



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 10:11 pm GMT

PDB ID : 4XK8
Title : Crystal structure of plant photosystem I-LHCI super-complex at 2.8 angstrom resolution
Authors : Suga, M.; Qin, X.; Kuang, T.; Shen, J.R.
Deposited on : 2015-01-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk28620

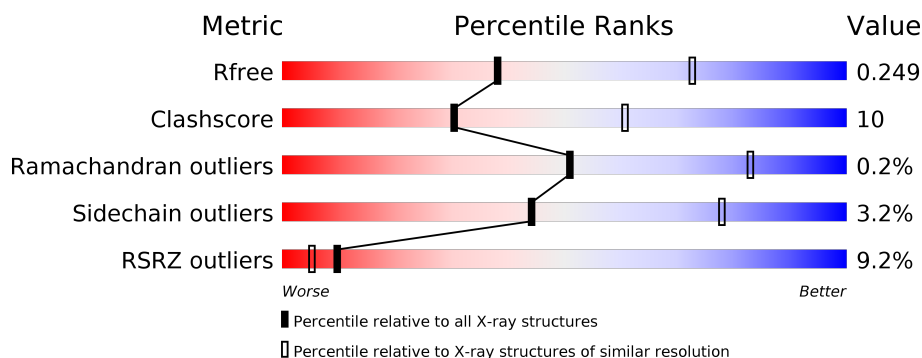
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	742	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>24%</div> </div> <div></div> </div>
1	a	742	<div> <div>4%</div> <div> <div></div> <div>98%</div> </div> <div></div> </div>
2	B	733	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>24%</div> </div> <div></div> </div>
2	b	733	<div> <div>7%</div> <div> <div></div> <div>98%</div> </div> <div></div> </div>
3	C	80	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>19%</div> </div> <div></div> </div>
3	c	80	<div> <div></div> <div> <div></div> <div>98%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
4	D	141	
4	d	141	
5	E	64	
5	e	64	
6	F	151	
6	f	151	
7	G	95	
7	g	95	
8	H	90	
8	h	90	
9	I	30	
9	i	30	
10	J	39	
10	j	39	
11	K	84	
11	k	84	
12	L	153	
12	l	153	
13	1	195	
13	6	195	
14	2	206	
14	7	206	
15	3	218	
15	8	218	
16	4	196	

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Mol	Chain	Length	Quality of chain
16	9	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	1	303	X	-	-	-
17	CLA	1	304	X	-	-	-
17	CLA	1	305	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	308	X	-	-	-
17	CLA	1	309	X	-	-	-
17	CLA	1	310	X	-	-	-
17	CLA	1	311	X	-	-	-
17	CLA	1	312	X	-	-	-
17	CLA	1	313	X	-	-	-
17	CLA	1	314	X	-	-	-
17	CLA	1	315	X	-	-	-
17	CLA	2	602	X	-	-	-
17	CLA	2	603	X	-	-	-
17	CLA	2	604	X	-	-	-
17	CLA	2	608	X	-	-	-
17	CLA	2	609	X	-	-	-
17	CLA	2	610	X	-	-	-
17	CLA	2	611	X	-	-	-
17	CLA	2	612	X	-	-	-
17	CLA	2	613	X	-	-	-
17	CLA	3	301	X	-	-	X
17	CLA	3	302	X	-	-	-
17	CLA	3	303	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	X
17	CLA	3	314	X	-	-	-
17	CLA	3	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	4	601	X	-	-	-
17	CLA	4	602	X	-	-	-
17	CLA	4	603	X	-	-	-
17	CLA	4	604	X	-	-	-
17	CLA	4	608	X	-	-	-
17	CLA	4	609	X	-	-	-
17	CