231:VAL:HG11	1:A:236:ILE:HG12	1.99	0.43
13:B:1205:CLA:O1A	13:B:1224:CLA:HBD	2.19	0.43
2:B:24:ILE:HA	13:B:1201:CLA:HMD3	2.01	0.43
4:D:18:LEU:HA	4:D:18:LEU:HD23	1.86	0.43
5:E:6:LYS:NZ	5:E:22:THR:HG21	2.34	0.43
13:A:1237:CLA:H41	13:A:1237:CLA:H62	1.62	0.42
13:A:1402:CLA:H3A	13:A:1402:CLA:HBA2	1.74	0.42
2:B:325:ILE:HD12	2:B:409:ASN:ND2	2.34	0.42
2:B:36:MET:HE1	2:B:40:ASN:C	2.39	0.42
4:D:73:ARG:HB2	4:D:74:PRO:HD3	2.00	0.42
13:A:1117:CLA:O1A	13:A:1127:CLA:HMD1	2.20	0.42
1:A:257:ASP:OD1	1:A:262:SER:CB	2.66	0.42
1:A:514:GLY:HA2	1:A:528:PRO:HB3	2.01	0.42
2:B:360:PRO:HG3	13:B:1215:CLA:HBA1	2.00	0.42
13:B:1207:CLA:CBB	7:I:19:CYS:HB3	2.50	0.42
8:J:39:HIS:HA	16:J:4015:BCR:H21C	2.00	0.42
1:A:683:TRP:CE3	13:A:1011:CLA:HMA1	2.54	0.42
1:A:403:PHE:CB	13:A:1104:CLA:H112	2.49	0.42
1:A:215:HIS:CD2	1:A:215:HIS:C	2.92	0.42
1:A:711:LEU:O	1:A:713:VAL:HG22	2.20	0.42
13:B:1214:CLA:HBA2	13:B:1214:CLA:H3A	1.39	0.42
13:B:1229:CLA:H61	16:F:4016:BCR:H312	2.00	0.42
2:B:357:SER:C	2:B:359:PRO:HD3	2.39	0.42
2:B:103:PHE:HZ	2:B:651:VAL:HG22	1.82	0.42
1:A:360:LEU:HD11	13:A:1128:CLA:HBB1	2.01	0.42
1:A:234:LYS:H	1:A:234:LYS:HG2	1.68	0.42
13:A:1107:CLA:H11	16:J:4012:BCR:H19C	2.01	0.42
13:A:1124:CLA:H51	13:A:1135:CLA:H43	2.00	0.42
1:A:679:ALA:HB1	1:A:738:GLY:O	2.20	0.42
2:B:588:TRP:CH2	13:B:1012:CLA:CBB	3.02	0.42
13:B:1226:CLA:CBB	13:B:1226:CLA:HMB1	2.48	0.42
2:B:325:ILE:CD1	2:B:409:ASN:ND2	2.82	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.20	0.42
10:L:4:LEU:HD22	10:L:4:LEU:N	2.35	0.42
2:B:341:LEU:HD21	13:B:1226:CLA:HAB	2.02	0.42
2:B:458:ILE:CD1	2:B:458:ILE:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:TRP:CZ3	13:B:1233:CLA:HMD3	2.54	0.42
2:B:6:LYS:HD2	11:M:31:LYS:HB3	2.02	0.42
4:D:95:HIS:HA	4:D:97:LYS:N	2.35	0.42
13:A:1128:CLA:H41	13:A:1128:CLA:H62	1.90	0.42
1:A:120:ILE:O	1:A:122:GLY:N	2.52	0.42
1:A:256:VAL:HG12	1:A:257:ASP:N	2.35	0.42
1:A:542:HIS:HD2	20:A:5029:HOH:O	2.03	0.42
13:A:1122:CLA:H92	16:A:4007:BCR:H14C	2.01	0.42
1:A:145:GLN:CD	1:A:145:GLN:H	2.22	0.42
16:A:4011:BCR:H362	13:B:1012:CLA:C4	2.38	0.42
2:B:372:ALA:HA	2:B:600:TRP:CZ3	2.55	0.42
17:B:5004:LHG:HC5	12:X:12:ARG:HB3	2.02	0.42
2:B:589:MET:HE1	2:B:590:LEU:N	2.35	0.42
13:A:1126:CLA:H93	16:J:4012:BCR:H20C	2.01	0.42
2:B:527:HIS:CD2	16:J:4015:BCR:H322	2.55	0.42
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.70	0.42
1:A:47:TRP:CZ3	1:A:51:LEU:HD12	2.54	0.42
1:A:511:VAL:HB	1:A:526:MET:HG3	2.02	0.42
13:B:1203:CLA:H143	13:B:1225:CLA:CBB	2.50	0.42
2:B:261:HIS:HD2	2:B:264:THR:H	1.67	0.42
2:B:414:VAL:HG11	16:B:4009:BCR:C40	2.50	0.42
6:F:103:VAL:O	6:F:107:ILE:HG13	2.20	0.42
13:A:1108:CLA:HBA2	13:A:1108:CLA:H3A	1.64	0.42
1:A:346:GLU:N	1:A:346:GLU:OE1	2.47	0.42
1:A:741:ALA:CB	16:A:4011:BCR:H323	2.50	0.42
2:B:136:GLN:HE21	13:B:1211:CLA:HAA1	1.85	0.42
8:J:19:MET:HE2	8:J:19:MET:HA	2.00	0.42
3:C:28:VAL:HG12	4:D:109:ARG:HB3	2.02	0.41
1:A:423:ALA:HA	4:D:38:VAL:HG11	2.02	0.41
1:A:42:PRO:CG	6:F:99:ILE:HD13	2.50	0.41
1:A:336:PHE:CD2	10:L:4:LEU:HD21	2.55	0.41
1:A:203:GLY:HA3	13:A:1111:CLA:HBB1	2.02	0.41
1:A:156:PHE:CE2	13:A:1114:CLA:HAA2	2.55	0.41
1:A:686:SER:HB2	1:A:731:GLY:O	2.20	0.41
1:A:744:TRP:NE1	13:A:1126:CLA:H11	2.35	0.41
2:B:189:TRP:HA	13:B:1211:CLA:HBB1	2.02	0.41
3:C:25:LEU:HA	3:C:40:SER:O	2.20	0.41
7:I:22:MET:O	7:I:26:VAL:HG13	2.19	0.41
11:M:9:TYR:HB3	16:M:4021:BCR:H401	2.02	0.41
1:A:685:PHE:HA	13:A:1013:CLA:HAB	2.01	0.41
13:A:1801:CLA:H12	13:A:1801:CLA:HBA2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TRP:HA	13:A:1112:CLA:HBB1	2.01	0.41
1:A:710:LYS:O	1:A:710:LYS:HD2	2.20	0.41
2:B:663:TRP:CE3	13:B:1021:CLA:HMA1	2.56	0.41
2:B:178:LEU:O	2:B:283:PHE:HB3	2.21	0.41
4:D:50:ARG:HG3	4:D:50:ARG:NH1	2.35	0.41
13:A:1134:CLA:H3A	13:A:1134:CLA:HBA2	1.73	0.41
1:A:202:ALA:C	13:A:1118:CLA:HBC3	2.41	0.41
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.83	0.41
1:A:49:TRP:CZ3	17:A:5001:LHG:H121	2.56	0.41
2:B:691:THR:HA	2:B:692:PRO:HD3	1.90	0.41
6:F:54:ASP:OD2	12:X:30:TYR:HE2	1.98	0.41
1:A:49:TRP:HZ3	17:A:5001:LHG:H121	1.86	0.41
13:B:1213:CLA:HBA2	13:B:1213:CLA:H3A	1.68	0.41
2:B:529:ILE:HG21	13:B:1234:CLA:CAB	2.51	0.41
1:A:161:THR:HG22	16:A:4002:BCR:HC32	2.01	0.41
13:L:1502:CLA:H111	13:L:1502:CLA:H152	1.99	0.41
13:A:1119:CLA:HMD1	13:A:1120:CLA:HBB1	2.02	0.41
1:A:112:PRO:HA	1:A:144:PHE:CE1	2.55	0.41
1:A:360:LEU:HD12	1:A:360:LEU:HA	1.93	0.41
13:B:1202:CLA:HBA1	13:B:1202:CLA:H3A	1.74	0.41
13:B:1222:CLA:HBA2	13:B:1222:CLA:H3A	1.69	0.41
4:D:104:LYS:H	4:D:104:LYS:HG2	1.51	0.41
6:F:73:ILE:O	6:F:77:ILE:HG13	2.21	0.41
13:B:1023:CLA:H122	16:I:4018:BCR:H281	2.03	0.41
13:A:1022:CLA:H3A	13:A:1022:CLA:O1A	2.21	0.41
13:A:1117:CLA:H3A	13:A:1117:CLA:HBA2	1.89	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.82	0.41
2:B:442:HIS:CD2	2:B:456:ILE:HG13	2.56	0.41
3:C:13:CYS:SG	3:C:15:GLN:HB2	2.61	0.41
6:F:24:THR:HG21	8:J:35:ASP:OD1	2.20	0.41
10:L:44:ILE:HG23	10:L:45:LEU:N	2.36	0.41
13:A:1140:CLA:H52	13:A:1140:CLA:NC	2.36	0.41
1:A:260:PHE:O	1:A:261:PHE:HB2	2.21	0.41
13:B:1207:CLA:H2A	13:B:1207:CLA:O2A	2.20	0.41
2:B:30:PHE:CD1	2:B:45:ILE:HD13	2.56	0.41
2:B:440:TYR:CZ	2:B:524:LEU:HB3	2.56	0.41
13:B:1206:CLA:H203	7:I:26:VAL:CG2	2.51	0.41
1:A:118:TRP:HB3	16:J:4013:BCR:C32	2.51	0.41
13:A:1013:CLA:C14	16:A:4011:BCR:H402	2.51	0.41
2:B:459:GLU:HA	2:B:460:PRO:HD3	1.81	0.41
2:B:629:TYR:O	2:B:633:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:THR:O	4:D:44:ALA:CB	2.68	0.41
13:A:1132:CLA:HED2	10:L:65:LEU:O	2.21	0.41
13:A:1140:CLA:H203	13:F:1301:CLA:CBB	2.52	0.40
1:A:502:ALA:N	1:A:503:PRO:HD3	2.36	0.40
13:B:1214:CLA:O1D	13:B:1215:CLA:HMA1	2.21	0.40
13:B:1215:CLA:H3A	13:B:1215:CLA:CGA	2.51	0.40
13:B:1211:CLA:HMA2	16:B:4006:BCR:H282	2.03	0.40
6:F:80:VAL:HG21	6:F:110:MET:HA	2.03	0.40
20:A:5047:HOH:O	10:L:16:HIS:HE1	2.04	0.40
1:A:713:VAL:HG11	13:A:1138:CLA:HMB3	2.03	0.40
1:A:114:ALA:O	1:A:115:GLN:O	2.39	0.40
2:B:279:ILE:HD11	13:B:1214:CLA:HBC3	2.02	0.40
2:B:33:HIS:HE1	13:B:1201:CLA:HED1	1.85	0.40
2:B:490:THR:O	2:B:495:TYR:HA	2.21	0.40
2:B:53:LEU:HD12	2:B:53:LEU:HA	1.83	0.40
2:B:605:LEU:HA	2:B:605:LEU:HD12	1.80	0.40
5:E:19:GLU:OE1	5:E:42:LYS:NZ	2.52	0.40
13:A:1126:CLA:H62	13:A:1126:CLA:H41	1.75	0.40
13:A:1130:CLA:HMC2	13:A:1136:CLA:H203	2.03	0.40
13:A:1122:CLA:HHB	13:A:1801:CLA:HBB1	2.02	0.40
1:A:212:TRP:O	1:A:216:GLN:HG3	2.22	0.40
2:B:176:HIS:CG	13:B:1210:CLA:HMC2	2.56	0.40
2:B:193:LEU:HA	2:B:197:ALA:HB3	2.03	0.40
2:B:269:LEU:HD23	2:B:272:MET:HE3	2.02	0.40
2:B:377:HIS:HE2	13:B:1225:CLA:C1B	2.35	0.40
2:B:564:PRO:O	2:B:565:CYS:HB3	2.22	0.40
16:L:4022:BCR:H361	16:L:4022:BCR:H20C	1.88	0.40
10:L:44:ILE:HB	20:L:4045:HOH:O	2.21	0.40
13:A:1116:CLA:H3A	13:A:1116:CLA:CGA	2.52	0.40
2:B:318:PHE:H	13:B:1219:CLA:C2B	2.34	0.40
2:B:313:LYS:O	2:B:314:VAL:CG1	2.68	0.40
2:B:548:ARG:HD3	6:F:141:ARG:O	2.21	0.40
3:C:40:SER:HA	20:C:3012:HOH:O	2.21	0.40
4:D:67:LEU:HD12	4:D:71:GLN:HG3	2.03	0.40
8:J:30:ASN:O	8:J:34:PRO:HG3	2.22	0.40
1:A:120:ILE:HG12	1:A:121:VAL:N	2.36	0.40
1:A:741:ALA:CB	16:A:4011:BCR:C32	2.99	0.40
13:B:1220:CLA:CBB	13:B:1227:CLA:HMD2	2.51	0.40
13:A:1107:CLA:CBB	13:B:1230:CLA:HMD2	2.51	0.40
2:B:36:MET:HE3	2:B:40:ASN:CB	2.47	0.40
2:B:496:GLY:O	2:B:497:ASN:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:3013:HOH:O	4:D:138:PRO:HG3	2.21	0.40
4:D:88:ASP:HB3	4:D:90:GLU:H	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:4048:HOH:O	20:L:4048:HOH:O[2_655]	1.94	0.26

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	736/755 (98%)	695 (94%)	31 (4%)	10 (1%)	13	23
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	15	27
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	14	25
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	8	12
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	2	1
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	8	12
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	1
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	14	25
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	4	5
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	4	5
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	11	18

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE
1	A	261	PHE
2	B	234	GLN
2	B	313	LYS
2	B	314	VAL
2	B	480	LEU
2	B	492	TRP
2	B	497	ASN
2	B	510	GLY
3	C	62	LEU
4	D	2	THR
6	F	91	SER
9	K	41	PRO
9	K	42	GLY
11	M	30	TYR
12	X	10	ALA
1	A	121	VAL
1	A	578	CYS
2	B	565	CYS
4	D	3	LEU
6	F	60	ALA
6	F	89	ARG
10	L	106	SER
1	A	234	LYS
4	D	44	ALA
5	E	53	SER
10	L	104	GLY
1	A	42	PRO
1	A	232	ALA
2	B	481	LEU
5	E	25	SER
5	E	54	GLY
1	A	276	SER
5	E	55	VAL
9	K	56	LEU

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	589/603 (98%)	565 (96%)	24 (4%)	35	61
2	B	595/597 (100%)	567 (95%)	28 (5%)	30	54
3	C	67/67 (100%)	66 (98%)	1 (2%)	70	89
4	D	115/115 (100%)	107 (93%)	8 (7%)	18	33
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	107 (98%)	2 (2%)	64	86
7	I	32/32 (100%)	30 (94%)	2 (6%)	21	38
8	J	36/36 (100%)	34 (94%)	2 (6%)	25	45
10	L	117/119 (98%)	109 (93%)	8 (7%)	18	34
11	M	26/26 (100%)	25 (96%)	1 (4%)	38	64
12	X	20/24 (83%)	18 (90%)	2 (10%)	9	17
All	All	1765/1811 (98%)	1687 (96%)	78 (4%)	33	57

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	147	TRP
1	A	155	GLU
1	A	172	MET
1	A	186	LYS
1	A	210	LEU
1	A	221	LEU
1	A	235	ASP
1	A	252	LEU
1	A	253	TYR
1	A	257	ASP
1	A	260	PHE
1	A	281	PHE
1	A	349	THR
1	A	360	LEU
1	A	372	GLN
1	A	395	THR
1	A	433	VAL
1	A	466	ARG
1	A	538	VAL

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Mol	Chain	Res	Type
1	A	587	CYS
1	A	632	SER
1	A	675	LEU
1	A	713	VAL
2	B	53	LEU
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU
2	B	211	PHE
2	B	214	THR
2	B	256	PHE
2	B	279	ILE
2	B	318	PHE
2	B	349	SER
2	B	370	THR
2	B	411	LEU
2	B	430	LEU
2	B	446	VAL
2	B	479	THR
2	B	525	VAL
2	B	574	CYS
2	B	582	PHE
2	B	589	MET
2	B	596	VAL
2	B	605	LEU
2	B	632	LEU
2	B	635	SER
2	B	647	ASN
2	B	648	ASN
2	B	651	VAL
2	B	697	VAL
2	B	698	ARG
3	C	61	PHE
4	D	1	THR
4	D	73	ARG
4	D	93	LEU
4	D	104	LYS
4	D	105	VAL
4	D	117	ARG
4	D	125	PRO
4	D	126	SER
6	F	56	ARG

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Mol	Chain	Res	Type
6	F	105	LEU
7	I	10	LEU
7	I	26	VAL
8	J	1	MET
8	J	19	MET
10	L	4	LEU
10	L	34	LEU
10	L	42	SER
10	L	44	ILE
10	L	48	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
11	M	17	LEU
12	X	8	THR
12	X	23	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	50	ASN
1	A	145	GLN
1	A	353	HIS
1	A	359	ASN
1	A	372	GLN
1	A	390	GLN
1	A	426	GLN
1	A	445	ASN
1	A	542	HIS
1	A	633	HIS
1	A	647	ASN
1	A	718	GLN
2	B	33	HIS
2	B	40	ASN
2	B	136	GLN
2	B	261	HIS
2	B	263	GLN
2	B	336	GLN
2	B	340	HIS
2	B	406	ASN
2	B	494	ASN

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Mol	Chain	Res	Type
2	B	611	ASN
2	B	614	GLN
2	B	616	ASN
2	B	639	ASN
2	B	647	ASN
2	B	648	ASN
2	B	678	GLN
2	B	688	HIS
3	C	37	GLN
4	D	54	ASN
4	D	71	GLN
4	D	95	HIS
5	E	18	ASN
6	F	40	GLN
6	F	95	ASN
10	L	16	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 128 ligands modelled in this entry, 1 is 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
13	CLA	A	1011	1	56,73,73	1.26	2 (3%)	65,113,113	2.02	12 (18%)
13	CLA	A	1013	1	56,73,73	1.25	5 (8%)	65,113,113	1.55	14 (21%)
13	CLA	A	1022	20	56,73,73	1.11	4 (7%)	65,113,113	1.46	10 (15%)
13	CLA	A	1101	1	56,73,73	1.13	4 (7%)	65,113,113	1.48	10 (15%)
13	CLA	A	1102	1,13	50,67,73	1.23	3 (6%)	57,105,113	1.62	15 (26%)
13	CLA	A	1103	1	56,73,73	1.20	3 (5%)	65,113,113	1.61	15 (23%)
13	CLA	A	1104	1	56,73,73	1.21	3 (5%)	65,113,113	1.74	17 (26%)
13	CLA	A	1105	1	42,59,73	1.48	4 (9%)	48,96,113	1.61	9 (18%)
13	CLA	A	1106	1	56,73,73	1.32	5 (8%)	65,113,113	1.51	11 (16%)
13	CLA	A	1107	1	56,73,73	1.13	3 (5%)	65,113,113	1.55	14 (21%)
13	CLA	A	1108	1	33,53,73	1.43	5 (15%)	37,89,113	1.60	9 (24%)
13	CLA	A	1109	1,13	56,73,73	1.18	5 (8%)	65,113,113	1.39	9 (13%)
13	CLA	A	1110	1	45,62,73	1.41	7 (15%)	51,99,113	1.64	11 (21%)
13	CLA	A	1111	1	51,68,73	1.21	3 (5%)	59,107,113	1.56	14 (23%)
13	CLA	A	1112	1	33,53,73	1.43	5 (15%)	37,89,113	1.72	10 (27%)
13	CLA	A	1113	1	33,53,73	1.53	2 (6%)	37,89,113	1.86	11 (29%)
13	CLA	A	1114	20	40,57,73	1.32	4 (10%)	46,93,113	1.67	11 (23%)
13	CLA	A	1115	1	45,62,73	1.28	4 (8%)	51,99,113	1.51	7 (13%)
13	CLA	A	1116	1	45,62,73	1.42	6 (13%)	51,99,113	1.64	13 (25%)
13	CLA	A	1117	1	56,73,73	1.19	7 (12%)	65,113,113	1.60	15 (23%)
13	CLA	A	1118	1	52,69,73	1.36	5 (9%)	60,108,113	1.65	13 (21%)
13	CLA	A	1119	20	56,73,73	1.15	5 (8%)	65,113,113	1.66	14 (21%)
13	CLA	A	1120	1	40,57,73	1.40	4 (10%)	46,93,113	1.82	14 (30%)
13	CLA	A	1121	1	42,59,73	1.39	6 (14%)	48,96,113	1.71	11 (22%)
13	CLA	A	1122	1	50,67,73	1.25	3 (6%)	57,105,113	1.52	12 (21%)
13	CLA	A	1123	20	56,73,73	1.23	3 (5%)	65,113,113	1.45	12 (18%)
13	CLA	A	1124	20	56,73,73	1.16	4 (7%)	65,113,113	1.44	10 (15%)
13	CLA	A	1125	1	56,73,73	1.29	3 (5%)	65,113,113	1.48	12 (18%)
13	CLA	A	1126	1	56,73,73	1.04	4 (7%)	65,113,113	1.39	11 (16%)
13	CLA	A	1127	1	56,73,73	1.25	3 (5%)	65,113,113	1.49	10 (15%)
13	CLA	A	1128	1	56,73,73	1.23	5 (8%)	65,113,113	1.45	11 (16%)
13	CLA	A	1129	1	41,58,73	1.39	4 (9%)	47,95,113	1.86	13 (27%)
13	CLA	A	1130	1	56,73,73	1.22	1 (1%)	65,113,113	1.55	14 (21%)
13	CLA	A	1131	1	56,73,73	1.09	1 (1%)	65,113,113	1.40	11 (16%)
13	CLA	A	1132	1	56,73,73	1.18	5 (8%)	65,113,113	1.50	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1133	1	45,62,73	1.40	5 (11%)	51,99,113	1.72	15 (29%)
13	CLA	A	1134	1	33,53,73	1.53	4 (12%)	37,89,113	1.75	10 (27%)
13	CLA	A	1135	1	42,59,73	1.46	1 (2%)	48,96,113	1.72	12 (25%)
13	CLA	A	1136	1	56,73,73	1.18	5 (8%)	65,113,113	1.35	9 (13%)
13	CLA	A	1137	1	38,55,73	1.51	4 (10%)	44,91,113	1.71	10 (22%)
13	CLA	A	1138	1	56,73,73	1.15	4 (7%)	65,113,113	1.44	12 (18%)
13	CLA	A	1139	20	42,59,73	1.53	4 (9%)	48,96,113	1.58	10 (20%)
13	CLA	A	1140	1	56,73,73	1.28	5 (8%)	65,113,113	1.54	15 (23%)
13	CLA	A	1237	20	56,73,73	1.28	6 (10%)	65,113,113	1.44	11 (16%)
13	CLA	A	1402	-	30,49,73	1.65	4 (13%)	33,83,113	1.57	7 (21%)
13	CLA	A	1801	17	43,60,73	1.43	7 (16%)	49,97,113	1.87	14 (28%)
14	PQN	A	2001	-	34,34,34	3.41	17 (50%)	43,45,45	2.15	3 (6%)
15	SF4	A	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
16	BCR	A	4001	-	41,41,41	1.35	5 (12%)	56,56,56	1.88	16 (28%)
16	BCR	A	4002	-	41,41,41	1.26	4 (9%)	56,56,56	1.77	17 (30%)
16	BCR	A	4003	-	41,41,41	1.39	6 (14%)	56,56,56	1.94	17 (30%)
16	BCR	A	4007	-	41,41,41	1.35	5 (12%)	56,56,56	1.79	14 (25%)
16	BCR	A	4008	-	41,41,41	1.25	7 (17%)	56,56,56	1.90	18 (32%)
16	BCR	A	4011	-	41,41,41	1.37	6 (14%)	56,56,56	2.04	19 (33%)
17	LHG	A	5001	-	48,48,48	1.69	6 (12%)	49,54,54	1.32	3 (6%)
17	LHG	A	5003	13	26,26,48	2.23	5 (19%)	27,32,54	1.57	5 (18%)
13	CLA	B	1012	20	56,73,73	1.19	2 (3%)	65,113,113	1.54	11 (16%)
13	CLA	B	1021	2	56,73,73	1.28	3 (5%)	65,113,113	1.44	10 (15%)
13	CLA	B	1023	2	56,73,73	1.26	5 (8%)	65,113,113	1.46	10 (15%)
13	CLA	B	1201	2	45,62,73	1.35	5 (11%)	51,99,113	1.69	11 (21%)
13	CLA	B	1202	2	56,73,73	1.21	4 (7%)	65,113,113	1.48	11 (16%)
13	CLA	B	1203	2	56,73,73	1.12	2 (3%)	65,113,113	1.39	10 (15%)
13	CLA	B	1204	2	56,73,73	1.29	5 (8%)	65,113,113	1.51	12 (18%)
13	CLA	B	1205	2	56,73,73	1.08	4 (7%)	65,113,113	1.55	12 (18%)
13	CLA	B	1206	2	56,73,73	1.05	2 (3%)	65,113,113	1.42	10 (15%)
13	CLA	B	1207	2	56,73,73	1.22	3 (5%)	65,113,113	1.38	12 (18%)
13	CLA	B	1208	2	33,53,73	1.40	5 (15%)	37,89,113	1.67	9 (24%)
13	CLA	B	1209	2	33,53,73	1.57	2 (6%)	37,89,113	1.77	9 (24%)
13	CLA	B	1210	2	56,73,73	1.09	4 (7%)	65,113,113	1.47	11 (16%)
13	CLA	B	1211	2	56,73,73	1.23	5 (8%)	65,113,113	1.54	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1212	2	33,53,73	1.42	4 (12%)	37,89,113	1.69	8 (21%)
13	CLA	B	1213	2	46,63,73	1.40	8 (17%)	53,101,113	1.60	13 (24%)
13	CLA	B	1214	2	50,67,73	1.28	5 (10%)	57,105,113	1.60	14 (24%)
13	CLA	B	1215	2	51,68,73	1.30	5 (9%)	59,107,113	1.68	11 (18%)
13	CLA	B	1216	20	56,73,73	1.19	4 (7%)	65,113,113	1.44	11 (16%)
13	CLA	B	1217	2	38,55,73	1.47	3 (7%)	44,91,113	1.85	12 (27%)
13	CLA	B	1218	2	33,53,73	1.47	2 (6%)	37,89,113	1.88	10 (27%)
13	CLA	B	1219	20	46,63,73	1.42	5 (10%)	53,101,113	1.64	12 (22%)
13	CLA	B	1220	2	33,53,73	1.42	3 (9%)	37,89,113	1.65	7 (18%)
13	CLA	B	1221	2	45,62,73	1.36	6 (13%)	51,99,113	1.69	13 (25%)
13	CLA	B	1222	20	37,54,73	1.33	3 (8%)	43,90,113	1.84	12 (27%)
13	CLA	B	1223	2	56,73,73	1.30	3 (5%)	65,113,113	1.49	12 (18%)
13	CLA	B	1224	2	56,73,73	1.29	4 (7%)	65,113,113	1.61	14 (21%)
13	CLA	B	1225	2	56,73,73	1.35	8 (14%)	65,113,113	1.47	13 (20%)
13	CLA	B	1226	2	56,73,73	1.26	5 (8%)	65,113,113	1.58	12 (18%)
13	CLA	B	1227	2	33,53,73	1.52	5 (15%)	37,89,113	1.81	10 (27%)
13	CLA	B	1228	2	40,57,73	1.34	4 (10%)	46,93,113	1.66	10 (21%)
13	CLA	B	1229	2	56,73,73	1.18	4 (7%)	65,113,113	1.52	11 (16%)
13	CLA	B	1230	2	49,66,73	1.47	5 (10%)	56,104,113	1.66	12 (21%)
13	CLA	B	1231	2	33,53,73	1.61	5 (15%)	37,89,113	1.81	12 (32%)
13	CLA	B	1232	20	33,53,73	1.47	5 (15%)	37,89,113	1.70	11 (29%)
13	CLA	B	1233	20	33,53,73	1.54	3 (9%)	37,89,113	1.66	8 (21%)
13	CLA	B	1234	2	51,68,73	1.40	5 (9%)	59,107,113	1.52	12 (20%)
13	CLA	B	1235	2	56,73,73	1.25	4 (7%)	65,113,113	1.56	14 (21%)
13	CLA	B	1236	2	38,55,73	1.34	4 (10%)	44,91,113	1.56	9 (20%)
13	CLA	B	1238	20	56,73,73	1.19	5 (8%)	65,113,113	1.36	11 (16%)
13	CLA	B	1239	2	56,73,73	1.21	5 (8%)	65,113,113	1.43	12 (18%)
14	PQN	B	2002	-	34,34,34	3.32	17 (50%)	43,45,45	2.04	4 (9%)
16	BCR	B	4004	-	41,41,41	1.50	5 (12%)	56,56,56	2.02	16 (28%)
16	BCR	B	4005	-	41,41,41	1.55	7 (17%)	56,56,56	2.09	19 (33%)
16	BCR	B	4006	-	41,41,41	1.24	5 (12%)	56,56,56	2.01	19 (33%)
16	BCR	B	4009	-	25,25,41	1.35	4 (16%)	32,33,56	1.86	11 (34%)
16	BCR	B	4010	-	41,41,41	1.23	5 (12%)	56,56,56	1.89	18 (32%)
16	BCR	B	4014	-	41,41,41	1.22	4 (9%)	56,56,56	2.00	20 (35%)
16	BCR	B	4017	-	41,41,41	1.26	4 (9%)	56,56,56	1.74	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	LMG	B	5002	-	55,55,55	0.88	2 (3%)	63,63,63	1.31	3 (4%)
17	LHG	B	5004	-	22,22,48	2.69	5 (22%)	23,28,54	1.08	1 (4%)
15	SF4	C	3002	3	0,12,12	0.00	-	0,24,24	0.00	-
15	SF4	C	3003	3	0,12,12	0.00	-	0,24,24	0.00	-
13	CLA	F	1301	20	33,53,73	1.47	4 (12%)	37,89,113	1.66	9 (24%)
16	BCR	F	4016	-	41,41,41	1.25	3 (7%)	56,56,56	1.81	17 (30%)
16	BCR	I	4018	-	41,41,41	1.28	7 (17%)	56,56,56	1.79	16 (28%)
16	BCR	I	4020	-	41,41,41	1.26	7 (17%)	56,56,56	1.83	17 (30%)
13	CLA	J	1302	8	33,53,73	1.61	4 (12%)	37,89,113	1.79	10 (27%)
13	CLA	J	1303	8	29,45,73	1.75	3 (10%)	33,78,113	1.86	11 (33%)
16	BCR	J	4012	-	41,41,41	1.27	5 (12%)	56,56,56	1.90	16 (28%)
16	BCR	J	4013	-	41,41,41	1.26	4 (9%)	56,56,56	1.84	20 (35%)
16	BCR	J	4015	-	41,41,41	1.39	5 (12%)	56,56,56	1.88	14 (25%)
13	CLA	K	1401	-	33,53,73	1.48	4 (12%)	37,89,113	1.64	9 (24%)
13	CLA	L	1501	10	56,73,73	1.22	4 (7%)	65,113,113	1.49	11 (16%)
13	CLA	L	1502	10	56,73,73	1.19	5 (8%)	65,113,113	1.48	11 (16%)
13	CLA	L	1503	20	56,73,73	1.19	3 (5%)	65,113,113	1.45	9 (13%)
16	BCR	L	4019	-	41,41,41	1.41	7 (17%)	56,56,56	1.82	15 (26%)
16	BCR	L	4022	-	41,41,41	1.59	7 (17%)	56,56,56	1.72	12 (21%)
13	CLA	M	1601	20	33,53,73	1.59	3 (9%)	37,89,113	1.78	10 (27%)
16	BCR	M	4021	-	41,41,41	1.33	6 (14%)	56,56,56	1.79	15 (26%)
13	CLA	X	1701	12	33,53,73	1.55	2 (6%)	37,89,113	1.75	11 (29%)

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
13	CLA	A	1011	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1013	1	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1022	20	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1101	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1102	1,13	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	A	1103	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1104	1	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1105	1	2/2/17/25	0/21/119/135	0/0/9/9
13	CLA	A	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1107	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1108	1	-	0/11/111/135	0/0/9/9
13	CLA	A	1109	1,13	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1110	1	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	1111	1	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	A	1112	1	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	1113	1	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	1114	20	3/3/16/25	1/18/116/135	0/0/9/9
13	CLA	A	1115	1	1/1/17/25	0/24/122/135	0/0/9/9
13	CLA	A	1116	1	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	1117	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1118	1	3/3/19/25	0/33/131/135	0/0/9/9
13	CLA	A	1119	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1120	1	3/3/16/25	0/18/116/135	0/0/9/9
13	CLA	A	1121	1	2/2/17/25	0/21/119/135	0/0/9/9
13	CLA	A	1122	1	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	A	1123	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1124	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1125	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1126	1	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1127	1	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1128	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1129	1	3/3/17/25	0/19/117/135	0/0/9/9
13	CLA	A	1130	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1131	1	-	0/37/135/135	0/0/9/9
13	CLA	A	1132	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1133	1	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	1134	1	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	1135	1	3/3/17/25	0/21/119/135	0/0/9/9
13	CLA	A	1136	1	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1137	1	1/1/16/25	0/16/114/135	0/0/9/9
13	CLA	A	1138	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1139	20	3/3/17/25	0/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1140	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1237	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	1402	-	3/3/14/25	0/5/101/135	0/0/9/9
13	CLA	A	1801	17	3/3/17/25	0/22/120/135	0/0/9/9
14	PQN	A	2001	-	-	0/23/43/43	0/2/2/2
15	SF4	A	3001	1,2	-	0/0/48/48	0/6/5/5
16	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
16	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
16	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
16	BCR	A	4008	-	-	0/29/63/63	0/2/2/2
16	BCR	A	4011	-	-	0/29/63/63	0/2/2/2
17	LHG	A	5001	-	-	0/53/53/53	0/0/0/0
17	LHG	A	5003	13	1/1/5/5	0/31/31/53	0/0/0/0
13	CLA	B	1012	20	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1021	2	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1023	2	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1201	2	2/2/17/25	0/24/122/135	0/0/9/9
13	CLA	B	1202	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1203	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1204	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1205	2	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1206	2	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1207	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1208	2	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	1209	2	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	1210	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1211	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1212	2	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	1213	2	3/3/18/25	0/25/123/135	0/0/9/9
13	CLA	B	1214	2	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	B	1215	2	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	B	1216	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1217	2	3/3/16/25	0/16/114/135	0/0/9/9
13	CLA	B	1218	2	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	1219	20	3/3/18/25	0/25/123/135	0/0/9/9
13	CLA	B	1220	2	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1221	2	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	B	1222	20	3/3/16/25	0/15/113/135	0/0/9/9
13	CLA	B	1223	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1224	2	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1225	2	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1226	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1227	2	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	1228	2	3/3/16/25	0/18/116/135	0/0/9/9
13	CLA	B	1229	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1230	2	3/3/18/25	0/29/127/135	0/0/9/9
13	CLA	B	1231	2	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	1232	20	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	1233	20	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	1234	2	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	B	1235	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1236	2	-	0/16/114/135	0/0/9/9
13	CLA	B	1238	20	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	1239	2	2/2/20/25	0/37/135/135	0/0/9/9
14	PQN	B	2002	-	-	0/23/43/43	0/2/2/2
16	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
16	BCR	B	4005	-	-	0/29/63/63	0/2/2/2
16	BCR	B	4006	-	-	0/29/63/63	0/2/2/2
16	BCR	B	4009	-	-	0/18/35/63	0/1/1/2
16	BCR	B	4010	-	-	0/29/63/63	0/2/2/2
16	BCR	B	4014	-	-	0/29/63/63	0/2/2/2
16	BCR	B	4017	-	-	0/29/63/63	0/2/2/2
18	LMG	B	5002	-	-	0/50/70/70	0/1/1/1
17	LHG	B	5004	-	-	0/26/26/53	0/0/0/0
15	SF4	C	3002	3	-	0/0/48/48	0/6/5/5
15	SF4	C	3003	3	-	0/0/48/48	0/6/5/5
13	CLA	F	1301	20	3/3/16/25	0/11/111/135	0/0/9/9
16	BCR	F	4016	-	-	0/29/63/63	0/2/2/2
16	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
16	BCR	I	4020	-	-	0/29/63/63	0/2/2/2
13	CLA	J	1302	8	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	J	1303	8	3/3/13/25	0/2/96/135	0/0/9/9
16	BCR	J	4012	-	-	0/29/63/63	0/2/2/2
16	BCR	J	4013	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	J	4015	-	-	0/29/63/63	0/2/2/2
13	CLA	K	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	L	1501	10	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	L	1502	10	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	L	1503	20	3/3/20/25	0/37/135/135	0/0/9/9
16	BCR	L	4019	-	-	0/29/63/63	0/2/2/2
16	BCR	L	4022	-	-	0/29/63/63	0/2/2/2
13	CLA	M	1601	20	3/3/16/25	0/11/111/135	0/0/9/9
16	BCR	M	4021	-	-	0/29/63/63	0/2/2/2
13	CLA	X	1701	12	3/3/16/25	0/11/111/135	0/0/9/9

All (564) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	2001	PQN	C2M-C2	-6.57	1.36	1.50
14	B	2002	PQN	C2M-C2	-6.23	1.37	1.50
14	B	2002	PQN	C16-C15	-4.63	1.34	1.52
14	A	2001	PQN	C16-C15	-4.51	1.35	1.52
13	B	1204	CLA	C3B-C2B	-3.74	1.35	1.40
13	A	1132	CLA	C3B-C2B	-3.63	1.35	1.40
13	B	1227	CLA	C3B-C2B	-3.59	1.35	1.40
13	B	1235	CLA	C3B-C2B	-3.30	1.36	1.40
13	B	1234	CLA	C3B-C2B	-3.20	1.36	1.40
13	B	1228	CLA	C3B-C2B	-3.17	1.36	1.40
13	B	1229	CLA	C3B-C2B	-3.12	1.36	1.40
13	A	1116	CLA	C3B-C2B	-3.09	1.36	1.40
13	A	1129	CLA	C3B-C2B	-3.02	1.36	1.40
13	B	1023	CLA	C3B-C2B	-2.92	1.36	1.40
13	A	1123	CLA	C3B-C2B	-2.92	1.36	1.40
13	A	1136	CLA	C3B-C2B	-2.88	1.36	1.40
13	A	1106	CLA	C3B-C2B	-2.87	1.36	1.40
13	B	1208	CLA	C3B-C2B	-2.85	1.36	1.40
13	A	1128	CLA	C3B-C2B	-2.84	1.36	1.40
13	B	1205	CLA	C3B-C2B	-2.79	1.36	1.40
13	A	1105	CLA	C3B-C2B	-2.77	1.36	1.40
13	B	1205	CLA	C1B-CHB	-2.75	1.32	1.40
13	B	1236	CLA	C3B-C2B	-2.74	1.36	1.40
13	A	1108	CLA	C3B-C2B	-2.73	1.36	1.40
13	B	1231	CLA	C3B-C2B	-2.72	1.36	1.40
13	B	1228	CLA	C1B-CHB	-2.72	1.32	1.40
13	B	1232	CLA	C3B-C2B	-2.71	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1121	CLA	C3B-C2B	-2.69	1.36	1.40
13	A	1013	CLA	C1B-CHB	-2.67	1.33	1.40
13	B	1216	CLA	C3B-C2B	-2.66	1.36	1.40
13	B	1225	CLA	C3B-C2B	-2.65	1.36	1.40
13	B	1238	CLA	C3B-C2B	-2.63	1.36	1.40
13	A	1129	CLA	C1B-CHB	-2.63	1.33	1.40
13	A	1119	CLA	C1B-CHB	-2.62	1.33	1.40
13	B	1023	CLA	C1B-CHB	-2.59	1.33	1.40
13	B	1207	CLA	C3B-C2B	-2.58	1.36	1.40
16	A	4011	BCR	C23-C22	-2.58	1.40	1.45
13	B	1204	CLA	C1B-CHB	-2.56	1.33	1.40
14	A	2001	PQN	C10-C1	-2.56	1.43	1.48
13	A	1120	CLA	C3B-C2B	-2.54	1.37	1.40
13	B	1214	CLA	C3B-C2B	-2.53	1.37	1.40
13	A	1112	CLA	C3B-C2B	-2.53	1.37	1.40
13	A	1137	CLA	C3B-C2B	-2.52	1.37	1.40
13	A	1237	CLA	C3B-C2B	-2.52	1.37	1.40
13	A	1124	CLA	C1B-CHB	-2.51	1.33	1.40
13	B	1021	CLA	C1B-CHB	-2.50	1.33	1.40
13	L	1502	CLA	C1B-CHB	-2.49	1.33	1.40
13	B	1212	CLA	C3B-C2B	-2.48	1.37	1.40
13	B	1214	CLA	C1B-CHB	-2.48	1.33	1.40
13	B	1236	CLA	C1B-CHB	-2.48	1.33	1.40
13	B	1208	CLA	C1B-CHB	-2.48	1.33	1.40
13	A	1106	CLA	C1B-CHB	-2.48	1.33	1.40
13	B	1221	CLA	C3B-C2B	-2.47	1.37	1.40
13	A	1801	CLA	C3B-C2B	-2.46	1.37	1.40
13	A	1022	CLA	C3B-C2B	-2.46	1.37	1.40
13	A	1138	CLA	C1B-CHB	-2.44	1.33	1.40
13	B	1221	CLA	C1B-CHB	-2.44	1.33	1.40
13	A	1109	CLA	C3B-C2B	-2.42	1.37	1.40
13	B	1213	CLA	C3B-C2B	-2.41	1.37	1.40
16	M	4021	BCR	C23-C22	-2.41	1.40	1.45
16	L	4019	BCR	C19-C18	-2.39	1.40	1.45
18	B	5002	LMG	O7-C8	-2.39	1.40	1.46
13	A	1110	CLA	C3B-C2B	-2.39	1.37	1.40
13	A	1101	CLA	C3B-C2B	-2.39	1.37	1.40
13	A	1112	CLA	C1B-CHB	-2.38	1.33	1.40
13	A	1101	CLA	C1B-CHB	-2.38	1.33	1.40
13	B	1235	CLA	C1B-CHB	-2.38	1.33	1.40
13	A	1118	CLA	C3B-C2B	-2.38	1.37	1.40
13	A	1132	CLA	C1B-CHB	-2.38	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1136	CLA	C1B-CHB	-2.35	1.33	1.40
13	A	1111	CLA	C1B-CHB	-2.34	1.33	1.40
13	B	1232	CLA	C1B-CHB	-2.34	1.34	1.40
13	B	1210	CLA	C1B-CHB	-2.34	1.34	1.40
13	A	1103	CLA	C1B-CHB	-2.34	1.34	1.40
13	A	1115	CLA	C1B-CHB	-2.33	1.34	1.40
13	A	1109	CLA	C1B-CHB	-2.32	1.34	1.40
13	K	1401	CLA	C3B-C2B	-2.32	1.37	1.40
13	A	1122	CLA	C1B-CHB	-2.31	1.34	1.40
13	B	1216	CLA	C1B-CHB	-2.31	1.34	1.40
16	B	4009	BCR	C23-C22	-2.31	1.40	1.45
16	B	4017	BCR	C23-C22	-2.31	1.40	1.45
13	B	1231	CLA	C1B-CHB	-2.30	1.34	1.40
16	B	4014	BCR	C23-C22	-2.30	1.40	1.45
13	A	1139	CLA	C3B-C2B	-2.30	1.37	1.40
13	B	1227	CLA	C1B-CHB	-2.29	1.34	1.40
13	B	1211	CLA	C1B-CHB	-2.27	1.34	1.40
13	A	1133	CLA	C3B-C2B	-2.27	1.37	1.40
14	B	2002	PQN	C5-C4	-2.26	1.43	1.48
13	K	1401	CLA	C1B-CHB	-2.25	1.34	1.40
13	A	1022	CLA	C1B-CHB	-2.23	1.34	1.40
13	A	1126	CLA	C1B-CHB	-2.23	1.34	1.40
16	I	4020	BCR	C19-C18	-2.23	1.41	1.45
13	A	1237	CLA	C1B-CHB	-2.22	1.34	1.40
13	B	1212	CLA	C1B-CHB	-2.22	1.34	1.40
13	A	1801	CLA	C1B-CHB	-2.22	1.34	1.40
13	A	1115	CLA	C3B-C2B	-2.20	1.37	1.40
13	B	1211	CLA	C3B-C2B	-2.19	1.37	1.40
16	L	4022	BCR	C23-C22	-2.17	1.41	1.45
13	B	1233	CLA	C3B-C2B	-2.17	1.37	1.40
13	A	1114	CLA	C3B-C2B	-2.17	1.37	1.40
13	A	1114	CLA	C1B-CHB	-2.16	1.34	1.40
13	B	1220	CLA	C3B-C2B	-2.16	1.37	1.40
13	B	1239	CLA	C3B-C2B	-2.16	1.37	1.40
13	A	1121	CLA	C1B-CHB	-2.15	1.34	1.40
16	I	4018	BCR	C19-C18	-2.15	1.41	1.45
14	A	2001	PQN	C5-C4	-2.15	1.43	1.48
13	B	1229	CLA	C1B-CHB	-2.13	1.34	1.40
13	A	1120	CLA	C1B-CHB	-2.13	1.34	1.40
13	B	1213	CLA	C1B-CHB	-2.13	1.34	1.40
16	B	4005	BCR	C29-C28	-2.13	1.47	1.52
13	B	1225	CLA	C1B-CHB	-2.13	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	4018	BCR	C2-C3	-2.12	1.47	1.52
13	A	1110	CLA	C1B-CHB	-2.11	1.34	1.40
13	A	1108	CLA	C1B-CHB	-2.11	1.34	1.40
13	B	1239	CLA	CAA-CBA	-2.11	1.45	1.52
13	A	1117	CLA	C1B-CHB	-2.11	1.34	1.40
14	B	2002	PQN	C10-C1	-2.11	1.44	1.48
13	A	1107	CLA	C1B-CHB	-2.09	1.34	1.40
16	A	4008	BCR	C19-C18	-2.09	1.41	1.45
13	B	1207	CLA	C1B-CHB	-2.08	1.34	1.40
13	A	1134	CLA	C3B-C2B	-2.08	1.37	1.40
13	F	1301	CLA	C3B-C2B	-2.06	1.37	1.40
13	J	1302	CLA	C3B-C2B	-2.04	1.37	1.40
16	A	4003	BCR	C29-C28	-2.04	1.47	1.52
16	L	4019	BCR	C29-C28	-2.03	1.47	1.52
13	B	1201	CLA	C1B-CHB	-2.03	1.34	1.40
13	A	1116	CLA	C1B-CHB	-2.03	1.34	1.40
13	B	1238	CLA	C1B-CHB	-2.02	1.34	1.40
16	M	4021	BCR	C2-C3	-2.02	1.47	1.52
13	B	1239	CLA	C1C-NC	-2.02	1.34	1.37
13	L	1503	CLA	CBA-CGA	-2.02	1.44	1.50
13	B	1219	CLA	C1B-CHB	-2.02	1.34	1.40
17	A	5001	LHG	O8-C6	-2.02	1.40	1.45
13	A	1104	CLA	CAA-CBA	-2.01	1.46	1.52
13	F	1301	CLA	C1B-CHB	-2.01	1.34	1.40
13	B	1215	CLA	C1B-CHB	-2.01	1.34	1.40
13	B	1206	CLA	CHC-C1C	2.00	1.41	1.35
13	A	1121	CLA	C1-C2	2.00	1.55	1.49
13	B	1210	CLA	CMD-C2D	2.00	1.55	1.51
13	A	1127	CLA	C3B-CAB	2.01	1.51	1.47
14	B	2002	PQN	C15-C13	2.01	1.55	1.51
13	B	1234	CLA	C4-C3	2.02	1.55	1.50
13	B	1219	CLA	C3B-CAB	2.02	1.51	1.47
13	A	1110	CLA	C4-C3	2.02	1.55	1.50
17	B	5004	LHG	O8-C23	2.02	1.43	1.33
13	A	1132	CLA	C1-C2	2.02	1.55	1.49
13	A	1013	CLA	CMD-C2D	2.02	1.55	1.51
13	B	1230	CLA	C4-C3	2.03	1.55	1.50
16	I	4020	BCR	C14-C13	2.03	1.38	1.35
13	A	1110	CLA	C5-C3	2.03	1.55	1.51
13	B	1238	CLA	CHC-C1C	2.03	1.41	1.35
16	A	4008	BCR	C26-C25	2.03	1.37	1.34
13	B	1201	CLA	C1-C2	2.04	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	4007	BCR	C14-C13	2.04	1.38	1.35
13	L	1501	CLA	C1C-C2C	2.04	1.48	1.44
13	A	1112	CLA	CAA-C2A	2.04	1.58	1.54
14	B	2002	PQN	C7-C6	2.04	1.42	1.38
13	A	1140	CLA	OBD-CAD	2.05	1.25	1.22
13	A	1117	CLA	CHC-C1C	2.05	1.41	1.35
13	B	1201	CLA	CAA-C2A	2.05	1.58	1.54
13	B	1204	CLA	C5-C3	2.05	1.55	1.51
13	A	1140	CLA	C5-C3	2.05	1.55	1.51
13	A	1402	CLA	CAA-C2A	2.06	1.58	1.54
13	A	1136	CLA	CAA-C2A	2.06	1.58	1.54
13	B	1234	CLA	C5-C3	2.06	1.55	1.51
16	J	4013	BCR	C1-C6	2.06	1.56	1.53
13	B	1023	CLA	C4-C3	2.07	1.56	1.50
16	B	4010	BCR	C5-C6	2.07	1.38	1.34
13	A	1128	CLA	CAA-C2A	2.07	1.58	1.54
16	I	4018	BCR	C26-C25	2.07	1.38	1.34
13	A	1126	CLA	C4-C3	2.07	1.56	1.50
13	B	1231	CLA	CAA-C2A	2.08	1.58	1.54
13	B	1222	CLA	CAA-C2A	2.08	1.58	1.54
13	B	1227	CLA	CAA-C2A	2.08	1.58	1.54
13	A	1801	CLA	C4-C3	2.08	1.56	1.50
13	A	1109	CLA	CAA-C2A	2.09	1.58	1.54
13	B	1226	CLA	C3B-CAB	2.10	1.52	1.47
16	A	4008	BCR	C33-C5	2.10	1.54	1.51
13	J	1302	CLA	CAA-C2A	2.10	1.58	1.54
13	B	1221	CLA	C1-C2	2.11	1.55	1.49
13	A	1117	CLA	C3B-CAB	2.11	1.52	1.47
13	A	1119	CLA	C1-C2	2.11	1.55	1.49
13	B	1213	CLA	C1-C2	2.12	1.55	1.49
13	B	1202	CLA	C5-C3	2.12	1.55	1.51
13	B	1202	CLA	CMD-C2D	2.12	1.56	1.51
13	A	1134	CLA	CAA-C2A	2.13	1.58	1.54
13	A	1126	CLA	CHC-C1C	2.13	1.41	1.35
13	A	1124	CLA	CHC-C1C	2.13	1.41	1.35
13	A	1105	CLA	C1-C2	2.13	1.55	1.49
13	A	1133	CLA	C1-C2	2.14	1.55	1.49
16	A	4003	BCR	C26-C25	2.15	1.38	1.34
16	I	4020	BCR	C26-C25	2.16	1.38	1.34
13	A	1132	CLA	CHC-C1C	2.16	1.41	1.35
13	A	1124	CLA	CAA-C2A	2.17	1.58	1.54
13	A	1139	CLA	CHC-C1C	2.17	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1138	CLA	CAA-C2A	2.17	1.58	1.54
16	I	4020	BCR	C33-C5	2.17	1.54	1.51
16	B	4006	BCR	C5-C6	2.18	1.38	1.34
13	B	1213	CLA	C4-C3	2.18	1.56	1.50
16	L	4019	BCR	C26-C25	2.19	1.38	1.34
13	B	1203	CLA	CHC-C1C	2.19	1.41	1.35
13	B	1021	CLA	CHC-C1C	2.19	1.41	1.35
16	L	4019	BCR	C38-C26	2.19	1.54	1.51
16	J	4012	BCR	C26-C25	2.19	1.38	1.34
13	B	1211	CLA	C5-C3	2.20	1.56	1.51
13	L	1502	CLA	CMD-C2D	2.20	1.56	1.51
13	B	1208	CLA	CAA-C2A	2.21	1.58	1.54
13	B	1215	CLA	CHC-C1C	2.21	1.41	1.35
13	A	1801	CLA	C5-C3	2.21	1.56	1.51
16	A	4008	BCR	C2-C1	2.21	1.59	1.54
13	B	1226	CLA	OBD-CAD	2.21	1.25	1.22
13	B	1238	CLA	CAA-C2A	2.22	1.58	1.54
13	B	1202	CLA	CHC-C1C	2.22	1.41	1.35
13	B	1230	CLA	CAA-C2A	2.25	1.58	1.54
16	I	4018	BCR	C33-C5	2.26	1.54	1.51
13	B	1239	CLA	CHC-C1C	2.26	1.41	1.35
16	B	4009	BCR	C14-C13	2.27	1.40	1.34
13	L	1501	CLA	CAA-C2A	2.27	1.58	1.54
13	B	1223	CLA	C3B-CAB	2.27	1.52	1.47
16	B	4014	BCR	C5-C6	2.28	1.38	1.34
13	B	1225	CLA	C1-C2	2.28	1.56	1.49
13	A	1118	CLA	CAA-C2A	2.29	1.58	1.54
13	A	1237	CLA	C4-C3	2.29	1.56	1.50
13	A	1110	CLA	CAA-C2A	2.30	1.58	1.54
13	B	1204	CLA	CAA-C2A	2.30	1.58	1.54
13	A	1139	CLA	C5-C3	2.31	1.58	1.51
14	A	2001	PQN	C7-C6	2.31	1.43	1.38
13	B	1226	CLA	CHC-C1C	2.32	1.42	1.35
14	B	2002	PQN	C8-C7	2.32	1.43	1.38
16	B	4005	BCR	C38-C26	2.33	1.54	1.51
16	L	4022	BCR	C38-C26	2.33	1.54	1.51
13	B	1225	CLA	CAA-C2A	2.33	1.58	1.54
14	A	2001	PQN	C9-C10	2.34	1.43	1.39
14	A	2001	PQN	C11-C3	2.34	1.55	1.51
13	A	1121	CLA	CAA-C2A	2.34	1.58	1.54
13	A	1117	CLA	CAA-C2A	2.35	1.58	1.54
13	L	1502	CLA	CAA-C2A	2.35	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1108	CLA	CAA-C2A	2.36	1.58	1.54
13	A	1118	CLA	C5-C3	2.37	1.56	1.51
16	L	4022	BCR	C26-C25	2.37	1.38	1.34
13	B	1225	CLA	CHC-C1C	2.38	1.42	1.35
16	A	4003	BCR	C29-C30	2.38	1.59	1.54
13	A	1128	CLA	C5-C3	2.38	1.56	1.51
13	A	1117	CLA	C2-C3	2.39	1.38	1.33
16	I	4018	BCR	C30-C25	2.39	1.57	1.53
13	A	1133	CLA	C5-C3	2.40	1.56	1.51
13	J	1303	CLA	CBD-CAD	2.40	1.57	1.51
13	A	1117	CLA	C1-C2	2.40	1.56	1.49
13	A	1110	CLA	CHC-C1C	2.40	1.42	1.35
13	B	1217	CLA	CAA-C2A	2.40	1.58	1.54
16	B	4010	BCR	C29-C30	2.41	1.59	1.54
13	B	1215	CLA	C3B-CAB	2.41	1.52	1.47
13	M	1601	CLA	CAA-C2A	2.41	1.58	1.54
13	A	1013	CLA	CAA-C2A	2.41	1.58	1.54
13	A	1116	CLA	C5-C3	2.41	1.56	1.51
13	A	1108	CLA	CHC-C1C	2.42	1.42	1.35
16	A	4001	BCR	C26-C25	2.42	1.38	1.34
14	B	2002	PQN	C8-C9	2.44	1.43	1.38
14	A	2001	PQN	C8-C7	2.44	1.44	1.38
13	A	1127	CLA	CHC-C1C	2.45	1.42	1.35
16	B	4005	BCR	C29-C30	2.45	1.59	1.54
16	I	4018	BCR	C2-C1	2.45	1.59	1.54
16	L	4019	BCR	C2-C1	2.45	1.59	1.54
13	A	1402	CLA	CHC-C1C	2.46	1.42	1.35
14	A	2001	PQN	C8-C9	2.47	1.43	1.38
13	A	1237	CLA	CMD-C2D	2.48	1.56	1.51
13	A	1102	CLA	CAA-C2A	2.48	1.58	1.54
13	A	1109	CLA	CHC-C1C	2.49	1.42	1.35
13	B	1222	CLA	CHC-C1C	2.49	1.42	1.35
14	B	2002	PQN	C9-C10	2.49	1.43	1.39
16	A	4011	BCR	C14-C13	2.50	1.39	1.35
13	A	1237	CLA	CAA-C2A	2.50	1.58	1.54
13	B	1225	CLA	C5-C3	2.50	1.56	1.51
14	A	2001	PQN	C11-C12	2.51	1.54	1.50
16	A	4008	BCR	C29-C30	2.52	1.60	1.54
13	A	1111	CLA	CHC-C1C	2.53	1.42	1.35
16	J	4015	BCR	C5-C6	2.53	1.38	1.34
13	A	1121	CLA	CHC-C1C	2.54	1.42	1.35
13	A	1114	CLA	CHC-C1C	2.55	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1140	CLA	C1-C2	2.55	1.57	1.49
13	A	1013	CLA	CHC-C1C	2.55	1.42	1.35
13	B	1230	CLA	CHC-C1C	2.56	1.42	1.35
13	A	1133	CLA	CHC-C1C	2.56	1.42	1.35
13	B	1215	CLA	CAA-C2A	2.56	1.59	1.54
13	B	1205	CLA	CHC-C1C	2.57	1.42	1.35
14	A	2001	PQN	C15-C13	2.58	1.56	1.51
17	A	5001	LHG	O7-C7	2.58	1.41	1.34
13	A	1402	CLA	CBD-CAD	2.58	1.57	1.51
13	B	1230	CLA	C5-C3	2.58	1.57	1.51
13	A	1101	CLA	CHC-C1C	2.59	1.42	1.35
13	B	1210	CLA	CHC-C1C	2.59	1.42	1.35
14	B	2002	PQN	C11-C3	2.59	1.55	1.51
13	B	1233	CLA	CHC-C1C	2.59	1.42	1.35
13	A	1113	CLA	CHC-C1C	2.60	1.42	1.35
13	A	1011	CLA	CHC-C1C	2.60	1.42	1.35
16	B	4014	BCR	C2-C1	2.60	1.60	1.54
16	A	4007	BCR	C2-C1	2.61	1.60	1.54
13	B	1214	CLA	CAA-C2A	2.62	1.59	1.54
16	B	4010	BCR	C1-C6	2.62	1.57	1.53
13	B	1208	CLA	CHC-C1C	2.64	1.43	1.35
13	A	1107	CLA	CHC-C1C	2.64	1.43	1.35
16	L	4022	BCR	C29-C30	2.64	1.60	1.54
13	B	1216	CLA	CHC-C1C	2.64	1.43	1.35
16	I	4020	BCR	C29-C30	2.66	1.60	1.54
13	B	1213	CLA	CHC-C1C	2.66	1.43	1.35
13	K	1401	CLA	CHC-C1C	2.67	1.43	1.35
16	A	4008	BCR	C30-C25	2.68	1.57	1.53
13	B	1236	CLA	CHC-C1C	2.68	1.43	1.35
13	B	1226	CLA	CAA-C2A	2.68	1.59	1.54
16	A	4001	BCR	C2-C1	2.69	1.60	1.54
13	B	1211	CLA	CHC-C1C	2.69	1.43	1.35
13	A	1119	CLA	CAA-C2A	2.69	1.59	1.54
16	A	4007	BCR	C1-C6	2.70	1.57	1.53
13	A	1022	CLA	CHC-C1C	2.70	1.43	1.35
16	A	4002	BCR	C1-C6	2.71	1.57	1.53
13	B	1209	CLA	CHC-C1C	2.71	1.43	1.35
13	A	1122	CLA	CHC-C1C	2.71	1.43	1.35
16	I	4018	BCR	C29-C30	2.72	1.60	1.54
13	B	1224	CLA	CAA-C2A	2.72	1.59	1.54
13	B	1232	CLA	CAA-C2A	2.72	1.59	1.54
17	A	5001	LHG	O8-C23	2.72	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1104	CLA	CHC-C1C	2.73	1.43	1.35
13	A	1115	CLA	CHC-C1C	2.74	1.43	1.35
13	A	1801	CLA	CAA-C2A	2.74	1.59	1.54
16	M	4021	BCR	C30-C25	2.75	1.57	1.53
18	B	5002	LMG	O8-C28	2.75	1.41	1.33
13	B	1213	CLA	CAA-C2A	2.75	1.59	1.54
13	B	1221	CLA	C5-C3	2.75	1.57	1.51
16	L	4019	BCR	C29-C30	2.76	1.60	1.54
13	B	1229	CLA	CHC-C1C	2.76	1.43	1.35
16	B	4009	BCR	C30-C25	2.76	1.57	1.53
13	A	1134	CLA	CHC-C1C	2.76	1.43	1.35
13	B	1227	CLA	CHC-C1C	2.76	1.43	1.35
13	J	1303	CLA	CHC-C1C	2.77	1.43	1.35
13	B	1219	CLA	CHC-C1C	2.77	1.43	1.35
13	B	1217	CLA	CHC-C1C	2.77	1.43	1.35
16	J	4012	BCR	C2-C1	2.78	1.60	1.54
13	A	1137	CLA	CAA-C2A	2.78	1.59	1.54
13	B	1213	CLA	C5-C3	2.79	1.57	1.51
16	A	4011	BCR	C29-C30	2.81	1.60	1.54
16	I	4020	BCR	C2-C1	2.81	1.60	1.54
13	B	1219	CLA	CAA-C2A	2.81	1.59	1.54
13	A	1103	CLA	CHC-C1C	2.81	1.43	1.35
13	A	1105	CLA	CHC-C1C	2.81	1.43	1.35
16	J	4012	BCR	C30-C25	2.82	1.57	1.53
16	B	4006	BCR	C30-C25	2.83	1.57	1.53
16	B	4006	BCR	C1-C6	2.83	1.57	1.53
16	B	4004	BCR	C29-C30	2.83	1.60	1.54
13	B	1224	CLA	OBD-CAD	2.83	1.26	1.22
13	B	1214	CLA	CHC-C1C	2.83	1.43	1.35
13	A	1116	CLA	CHC-C1C	2.84	1.43	1.35
16	B	4005	BCR	C26-C25	2.84	1.39	1.34
13	M	1601	CLA	CHC-C1C	2.85	1.43	1.35
16	B	4017	BCR	C30-C25	2.85	1.57	1.53
16	B	4006	BCR	C29-C30	2.85	1.60	1.54
17	A	5003	LHG	O8-C23	2.86	1.41	1.33
13	A	1116	CLA	CAA-C2A	2.86	1.59	1.54
16	J	4015	BCR	C29-C30	2.86	1.60	1.54
16	A	4001	BCR	C29-C30	2.87	1.60	1.54
16	B	4010	BCR	C2-C1	2.87	1.60	1.54
13	B	1228	CLA	CHC-C1C	2.88	1.43	1.35
13	A	1140	CLA	CHC-C1C	2.88	1.43	1.35
13	B	1201	CLA	CHC-C1C	2.89	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1223	CLA	CHC-C1C	2.89	1.43	1.35
16	B	4006	BCR	C2-C1	2.90	1.60	1.54
16	F	4016	BCR	C29-C30	2.90	1.60	1.54
13	A	1125	CLA	C5-C3	2.90	1.57	1.51
16	B	4017	BCR	C29-C30	2.90	1.60	1.54
16	B	4009	BCR	C29-C30	2.91	1.60	1.54
16	B	4005	BCR	C2-C1	2.91	1.60	1.54
13	A	1136	CLA	CHC-C1C	2.92	1.43	1.35
16	J	4012	BCR	C1-C6	2.92	1.57	1.53
13	A	1137	CLA	CHC-C1C	2.92	1.43	1.35
13	A	1102	CLA	CHC-C1C	2.93	1.43	1.35
13	A	1106	CLA	CAA-C2A	2.94	1.59	1.54
16	M	4021	BCR	C29-C30	2.94	1.61	1.54
13	F	1301	CLA	CHC-C1C	2.95	1.43	1.35
16	M	4021	BCR	C2-C1	2.96	1.61	1.54
16	B	4005	BCR	C30-C25	2.97	1.57	1.53
13	J	1302	CLA	CHC-C1C	2.97	1.44	1.35
13	B	1012	CLA	CHC-C1C	2.98	1.44	1.35
13	L	1503	CLA	CHC-C1C	2.98	1.44	1.35
16	A	4002	BCR	C29-C30	2.99	1.61	1.54
16	B	4014	BCR	C29-C30	2.99	1.61	1.54
16	A	4003	BCR	C2-C1	2.99	1.61	1.54
13	A	1129	CLA	CHC-C1C	3.00	1.44	1.35
13	B	1234	CLA	CHC-C1C	3.03	1.44	1.35
13	A	1120	CLA	CHC-C1C	3.04	1.44	1.35
13	A	1123	CLA	CHC-C1C	3.04	1.44	1.35
13	B	1225	CLA	C2-C3	3.05	1.40	1.33
13	A	1119	CLA	CHC-C1C	3.05	1.44	1.35
13	B	1232	CLA	CHC-C1C	3.05	1.44	1.35
16	A	4011	BCR	C2-C1	3.05	1.61	1.54
16	A	4002	BCR	C2-C1	3.06	1.61	1.54
14	A	2001	PQN	C6-C5	3.06	1.44	1.39
13	A	1118	CLA	CHC-C1C	3.07	1.44	1.35
16	F	4016	BCR	C30-C25	3.07	1.58	1.53
13	B	1212	CLA	CHC-C1C	3.08	1.44	1.35
16	J	4015	BCR	C2-C1	3.08	1.61	1.54
13	B	1220	CLA	CHC-C1C	3.09	1.44	1.35
14	A	2001	PQN	C10-C5	3.10	1.46	1.40
16	B	4017	BCR	C2-C1	3.10	1.61	1.54
13	A	1112	CLA	CHC-C1C	3.10	1.44	1.35
16	J	4012	BCR	C29-C30	3.11	1.61	1.54
16	A	4007	BCR	C29-C30	3.11	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	1701	CLA	CHC-C1C	3.12	1.44	1.35
14	B	2002	PQN	C6-C5	3.12	1.44	1.39
13	A	1125	CLA	CHC-C1C	3.13	1.44	1.35
13	B	1231	CLA	CHC-C1C	3.14	1.44	1.35
16	B	4010	BCR	C30-C25	3.15	1.58	1.53
16	J	4013	BCR	C30-C25	3.16	1.58	1.53
13	A	1106	CLA	CHC-C1C	3.16	1.44	1.35
13	A	1801	CLA	CHC-C1C	3.16	1.44	1.35
13	B	1221	CLA	CHC-C1C	3.16	1.44	1.35
13	L	1502	CLA	CHC-C1C	3.17	1.44	1.35
13	B	1224	CLA	CHC-C1C	3.17	1.44	1.35
13	A	1138	CLA	CHC-C1C	3.17	1.44	1.35
13	A	1128	CLA	CHC-C1C	3.19	1.44	1.35
16	B	4004	BCR	C2-C1	3.20	1.61	1.54
14	B	2002	PQN	C11-C12	3.21	1.55	1.50
16	B	4004	BCR	C26-C25	3.23	1.40	1.34
16	A	4008	BCR	C1-C6	3.24	1.58	1.53
16	J	4015	BCR	C1-C6	3.24	1.58	1.53
16	I	4020	BCR	C30-C25	3.25	1.58	1.53
13	B	1218	CLA	CHC-C1C	3.25	1.44	1.35
16	A	4011	BCR	C1-C6	3.28	1.58	1.53
16	B	4004	BCR	C1-C6	3.29	1.58	1.53
13	B	1023	CLA	CHC-C1C	3.30	1.44	1.35
16	L	4022	BCR	C2-C1	3.33	1.61	1.54
16	M	4021	BCR	C1-C6	3.37	1.58	1.53
13	L	1501	CLA	CHC-C1C	3.37	1.45	1.35
16	A	4002	BCR	C30-C25	3.43	1.58	1.53
13	B	1235	CLA	CHC-C1C	3.44	1.45	1.35
16	A	4011	BCR	C30-C25	3.48	1.58	1.53
16	F	4016	BCR	C2-C1	3.49	1.62	1.54
17	B	5004	LHG	O7-C7	3.49	1.44	1.34
16	A	4001	BCR	C1-C6	3.51	1.58	1.53
14	B	2002	PQN	C10-C5	3.56	1.46	1.40
16	J	4013	BCR	C2-C1	3.58	1.62	1.54
16	A	4001	BCR	C30-C25	3.58	1.58	1.53
16	J	4015	BCR	C30-C25	3.61	1.58	1.53
16	A	4003	BCR	C30-C25	3.65	1.58	1.53
16	A	4003	BCR	C1-C6	3.69	1.58	1.53
17	A	5003	LHG	O7-C7	3.71	1.45	1.34
16	J	4013	BCR	C29-C30	3.72	1.62	1.54
17	A	5001	LHG	P-O6	3.95	1.76	1.59
13	B	1205	CLA	CHB-C4A	4.15	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5003	LHG	P-O3	4.27	1.77	1.59
13	B	1023	CLA	CHB-C4A	4.34	1.39	1.33
13	L	1502	CLA	CHB-C4A	4.44	1.39	1.33
16	A	4007	BCR	C30-C25	4.47	1.59	1.53
13	A	1126	CLA	CHB-C4A	4.57	1.39	1.33
16	L	4022	BCR	C30-C25	4.58	1.60	1.53
13	B	1221	CLA	CHB-C4A	4.65	1.39	1.33
16	B	4004	BCR	C30-C25	4.70	1.60	1.53
17	A	5003	LHG	P-O6	4.72	1.79	1.59
16	L	4019	BCR	C30-C25	4.75	1.60	1.53
13	A	1132	CLA	CHB-C4A	4.79	1.39	1.33
16	B	4005	BCR	C1-C6	4.81	1.60	1.53
13	B	1228	CLA	CHB-C4A	4.92	1.39	1.33
13	A	1136	CLA	CHB-C4A	4.93	1.39	1.33
13	B	1210	CLA	CHB-C4A	4.95	1.39	1.33
16	L	4022	BCR	C1-C6	4.95	1.60	1.53
17	A	5001	LHG	P-O3	4.99	1.80	1.59
13	A	1022	CLA	CHB-C4A	5.01	1.39	1.33
17	B	5004	LHG	P-O3	5.07	1.80	1.59
13	A	1117	CLA	CHB-C4A	5.07	1.40	1.33
13	B	1229	CLA	CHB-C4A	5.08	1.40	1.33
13	B	1232	CLA	CHB-C4A	5.11	1.40	1.33
13	B	1208	CLA	CHB-C4A	5.19	1.40	1.33
13	B	1236	CLA	CHB-C4A	5.21	1.40	1.33
13	A	1112	CLA	CHB-C4A	5.22	1.40	1.33
14	B	2002	PQN	C3-C2	5.23	1.46	1.35
13	B	1214	CLA	CHB-C4A	5.24	1.40	1.33
14	A	2001	PQN	C3-C2	5.27	1.46	1.35
13	A	1119	CLA	CHB-C4A	5.29	1.40	1.33
13	A	1129	CLA	CHB-C4A	5.32	1.40	1.33
13	A	1138	CLA	CHB-C4A	5.34	1.40	1.33
13	A	1128	CLA	CHB-C4A	5.35	1.40	1.33
13	A	1115	CLA	CHB-C4A	5.35	1.40	1.33
13	B	1212	CLA	CHB-C4A	5.37	1.40	1.33
13	B	1238	CLA	CHB-C4A	5.39	1.40	1.33
13	A	1801	CLA	CHB-C4A	5.39	1.40	1.33
13	A	1101	CLA	CHB-C4A	5.53	1.40	1.33
13	B	1216	CLA	CHB-C4A	5.57	1.40	1.33
13	A	1114	CLA	CHB-C4A	5.62	1.40	1.33
13	L	1503	CLA	CHB-C4A	5.63	1.40	1.33
17	B	5004	LHG	P-O6	5.63	1.83	1.59
13	B	1201	CLA	CHB-C4A	5.65	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1124	CLA	CHB-C4A	5.67	1.40	1.33
13	A	1237	CLA	CHB-C4A	5.67	1.40	1.33
13	B	1224	CLA	CHB-C4A	5.69	1.40	1.33
13	B	1213	CLA	CHB-C4A	5.72	1.40	1.33
13	A	1109	CLA	CHB-C4A	5.73	1.40	1.33
13	B	1206	CLA	CHB-C4A	5.76	1.40	1.33
13	A	1106	CLA	CHB-C4A	5.78	1.40	1.33
13	B	1203	CLA	CHB-C4A	5.78	1.40	1.33
13	A	1013	CLA	CHB-C4A	5.80	1.40	1.33
13	A	1108	CLA	CHB-C4A	5.80	1.40	1.33
13	B	1211	CLA	CHB-C4A	5.81	1.40	1.33
13	A	1102	CLA	CHB-C4A	5.82	1.40	1.33
13	K	1401	CLA	CHB-C4A	5.86	1.41	1.33
13	B	1215	CLA	CHB-C4A	5.87	1.41	1.33
13	A	1111	CLA	CHB-C4A	5.87	1.41	1.33
13	B	1220	CLA	CHB-C4A	5.89	1.41	1.33
13	A	1140	CLA	CHB-C4A	5.93	1.41	1.33
13	A	1131	CLA	CHB-C4A	5.93	1.41	1.33
13	B	1235	CLA	CHB-C4A	5.93	1.41	1.33
13	B	1227	CLA	CHB-C4A	5.94	1.41	1.33
13	B	1225	CLA	CHB-C4A	5.94	1.41	1.33
13	A	1121	CLA	CHB-C4A	5.94	1.41	1.33
13	A	1107	CLA	CHB-C4A	5.95	1.41	1.33
13	A	1122	CLA	CHB-C4A	5.97	1.41	1.33
13	A	1116	CLA	CHB-C4A	5.98	1.41	1.33
13	A	1123	CLA	CHB-C4A	6.01	1.41	1.33
13	B	1012	CLA	CHB-C4A	6.06	1.41	1.33
13	L	1501	CLA	CHB-C4A	6.07	1.41	1.33
13	B	1222	CLA	CHB-C4A	6.08	1.41	1.33
13	A	1120	CLA	CHB-C4A	6.11	1.41	1.33
13	A	1104	CLA	CHB-C4A	6.12	1.41	1.33
13	B	1218	CLA	CHB-C4A	6.23	1.41	1.33
13	B	1202	CLA	CHB-C4A	6.28	1.41	1.33
13	A	1103	CLA	CHB-C4A	6.31	1.41	1.33
13	A	1110	CLA	CHB-C4A	6.35	1.41	1.33
13	A	1137	CLA	CHB-C4A	6.39	1.41	1.33
13	F	1301	CLA	CHB-C4A	6.40	1.41	1.33
13	B	1239	CLA	CHB-C4A	6.44	1.41	1.33
13	B	1204	CLA	CHB-C4A	6.44	1.41	1.33
13	A	1133	CLA	CHB-C4A	6.50	1.41	1.33
13	B	1219	CLA	CHB-C4A	6.51	1.41	1.33
13	A	1011	CLA	CHB-C4A	6.52	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1021	CLA	CHB-C4A	6.53	1.41	1.33
13	A	1105	CLA	CHB-C4A	6.53	1.41	1.33
13	A	1118	CLA	CHB-C4A	6.55	1.41	1.33
13	B	1231	CLA	CHB-C4A	6.55	1.41	1.33
13	A	1125	CLA	CHB-C4A	6.56	1.41	1.33
13	B	1207	CLA	CHB-C4A	6.57	1.41	1.33
13	B	1234	CLA	CHB-C4A	6.66	1.42	1.33
13	B	1226	CLA	CHB-C4A	6.72	1.42	1.33
13	A	1134	CLA	CHB-C4A	6.73	1.42	1.33
13	A	1402	CLA	CHB-C4A	6.76	1.42	1.33
13	A	1130	CLA	CHB-C4A	6.93	1.42	1.33
13	M	1601	CLA	CHB-C4A	6.97	1.42	1.33
13	J	1302	CLA	CHB-C4A	6.99	1.42	1.33
13	B	1217	CLA	CHB-C4A	7.03	1.42	1.33
13	B	1233	CLA	CHB-C4A	7.04	1.42	1.33
13	A	1127	CLA	CHB-C4A	7.10	1.42	1.33
13	A	1113	CLA	CHB-C4A	7.11	1.42	1.33
13	X	1701	CLA	CHB-C4A	7.21	1.42	1.33
17	A	5003	LHG	P-O5	7.25	1.78	1.50
13	J	1303	CLA	CHB-C4A	7.28	1.42	1.33
13	A	1139	CLA	CHB-C4A	7.29	1.42	1.33
13	B	1230	CLA	CHB-C4A	7.31	1.42	1.33
13	B	1209	CLA	CHB-C4A	7.35	1.42	1.33
13	B	1223	CLA	CHB-C4A	7.37	1.42	1.33
13	A	1135	CLA	CHB-C4A	7.71	1.43	1.33
17	A	5001	LHG	P-O5	7.73	1.79	1.50
14	B	2002	PQN	C12-C13	7.92	1.52	1.33
14	A	2001	PQN	C12-C13	7.92	1.52	1.33
17	B	5004	LHG	P-O5	8.14	1.81	1.50
14	B	2002	PQN	O1-C1	8.18	1.41	1.23
14	A	2001	PQN	O1-C1	8.68	1.42	1.23
14	B	2002	PQN	O4-C4	8.71	1.42	1.23
14	A	2001	PQN	O4-C4	9.02	1.42	1.23

All (1468) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2002	PQN	C11-C12-C13	-8.11	113.14	126.71
14	A	2001	PQN	C11-C12-C13	-8.00	113.34	126.71
14	A	2001	PQN	C15-C13-C12	-7.18	106.41	121.10
13	A	1011	CLA	C3D-CAD-CBD	-6.23	98.79	107.60
13	A	1011	CLA	O1D-CGD-CBD	-6.10	113.64	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2002	PQN	C15-C13-C12	-6.10	108.62	121.10
13	A	1104	CLA	CAA-C2A-C3A	-4.73	99.84	112.81
13	A	1119	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
13	A	1117	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
13	B	1215	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
13	B	1226	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
13	A	1127	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
16	A	4008	BCR	C38-C26-C27	-3.96	105.95	113.45
16	B	4004	BCR	C38-C26-C27	-3.86	106.14	113.45
13	B	1223	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
13	A	1104	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
13	J	1303	CLA	CAA-C2A-C3A	-3.64	109.01	116.38
16	B	4005	BCR	C30-C25-C26	-3.63	117.49	122.59
13	B	1012	CLA	OBD-CAD-CBD	-3.61	120.48	125.94
16	B	4014	BCR	C33-C5-C4	-3.61	106.61	113.45
13	A	1022	CLA	OBD-CAD-CBD	-3.60	120.50	125.94
16	B	4005	BCR	C38-C26-C27	-3.59	106.64	113.45
13	B	1205	CLA	O1D-CGD-CBD	-3.56	118.20	124.60
13	B	1206	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
13	B	1232	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
16	A	4003	BCR	C38-C26-C27	-3.54	106.74	113.45
16	A	4001	BCR	C38-C26-C27	-3.51	106.80	113.45
16	J	4012	BCR	C38-C26-C27	-3.50	106.81	113.45
13	B	1210	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
13	A	1124	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
16	B	4006	BCR	C38-C26-C27	-3.48	106.86	113.45
13	A	1129	CLA	C2C-C1C-NC	-3.41	107.88	110.22
13	B	1222	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
16	I	4020	BCR	C33-C5-C4	-3.40	107.00	113.45
16	I	4020	BCR	C38-C26-C27	-3.40	107.01	113.45
16	A	4002	BCR	C38-C26-C27	-3.39	107.02	113.45
16	L	4019	BCR	C33-C5-C4	-3.35	107.09	113.45
13	B	1202	CLA	OBD-CAD-CBD	-3.35	120.88	125.94
13	B	1239	CLA	OBD-CAD-CBD	-3.35	120.89	125.94
13	A	1113	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
13	B	1202	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
13	A	1107	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
13	B	1204	CLA	OBD-CAD-CBD	-3.33	120.91	125.94
16	B	4010	BCR	C33-C5-C4	-3.32	107.16	113.45
16	B	4006	BCR	C33-C5-C4	-3.31	107.17	113.45
16	J	4015	BCR	C33-C5-C4	-3.30	107.19	113.45
13	B	1219	CLA	CMB-C2B-C1B	-3.30	123.40	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	4009	BCR	C38-C26-C27	-3.27	107.24	113.45
16	I	4018	BCR	C38-C26-C27	-3.27	107.25	113.45
16	J	4015	BCR	C38-C26-C27	-3.26	107.26	113.45
13	A	1103	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
13	A	1237	CLA	O2A-CGA-O1A	-3.24	115.50	123.55
16	B	4014	BCR	C38-C26-C27	-3.23	107.33	113.45
13	A	1126	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
16	B	4004	BCR	C30-C25-C26	-3.21	118.08	122.59
13	A	1131	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
13	A	1102	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
16	B	4004	BCR	C33-C5-C4	-3.19	107.40	113.45
16	L	4022	BCR	C33-C5-C4	-3.19	107.41	113.45
13	A	1114	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
16	A	4007	BCR	C38-C26-C27	-3.17	107.44	113.45
13	B	1210	CLA	O1D-CGD-CBD	-3.17	118.91	124.60
13	A	1013	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
16	F	4016	BCR	C33-C5-C4	-3.15	107.47	113.45
16	A	4001	BCR	C30-C25-C26	-3.14	118.17	122.59
13	A	1013	CLA	O2A-CGA-O1A	-3.14	115.76	123.55
13	A	1801	CLA	C2C-C1C-NC	-3.14	108.07	110.22
16	L	4019	BCR	C38-C26-C27	-3.14	107.50	113.45
13	A	1108	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
16	F	4016	BCR	C38-C26-C27	-3.13	107.51	113.45
16	A	4003	BCR	C33-C5-C4	-3.11	107.55	113.45
16	A	4011	BCR	C33-C5-C4	-3.10	107.56	113.45
16	A	4001	BCR	C33-C5-C4	-3.10	107.56	113.45
16	J	4012	BCR	C30-C25-C26	-3.10	118.23	122.59
13	A	1801	CLA	O1D-CGD-CBD	-3.10	119.04	124.60
13	B	1230	CLA	O1D-CGD-CBD	-3.09	119.04	124.60
13	B	1214	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
13	A	1102	CLA	O1D-CGD-CBD	-3.08	119.06	124.60
16	A	4008	BCR	C30-C25-C26	-3.07	118.27	122.59
13	A	1140	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
13	A	1123	CLA	O1D-CGD-CBD	-3.06	119.11	124.60
13	A	1111	CLA	O1D-CGD-CBD	-3.05	119.11	124.60
13	A	1135	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
16	B	4005	BCR	C33-C5-C4	-3.05	107.66	113.45
13	A	1111	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
13	B	1211	CLA	O1D-CGD-CBD	-3.05	119.13	124.60
13	B	1227	CLA	O1D-CGD-CBD	-3.04	119.13	124.60
13	B	1224	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
13	A	1135	CLA	O2A-CGA-O1A	-3.02	116.04	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1103	CLA	CAA-C2A-C3A	-3.02	104.53	112.81
16	J	4015	BCR	C1-C6-C5	-3.01	118.35	122.59
16	B	4010	BCR	C38-C26-C27	-3.01	107.73	113.45
16	M	4021	BCR	C38-C26-C27	-3.01	107.73	113.45
13	A	1106	CLA	O1D-CGD-CBD	-3.01	119.19	124.60
13	B	1229	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
13	B	1224	CLA	OBD-CAD-CBD	-3.01	121.40	125.94
13	B	1203	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
13	B	1216	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
13	A	1129	CLA	O1D-CGD-CBD	-3.00	119.21	124.60
17	A	5003	LHG	C6-C5-C4	-3.00	105.09	111.86
13	A	1103	CLA	OBD-CAD-CBD	-3.00	121.41	125.94
13	A	1120	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
13	L	1501	CLA	OBD-CAD-CBD	-2.99	121.42	125.94
13	B	1218	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
13	B	1212	CLA	O1D-CGD-CBD	-2.99	119.23	124.60
16	B	4017	BCR	C38-C26-C27	-2.99	107.78	113.45
16	A	4002	BCR	C33-C5-C4	-2.99	107.78	113.45
13	A	1115	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
16	B	4014	BCR	C8-C9-C10	-2.98	114.36	118.94
13	B	1214	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
16	A	4011	BCR	C38-C26-C27	-2.97	107.81	113.45
13	B	1235	CLA	OBD-CAD-CBD	-2.97	121.46	125.94
13	A	1119	CLA	OBD-CAD-CBD	-2.96	121.46	125.94
13	A	1134	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
13	B	1229	CLA	OBD-CAD-CBD	-2.96	121.48	125.94
13	A	1128	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
13	A	1129	CLA	OBD-CAD-CBD	-2.95	121.48	125.94
16	B	4005	BCR	C1-C6-C5	-2.95	118.45	122.59
13	B	1201	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
13	A	1101	CLA	CMB-C2B-C1B	-2.95	123.94	128.46
13	B	1218	CLA	O1D-CGD-CBD	-2.94	119.31	124.60
13	A	1133	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
16	B	4004	BCR	C1-C6-C5	-2.94	118.46	122.59
13	B	1021	CLA	C7-C6-C5	-2.94	104.94	113.11
13	B	1205	CLA	CAA-C2A-C3A	-2.94	104.75	112.81
13	B	1212	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
13	B	1218	CLA	C2C-C1C-NC	-2.94	108.21	110.22
13	A	1137	CLA	O2A-CGA-O1A	-2.93	116.26	123.55
13	X	1701	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
13	B	1220	CLA	OBD-CAD-CBD	-2.93	121.52	125.94
13	A	1121	CLA	CMB-C2B-C1B	-2.92	123.97	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1220	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
13	A	1112	CLA	OBD-CAD-CBD	-2.92	121.53	125.94
13	A	1801	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
13	B	1213	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
13	A	1125	CLA	O1D-CGD-CBD	-2.91	119.37	124.60
13	L	1503	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
16	A	4007	BCR	C30-C25-C26	-2.91	118.50	122.59
13	A	1106	CLA	C2C-C1C-NC	-2.90	108.23	110.22
16	J	4013	BCR	C33-C5-C4	-2.90	107.94	113.45
13	L	1501	CLA	O1D-CGD-CBD	-2.90	119.39	124.60
13	B	1209	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
13	J	1302	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
13	B	1012	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
13	A	1116	CLA	OBD-CAD-CBD	-2.89	121.57	125.94
13	B	1213	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
16	B	4014	BCR	C12-C13-C14	-2.89	114.50	118.94
13	L	1503	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
13	B	1238	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
13	B	1221	CLA	OBD-CAD-CBD	-2.88	121.59	125.94
13	A	1126	CLA	OBD-CAD-CBD	-2.88	121.59	125.94
13	B	1225	CLA	CMB-C2B-C1B	-2.88	124.05	128.46
13	B	1217	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
16	A	4007	BCR	C33-C5-C4	-2.86	108.02	113.45
16	B	4017	BCR	C33-C5-C4	-2.86	108.03	113.45
13	A	1116	CLA	CMB-C2B-C1B	-2.86	124.08	128.46
13	B	1226	CLA	O1D-CGD-CBD	-2.85	119.47	124.60
16	M	4021	BCR	C1-C6-C5	-2.85	118.58	122.59
13	B	1023	CLA	OBD-CAD-CBD	-2.85	121.63	125.94
13	B	1205	CLA	O2A-CGA-O1A	-2.85	116.48	123.55
13	A	1132	CLA	O1D-CGD-CBD	-2.84	119.49	124.60
13	A	1108	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
16	B	4006	BCR	C1-C6-C5	-2.84	118.59	122.59
13	A	1113	CLA	O1D-CGD-CBD	-2.84	119.50	124.60
13	B	1231	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
13	A	1118	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
13	B	1215	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
16	B	4006	BCR	C30-C25-C26	-2.84	118.60	122.59
16	J	4012	BCR	C33-C5-C4	-2.84	108.07	113.45
13	B	1236	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
13	A	1022	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
13	B	1232	CLA	OBD-CAD-CBD	-2.83	121.67	125.94
13	B	1021	CLA	OBD-CAD-CBD	-2.83	121.67	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1211	CLA	OBD-CAD-CBD	-2.83	121.67	125.94
13	B	1201	CLA	O1D-CGD-CBD	-2.82	119.53	124.60
13	B	1239	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
13	A	1138	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
13	A	1112	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
13	K	1401	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
13	A	1136	CLA	OBD-CAD-CBD	-2.80	121.71	125.94
13	B	1211	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
13	A	1103	CLA	O1D-CGD-CBD	-2.80	119.58	124.60
13	A	1122	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
13	B	1222	CLA	O1D-CGD-CBD	-2.79	119.58	124.60
16	M	4021	BCR	C33-C5-C4	-2.79	108.15	113.45
13	A	1132	CLA	OBD-CAD-CBD	-2.79	121.72	125.94
13	L	1502	CLA	OBD-CAD-CBD	-2.79	121.73	125.94
13	A	1138	CLA	C2C-C1C-NC	-2.79	108.31	110.22
13	B	1205	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
13	A	1237	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
16	A	4001	BCR	C1-C6-C5	-2.78	118.69	122.59
13	B	1236	CLA	OBD-CAD-CBD	-2.78	121.74	125.94
13	B	1228	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
16	I	4018	BCR	C33-C5-C4	-2.78	108.18	113.45
13	B	1225	CLA	C4-C3-C5	-2.78	110.47	115.29
16	A	4002	BCR	C30-C25-C26	-2.78	118.69	122.59
13	A	1119	CLA	CAA-C2A-C3A	-2.77	105.20	112.81
13	B	1217	CLA	O1D-CGD-CBD	-2.77	119.62	124.60
13	A	1120	CLA	C2C-C1C-NC	-2.77	108.32	110.22
16	L	4022	BCR	C38-C26-C27	-2.76	108.21	113.45
13	B	1206	CLA	OBD-CAD-CBD	-2.76	121.77	125.94
13	B	1230	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
13	M	1601	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
13	B	1221	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
16	A	4003	BCR	C1-C6-C5	-2.74	118.74	122.59
13	A	1106	CLA	OBD-CAD-CBD	-2.74	121.80	125.94
16	I	4020	BCR	C30-C25-C26	-2.74	118.74	122.59
16	J	4013	BCR	C38-C26-C27	-2.74	108.25	113.45
16	J	4015	BCR	C30-C25-C26	-2.74	118.75	122.59
13	A	1131	CLA	OBD-CAD-CBD	-2.73	121.82	125.94
13	A	1130	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
13	A	1104	CLA	O2A-CGA-O1A	-2.73	116.78	123.55
13	A	1135	CLA	C4-C3-C5	-2.73	112.62	115.85
13	J	1302	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
13	A	1118	CLA	C2C-C1C-NC	-2.72	108.36	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	4019	BCR	C30-C25-C26	-2.72	118.78	122.59
13	B	1234	CLA	O1D-CGD-CBD	-2.71	119.73	124.60
13	A	1128	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
13	A	1011	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
13	B	1208	CLA	CAA-C2A-C3A	-2.70	105.41	112.81
13	A	1120	CLA	OBD-CAD-CBD	-2.70	121.87	125.94
13	F	1301	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
13	J	1303	CLA	CMA-C3A-C2A	-2.69	110.94	116.38
13	A	1111	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
13	B	1235	CLA	C2C-C1C-NC	-2.69	108.38	110.22
13	A	1101	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
13	J	1303	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
13	A	1109	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
13	A	1110	CLA	CMB-C2B-C1B	-2.67	124.35	128.46
13	A	1402	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
13	A	1119	CLA	C2C-C1C-NC	-2.67	108.39	110.22
13	A	1125	CLA	CMB-C2B-C1B	-2.67	124.37	128.46
13	B	1228	CLA	C2C-C1C-NC	-2.66	108.39	110.22
13	A	1105	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
16	F	4016	BCR	C1-C6-C5	-2.66	118.85	122.59
16	A	4003	BCR	C30-C25-C26	-2.66	118.86	122.59
13	A	1128	CLA	C2C-C1C-NC	-2.66	108.40	110.22
16	B	4010	BCR	C30-C25-C26	-2.66	118.86	122.59
13	A	1237	CLA	CAA-C2A-C3A	-2.65	105.53	112.81
13	A	1237	CLA	OBD-CAD-CBD	-2.65	121.94	125.94
13	X	1701	CLA	OBD-CAD-CBD	-2.65	121.95	125.94
13	A	1114	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
13	A	1120	CLA	O1D-CGD-CBD	-2.64	119.86	124.60
16	L	4022	BCR	C30-C25-C26	-2.64	118.88	122.59
13	B	1205	CLA	OBD-CAD-CBD	-2.64	121.96	125.94
16	B	4014	BCR	C30-C25-C26	-2.64	118.88	122.59
13	B	1208	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
13	A	1125	CLA	C2C-C1C-NC	-2.63	108.42	110.22
13	A	1116	CLA	C2C-C1C-NC	-2.63	108.42	110.22
13	B	1224	CLA	O1D-CGD-CBD	-2.63	119.88	124.60
13	B	1218	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
16	F	4016	BCR	C30-C25-C26	-2.62	118.90	122.59
13	A	1136	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
13	A	1123	CLA	OBD-CAD-CBD	-2.62	121.98	125.94
13	B	1238	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
13	B	1208	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
13	B	1221	CLA	O1D-CGD-CBD	-2.61	119.91	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1118	CLA	O1D-CGD-CBD	-2.61	119.92	124.60
16	B	4017	BCR	C8-C9-C10	-2.61	114.94	118.94
13	L	1501	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
13	A	1132	CLA	CAA-C2A-C3A	-2.60	105.69	112.81
13	B	1230	CLA	C2C-C1C-NC	-2.60	108.44	110.22
13	B	1023	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
16	J	4012	BCR	C1-C6-C5	-2.60	118.94	122.59
13	A	1139	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
13	A	1022	CLA	C2C-C1C-NC	-2.59	108.44	110.22
13	A	1121	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
13	B	1216	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
13	A	1112	CLA	O1D-CGD-CBD	-2.59	119.95	124.60
13	A	1124	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
13	M	1601	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
13	X	1701	CLA	C2C-C1C-NC	-2.59	108.45	110.22
16	J	4013	BCR	C30-C25-C26	-2.59	118.96	122.59
13	B	1233	CLA	CMB-C2B-C1B	-2.58	124.49	128.46
13	A	1118	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
13	B	1216	CLA	CAA-C2A-C3A	-2.58	105.75	112.81
13	A	1137	CLA	OBD-CAD-CBD	-2.57	122.05	125.94
13	A	1133	CLA	O2A-CGA-O1A	-2.57	117.16	123.55
13	L	1502	CLA	CAA-C2A-C3A	-2.57	105.76	112.81
13	A	1123	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
16	A	4011	BCR	C30-C25-C26	-2.57	118.98	122.59
13	A	1129	CLA	CAA-C2A-C3A	-2.57	105.77	112.81
13	A	1122	CLA	OBD-CAD-CBD	-2.56	122.07	125.94
13	A	1127	CLA	OBD-CAD-CBD	-2.56	122.07	125.94
16	L	4022	BCR	C1-C6-C5	-2.56	119.00	122.59
13	A	1137	CLA	CMB-C2B-C1B	-2.56	124.54	128.46
16	M	4021	BCR	C30-C25-C26	-2.55	119.00	122.59
13	A	1140	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
13	A	1134	CLA	C2C-C1C-NC	-2.55	108.47	110.22
13	A	1117	CLA	OBD-CAD-CBD	-2.55	122.10	125.94
13	B	1228	CLA	OBD-CAD-CBD	-2.54	122.10	125.94
13	B	1226	CLA	O2A-CGA-O1A	-2.54	117.24	123.55
13	A	1128	CLA	CAA-C2A-C3A	-2.54	105.84	112.81
16	J	4013	BCR	C1-C6-C5	-2.54	119.02	122.59
13	B	1212	CLA	C2C-C1C-NC	-2.54	108.48	110.22
13	L	1502	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
16	A	4002	BCR	C1-C6-C5	-2.53	119.03	122.59
13	B	1207	CLA	O1D-CGD-CBD	-2.53	120.06	124.60
13	B	1223	CLA	O1D-CGD-CBD	-2.53	120.06	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	4018	BCR	C1-C6-C5	-2.52	119.05	122.59
13	B	1221	CLA	C2C-C1C-NC	-2.52	108.50	110.22
16	A	4008	BCR	C33-C5-C4	-2.51	108.68	113.45
13	F	1301	CLA	OBD-CAD-CBD	-2.51	122.16	125.94
13	B	1235	CLA	CMB-C2B-C1B	-2.50	124.61	128.46
13	B	1012	CLA	O1D-CGD-CBD	-2.50	120.11	124.60
13	L	1502	CLA	C2C-C1C-NC	-2.50	108.51	110.22
13	A	1117	CLA	O2A-CGA-O1A	-2.50	117.34	123.55
13	B	1233	CLA	OBD-CAD-CBD	-2.50	122.17	125.94
13	B	1234	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
13	A	1135	CLA	O1D-CGD-CBD	-2.50	120.11	124.60
13	B	1208	CLA	C2C-C1C-NC	-2.50	108.51	110.22
13	B	1227	CLA	CMB-C2B-C1B	-2.49	124.63	128.46
13	A	1126	CLA	O2A-CGA-O1A	-2.49	117.37	123.55
13	A	1129	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
13	B	1213	CLA	O2A-CGA-O1A	-2.49	117.38	123.55
13	B	1234	CLA	OBD-CAD-CBD	-2.49	122.19	125.94
13	B	1012	CLA	O2A-CGA-O1A	-2.48	117.40	123.55
13	B	1207	CLA	OBD-CAD-CBD	-2.48	122.20	125.94
13	A	1106	CLA	O2A-CGA-O1A	-2.48	117.40	123.55
13	B	1227	CLA	C2C-C1C-NC	-2.48	108.52	110.22
16	A	4011	BCR	C23-C22-C21	-2.47	115.15	118.94
13	A	1801	CLA	O2A-CGA-O1A	-2.47	117.41	123.55
13	J	1302	CLA	O1D-CGD-CBD	-2.47	120.16	124.60
13	A	1135	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
13	B	1217	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
13	A	1110	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
13	B	1023	CLA	C2C-C1C-NC	-2.46	108.53	110.22
13	B	1224	CLA	C2C-C1C-NC	-2.45	108.54	110.22
13	A	1126	CLA	CAA-C2A-C3A	-2.45	106.08	112.81
13	B	1231	CLA	C2C-C1C-NC	-2.45	108.54	110.22
13	A	1106	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
13	B	1235	CLA	O1D-CGD-CBD	-2.45	120.20	124.60
13	A	1118	CLA	O2A-CGA-O1A	-2.45	117.47	123.55
13	B	1231	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
13	J	1302	CLA	C2C-C1C-NC	-2.44	108.55	110.22
13	B	1215	CLA	O2A-CGA-O1A	-2.43	117.50	123.55
13	A	1102	CLA	C2C-C1C-NC	-2.43	108.55	110.22
13	A	1109	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
16	B	4009	BCR	C30-C25-C26	-2.43	119.18	122.59
16	A	4011	BCR	C1-C6-C5	-2.40	119.22	122.59
13	B	1222	CLA	OBD-CAD-CBD	-2.39	122.33	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	4018	BCR	C30-C25-C26	-2.39	119.23	122.59
16	B	4010	BCR	C1-C6-C5	-2.39	119.23	122.59
13	A	1105	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
13	A	1115	CLA	OBD-CAD-CBD	-2.38	122.34	125.94
13	B	1227	CLA	C3C-C4C-NC	-2.38	107.80	110.21
13	A	1102	CLA	OBD-CAD-CBD	-2.38	122.35	125.94
13	B	1219	CLA	OBD-CAD-CBD	-2.38	122.35	125.94
13	L	1501	CLA	C2C-C1C-NC	-2.38	108.59	110.22
13	A	1134	CLA	OBD-CAD-CBD	-2.37	122.35	125.94
13	A	1131	CLA	O1D-CGD-CBD	-2.37	120.34	124.60
13	A	1138	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
16	A	4008	BCR	C8-C9-C10	-2.36	115.32	118.94
13	B	1021	CLA	CAA-C2A-C3A	-2.35	106.36	112.81
16	I	4020	BCR	C1-C6-C5	-2.35	119.29	122.59
13	A	1104	CLA	OBD-CAD-CBD	-2.35	122.40	125.94
13	A	1107	CLA	OBD-CAD-CBD	-2.35	122.40	125.94
13	A	1133	CLA	OBD-CAD-CBD	-2.35	122.40	125.94
13	A	1140	CLA	C2C-C1C-NC	-2.35	108.61	110.22
13	A	1110	CLA	O2A-CGA-O1A	-2.34	117.73	123.55
13	A	1129	CLA	O2A-CGA-O1A	-2.34	117.74	123.55
13	B	1215	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
13	A	1113	CLA	OBD-CAD-CBD	-2.34	122.41	125.94
13	A	1128	CLA	O1D-CGD-CBD	-2.34	120.41	124.60
13	B	1204	CLA	CMB-C2B-C1B	-2.33	124.88	128.46
13	A	1119	CLA	C12-C11-C10	-2.33	101.97	113.25
13	A	1139	CLA	O1D-CGD-CBD	-2.33	120.42	124.60
13	B	1204	CLA	C3C-C4C-NC	-2.33	107.85	110.21
13	A	1101	CLA	C2C-C1C-NC	-2.33	108.63	110.22
13	A	1107	CLA	C2C-C1C-NC	-2.33	108.63	110.22
13	A	1130	CLA	O2A-CGA-O1A	-2.32	117.78	123.55
13	B	1202	CLA	O1D-CGD-CBD	-2.32	120.43	124.60
13	A	1130	CLA	OBD-CAD-CBD	-2.32	122.44	125.94
13	A	1130	CLA	CAA-C2A-C3A	-2.32	106.46	112.81
16	A	4007	BCR	C1-C6-C5	-2.32	119.34	122.59
13	L	1503	CLA	C2C-C1C-NC	-2.31	108.64	110.22
13	A	1128	CLA	O2A-CGA-O1A	-2.30	117.83	123.55
13	A	1122	CLA	CAA-C2A-C3A	-2.30	106.50	112.81
13	A	1139	CLA	OBD-CAD-CBD	-2.30	122.47	125.94
13	A	1137	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
13	A	1132	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
13	B	1209	CLA	OBD-CAD-CBD	-2.29	122.48	125.94
13	A	1013	CLA	CAA-C2A-C3A	-2.29	106.54	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1234	CLA	C2C-C1C-NC	-2.29	108.65	110.22
13	A	1121	CLA	O2A-CGA-O1A	-2.28	117.88	123.55
13	A	1133	CLA	O1D-CGD-CBD	-2.28	120.50	124.60
13	A	1125	CLA	O2A-CGA-O1A	-2.28	117.88	123.55
13	B	1210	CLA	OBD-CAD-CBD	-2.28	122.50	125.94
16	B	4017	BCR	C30-C25-C26	-2.28	119.39	122.59
16	L	4019	BCR	C1-C6-C5	-2.28	119.39	122.59
13	B	1223	CLA	OBD-CAD-CBD	-2.28	122.50	125.94
13	B	1206	CLA	C12-C11-C10	-2.27	102.26	113.25
13	A	1117	CLA	C4-C3-C5	-2.27	111.34	115.29
13	A	1122	CLA	O2A-CGA-O1A	-2.27	117.92	123.55
13	L	1502	CLA	O2A-CGA-O1A	-2.27	117.93	123.55
13	M	1601	CLA	O1D-CGD-CBD	-2.26	120.53	124.60
13	A	1011	CLA	CAA-C2A-C3A	-2.26	106.61	112.81
13	B	1207	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
13	L	1502	CLA	C3C-C4C-NC	-2.26	107.92	110.21
13	B	1220	CLA	C2C-C1C-NC	-2.26	108.67	110.22
16	A	4008	BCR	C23-C22-C21	-2.26	115.47	118.94
13	B	1205	CLA	C7-C6-C5	-2.26	106.83	113.11
13	A	1136	CLA	C3C-C4C-NC	-2.26	107.92	110.21
13	A	1130	CLA	O1D-CGD-CBD	-2.26	120.55	124.60
13	B	1219	CLA	C2C-C1C-NC	-2.26	108.67	110.22
13	B	1211	CLA	CAA-C2A-C3A	-2.25	106.63	112.81
13	B	1236	CLA	O2A-CGA-O1A	-2.25	117.96	123.55
13	A	1107	CLA	O2A-CGA-O1A	-2.25	117.97	123.55
13	B	1234	CLA	O2A-CGA-O1A	-2.24	117.99	123.55
13	B	1226	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
13	A	1127	CLA	O1D-CGD-CBD	-2.24	120.58	124.60
13	A	1120	CLA	O2A-CGA-O1A	-2.24	117.99	123.55
13	B	1021	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
13	A	1125	CLA	OBD-CAD-CBD	-2.23	122.57	125.94
16	A	4008	BCR	C1-C6-C5	-2.23	119.45	122.59
13	B	1217	CLA	O2A-CGA-O1A	-2.23	118.01	123.55
13	A	1121	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
13	B	1222	CLA	CAA-C2A-C3A	-2.23	106.70	112.81
13	B	1229	CLA	C12-C11-C10	-2.23	102.47	113.25
16	B	4017	BCR	C23-C22-C21	-2.23	115.52	118.94
16	I	4018	BCR	C19-C18-C17	-2.23	115.52	118.94
13	B	1214	CLA	CAA-C2A-C3A	-2.22	106.72	112.81
13	B	1217	CLA	C2C-C1C-NC	-2.22	108.70	110.22
16	I	4020	BCR	C19-C18-C17	-2.22	115.54	118.94
13	B	1229	CLA	C2C-C1C-NC	-2.21	108.70	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1203	CLA	OBD-CAD-CBD	-2.21	122.60	125.94
13	B	1214	CLA	C2C-C1C-NC	-2.21	108.70	110.22
13	A	1139	CLA	O2A-CGA-O1A	-2.21	118.06	123.55
13	L	1501	CLA	O2A-CGA-O1A	-2.21	118.07	123.55
13	K	1401	CLA	O1D-CGD-CBD	-2.21	120.64	124.60
13	B	1201	CLA	C2C-C1C-NC	-2.21	108.71	110.22
13	B	1225	CLA	OBD-CAD-CBD	-2.20	122.61	125.94
13	B	1230	CLA	OBD-CAD-CBD	-2.20	122.61	125.94
16	B	4014	BCR	C1-C6-C5	-2.20	119.50	122.59
13	B	1219	CLA	C3C-C4C-NC	-2.20	107.99	110.21
16	B	4017	BCR	C1-C6-C5	-2.20	119.51	122.59
13	B	1231	CLA	C3C-C4C-NC	-2.19	107.99	110.21
13	A	1101	CLA	O1D-CGD-CBD	-2.19	120.67	124.60
13	B	1238	CLA	C3C-C4C-NC	-2.19	108.00	110.21
13	A	1801	CLA	OBD-CAD-CBD	-2.18	122.64	125.94
13	B	1229	CLA	O1D-CGD-CBD	-2.18	120.68	124.60
13	B	1227	CLA	OBD-CAD-CBD	-2.18	122.64	125.94
13	A	1102	CLA	O2A-CGA-O1A	-2.18	118.13	123.55
13	A	1237	CLA	CMA-C3A-C2A	-2.18	104.92	113.77
13	A	1109	CLA	O2A-CGA-O1A	-2.18	118.13	123.55
13	M	1601	CLA	C2C-C1C-NC	-2.18	108.73	110.22
13	F	1301	CLA	C2C-C1C-NC	-2.18	108.73	110.22
13	A	1123	CLA	C2C-C1C-NC	-2.17	108.73	110.22
13	A	1131	CLA	O2A-CGA-O1A	-2.17	118.17	123.55
13	A	1103	CLA	C3C-C4C-NC	-2.17	108.02	110.21
13	A	1133	CLA	C2C-C1C-NC	-2.16	108.74	110.22
13	A	1134	CLA	O1D-CGD-CBD	-2.16	120.72	124.60
13	B	1023	CLA	C12-C11-C10	-2.16	102.81	113.25
13	B	1223	CLA	C2C-C1C-NC	-2.16	108.74	110.22
13	B	1239	CLA	O1D-CGD-CBD	-2.16	120.73	124.60
13	J	1303	CLA	C2C-C1C-NC	-2.15	108.75	110.22
13	B	1214	CLA	O2A-CGA-O1A	-2.15	118.21	123.55
13	A	1116	CLA	O2A-CGA-O1A	-2.15	118.22	123.55
13	B	1216	CLA	O1D-CGD-CBD	-2.15	120.75	124.60
13	A	1126	CLA	O1D-CGD-CBD	-2.14	120.75	124.60
13	A	1113	CLA	C2C-C1C-NC	-2.14	108.75	110.22
13	A	1112	CLA	C2C-C1C-NC	-2.13	108.76	110.22
13	A	1138	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
13	B	1201	CLA	O2A-CGA-O1A	-2.13	118.27	123.55
13	J	1303	CLA	OBD-CAD-CBD	-2.12	121.71	125.98
13	A	1117	CLA	C3C-C4C-NC	-2.12	108.06	110.21
13	B	1207	CLA	O2A-CGA-O1A	-2.12	118.29	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1120	CLA	C3C-C4C-NC	-2.12	108.07	110.21
13	A	1116	CLA	O1D-CGD-CBD	-2.12	120.80	124.60
13	A	1102	CLA	C12-C11-C10	-2.12	106.11	113.63
13	A	1122	CLA	O1D-CGD-CBD	-2.11	120.80	124.60
16	J	4013	BCR	C19-C18-C17	-2.11	115.70	118.94
13	K	1401	CLA	OBD-CAD-CBD	-2.11	122.76	125.94
13	A	1138	CLA	O1D-CGD-CBD	-2.11	120.82	124.60
16	B	4010	BCR	C19-C18-C17	-2.10	115.71	118.94
13	B	1231	CLA	CAA-C2A-C3A	-2.10	107.05	112.81
13	A	1110	CLA	C3C-C4C-NC	-2.10	108.08	110.21
13	B	1224	CLA	O2A-CGA-O1A	-2.10	118.34	123.55
13	A	1107	CLA	O1D-CGD-CBD	-2.09	120.84	124.60
13	B	1235	CLA	C3C-C4C-NC	-2.08	108.10	110.21
13	B	1201	CLA	CAA-C2A-C3A	-2.08	107.10	112.81
13	B	1213	CLA	C2C-C1C-NC	-2.08	108.80	110.22
14	B	2002	PQN	C17-C16-C15	-2.08	107.33	113.11
13	B	1213	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
13	A	1117	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
13	B	1209	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
13	A	1104	CLA	C3C-C4C-NC	-2.07	108.11	110.21
13	A	1114	CLA	O1D-CGD-CBD	-2.07	120.89	124.60
13	X	1701	CLA	O1D-CGD-CBD	-2.07	120.89	124.60
13	A	1022	CLA	C6-C5-C3	-2.07	107.97	112.66
13	A	1133	CLA	C3C-C4C-NC	-2.06	108.12	110.21
13	B	1204	CLA	O1D-CGD-CBD	-2.06	120.89	124.60
13	B	1206	CLA	CAA-C2A-C3A	-2.06	107.16	112.81
13	B	1225	CLA	O1D-CGD-CBD	-2.06	120.90	124.60
13	A	1013	CLA	OBD-CAD-CBD	-2.06	122.83	125.94
13	A	1105	CLA	C4-C3-C5	-2.05	113.42	115.85
13	B	1209	CLA	C2C-C1C-NC	-2.05	108.82	110.22
13	B	1235	CLA	CAA-C2A-C3A	-2.05	107.20	112.81
13	B	1235	CLA	O2A-CGA-O1A	-2.05	118.47	123.55
16	J	4012	BCR	C19-C18-C17	-2.05	115.80	118.94
13	B	1223	CLA	O2A-CGA-O1A	-2.04	118.47	123.55
13	A	1103	CLA	O2A-CGA-O1A	-2.04	118.48	123.55
13	B	1232	CLA	C2C-C1C-NC	-2.04	108.82	110.22
13	A	1111	CLA	O2A-CGA-O1A	-2.04	118.49	123.55
13	K	1401	CLA	C2C-C1C-NC	-2.04	108.83	110.22
13	A	1113	CLA	CAA-C2A-C3A	-2.04	107.23	112.81
13	B	1225	CLA	O2A-CGA-O1A	-2.03	118.50	123.55
13	A	1114	CLA	O2A-CGA-O1A	-2.03	118.51	123.55
13	L	1501	CLA	C12-C11-C10	-2.02	103.46	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1212	CLA	OBD-CAD-CBD	-2.02	122.88	125.94
13	J	1303	CLA	C3C-C4C-NC	-2.02	108.16	110.21
13	A	1138	CLA	CAA-C2A-C3A	-2.02	107.26	112.81
13	B	1228	CLA	O1D-CGD-CBD	-2.02	120.97	124.60
13	B	1204	CLA	O2A-CGA-O1A	-2.02	118.54	123.55
13	B	1012	CLA	C2C-C1C-NC	-2.02	108.84	110.22
13	B	1231	CLA	CMA-C3A-C4A	-2.01	106.36	111.77
13	A	1140	CLA	C12-C11-C10	-2.01	103.52	113.25
16	F	4016	BCR	C35-C13-C14	-2.01	120.10	122.92
13	A	1402	CLA	OBD-CAD-CBD	-2.00	121.96	125.98
13	A	1108	CLA	O1D-CGD-CBD	-2.00	121.01	124.60
16	B	4009	BCR	C19-C18-C17	-2.00	115.87	118.94
13	B	1225	CLA	C3A-C2A-C1A	2.00	104.33	101.34
13	A	1111	CLA	C2A-C3A-C4A	2.00	105.10	101.87
13	B	1226	CLA	C2A-C3A-C4A	2.00	105.10	101.87
16	A	4003	BCR	C15-C14-C13	2.00	130.17	127.31
13	A	1127	CLA	CMD-C2D-C3D	2.01	128.62	124.89
16	I	4018	BCR	C30-C25-C24	2.01	121.38	115.73
16	B	4005	BCR	C8-C7-C6	2.01	132.88	127.25
13	B	1214	CLA	CMB-C2B-C3B	2.01	128.62	124.89
13	B	1232	CLA	C2A-C3A-C4A	2.01	105.12	101.87
16	A	4003	BCR	C28-C27-C26	2.01	117.24	113.78
13	A	1102	CLA	C1-C2-C3	2.01	129.66	125.96
13	A	1124	CLA	CED-O2D-CGD	2.01	120.69	115.97
13	A	1011	CLA	CGD-CBD-CAD	2.01	117.46	110.71
16	F	4016	BCR	C40-C30-C25	2.01	113.58	110.31
13	A	1108	CLA	C1C-NC-C4C	2.01	108.21	107.06
16	M	4021	BCR	C32-C1-C6	2.02	113.58	110.31
16	J	4015	BCR	C40-C30-C25	2.02	113.58	110.31
16	J	4015	BCR	C37-C22-C23	2.02	121.31	118.10
13	X	1701	CLA	C2A-C3A-C4A	2.02	105.13	101.87
13	A	1104	CLA	O2D-CGD-CBD	2.02	114.91	111.30
13	L	1503	CLA	CMB-C2B-C3B	2.02	128.64	124.89
13	A	1121	CLA	CMB-C2B-C3B	2.02	128.64	124.89
16	A	4002	BCR	C32-C1-C6	2.02	113.58	110.31
13	A	1120	CLA	C2A-C1A-CHA	2.02	127.50	123.92
13	B	1214	CLA	C2A-C3A-C4A	2.02	105.13	101.87
16	B	4014	BCR	C11-C10-C9	2.02	130.19	127.31
13	A	1801	CLA	CMB-C2B-C3B	2.02	128.64	124.89
13	B	1212	CLA	C1C-NC-C4C	2.02	108.22	107.06
13	A	1107	CLA	C1-C2-C3	2.02	129.69	125.96
16	B	4010	BCR	C23-C24-C25	2.03	132.93	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1012	CLA	C1C-NC-C4C	2.03	108.22	107.06
13	B	1239	CLA	OBD-CAD-C3D	2.03	131.77	128.03
13	X	1701	CLA	CMB-C2B-C3B	2.03	128.66	124.89
16	I	4020	BCR	C35-C13-C12	2.03	121.33	118.10
13	A	1123	CLA	C2A-C1A-CHA	2.03	127.52	123.92
13	B	1021	CLA	C6-C5-C3	2.03	117.27	112.66
13	A	1102	CLA	C2A-C1A-CHA	2.04	127.53	123.92
13	B	1236	CLA	CMB-C2B-C3B	2.04	128.67	124.89
16	A	4002	BCR	C35-C13-C12	2.04	121.34	118.10
13	A	1122	CLA	CED-O2D-CGD	2.04	120.75	115.97
13	A	1122	CLA	C1-C2-C3	2.04	129.71	125.96
16	M	4021	BCR	C37-C22-C23	2.05	121.36	118.10
13	A	1125	CLA	C2A-C3A-C4A	2.05	105.17	101.87
13	A	1133	CLA	C6-C5-C3	2.05	117.30	112.66
13	B	1224	CLA	CED-O2D-CGD	2.05	120.77	115.97
16	B	4005	BCR	C15-C14-C13	2.05	130.23	127.31
13	B	1210	CLA	C2A-C1A-CHA	2.05	127.55	123.92
16	B	4004	BCR	C37-C22-C23	2.05	121.36	118.10
16	F	4016	BCR	C36-C18-C19	2.05	121.36	118.10
13	B	1213	CLA	CMB-C2B-C3B	2.05	128.70	124.89
13	B	1207	CLA	C3A-C2A-C1A	2.05	104.41	101.34
13	B	1238	CLA	CMB-C2B-C3B	2.05	128.70	124.89
13	A	1112	CLA	C2A-C1A-CHA	2.05	127.56	123.92
16	I	4018	BCR	C32-C1-C6	2.05	113.64	110.31
13	A	1111	CLA	C2A-C1A-CHA	2.05	127.56	123.92
16	B	4006	BCR	C20-C21-C22	2.06	130.24	127.31
16	J	4015	BCR	C16-C17-C18	2.06	130.25	127.31
16	F	4016	BCR	C8-C7-C6	2.06	133.02	127.25
13	A	1131	CLA	CED-O2D-CGD	2.06	120.80	115.97
13	B	1224	CLA	CAA-CBA-CGA	2.06	119.55	113.35
16	A	4002	BCR	C15-C14-C13	2.06	130.25	127.31
16	L	4022	BCR	C23-C24-C25	2.06	133.03	127.25
13	A	1108	CLA	CMB-C2B-C3B	2.06	128.72	124.89
16	B	4004	BCR	C20-C21-C22	2.06	130.25	127.31
16	L	4022	BCR	C32-C1-C6	2.06	113.65	110.31
16	B	4017	BCR	C30-C25-C24	2.06	121.53	115.73
13	A	1134	CLA	C2A-C1A-CHA	2.07	127.58	123.92
16	B	4014	BCR	C40-C30-C25	2.07	113.66	110.31
16	B	4004	BCR	C34-C9-C8	2.07	121.39	118.10
13	A	1133	CLA	CMB-C2B-C3B	2.07	128.73	124.89
13	B	1204	CLA	C1-C2-C3	2.07	129.77	125.96
13	A	1131	CLA	C2A-C3A-C4A	2.07	105.21	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1135	CLA	C2A-C1A-CHA	2.07	127.59	123.92
13	A	1107	CLA	CMB-C2B-C3B	2.07	128.74	124.89
13	B	1232	CLA	CMB-C2B-C3B	2.07	128.74	124.89
13	A	1106	CLA	CED-O2D-CGD	2.07	120.83	115.97
13	A	1107	CLA	CBA-CAA-C2A	2.07	120.00	113.80
13	A	1140	CLA	CBA-CAA-C2A	2.08	120.01	113.80
16	J	4013	BCR	C15-C14-C13	2.08	130.27	127.31
13	M	1601	CLA	C2A-C1A-CHA	2.08	127.60	123.92
13	A	1140	CLA	C1C-NC-C4C	2.08	108.25	107.06
13	A	1022	CLA	CED-O2D-CGD	2.08	120.84	115.97
17	A	5003	LHG	O8-C6-C5	2.08	113.88	108.66
16	A	4001	BCR	C30-C25-C24	2.08	121.58	115.73
13	A	1013	CLA	C2A-C3A-C4A	2.08	105.23	101.87
16	B	4010	BCR	C34-C9-C8	2.08	121.42	118.10
13	A	1123	CLA	C1-C2-C3	2.09	129.80	125.96
13	B	1239	CLA	CED-O2D-CGD	2.09	120.87	115.97
13	B	1206	CLA	C1-C2-C3	2.09	129.81	125.96
13	B	1205	CLA	CMB-C2B-C3B	2.09	128.78	124.89
16	B	4006	BCR	C40-C30-C25	2.09	113.70	110.31
13	B	1203	CLA	C1C-NC-C4C	2.09	108.26	107.06
16	B	4017	BCR	C11-C10-C9	2.09	130.30	127.31
13	B	1230	CLA	CBA-CAA-C2A	2.09	120.06	113.80
13	B	1222	CLA	O2A-CGA-CBA	2.10	120.97	112.33
16	M	4021	BCR	C30-C25-C24	2.10	121.62	115.73
13	B	1205	CLA	CED-O2D-CGD	2.10	120.89	115.97
13	B	1223	CLA	CED-O2D-CGD	2.10	120.89	115.97
13	A	1402	CLA	C2A-C3A-C4A	2.10	105.26	101.87
13	B	1023	CLA	OBD-CAD-C3D	2.10	131.89	128.03
13	A	1114	CLA	CMB-C2B-C3B	2.10	128.80	124.89
16	J	4013	BCR	C28-C27-C26	2.11	117.40	113.78
16	A	4008	BCR	C8-C7-C6	2.11	133.15	127.25
16	M	4021	BCR	C35-C13-C12	2.11	121.46	118.10
16	B	4017	BCR	C15-C14-C13	2.11	130.32	127.31
13	B	1233	CLA	C2A-C1A-CHA	2.11	127.66	123.92
13	A	1120	CLA	C2A-C3A-C4A	2.11	105.28	101.87
13	A	1117	CLA	CBA-CAA-C2A	2.12	120.13	113.80
13	A	1118	CLA	C2A-C1A-CHA	2.12	127.67	123.92
16	A	4003	BCR	C35-C13-C12	2.12	121.47	118.10
16	A	4011	BCR	C37-C22-C23	2.12	121.47	118.10
13	A	1131	CLA	C1D-CHD-C4C	2.12	125.38	122.48
13	A	1140	CLA	CMB-C2B-C3B	2.13	128.84	124.89
13	A	1110	CLA	CED-O2D-CGD	2.13	120.96	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	4019	BCR	C37-C22-C23	2.13	121.49	118.10
16	A	4002	BCR	C40-C30-C25	2.13	113.77	110.31
16	F	4016	BCR	C1-C6-C7	2.14	121.74	115.73
13	A	1130	CLA	C2A-C3A-C4A	2.14	105.33	101.87
13	A	1140	CLA	C6-C5-C3	2.15	117.52	112.66
13	B	1221	CLA	C6-C5-C3	2.15	117.52	112.66
13	A	1104	CLA	CAA-CBA-CGA	2.15	119.81	113.35
13	B	1224	CLA	OBD-CAD-C3D	2.15	131.99	128.03
13	B	1202	CLA	C2A-C3A-C4A	2.15	105.34	101.87
16	J	4013	BCR	C34-C9-C8	2.15	121.53	118.10
16	J	4013	BCR	C35-C13-C12	2.16	121.53	118.10
13	A	1102	CLA	CED-O2D-CGD	2.16	121.03	115.97
16	L	4019	BCR	C23-C24-C25	2.16	133.31	127.25
13	A	1116	CLA	C1-C2-C3	2.16	129.94	125.96
13	A	1013	CLA	C1C-NC-C4C	2.17	108.30	107.06
13	B	1239	CLA	CBA-CAA-C2A	2.17	120.29	113.80
13	X	1701	CLA	CED-O2D-CGD	2.17	121.06	115.97
16	A	4001	BCR	C32-C1-C6	2.17	113.83	110.31
16	B	4006	BCR	C1-C6-C7	2.17	121.83	115.73
13	B	1226	CLA	CED-O2D-CGD	2.17	121.06	115.97
16	J	4012	BCR	C37-C22-C23	2.17	121.56	118.10
13	A	1117	CLA	C1-C2-C3	2.17	129.96	125.96
13	A	1139	CLA	CED-O2D-CGD	2.17	121.07	115.97
13	B	1207	CLA	CAA-C2A-C1A	2.18	119.11	111.97
16	B	4010	BCR	C1-C6-C7	2.18	121.86	115.73
16	B	4009	BCR	C36-C18-C19	2.18	121.57	118.10
16	A	4011	BCR	C34-C9-C8	2.18	121.57	118.10
13	B	1232	CLA	C2A-C1A-CHA	2.18	127.79	123.92
16	B	4006	BCR	C36-C18-C19	2.18	121.58	118.10
16	B	4006	BCR	C34-C9-C8	2.19	121.58	118.10
16	A	4003	BCR	C8-C7-C6	2.19	133.38	127.25
16	B	4014	BCR	C24-C23-C22	2.19	129.50	126.21
16	A	4001	BCR	C35-C13-C12	2.19	121.59	118.10
13	A	1116	CLA	CBA-CAA-C2A	2.19	120.36	113.80
16	A	4001	BCR	C37-C22-C23	2.19	121.59	118.10
16	I	4018	BCR	C34-C9-C8	2.20	121.60	118.10
13	A	1013	CLA	O2D-CGD-CBD	2.20	115.23	111.30
16	A	4008	BCR	C7-C8-C9	2.20	129.52	126.21
13	B	1218	CLA	C2A-C1A-CHA	2.20	127.83	123.92
16	I	4018	BCR	C1-C6-C7	2.20	121.92	115.73
13	B	1238	CLA	C1D-CHD-C4C	2.20	125.50	122.48
13	A	1118	CLA	CED-O2D-CGD	2.21	121.15	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1101	CLA	C1-C2-C3	2.21	130.03	125.96
16	B	4005	BCR	C36-C18-C19	2.21	121.62	118.10
16	J	4013	BCR	C1-C6-C7	2.21	121.95	115.73
13	A	1237	CLA	C1C-NC-C4C	2.22	108.33	107.06
16	B	4005	BCR	C34-C9-C8	2.22	121.64	118.10
13	K	1401	CLA	C1C-NC-C4C	2.22	108.33	107.06
16	B	4006	BCR	C30-C25-C24	2.22	121.98	115.73
13	B	1217	CLA	C2A-C1A-CHA	2.22	127.86	123.92
13	B	1222	CLA	CED-O2D-CGD	2.23	121.19	115.97
13	B	1201	CLA	C1-C2-C3	2.23	130.06	125.96
16	B	4009	BCR	C30-C25-C24	2.23	122.01	115.73
13	L	1501	CLA	C1C-NC-C4C	2.24	108.34	107.06
16	B	4004	BCR	C1-C6-C7	2.24	122.02	115.73
13	B	1234	CLA	CED-O2D-CGD	2.24	121.22	115.97
16	B	4005	BCR	C35-C13-C12	2.24	121.67	118.10
13	J	1302	CLA	C2A-C1A-CHA	2.24	127.89	123.92
16	B	4017	BCR	C23-C24-C25	2.24	133.53	127.25
16	F	4016	BCR	C30-C25-C24	2.25	122.04	115.73
13	B	1238	CLA	C1C-NC-C4C	2.25	108.35	107.06
13	F	1301	CLA	C2A-C1A-CHA	2.25	127.90	123.92
16	J	4013	BCR	C24-C23-C22	2.25	129.59	126.21
16	L	4022	BCR	C30-C25-C24	2.26	122.07	115.73
13	A	1136	CLA	CED-O2D-CGD	2.26	121.26	115.97
13	F	1301	CLA	C1C-NC-C4C	2.26	108.35	107.06
16	B	4004	BCR	C8-C7-C6	2.26	133.57	127.25
13	B	1239	CLA	CMB-C2B-C3B	2.26	129.08	124.89
16	J	4013	BCR	C40-C30-C25	2.26	113.98	110.31
13	A	1801	CLA	C2A-C1A-CHA	2.27	127.94	123.92
13	B	1205	CLA	C1D-CHD-C4C	2.27	125.59	122.48
13	A	1102	CLA	CMB-C2B-C3B	2.27	129.10	124.89
13	B	1239	CLA	C1C-NC-C4C	2.27	108.36	107.06
16	I	4020	BCR	C1-C6-C7	2.27	122.12	115.73
13	A	1103	CLA	C1-C2-C3	2.28	130.15	125.96
13	B	1227	CLA	CED-O2D-CGD	2.28	121.31	115.97
13	A	1121	CLA	C1C-NC-C4C	2.29	108.37	107.06
16	A	4007	BCR	C23-C24-C25	2.29	133.67	127.25
13	A	1109	CLA	C1-C2-C3	2.29	130.18	125.96
13	A	1106	CLA	C1C-NC-C4C	2.29	108.38	107.06
13	B	1213	CLA	C1C-NC-C4C	2.30	108.38	107.06
13	B	1203	CLA	CED-O2D-CGD	2.30	121.36	115.97
13	B	1221	CLA	C2A-C1A-CHA	2.30	128.00	123.92
13	A	1137	CLA	C1C-NC-C4C	2.30	108.38	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1237	CLA	CED-O2D-CGD	2.31	121.38	115.97
13	A	1128	CLA	CED-O2D-CGD	2.31	121.38	115.97
16	A	4002	BCR	C23-C24-C25	2.31	133.72	127.25
13	A	1139	CLA	C1D-CHD-C4C	2.31	125.64	122.48
13	A	1111	CLA	CMB-C2B-C3B	2.31	129.18	124.89
16	A	4002	BCR	C1-C6-C7	2.31	122.23	115.73
13	A	1127	CLA	CED-O2D-CGD	2.31	121.39	115.97
16	A	4007	BCR	C40-C30-C25	2.32	114.06	110.31
13	B	1225	CLA	CBA-CAA-C2A	2.32	120.73	113.80
16	B	4017	BCR	C24-C23-C22	2.32	129.69	126.21
13	B	1233	CLA	CED-O2D-CGD	2.32	121.40	115.97
16	A	4008	BCR	C34-C9-C8	2.32	121.79	118.10
13	A	1117	CLA	C1C-NC-C4C	2.32	108.39	107.06
13	A	1136	CLA	O2D-CGD-CBD	2.33	115.46	111.30
13	A	1013	CLA	C1-C2-C3	2.33	130.24	125.96
13	B	1204	CLA	CED-O2D-CGD	2.33	121.44	115.97
13	A	1402	CLA	C1C-NC-C4C	2.34	108.40	107.06
16	I	4020	BCR	C29-C30-C25	2.34	114.14	110.48
16	J	4015	BCR	C30-C25-C24	2.35	122.34	115.73
13	F	1301	CLA	CED-O2D-CGD	2.35	121.48	115.97
13	A	1011	CLA	C2A-C3A-C4A	2.35	105.67	101.87
13	A	1126	CLA	CED-O2D-CGD	2.35	121.49	115.97
13	A	1123	CLA	CED-O2D-CGD	2.35	121.49	115.97
16	B	4014	BCR	C36-C18-C19	2.35	121.85	118.10
13	A	1129	CLA	C1-C2-C3	2.36	130.40	126.68
13	A	1111	CLA	C1C-NC-C4C	2.36	108.41	107.06
16	A	4001	BCR	C1-C6-C7	2.36	122.37	115.73
13	A	1136	CLA	C1C-NC-C4C	2.36	108.41	107.06
13	B	1214	CLA	C1-C2-C3	2.37	130.31	125.96
13	B	1231	CLA	C2A-C3A-C4A	2.37	105.69	101.87
13	A	1135	CLA	CMB-C2B-C3B	2.37	129.29	124.89
13	A	1103	CLA	C2A-C3A-C4A	2.37	105.70	101.87
13	B	1207	CLA	C1-C2-C3	2.37	130.32	125.96
16	A	4007	BCR	C1-C6-C7	2.37	122.40	115.73
13	K	1401	CLA	CED-O2D-CGD	2.38	121.54	115.97
13	B	1236	CLA	CED-O2D-CGD	2.38	121.54	115.97
16	L	4019	BCR	C36-C18-C19	2.38	121.89	118.10
13	B	1211	CLA	CED-O2D-CGD	2.38	121.56	115.97
13	A	1140	CLA	C1-C2-C3	2.39	130.35	125.96
13	B	1202	CLA	CED-O2D-CGD	2.39	121.57	115.97
13	A	1139	CLA	C1-C2-C3	2.39	130.36	125.96
13	A	1114	CLA	C1C-NC-C4C	2.39	108.43	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	4012	BCR	C24-C23-C22	2.39	129.80	126.21
13	A	1130	CLA	CMB-C2B-C3B	2.39	129.33	124.89
16	F	4016	BCR	C7-C8-C9	2.39	129.81	126.21
13	B	1213	CLA	CED-O2D-CGD	2.39	121.58	115.97
16	A	4008	BCR	C37-C22-C23	2.39	121.91	118.10
13	B	1229	CLA	C1-C2-C3	2.40	130.38	125.96
13	A	1104	CLA	C2A-C1A-CHA	2.40	128.18	123.92
13	L	1502	CLA	C1D-CHD-C4C	2.40	125.77	122.48
16	A	4007	BCR	C32-C1-C6	2.40	114.20	110.31
13	A	1132	CLA	CED-O2D-CGD	2.40	121.60	115.97
16	J	4012	BCR	C35-C13-C12	2.41	121.94	118.10
13	A	1137	CLA	CED-O2D-CGD	2.41	121.62	115.97
13	A	1105	CLA	C1-C2-C3	2.42	130.41	125.96
13	A	1123	CLA	C1C-NC-C4C	2.42	108.44	107.06
13	A	1111	CLA	C1-C2-C3	2.42	130.41	125.96
13	A	1124	CLA	C1C-NC-C4C	2.42	108.45	107.06
13	B	1215	CLA	CED-O2D-CGD	2.43	121.66	115.97
13	B	1232	CLA	O2D-CGD-CBD	2.43	115.64	111.30
13	A	1113	CLA	CED-O2D-CGD	2.43	121.67	115.97
13	A	1011	CLA	C1-C2-C3	2.43	130.44	125.96
16	I	4020	BCR	C36-C18-C19	2.43	121.98	118.10
13	B	1012	CLA	C2A-C1A-CHA	2.44	128.24	123.92
13	A	1125	CLA	C1C-NC-C4C	2.44	108.46	107.06
13	B	1215	CLA	C1C-NC-C4C	2.45	108.46	107.06
13	A	1119	CLA	CAA-CBA-CGA	2.45	120.74	113.35
13	A	1120	CLA	CED-O2D-CGD	2.46	121.73	115.97
16	B	4014	BCR	C35-C13-C12	2.46	122.01	118.10
16	B	4017	BCR	C34-C9-C8	2.46	122.01	118.10
13	B	1224	CLA	C1-C2-C3	2.46	130.49	125.96
16	A	4002	BCR	C24-C23-C22	2.46	129.91	126.21
13	B	1216	CLA	C1-C2-C3	2.46	130.49	125.96
13	A	1116	CLA	C1C-NC-C4C	2.47	108.47	107.06
13	J	1303	CLA	C2A-C3A-C4A	2.47	104.93	101.82
13	B	1228	CLA	CED-O2D-CGD	2.47	121.76	115.97
13	A	1138	CLA	O2D-CGD-CBD	2.47	115.72	111.30
16	A	4003	BCR	C30-C25-C24	2.47	122.68	115.73
13	B	1223	CLA	C1-C2-C3	2.48	130.52	125.96
16	I	4020	BCR	C30-C25-C24	2.48	122.69	115.73
16	A	4002	BCR	C30-C25-C24	2.48	122.69	115.73
13	B	1219	CLA	CMB-C2B-C3B	2.48	129.49	124.89
16	A	4002	BCR	C7-C8-C9	2.48	129.94	126.21
16	J	4013	BCR	C36-C18-C19	2.48	122.05	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1111	CLA	CED-O2D-CGD	2.48	121.79	115.97
13	A	1135	CLA	C1D-CHD-C4C	2.48	125.88	122.48
13	A	1022	CLA	C1D-CHD-C4C	2.49	125.88	122.48
13	B	1222	CLA	C2A-C3A-C4A	2.49	105.89	101.87
13	B	1209	CLA	CED-O2D-CGD	2.49	121.80	115.97
13	A	1126	CLA	CMB-C2B-C3B	2.49	129.51	124.89
16	A	4003	BCR	C1-C6-C7	2.49	122.73	115.73
16	B	4005	BCR	C32-C1-C6	2.49	114.35	110.31
13	A	1105	CLA	CED-O2D-CGD	2.50	121.82	115.97
16	B	4010	BCR	C32-C1-C6	2.50	114.36	110.31
13	A	1130	CLA	C1C-NC-C4C	2.50	108.49	107.06
13	A	1124	CLA	C1-C2-C3	2.50	130.56	125.96
13	B	1235	CLA	C1-C2-C3	2.50	130.56	125.96
16	A	4008	BCR	C1-C6-C7	2.50	122.76	115.73
13	B	1207	CLA	CED-O2D-CGD	2.50	121.84	115.97
16	B	4014	BCR	C23-C24-C25	2.50	134.26	127.25
13	A	1104	CLA	C1C-NC-C4C	2.51	108.50	107.06
16	B	4006	BCR	C23-C24-C25	2.51	134.27	127.25
13	B	1203	CLA	CMB-C2B-C3B	2.51	129.54	124.89
16	B	4006	BCR	C35-C13-C12	2.51	122.09	118.10
13	A	1129	CLA	CED-O2D-CGD	2.51	121.86	115.97
13	B	1202	CLA	CMB-C2B-C3B	2.52	129.57	124.89
13	B	1210	CLA	CED-O2D-CGD	2.53	121.89	115.97
16	I	4020	BCR	C3-C4-C5	2.53	118.13	113.78
16	M	4021	BCR	C8-C7-C6	2.53	134.33	127.25
16	A	4011	BCR	C1-C6-C7	2.53	122.83	115.73
13	A	1103	CLA	CMB-C2B-C3B	2.53	129.59	124.89
13	A	1119	CLA	O2D-CGD-CBD	2.54	115.84	111.30
13	B	1225	CLA	CED-O2D-CGD	2.55	121.94	115.97
13	B	1221	CLA	C1-C2-C3	2.55	130.65	125.96
13	A	1102	CLA	C1C-NC-C4C	2.55	108.52	107.06
16	A	4011	BCR	C15-C14-C13	2.55	130.95	127.31
13	B	1021	CLA	C1-C2-C3	2.55	130.66	125.96
16	L	4019	BCR	C29-C30-C25	2.56	114.47	110.48
13	A	1013	CLA	CMB-C2B-C3B	2.56	129.63	124.89
13	A	1134	CLA	CED-O2D-CGD	2.56	121.96	115.97
13	A	1801	CLA	CED-O2D-CGD	2.56	121.97	115.97
16	B	4014	BCR	C34-C9-C8	2.56	122.18	118.10
13	A	1140	CLA	C1-O2A-CGA	2.56	122.92	116.77
13	A	1128	CLA	C1D-CHD-C4C	2.56	125.99	122.48
13	B	1216	CLA	CED-O2D-CGD	2.57	121.99	115.97
13	B	1206	CLA	CED-O2D-CGD	2.57	122.00	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1115	CLA	CED-O2D-CGD	2.57	122.00	115.97
16	B	4010	BCR	C16-C17-C18	2.57	130.98	127.31
13	B	1216	CLA	C1C-NC-C4C	2.58	108.54	107.06
13	B	1203	CLA	C1-C2-C3	2.58	130.72	125.96
13	A	1107	CLA	C2A-C1A-CHA	2.58	128.50	123.92
13	B	1208	CLA	C1D-CHD-C4C	2.59	126.03	122.48
13	A	1013	CLA	C1-O2A-CGA	2.60	123.00	116.77
13	B	1201	CLA	C1C-NC-C4C	2.60	108.55	107.06
13	A	1131	CLA	CMB-C2B-C3B	2.60	129.72	124.89
13	B	1214	CLA	CED-O2D-CGD	2.61	122.08	115.97
13	A	1108	CLA	CED-O2D-CGD	2.61	122.08	115.97
13	B	1232	CLA	C1C-NC-C4C	2.61	108.56	107.06
16	I	4018	BCR	C29-C30-C25	2.61	114.56	110.48
13	A	1113	CLA	CMB-C2B-C3B	2.61	129.73	124.89
16	J	4013	BCR	C23-C24-C25	2.62	134.57	127.25
16	B	4009	BCR	C35-C13-C12	2.62	120.71	114.60
13	A	1133	CLA	CED-O2D-CGD	2.62	122.10	115.97
16	I	4020	BCR	C37-C22-C23	2.62	122.27	118.10
13	B	1238	CLA	O2D-CGD-CBD	2.62	115.98	111.30
13	A	1132	CLA	C1C-NC-C4C	2.62	108.56	107.06
16	B	4006	BCR	C28-C27-C26	2.62	118.29	113.78
13	A	1109	CLA	O2D-CGD-CBD	2.62	115.98	111.30
16	A	4008	BCR	C11-C10-C9	2.62	131.05	127.31
16	B	4010	BCR	C36-C18-C19	2.63	122.28	118.10
13	A	1126	CLA	C1D-CHD-C4C	2.63	126.08	122.48
13	A	1125	CLA	C1-C2-C3	2.63	130.80	125.96
18	B	5002	LMG	C7-O1-C1	2.63	119.15	113.76
13	B	1023	CLA	C1D-CHD-C4C	2.63	126.08	122.48
13	B	1221	CLA	C1C-NC-C4C	2.64	108.57	107.06
13	B	1214	CLA	C1C-NC-C4C	2.64	108.57	107.06
13	B	1207	CLA	C2A-C1A-CHA	2.64	128.60	123.92
16	B	4010	BCR	C30-C25-C24	2.64	123.15	115.73
13	B	1225	CLA	C1D-CHD-C4C	2.64	126.10	122.48
13	B	1202	CLA	C1D-CHD-C4C	2.64	126.10	122.48
13	B	1203	CLA	C1D-CHD-C4C	2.65	126.10	122.48
13	A	1119	CLA	O2A-CGA-CBA	2.65	119.61	111.90
13	A	1112	CLA	CED-O2D-CGD	2.65	122.18	115.97
13	A	1138	CLA	C1D-CHD-C4C	2.65	126.11	122.48
13	A	1116	CLA	CED-O2D-CGD	2.65	122.19	115.97
13	A	1102	CLA	C1D-CHD-C4C	2.66	126.12	122.48
13	A	1109	CLA	CED-O2D-CGD	2.66	122.21	115.97
13	A	1140	CLA	CED-O2D-CGD	2.66	122.21	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1022	CLA	O2A-CGA-CBA	2.67	119.66	111.90
16	B	4014	BCR	C32-C1-C6	2.67	114.63	110.31
13	B	1208	CLA	C1C-NC-C4C	2.67	108.59	107.06
13	B	1211	CLA	C1C-NC-C4C	2.67	108.59	107.06
13	A	1101	CLA	C1C-NC-C4C	2.67	108.59	107.06
13	A	1103	CLA	CED-O2D-CGD	2.67	122.23	115.97
16	J	4012	BCR	C1-C6-C7	2.67	123.24	115.73
13	B	1223	CLA	C1D-CHD-C4C	2.67	126.14	122.48
13	A	1130	CLA	CED-O2D-CGD	2.68	122.25	115.97
16	B	4010	BCR	C29-C30-C25	2.68	114.67	110.48
13	A	1107	CLA	C1C-NC-C4C	2.68	108.60	107.06
13	B	1206	CLA	C1D-CHD-C4C	2.68	126.16	122.48
16	L	4019	BCR	C40-C30-C25	2.69	114.66	110.31
13	B	1232	CLA	CED-O2D-CGD	2.69	122.28	115.97
13	B	1021	CLA	CED-O2D-CGD	2.69	122.28	115.97
13	A	1103	CLA	C1C-NC-C4C	2.69	108.60	107.06
16	I	4018	BCR	C23-C24-C25	2.69	134.79	127.25
16	I	4018	BCR	C36-C18-C19	2.70	122.40	118.10
13	A	1136	CLA	C1D-CHD-C4C	2.70	126.17	122.48
13	A	1105	CLA	C1D-CHD-C4C	2.70	126.17	122.48
13	A	1237	CLA	O2D-CGD-CBD	2.70	116.13	111.30
16	L	4019	BCR	C8-C7-C6	2.71	134.83	127.25
16	L	4022	BCR	C29-C30-C25	2.71	114.72	110.48
13	A	1117	CLA	CED-O2D-CGD	2.71	122.33	115.97
16	A	4001	BCR	C8-C7-C6	2.71	134.85	127.25
13	A	1112	CLA	C1C-NC-C4C	2.72	108.62	107.06
13	J	1302	CLA	CED-O2D-CGD	2.72	122.34	115.97
13	B	1218	CLA	CED-O2D-CGD	2.72	122.35	115.97
13	B	1213	CLA	C1-C2-C3	2.72	130.97	125.96
16	A	4008	BCR	C23-C24-C25	2.72	134.87	127.25
13	A	1110	CLA	C1C-NC-C4C	2.72	108.62	107.06
13	J	1302	CLA	C1C-NC-C4C	2.72	108.62	107.06
13	A	1124	CLA	C1D-CHD-C4C	2.73	126.22	122.48
13	B	1234	CLA	C1C-NC-C4C	2.73	108.63	107.06
13	A	1104	CLA	C1-C2-C3	2.73	130.99	125.96
13	B	1236	CLA	C1D-CHD-C4C	2.73	126.22	122.48
13	B	1219	CLA	CED-O2D-CGD	2.73	122.38	115.97
16	A	4011	BCR	C30-C25-C24	2.74	123.42	115.73
16	B	4005	BCR	C20-C21-C22	2.74	131.22	127.31
13	B	1210	CLA	CMB-C2B-C3B	2.74	129.98	124.89
13	A	1132	CLA	C1D-CHD-C4C	2.74	126.23	122.48
13	B	1210	CLA	C1-C2-C3	2.74	131.01	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1231	CLA	CED-O2D-CGD	2.75	122.41	115.97
13	L	1503	CLA	C1C-NC-C4C	2.75	108.64	107.06
13	B	1239	CLA	C1D-CHD-C4C	2.75	126.25	122.48
13	B	1201	CLA	C1D-CHD-C4C	2.76	126.25	122.48
16	L	4022	BCR	C8-C7-C6	2.76	134.97	127.25
13	B	1230	CLA	CED-O2D-CGD	2.76	122.44	115.97
16	A	4011	BCR	C32-C1-C6	2.76	114.78	110.31
13	L	1501	CLA	C1D-CHD-C4C	2.76	126.26	122.48
13	B	1229	CLA	C1C-NC-C4C	2.76	108.64	107.06
13	B	1225	CLA	O2D-CGD-CBD	2.76	116.24	111.30
13	B	1223	CLA	CMB-C2B-C3B	2.77	130.03	124.89
16	I	4020	BCR	C32-C1-C6	2.77	114.80	110.31
13	B	1222	CLA	CMB-C2B-C3B	2.77	130.03	124.89
13	B	1233	CLA	C1C-NC-C4C	2.77	108.65	107.06
16	B	4009	BCR	C40-C30-C25	2.78	114.81	110.31
13	B	1217	CLA	CED-O2D-CGD	2.78	122.48	115.97
13	B	1212	CLA	C1D-CHD-C4C	2.78	126.28	122.48
13	A	1110	CLA	C1-C2-C3	2.78	131.07	125.96
13	A	1121	CLA	C1D-CHD-C4C	2.78	126.28	122.48
13	A	1109	CLA	C1D-CHD-C4C	2.78	126.28	122.48
13	B	1226	CLA	C1-C2-C3	2.78	131.09	125.96
13	A	1126	CLA	O2D-CGD-CBD	2.78	116.27	111.30
13	A	1106	CLA	C1D-CHD-C4C	2.79	126.30	122.48
13	B	1225	CLA	C5-C3-C2	2.79	126.81	121.10
13	B	1221	CLA	CED-O2D-CGD	2.79	122.51	115.97
13	B	1238	CLA	O2A-CGA-CBA	2.79	120.02	111.90
16	B	4014	BCR	C15-C14-C13	2.80	131.30	127.31
13	A	1108	CLA	C1D-CHD-C4C	2.80	126.31	122.48
16	A	4008	BCR	C2-C1-C6	2.80	114.86	110.48
16	B	4005	BCR	C1-C6-C7	2.80	123.60	115.73
13	A	1140	CLA	C1D-CHD-C4C	2.80	126.31	122.48
13	A	1122	CLA	C1D-CHD-C4C	2.81	126.33	122.48
16	I	4020	BCR	C7-C8-C9	2.81	130.44	126.21
16	J	4012	BCR	C36-C18-C19	2.81	122.58	118.10
13	A	1119	CLA	C1-C2-C3	2.81	131.14	125.96
13	A	1113	CLA	C1C-NC-C4C	2.81	108.67	107.06
13	B	1208	CLA	CED-O2D-CGD	2.81	122.57	115.97
13	A	1125	CLA	C1D-CHD-C4C	2.82	126.33	122.48
13	A	1137	CLA	C1D-CHD-C4C	2.82	126.34	122.48
13	A	1117	CLA	CMB-C2B-C3B	2.82	130.12	124.89
13	B	1023	CLA	CED-O2D-CGD	2.82	122.58	115.97
13	A	1124	CLA	CMB-C2B-C3B	2.82	130.13	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1230	CLA	C1D-CHD-C4C	2.83	126.35	122.48
13	A	1104	CLA	CBA-CAA-C2A	2.83	122.26	113.80
13	A	1123	CLA	C1D-CHD-C4C	2.83	126.36	122.48
16	A	4007	BCR	C30-C25-C24	2.84	123.70	115.73
13	A	1117	CLA	O2D-CGD-CBD	2.84	116.37	111.30
13	B	1213	CLA	C1D-CHD-C4C	2.84	126.37	122.48
13	B	1214	CLA	O2D-CGD-CBD	2.85	116.38	111.30
13	A	1104	CLA	CMB-C2B-C3B	2.85	130.18	124.89
13	B	1235	CLA	CED-O2D-CGD	2.85	122.66	115.97
13	B	1220	CLA	C1C-NC-C4C	2.85	108.70	107.06
16	A	4001	BCR	C24-C23-C22	2.86	130.51	126.21
13	B	1208	CLA	O2D-CGD-CBD	2.86	116.41	111.30
16	A	4002	BCR	C29-C30-C25	2.86	114.95	110.48
16	A	4001	BCR	C23-C24-C25	2.86	135.26	127.25
16	B	4017	BCR	C29-C30-C25	2.86	114.95	110.48
13	A	1128	CLA	O2A-CGA-CBA	2.86	120.23	111.90
13	A	1104	CLA	CED-O2D-CGD	2.87	122.69	115.97
13	A	1013	CLA	C1D-CHD-C4C	2.87	126.41	122.48
13	B	1203	CLA	O2D-CGD-CBD	2.87	116.43	111.30
13	A	1140	CLA	O2D-CGD-CBD	2.88	116.44	111.30
13	A	1122	CLA	C1C-NC-C4C	2.88	108.71	107.06
16	J	4012	BCR	C8-C7-C6	2.88	135.31	127.25
13	M	1601	CLA	CED-O2D-CGD	2.88	122.73	115.97
16	J	4013	BCR	C30-C25-C24	2.89	123.85	115.73
13	B	1021	CLA	C1D-CHD-C4C	2.89	126.44	122.48
13	A	1801	CLA	C1C-NC-C4C	2.89	108.72	107.06
16	F	4016	BCR	C24-C23-C22	2.89	130.56	126.21
13	B	1228	CLA	C1D-CHD-C4C	2.89	126.44	122.48
16	A	4003	BCR	C7-C8-C9	2.89	130.56	126.21
13	A	1114	CLA	CED-O2D-CGD	2.90	122.77	115.97
13	B	1211	CLA	C1D-CHD-C4C	2.90	126.45	122.48
16	L	4019	BCR	C2-C1-C6	2.90	115.02	110.48
16	M	4021	BCR	C1-C6-C7	2.90	123.89	115.73
13	B	1234	CLA	O2A-CGA-CBA	2.91	120.36	111.90
13	J	1303	CLA	C1C-NC-C4C	2.91	108.73	107.06
13	A	1115	CLA	C1D-CHD-C4C	2.91	126.46	122.48
13	M	1601	CLA	C1C-NC-C4C	2.91	108.73	107.06
16	B	4005	BCR	C23-C24-C25	2.91	135.40	127.25
13	B	1236	CLA	O2D-CGD-CBD	2.91	116.51	111.30
16	A	4003	BCR	C40-C30-C25	2.92	115.04	110.31
13	A	1112	CLA	C1D-CHD-C4C	2.92	126.47	122.48
13	A	1237	CLA	C1D-CHD-C4C	2.92	126.48	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1210	CLA	C1D-CHD-C4C	2.93	126.48	122.48
13	B	1235	CLA	C1D-CHD-C4C	2.93	126.49	122.48
13	A	1011	CLA	C1D-CHD-C4C	2.93	126.49	122.48
13	B	1226	CLA	C1D-CHD-C4C	2.94	126.50	122.48
13	A	1013	CLA	CED-O2D-CGD	2.94	122.85	115.97
13	A	1118	CLA	C1-C2-C3	2.94	131.37	125.96
13	A	1110	CLA	C1D-CHD-C4C	2.94	126.50	122.48
13	B	1203	CLA	O2A-CGA-CBA	2.94	120.47	111.90
16	B	4009	BCR	C29-C30-C25	2.95	115.08	110.48
13	A	1127	CLA	CMB-C2B-C3B	2.95	130.36	124.89
16	A	4011	BCR	C16-C17-C18	2.95	131.51	127.31
16	I	4018	BCR	C7-C8-C9	2.95	130.64	126.21
13	A	1402	CLA	OBD-CAD-C3D	2.95	130.35	127.24
13	A	1133	CLA	C1D-CHD-C4C	2.95	126.52	122.48
13	A	1104	CLA	C2A-C3A-C4A	2.95	106.64	101.87
13	A	1108	CLA	O2D-CGD-CBD	2.96	116.58	111.30
13	A	1116	CLA	C1D-CHD-C4C	2.96	126.53	122.48
17	A	5003	LHG	O7-C7-C8	2.96	117.69	111.55
13	A	1104	CLA	C1D-CHD-C4C	2.96	126.53	122.48
16	L	4019	BCR	C30-C25-C24	2.96	124.05	115.73
13	A	1132	CLA	O2A-CGA-CBA	2.97	120.54	111.90
13	B	1228	CLA	C1C-NC-C4C	2.97	108.76	107.06
16	B	4006	BCR	C24-C23-C22	2.97	130.67	126.21
13	A	1121	CLA	C1-C2-C3	2.97	131.43	125.96
13	B	1234	CLA	C1D-CHD-C4C	2.97	126.55	122.48
13	A	1133	CLA	C1C-NC-C4C	2.98	108.77	107.06
13	B	1230	CLA	C1-C2-C3	2.98	131.44	125.96
16	B	4005	BCR	C2-C1-C6	2.98	115.14	110.48
13	A	1127	CLA	C1D-CHD-C4C	2.98	126.56	122.48
13	A	1116	CLA	O2D-CGD-CBD	2.98	116.63	111.30
16	B	4010	BCR	C24-C23-C22	2.99	130.70	126.21
13	B	1204	CLA	C1C-NC-C4C	2.99	108.77	107.06
13	B	1219	CLA	O2D-CGD-CBD	2.99	116.64	111.30
16	A	4001	BCR	C2-C1-C6	2.99	115.16	110.48
13	A	1114	CLA	C1D-CHD-C4C	2.99	126.58	122.48
13	A	1022	CLA	C1-C2-C3	3.00	131.48	125.96
13	B	1012	CLA	C1D-CHD-C4C	3.00	126.59	122.48
13	B	1224	CLA	C1D-CHD-C4C	3.00	126.59	122.48
16	B	4009	BCR	C24-C23-C22	3.01	130.73	126.21
13	A	1138	CLA	CED-O2D-CGD	3.01	123.03	115.97
13	X	1701	CLA	C1C-NC-C4C	3.01	108.79	107.06
13	B	1230	CLA	C1C-NC-C4C	3.02	108.79	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1216	CLA	O2D-CGD-CBD	3.03	116.71	111.30
13	A	1101	CLA	C1D-CHD-C4C	3.03	126.63	122.48
17	A	5001	LHG	O7-C7-C8	3.04	117.86	111.55
13	B	1220	CLA	C1D-CHD-C4C	3.04	126.64	122.48
13	A	1119	CLA	CED-O2D-CGD	3.04	123.09	115.97
13	A	1122	CLA	O2D-CGD-CBD	3.04	116.73	111.30
13	B	1231	CLA	C1D-CHD-C4C	3.04	126.64	122.48
13	B	1207	CLA	O2D-CGD-CBD	3.05	116.74	111.30
16	A	4007	BCR	C2-C1-C6	3.05	115.24	110.48
13	A	1402	CLA	C1D-CHD-C4C	3.05	126.66	122.48
13	B	1221	CLA	C1D-CHD-C4C	3.05	126.66	122.48
16	B	4004	BCR	C7-C8-C9	3.05	130.80	126.21
16	B	4017	BCR	C7-C8-C9	3.05	130.80	126.21
13	B	1238	CLA	CED-O2D-CGD	3.06	123.13	115.97
13	A	1131	CLA	O2A-CGA-CBA	3.06	120.80	111.90
13	K	1401	CLA	C1D-CHD-C4C	3.06	126.67	122.48
16	A	4003	BCR	C2-C1-C6	3.07	115.27	110.48
13	F	1301	CLA	O2D-CGD-CBD	3.07	116.78	111.30
13	B	1232	CLA	C1D-CHD-C4C	3.07	126.68	122.48
13	A	1138	CLA	C1C-NC-C4C	3.08	108.82	107.06
13	A	1117	CLA	C1D-CHD-C4C	3.08	126.69	122.48
13	B	1216	CLA	C1D-CHD-C4C	3.08	126.69	122.48
13	B	1215	CLA	C1D-CHD-C4C	3.08	126.69	122.48
13	A	1124	CLA	O2A-CGA-CBA	3.08	120.87	111.90
16	L	4019	BCR	C24-C23-C22	3.08	130.84	126.21
13	A	1134	CLA	C1C-NC-C4C	3.09	108.83	107.06
17	B	5004	LHG	O7-C7-C8	3.09	117.98	111.55
13	A	1111	CLA	C1D-CHD-C4C	3.10	126.72	122.48
16	B	4004	BCR	C29-C30-C25	3.10	115.33	110.48
16	A	4007	BCR	C29-C30-C25	3.10	115.33	110.48
13	B	1211	CLA	O2A-CGA-CBA	3.10	120.93	111.90
13	B	1202	CLA	C1-C2-C3	3.10	131.67	125.96
13	B	1206	CLA	O2D-CGD-CBD	3.10	116.85	111.30
13	A	1107	CLA	O2D-CGD-CBD	3.11	116.85	111.30
13	B	1204	CLA	C1D-CHD-C4C	3.11	126.74	122.48
13	B	1233	CLA	O2D-CGD-CBD	3.12	116.87	111.30
13	B	1238	CLA	C1-C2-C3	3.12	131.70	125.96
13	B	1214	CLA	C1D-CHD-C4C	3.12	126.75	122.48
13	B	1219	CLA	C1D-CHD-C4C	3.13	126.76	122.48
13	B	1219	CLA	C1-C2-C3	3.13	131.73	125.96
13	L	1503	CLA	O2A-CGA-CBA	3.14	121.04	111.90
13	B	1215	CLA	CMB-C2B-C3B	3.14	130.72	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	4016	BCR	C29-C30-C25	3.15	115.40	110.48
13	A	1135	CLA	C1-C2-C3	3.15	131.76	125.96
13	L	1502	CLA	O2A-CGA-CBA	3.15	121.08	111.90
16	M	4021	BCR	C29-C30-C25	3.15	115.41	110.48
13	A	1115	CLA	O2A-CGA-CBA	3.16	121.09	111.90
13	B	1234	CLA	C1-C2-C3	3.16	131.78	125.96
13	B	1233	CLA	C1D-CHD-C4C	3.16	126.81	122.48
13	B	1230	CLA	O2A-CGA-CBA	3.18	121.14	111.90
13	B	1206	CLA	O2A-CGA-CBA	3.18	121.15	111.90
13	B	1229	CLA	C1D-CHD-C4C	3.18	126.83	122.48
16	A	4008	BCR	C29-C30-C25	3.18	115.46	110.48
13	A	1122	CLA	O2A-CGA-CBA	3.18	121.17	111.90
13	B	1228	CLA	O2A-CGA-CBA	3.19	121.18	111.90
13	A	1119	CLA	C1D-CHD-C4C	3.19	126.85	122.48
13	A	1801	CLA	C1D-CHD-C4C	3.19	126.85	122.48
13	B	1219	CLA	C1C-NC-C4C	3.19	108.89	107.06
16	J	4013	BCR	C7-C8-C9	3.20	131.02	126.21
13	B	1239	CLA	O2A-CGA-CBA	3.21	121.23	111.90
13	B	1218	CLA	C1D-CHD-C4C	3.21	126.87	122.48
13	A	1133	CLA	O2D-CGD-CBD	3.21	117.04	111.30
16	F	4016	BCR	C2-C1-C6	3.22	115.51	110.48
13	A	1103	CLA	C1D-CHD-C4C	3.22	126.89	122.48
16	L	4022	BCR	C2-C1-C6	3.22	115.52	110.48
13	F	1301	CLA	C1D-CHD-C4C	3.23	126.90	122.48
13	A	1113	CLA	C1D-CHD-C4C	3.23	126.90	122.48
13	A	1120	CLA	C1D-CHD-C4C	3.23	126.90	122.48
13	B	1219	CLA	O2A-CGA-CBA	3.23	121.31	111.90
13	B	1216	CLA	O2A-CGA-CBA	3.23	121.31	111.90
16	J	4013	BCR	C38-C26-C25	3.24	128.13	124.51
13	A	1133	CLA	C1-C2-C3	3.24	131.93	125.96
16	J	4015	BCR	C29-C30-C25	3.25	115.56	110.48
13	A	1105	CLA	O2D-CGD-CBD	3.25	117.11	111.30
16	B	4010	BCR	C2-C1-C6	3.26	115.57	110.48
13	B	1226	CLA	CMB-C2B-C3B	3.26	130.94	124.89
13	A	1115	CLA	O2D-CGD-CBD	3.26	117.12	111.30
13	A	1134	CLA	O2D-CGD-CBD	3.26	117.12	111.30
13	B	1221	CLA	O2A-CGA-CBA	3.26	121.38	111.90
13	L	1502	CLA	C1C-NC-C4C	3.26	108.93	107.06
13	B	1023	CLA	C1C-NC-C4C	3.26	108.93	107.06
16	B	4006	BCR	C2-C1-C6	3.26	115.58	110.48
13	A	1110	CLA	O2D-CGD-CBD	3.26	117.13	111.30
13	B	1021	CLA	O2A-CGA-CBA	3.27	121.40	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	4021	BCR	C2-C1-C6	3.27	115.59	110.48
16	B	4017	BCR	C2-C1-C6	3.27	115.59	110.48
16	B	4004	BCR	C24-C23-C22	3.27	131.13	126.21
13	A	1123	CLA	O2A-CGA-CBA	3.27	121.43	111.90
13	B	1226	CLA	O2A-CGA-CBA	3.28	121.45	111.90
13	L	1503	CLA	C1D-CHD-C4C	3.28	126.97	122.48
16	A	4001	BCR	C29-C30-C25	3.29	115.62	110.48
13	A	1107	CLA	C1D-CHD-C4C	3.29	126.98	122.48
13	B	1231	CLA	C1C-NC-C4C	3.30	108.95	107.06
16	B	4014	BCR	C29-C30-C25	3.30	115.64	110.48
16	B	4004	BCR	C23-C24-C25	3.30	136.49	127.25
13	B	1235	CLA	C1C-NC-C4C	3.30	108.95	107.06
16	B	4014	BCR	C2-C1-C6	3.30	115.64	110.48
13	B	1023	CLA	O2A-CGA-CBA	3.31	121.53	111.90
16	A	4002	BCR	C2-C1-C6	3.31	115.66	110.48
13	B	1217	CLA	C1C-NC-C4C	3.32	108.96	107.06
13	J	1303	CLA	OBD-CAD-C3D	3.32	130.75	127.24
13	A	1130	CLA	C1-C2-C3	3.32	132.08	125.96
16	A	4011	BCR	C29-C30-C25	3.33	115.69	110.48
13	X	1701	CLA	C1D-CHD-C4C	3.33	127.04	122.48
18	B	5002	LMG	O8-C28-C29	3.33	121.60	111.90
13	A	1022	CLA	O2D-CGD-CBD	3.34	117.26	111.30
13	B	1236	CLA	O2A-CGA-CBA	3.34	121.61	111.90
16	J	4012	BCR	C23-C24-C25	3.34	136.60	127.25
13	B	1227	CLA	C1D-CHD-C4C	3.34	127.05	122.48
13	B	1215	CLA	O2D-CGD-CBD	3.35	117.29	111.30
13	A	1135	CLA	O2D-CGD-CBD	3.36	117.31	111.30
13	B	1220	CLA	O2D-CGD-CBD	3.36	117.31	111.30
13	J	1303	CLA	C1D-CHD-C4C	3.37	127.09	122.48
13	B	1012	CLA	O2A-CGA-CBA	3.37	121.70	111.90
13	A	1129	CLA	C1C-NC-C4C	3.37	108.99	107.06
16	J	4012	BCR	C2-C1-C6	3.37	115.75	110.48
13	B	1205	CLA	C4A-NA-C1A	3.38	110.65	106.45
13	J	1302	CLA	C1D-CHD-C4C	3.38	127.11	122.48
13	A	1139	CLA	O2D-CGD-CBD	3.38	117.34	111.30
13	B	1217	CLA	C1D-CHD-C4C	3.39	127.11	122.48
13	B	1235	CLA	O2D-CGD-CBD	3.39	117.36	111.30
13	B	1210	CLA	O2A-CGA-CBA	3.39	121.77	111.90
13	B	1202	CLA	O2A-CGA-CBA	3.39	121.77	111.90
13	B	1229	CLA	O2A-CGA-CBA	3.39	121.78	111.90
13	B	1209	CLA	C1C-NC-C4C	3.40	109.01	107.06
13	A	1119	CLA	CMB-C2B-C3B	3.40	131.20	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1239	CLA	O2D-CGD-CBD	3.40	117.38	111.30
16	B	4009	BCR	C20-C21-C22	3.41	132.17	127.31
16	B	4005	BCR	C29-C30-C25	3.41	115.81	110.48
13	B	1222	CLA	C1D-CHD-C4C	3.41	127.15	122.48
13	A	1136	CLA	O2A-CGA-CBA	3.41	121.82	111.90
13	A	1124	CLA	O2D-CGD-CBD	3.41	117.39	111.30
16	A	4008	BCR	C24-C23-C22	3.41	131.34	126.21
13	B	1225	CLA	C4A-NA-C1A	3.41	110.69	106.45
13	M	1601	CLA	C1D-CHD-C4C	3.41	127.15	122.48
16	F	4016	BCR	C15-C14-C13	3.41	132.18	127.31
13	A	1103	CLA	O2A-CGA-CBA	3.41	121.84	111.90
13	A	1111	CLA	O2A-CGA-CBA	3.42	121.86	111.90
13	L	1502	CLA	O2D-CGD-CBD	3.42	117.42	111.30
13	A	1112	CLA	O2D-CGD-CBD	3.43	117.42	111.30
13	B	1223	CLA	O2A-CGA-CBA	3.43	121.88	111.90
13	A	1118	CLA	C1D-CHD-C4C	3.43	127.17	122.48
13	B	1224	CLA	O2D-CGD-CBD	3.43	117.44	111.30
17	A	5003	LHG	O8-C23-C24	3.44	120.59	111.35
13	A	1133	CLA	O2A-CGA-CBA	3.44	121.92	111.90
13	A	1119	CLA	C1C-NC-C4C	3.45	109.04	107.06
13	A	1134	CLA	C1D-CHD-C4C	3.45	127.20	122.48
13	A	1131	CLA	O2D-CGD-CBD	3.45	117.46	111.30
13	B	1222	CLA	C1C-NC-C4C	3.45	109.04	107.06
13	A	1118	CLA	C1C-NC-C4C	3.46	109.05	107.06
13	A	1130	CLA	O2A-CGA-CBA	3.47	121.99	111.90
13	A	1118	CLA	O2D-CGD-CBD	3.48	117.51	111.30
13	A	1011	CLA	O2A-CGA-CBA	3.48	122.02	111.90
13	B	1213	CLA	O2D-CGD-CBD	3.48	117.52	111.30
13	A	1138	CLA	O2A-CGA-CBA	3.48	122.04	111.90
13	X	1701	CLA	O2D-CGD-CBD	3.48	117.52	111.30
17	A	5001	LHG	O8-C23-C24	3.48	122.04	111.90
13	A	1022	CLA	C4A-NA-C1A	3.49	110.78	106.45
13	B	1204	CLA	O2A-CGA-CBA	3.49	122.05	111.90
13	B	1207	CLA	O2A-CGA-CBA	3.49	122.06	111.90
13	L	1503	CLA	O2D-CGD-CBD	3.50	117.55	111.30
16	J	4013	BCR	C29-C30-C25	3.50	115.95	110.48
13	A	1011	CLA	C4A-NA-C1A	3.51	110.81	106.45
13	A	1126	CLA	O2A-CGA-CBA	3.51	122.11	111.90
13	A	1129	CLA	O2A-CGA-CBA	3.51	122.12	111.90
13	B	1209	CLA	O2D-CGD-CBD	3.51	117.58	111.30
13	A	1114	CLA	O2A-CGA-CBA	3.52	122.14	111.90
16	J	4013	BCR	C2-C1-C6	3.52	115.98	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1101	CLA	O2A-CGA-CBA	3.52	122.14	111.90
13	A	1130	CLA	O2D-CGD-CBD	3.53	117.60	111.30
13	B	1209	CLA	C1D-CHD-C4C	3.53	127.31	122.48
13	A	1137	CLA	O2D-CGD-CBD	3.54	117.62	111.30
13	B	1202	CLA	C4A-NA-C1A	3.54	110.84	106.45
13	A	1114	CLA	O2D-CGD-CBD	3.55	117.64	111.30
16	J	4015	BCR	C24-C23-C22	3.56	131.56	126.21
13	B	1235	CLA	O2A-CGA-CBA	3.56	122.26	111.90
13	A	1120	CLA	C1C-NC-C4C	3.56	109.10	107.06
13	B	1218	CLA	C1C-NC-C4C	3.56	109.11	107.06
13	A	1130	CLA	C1D-CHD-C4C	3.57	127.36	122.48
13	B	1204	CLA	O2D-CGD-CBD	3.57	117.68	111.30
13	A	1127	CLA	O2D-CGD-CBD	3.57	117.68	111.30
13	A	1801	CLA	C1-C2-C3	3.57	132.53	125.96
13	L	1501	CLA	O2A-CGA-CBA	3.57	122.30	111.90
13	A	1102	CLA	O2A-CGA-CBA	3.58	122.31	111.90
13	B	1211	CLA	C1-C2-C3	3.58	132.56	125.96
16	A	4003	BCR	C24-C23-C22	3.59	131.60	126.21
16	A	4008	BCR	C33-C5-C6	3.59	128.53	124.51
13	B	1210	CLA	C4A-NA-C1A	3.61	110.93	106.45
13	A	1011	CLA	OBD-CAD-C3D	3.62	134.69	128.03
16	I	4020	BCR	C33-C5-C6	3.62	128.56	124.51
16	A	4007	BCR	C24-C23-C22	3.62	131.66	126.21
13	A	1237	CLA	C4A-NA-C1A	3.63	110.96	106.45
16	A	4003	BCR	C29-C30-C25	3.64	116.17	110.48
13	A	1109	CLA	O2A-CGA-CBA	3.64	122.50	111.90
13	A	1126	CLA	C4A-NA-C1A	3.65	110.98	106.45
16	B	4010	BCR	C7-C8-C9	3.66	131.71	126.21
13	A	1137	CLA	C4A-NA-C1A	3.66	110.99	106.45
13	B	1012	CLA	C4A-NA-C1A	3.66	111.00	106.45
13	B	1203	CLA	C4A-NA-C1A	3.66	111.00	106.45
16	J	4013	BCR	C33-C5-C6	3.67	128.61	124.51
13	A	1129	CLA	C1D-CHD-C4C	3.67	127.50	122.48
13	A	1013	CLA	C4A-NA-C1A	3.67	111.00	106.45
13	A	1132	CLA	C4A-NA-C1A	3.67	111.01	106.45
16	M	4021	BCR	C33-C5-C6	3.68	128.62	124.51
16	B	4004	BCR	C2-C1-C6	3.68	116.23	110.48
13	B	1236	CLA	C4A-NA-C1A	3.68	111.02	106.45
16	J	4012	BCR	C29-C30-C25	3.68	116.24	110.48
13	A	1125	CLA	O2A-CGA-CBA	3.68	122.62	111.90
16	B	4005	BCR	C24-C23-C22	3.70	131.77	126.21
16	A	4011	BCR	C2-C1-C6	3.70	116.26	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1231	CLA	O2D-CGD-CBD	3.70	117.91	111.30
13	B	1227	CLA	C1C-NC-C4C	3.72	109.19	107.06
13	A	1111	CLA	O2D-CGD-CBD	3.72	117.94	111.30
16	J	4015	BCR	C2-C1-C6	3.73	116.31	110.48
13	A	1128	CLA	C4A-NA-C1A	3.73	111.09	106.45
13	B	1213	CLA	O2A-CGA-CBA	3.74	122.79	111.90
13	B	1023	CLA	C4A-NA-C1A	3.75	111.10	106.45
16	A	4011	BCR	C40-C30-C25	3.75	116.39	110.31
13	B	1228	CLA	O2D-CGD-CBD	3.75	118.00	111.30
13	A	1103	CLA	C4A-NA-C1A	3.76	111.11	106.45
13	B	1238	CLA	C4A-NA-C1A	3.76	111.12	106.45
13	A	1115	CLA	C4A-NA-C1A	3.76	111.12	106.45
13	A	1131	CLA	C4A-NA-C1A	3.77	111.13	106.45
13	B	1221	CLA	O2D-CGD-CBD	3.78	118.05	111.30
13	B	1226	CLA	C4A-NA-C1A	3.78	111.15	106.45
13	B	1224	CLA	CBA-CAA-C2A	3.79	125.12	113.80
13	B	1201	CLA	O2A-CGA-CBA	3.79	122.92	111.90
13	A	1120	CLA	O2D-CGD-CBD	3.80	118.08	111.30
13	A	1106	CLA	O2A-CGA-CBA	3.80	122.95	111.90
13	A	1105	CLA	O2A-CGA-CBA	3.80	122.95	111.90
16	M	4021	BCR	C24-C23-C22	3.80	131.93	126.21
13	L	1503	CLA	C4A-NA-C1A	3.81	111.17	106.45
13	A	1103	CLA	O2D-CGD-CBD	3.81	118.11	111.30
13	K	1401	CLA	O2D-CGD-CBD	3.81	118.11	111.30
13	B	1234	CLA	C4A-NA-C1A	3.82	111.19	106.45
16	B	4014	BCR	C7-C8-C9	3.83	131.96	126.21
13	B	1223	CLA	O2D-CGD-CBD	3.83	118.14	111.30
13	A	1121	CLA	C4A-NA-C1A	3.84	111.22	106.45
13	A	1104	CLA	C4A-NA-C1A	3.84	111.22	106.45
13	A	1110	CLA	O2A-CGA-CBA	3.86	123.12	111.90
16	A	4011	BCR	C24-C23-C22	3.86	132.01	126.21
13	A	1116	CLA	O2A-CGA-CBA	3.86	123.13	111.90
13	B	1213	CLA	C4A-NA-C1A	3.86	111.25	106.45
13	B	1202	CLA	O2D-CGD-CBD	3.86	118.20	111.30
13	B	1210	CLA	O2D-CGD-CBD	3.87	118.21	111.30
13	B	1224	CLA	C4A-NA-C1A	3.87	111.26	106.45
13	K	1401	CLA	C4A-NA-C1A	3.87	111.26	106.45
16	A	4007	BCR	C33-C5-C6	3.89	128.86	124.51
13	A	1123	CLA	C4A-NA-C1A	3.89	111.28	106.45
13	B	1214	CLA	O2A-CGA-CBA	3.89	123.21	111.90
13	A	1108	CLA	C4A-NA-C1A	3.89	111.28	106.45
13	A	1136	CLA	C4A-NA-C1A	3.90	111.30	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	1501	CLA	C4A-NA-C1A	3.90	111.30	106.45
13	J	1302	CLA	O2D-CGD-CBD	3.91	118.29	111.30
16	B	4017	BCR	C38-C26-C25	3.91	128.89	124.51
16	B	4017	BCR	C33-C5-C6	3.92	128.89	124.51
13	A	1121	CLA	O2D-CGD-CBD	3.92	118.30	111.30
13	B	1206	CLA	C4A-NA-C1A	3.92	111.32	106.45
13	B	1218	CLA	O2D-CGD-CBD	3.93	118.31	111.30
16	B	4005	BCR	C7-C8-C9	3.93	132.12	126.21
13	A	1127	CLA	C4A-NA-C1A	3.93	111.33	106.45
13	B	1217	CLA	O2A-CGA-CBA	3.93	123.34	111.90
13	B	1208	CLA	C4A-NA-C1A	3.93	111.33	106.45
13	A	1127	CLA	O2A-CGA-CBA	3.94	123.37	111.90
13	B	1232	CLA	C4A-NA-C1A	3.95	111.35	106.45
13	B	1234	CLA	O2D-CGD-CBD	3.95	118.35	111.30
13	B	1221	CLA	C4A-NA-C1A	3.95	111.36	106.45
13	A	1139	CLA	C4A-NA-C1A	3.96	111.36	106.45
13	A	1121	CLA	O2A-CGA-CBA	3.96	123.42	111.90
13	A	1140	CLA	C4A-NA-C1A	3.96	111.37	106.45
13	A	1119	CLA	C4A-NA-C1A	3.96	111.37	106.45
16	B	4010	BCR	C38-C26-C25	3.96	128.94	124.51
16	A	4002	BCR	C33-C5-C6	3.96	128.95	124.51
16	A	4011	BCR	C38-C26-C25	3.97	128.95	124.51
13	L	1502	CLA	C4A-NA-C1A	3.97	111.38	106.45
13	A	1112	CLA	C4A-NA-C1A	3.97	111.38	106.45
13	A	1122	CLA	C4A-NA-C1A	3.98	111.39	106.45
13	B	1229	CLA	C4A-NA-C1A	3.98	111.40	106.45
13	B	1220	CLA	C4A-NA-C1A	3.98	111.40	106.45
13	B	1227	CLA	O2D-CGD-CBD	3.99	118.43	111.30
16	F	4016	BCR	C33-C5-C6	3.99	128.98	124.51
13	B	1229	CLA	O2D-CGD-CBD	4.00	118.44	111.30
13	A	1139	CLA	O2A-CGA-CBA	4.01	123.57	111.90
16	J	4015	BCR	C8-C7-C6	4.02	138.50	127.25
13	A	1129	CLA	O2D-CGD-CBD	4.02	118.48	111.30
13	A	1101	CLA	C4A-NA-C1A	4.02	111.44	106.45
16	I	4020	BCR	C24-C23-C22	4.02	132.26	126.21
13	B	1021	CLA	C4A-NA-C1A	4.03	111.45	106.45
13	B	1217	CLA	O2D-CGD-CBD	4.03	118.50	111.30
13	B	1211	CLA	C4A-NA-C1A	4.04	111.47	106.45
13	B	1214	CLA	C4A-NA-C1A	4.05	111.47	106.45
16	I	4018	BCR	C2-C1-C6	4.05	116.81	110.48
13	M	1601	CLA	O2D-CGD-CBD	4.05	118.54	111.30
13	A	1801	CLA	O2A-CGA-CBA	4.06	123.71	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1118	CLA	O2A-CGA-CBA	4.06	123.71	111.90
13	A	1124	CLA	C4A-NA-C1A	4.06	111.50	106.45
13	B	1231	CLA	C4A-NA-C1A	4.07	111.50	106.45
13	A	1128	CLA	O2D-CGD-CBD	4.07	118.57	111.30
13	B	1212	CLA	C4A-NA-C1A	4.07	111.50	106.45
13	A	1116	CLA	C4A-NA-C1A	4.07	111.51	106.45
13	A	1237	CLA	O2A-CGA-CBA	4.08	123.76	111.90
16	J	4012	BCR	C33-C5-C6	4.08	129.08	124.51
13	B	1228	CLA	C4A-NA-C1A	4.08	111.52	106.45
13	B	1215	CLA	O2A-CGA-CBA	4.08	123.78	111.90
16	I	4020	BCR	C38-C26-C25	4.08	129.08	124.51
13	A	1117	CLA	O2A-CGA-CBA	4.09	123.80	111.90
13	A	1120	CLA	O2A-CGA-CBA	4.09	123.81	111.90
13	B	1216	CLA	C4A-NA-C1A	4.09	111.53	106.45
13	B	1239	CLA	C4A-NA-C1A	4.11	111.55	106.45
13	A	1106	CLA	O2D-CGD-CBD	4.11	118.64	111.30
13	B	1205	CLA	O2A-CGA-CBA	4.11	123.86	111.90
13	A	1138	CLA	C4A-NA-C1A	4.12	111.56	106.45
13	A	1107	CLA	O2A-CGA-CBA	4.13	123.91	111.90
16	A	4011	BCR	C33-C5-C6	4.13	129.13	124.51
13	A	1125	CLA	C4A-NA-C1A	4.13	111.58	106.45
13	A	1140	CLA	O2A-CGA-CBA	4.13	123.93	111.90
13	A	1101	CLA	O2D-CGD-CBD	4.13	118.69	111.30
13	A	1102	CLA	C4A-NA-C1A	4.14	111.59	106.45
16	B	4005	BCR	C33-C5-C6	4.15	129.16	124.51
13	A	1402	CLA	C4A-NA-C1A	4.16	111.61	106.45
13	A	1106	CLA	C4A-NA-C1A	4.16	111.61	106.45
13	B	1235	CLA	C4A-NA-C1A	4.17	111.63	106.45
13	A	1105	CLA	C4A-NA-C1A	4.17	111.63	106.45
16	B	4009	BCR	C38-C26-C25	4.17	129.18	124.51
13	B	1223	CLA	C4A-NA-C1A	4.17	111.63	106.45
13	A	1135	CLA	C4A-NA-C1A	4.17	111.63	106.45
13	B	1222	CLA	O2D-CGD-CBD	4.18	118.77	111.30
13	A	1125	CLA	O2D-CGD-CBD	4.18	118.78	111.30
13	B	1201	CLA	C4A-NA-C1A	4.20	111.67	106.45
13	A	1113	CLA	O2D-CGD-CBD	4.20	118.81	111.30
13	B	1222	CLA	C4A-NA-C1A	4.21	111.67	106.45
13	A	1123	CLA	O2D-CGD-CBD	4.21	118.82	111.30
13	B	1207	CLA	C4A-NA-C1A	4.21	111.68	106.45
13	A	1111	CLA	C4A-NA-C1A	4.22	111.69	106.45
13	A	1117	CLA	C4A-NA-C1A	4.22	111.70	106.45
13	A	1129	CLA	C4A-NA-C1A	4.22	111.70	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	4019	BCR	C38-C26-C25	4.24	129.25	124.51
13	B	1204	CLA	C4A-NA-C1A	4.24	111.72	106.45
13	A	1133	CLA	C4A-NA-C1A	4.24	111.72	106.45
16	B	4006	BCR	C29-C30-C25	4.24	117.11	110.48
13	A	1107	CLA	C4A-NA-C1A	4.25	111.73	106.45
13	B	1219	CLA	C4A-NA-C1A	4.26	111.74	106.45
13	B	1225	CLA	O2A-CGA-CBA	4.27	124.32	111.90
16	B	4006	BCR	C38-C26-C25	4.28	129.30	124.51
13	A	1120	CLA	C4A-NA-C1A	4.29	111.77	106.45
13	B	1212	CLA	O2D-CGD-CBD	4.29	118.96	111.30
13	B	1215	CLA	C4A-NA-C1A	4.29	111.78	106.45
16	A	4011	BCR	C7-C8-C9	4.30	132.68	126.21
13	B	1230	CLA	C4A-NA-C1A	4.30	111.79	106.45
13	J	1303	CLA	C4A-NA-C1A	4.31	111.80	106.45
16	A	4007	BCR	C38-C26-C25	4.32	129.34	124.51
13	A	1109	CLA	C4A-NA-C1A	4.32	111.82	106.45
13	A	1114	CLA	C4A-NA-C1A	4.32	111.82	106.45
16	A	4003	BCR	C33-C5-C6	4.33	129.35	124.51
16	A	4001	BCR	C33-C5-C6	4.34	129.36	124.51
13	A	1137	CLA	O2A-CGA-CBA	4.34	124.53	111.90
13	F	1301	CLA	C4A-NA-C1A	4.35	111.85	106.45
13	A	1013	CLA	O2A-CGA-CBA	4.35	124.56	111.90
13	B	1227	CLA	C4A-NA-C1A	4.37	111.88	106.45
13	A	1135	CLA	O2A-CGA-CBA	4.37	124.62	111.90
16	M	4021	BCR	C38-C26-C25	4.40	129.43	124.51
13	B	1211	CLA	O2D-CGD-CBD	4.42	119.20	111.30
13	A	1134	CLA	C4A-NA-C1A	4.42	111.94	106.45
16	B	4014	BCR	C38-C26-C25	4.43	129.46	124.51
13	B	1233	CLA	C4A-NA-C1A	4.43	111.96	106.45
13	A	1801	CLA	O2D-CGD-CBD	4.44	119.22	111.30
13	X	1701	CLA	C4A-NA-C1A	4.44	111.96	106.45
13	A	1801	CLA	C4A-NA-C1A	4.44	111.96	106.45
16	I	4018	BCR	C38-C26-C25	4.45	129.49	124.51
13	J	1302	CLA	C4A-NA-C1A	4.47	112.00	106.45
16	B	4006	BCR	C7-C8-C9	4.47	132.93	126.21
16	A	4002	BCR	C38-C26-C25	4.47	129.51	124.51
13	B	1230	CLA	O2D-CGD-CBD	4.47	119.29	111.30
13	B	1205	CLA	O2D-CGD-CBD	4.48	119.31	111.30
13	B	1218	CLA	C4A-NA-C1A	4.49	112.03	106.45
13	A	1110	CLA	C4A-NA-C1A	4.50	112.04	106.45
13	B	1209	CLA	C4A-NA-C1A	4.50	112.04	106.45
16	F	4016	BCR	C38-C26-C25	4.50	129.55	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1118	CLA	C4A-NA-C1A	4.52	112.06	106.45
13	A	1102	CLA	O2D-CGD-CBD	4.52	119.38	111.30
16	L	4022	BCR	C38-C26-C25	4.53	129.57	124.51
13	A	1113	CLA	C4A-NA-C1A	4.55	112.10	106.45
16	A	4003	BCR	C38-C26-C25	4.59	129.65	124.51
13	M	1601	CLA	C4A-NA-C1A	4.62	112.18	106.45
13	L	1501	CLA	O2D-CGD-CBD	4.62	119.55	111.30
16	J	4015	BCR	C38-C26-C25	4.63	129.69	124.51
13	A	1130	CLA	C4A-NA-C1A	4.64	112.21	106.45
13	B	1217	CLA	C4A-NA-C1A	4.66	112.24	106.45
16	B	4004	BCR	C33-C5-C6	4.68	129.74	124.51
16	I	4018	BCR	C33-C5-C6	4.68	129.75	124.51
13	B	1201	CLA	O2D-CGD-CBD	4.70	119.70	111.30
16	B	4010	BCR	C33-C5-C6	4.71	129.78	124.51
17	A	5003	LHG	C25-C24-C23	4.71	137.56	114.06
13	B	1224	CLA	O2A-CGA-CBA	4.73	125.66	111.90
16	B	4006	BCR	C33-C5-C6	4.77	129.85	124.51
16	J	4015	BCR	C33-C5-C6	4.80	129.88	124.51
13	B	1226	CLA	O2D-CGD-CBD	4.81	119.90	111.30
13	A	1132	CLA	O2D-CGD-CBD	4.82	119.91	111.30
13	B	1012	CLA	O2D-CGD-CBD	4.83	119.94	111.30
16	L	4019	BCR	C33-C5-C6	4.92	130.02	124.51
13	A	1104	CLA	O2A-CGA-CBA	5.01	126.48	111.90
16	J	4012	BCR	C38-C26-C25	5.08	130.20	124.51
16	B	4014	BCR	C33-C5-C6	5.11	130.22	124.51
16	A	4001	BCR	C38-C26-C25	5.16	130.28	124.51
16	L	4022	BCR	C33-C5-C6	5.18	130.31	124.51
16	A	4008	BCR	C38-C26-C25	5.51	130.68	124.51
16	B	4005	BCR	C38-C26-C25	5.79	130.99	124.51
16	B	4004	BCR	C38-C26-C25	5.99	131.22	124.51
18	B	5002	LMG	C30-C29-C28	6.13	135.97	113.58
14	B	2002	PQN	C14-C13-C15	6.18	126.01	115.29
17	A	5001	LHG	C25-C24-C23	6.19	136.18	113.58
14	A	2001	PQN	C14-C13-C15	7.19	127.76	115.29
13	A	1011	CLA	O2D-CGD-CBD	8.49	126.47	111.30

All (249) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	F	1301	CLA	NC
13	F	1301	CLA	ND
13	F	1301	CLA	NA

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Mol	Chain	Res	Type	Atom
13	A	1115	CLA	NA
13	B	1206	CLA	ND
13	B	1227	CLA	NC
13	B	1227	CLA	ND
13	B	1227	CLA	NA
13	B	1023	CLA	NA
13	B	1204	CLA	NC
13	B	1204	CLA	ND
13	B	1204	CLA	NA
13	B	1208	CLA	ND
13	B	1208	CLA	NA
13	A	1137	CLA	ND
13	A	1237	CLA	NC
13	A	1237	CLA	ND
13	A	1237	CLA	NA
13	B	1230	CLA	NC
13	B	1230	CLA	ND
13	B	1230	CLA	NA
13	B	1203	CLA	NA
13	B	1203	CLA	NC
13	B	1203	CLA	ND
13	A	1011	CLA	NC
13	A	1011	CLA	ND
13	A	1011	CLA	NA
13	A	1134	CLA	NC
13	A	1134	CLA	ND
13	A	1134	CLA	NA
13	A	1139	CLA	NC
13	A	1139	CLA	ND
13	A	1139	CLA	NA
13	B	1219	CLA	NC
13	B	1219	CLA	ND
13	B	1219	CLA	NA
13	B	1229	CLA	NC
13	B	1229	CLA	ND
13	B	1229	CLA	NA
13	B	1228	CLA	NC
13	B	1228	CLA	ND
13	B	1228	CLA	NA
13	A	1124	CLA	NC
13	A	1124	CLA	ND
13	A	1124	CLA	NA

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Mol	Chain	Res	Type	Atom
13	B	1233	CLA	NC
13	B	1233	CLA	ND
13	B	1233	CLA	NA
13	B	1232	CLA	NC
13	B	1232	CLA	ND
13	B	1232	CLA	NA
13	A	1117	CLA	NC
13	A	1117	CLA	ND
13	A	1117	CLA	NA
13	A	1402	CLA	NA
13	A	1402	CLA	NC
13	A	1402	CLA	ND
13	A	1111	CLA	NC
13	A	1111	CLA	ND
13	A	1111	CLA	NA
13	A	1135	CLA	NC
13	A	1135	CLA	ND
13	A	1135	CLA	NA
13	B	1207	CLA	NC
13	B	1207	CLA	ND
13	B	1207	CLA	NA
13	A	1138	CLA	NC
13	A	1138	CLA	ND
13	A	1138	CLA	NA
13	L	1501	CLA	NC
13	L	1501	CLA	ND
13	L	1501	CLA	NA
13	A	1113	CLA	NC
13	A	1113	CLA	ND
13	A	1113	CLA	NA
13	B	1012	CLA	ND
13	B	1012	CLA	NA
13	B	1222	CLA	NC
13	B	1222	CLA	ND
13	B	1222	CLA	NA
13	B	1213	CLA	NC
13	B	1213	CLA	ND
13	B	1213	CLA	NA
13	A	1133	CLA	NC
13	A	1133	CLA	ND
13	A	1133	CLA	NA
13	A	1114	CLA	NC

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Mol	Chain	Res	Type	Atom
13	A	1114	CLA	ND
13	A	1114	CLA	NA
13	X	1701	CLA	NC
13	X	1701	CLA	ND
13	X	1701	CLA	NA
13	B	1239	CLA	NC
13	B	1239	CLA	NA
13	A	1129	CLA	NC
13	A	1129	CLA	ND
13	A	1129	CLA	NA
13	J	1303	CLA	NC
13	J	1303	CLA	ND
13	J	1303	CLA	NA
13	B	1021	CLA	ND
13	A	1126	CLA	ND
13	B	1238	CLA	NC
13	B	1238	CLA	ND
13	B	1226	CLA	NC
13	B	1226	CLA	ND
13	B	1226	CLA	NA
13	A	1125	CLA	NC
13	A	1125	CLA	ND
13	A	1125	CLA	NA
13	A	1120	CLA	NC
13	A	1120	CLA	ND
13	A	1120	CLA	NA
13	B	1205	CLA	ND
13	B	1205	CLA	NA
13	A	1013	CLA	ND
13	A	1013	CLA	NA
13	A	1022	CLA	ND
13	A	1022	CLA	NA
13	A	1118	CLA	NC
13	A	1118	CLA	ND
13	A	1118	CLA	NA
13	B	1224	CLA	ND
13	A	1130	CLA	NC
13	A	1130	CLA	ND
13	A	1130	CLA	NA
13	A	1140	CLA	NC
13	A	1140	CLA	ND
13	A	1140	CLA	NA

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Mol	Chain	Res	Type	Atom
13	A	1110	CLA	NC
13	A	1110	CLA	ND
13	A	1110	CLA	NA
13	L	1503	CLA	NC
13	L	1503	CLA	ND
13	L	1503	CLA	NA
13	B	1201	CLA	ND
13	B	1201	CLA	NA
13	B	1235	CLA	NC
13	B	1235	CLA	ND
13	B	1235	CLA	NA
13	A	1109	CLA	NC
13	A	1109	CLA	ND
13	A	1109	CLA	NA
13	B	1220	CLA	NC
13	B	1220	CLA	ND
13	B	1220	CLA	NA
13	B	1221	CLA	NC
13	B	1221	CLA	ND
13	B	1221	CLA	NA
13	B	1210	CLA	NA
13	B	1210	CLA	NC
13	B	1210	CLA	ND
13	A	1123	CLA	NC
13	A	1123	CLA	ND
13	A	1123	CLA	NA
13	A	1102	CLA	NC
13	A	1102	CLA	ND
13	A	1102	CLA	NA
13	L	1502	CLA	NC
13	L	1502	CLA	NA
13	A	1107	CLA	NC
13	A	1107	CLA	ND
13	A	1107	CLA	NA
13	A	1122	CLA	NC
13	A	1122	CLA	ND
13	A	1122	CLA	NA
13	B	1217	CLA	NC
13	B	1217	CLA	ND
13	B	1217	CLA	NA
13	A	1112	CLA	NC
13	A	1112	CLA	ND

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Mol	Chain	Res	Type	Atom
13	A	1112	CLA	NA
13	B	1209	CLA	NC
13	B	1209	CLA	ND
13	B	1209	CLA	NA
13	J	1302	CLA	NC
13	J	1302	CLA	ND
13	J	1302	CLA	NA
13	A	1119	CLA	NC
13	A	1119	CLA	ND
13	A	1119	CLA	NA
13	B	1225	CLA	NA
13	A	1801	CLA	NC
13	A	1801	CLA	ND
13	A	1801	CLA	NA
13	B	1202	CLA	NA
13	B	1202	CLA	NC
13	B	1202	CLA	ND
13	A	1127	CLA	NC
13	A	1127	CLA	ND
17	A	5003	LHG	C2
13	A	1116	CLA	NC
13	A	1116	CLA	ND
13	A	1116	CLA	NA
13	A	1136	CLA	ND
13	A	1136	CLA	NA
13	A	1105	CLA	ND
13	A	1105	CLA	NA
13	A	1132	CLA	NC
13	A	1132	CLA	ND
13	A	1132	CLA	NA
13	B	1216	CLA	NC
13	B	1216	CLA	ND
13	B	1216	CLA	NA
13	B	1211	CLA	NC
13	B	1211	CLA	ND
13	B	1211	CLA	NA
13	A	1128	CLA	NC
13	A	1128	CLA	ND
13	A	1128	CLA	NA
13	A	1106	CLA	NC
13	A	1106	CLA	ND
13	A	1106	CLA	NA

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Mol	Chain	Res	Type	Atom
13	B	1212	CLA	NC
13	B	1212	CLA	NA
13	B	1218	CLA	NC
13	B	1218	CLA	ND
13	B	1218	CLA	NA
13	A	1104	CLA	NC
13	A	1104	CLA	ND
13	A	1104	CLA	NA
13	B	1231	CLA	NC
13	B	1231	CLA	ND
13	B	1231	CLA	NA
13	A	1101	CLA	NC
13	A	1101	CLA	ND
13	A	1101	CLA	NA
13	A	1121	CLA	ND
13	A	1121	CLA	NA
13	M	1601	CLA	NC
13	M	1601	CLA	ND
13	M	1601	CLA	NA
13	B	1223	CLA	NC
13	B	1223	CLA	ND
13	B	1223	CLA	NA
13	A	1103	CLA	NA
13	A	1103	CLA	NC
13	A	1103	CLA	ND
13	B	1215	CLA	NC
13	B	1215	CLA	ND
13	B	1215	CLA	NA
13	K	1401	CLA	NC
13	K	1401	CLA	NA
13	B	1214	CLA	NC
13	B	1214	CLA	ND
13	B	1214	CLA	NA
13	B	1234	CLA	NC
13	B	1234	CLA	ND
13	B	1234	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1114	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

114 monomers are involved in 339 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1011	CLA	9	0
13	A	1013	CLA	10	0
13	A	1022	CLA	3	0
13	A	1101	CLA	2	0
13	A	1102	CLA	1	0
13	A	1103	CLA	6	0
13	A	1104	CLA	4	0
13	A	1105	CLA	2	0
13	A	1106	CLA	6	0
13	A	1107	CLA	4	0
13	A	1108	CLA	4	0
13	A	1109	CLA	1	0
13	A	1111	CLA	1	0
13	A	1112	CLA	5	0
13	A	1114	CLA	2	0
13	A	1116	CLA	5	0
13	A	1117	CLA	6	0
13	A	1118	CLA	5	0
13	A	1119	CLA	4	0
13	A	1120	CLA	2	0
13	A	1121	CLA	1	0
13	A	1122	CLA	2	0
13	A	1123	CLA	4	0
13	A	1124	CLA	5	0
13	A	1125	CLA	3	0
13	A	1126	CLA	14	0
13	A	1127	CLA	1	0
13	A	1128	CLA	7	0
13	A	1129	CLA	1	0
13	A	1130	CLA	2	0
13	A	1132	CLA	4	0
13	A	1133	CLA	4	0
13	A	1134	CLA	2	0
13	A	1135	CLA	2	0
13	A	1136	CLA	7	0
13	A	1137	CLA	3	0
13	A	1138	CLA	2	0
13	A	1140	CLA	8	0
13	A	1237	CLA	5	0
13	A	1402	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1801	CLA	5	0
14	A	2001	PQN	1	0
16	A	4001	BCR	2	0
16	A	4002	BCR	2	0
16	A	4003	BCR	1	0
16	A	4007	BCR	4	0
16	A	4008	BCR	1	0
16	A	4011	BCR	13	0
17	A	5001	LHG	4	0
17	A	5003	LHG	2	0
13	B	1012	CLA	17	0
13	B	1021	CLA	8	0
13	B	1023	CLA	4	0
13	B	1201	CLA	2	0
13	B	1202	CLA	3	0
13	B	1203	CLA	6	0
13	B	1204	CLA	1	0
13	B	1205	CLA	3	0
13	B	1206	CLA	2	0
13	B	1207	CLA	5	0
13	B	1208	CLA	1	0
13	B	1209	CLA	1	0
13	B	1210	CLA	6	0
13	B	1211	CLA	6	0
13	B	1212	CLA	2	0
13	B	1213	CLA	3	0
13	B	1214	CLA	8	0
13	B	1215	CLA	6	0
13	B	1216	CLA	5	0
13	B	1217	CLA	2	0
13	B	1218	CLA	1	0
13	B	1219	CLA	4	0
13	B	1220	CLA	3	0
13	B	1221	CLA	10	0
13	B	1222	CLA	2	0
13	B	1223	CLA	3	0
13	B	1224	CLA	5	0
13	B	1225	CLA	8	0
13	B	1226	CLA	7	0
13	B	1227	CLA	5	0
13	B	1228	CLA	2	0
13	B	1229	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1230	CLA	7	0
13	B	1232	CLA	3	0
13	B	1233	CLA	2	0
13	B	1234	CLA	3	0
13	B	1235	CLA	2	0
13	B	1236	CLA	4	0
13	B	1238	CLA	3	0
14	B	2002	PQN	1	0
16	B	4004	BCR	1	0
16	B	4005	BCR	1	0
16	B	4006	BCR	5	0
16	B	4009	BCR	5	0
16	B	4010	BCR	3	0
16	B	4014	BCR	1	0
16	B	4017	BCR	1	0
18	B	5002	LMG	5	0
17	B	5004	LHG	1	0
13	F	1301	CLA	1	0
16	F	4016	BCR	2	0
16	I	4018	BCR	3	0
13	J	1302	CLA	1	0
16	J	4012	BCR	4	0
16	J	4013	BCR	7	0
16	J	4015	BCR	5	0
13	K	1401	CLA	1	0
13	L	1501	CLA	2	0
13	L	1502	CLA	8	0
13	L	1503	CLA	2	0
16	L	4022	BCR	1	0
13	M	1601	CLA	1	0
16	M	4021	BCR	2	0
13	X	1701	CLA	1	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.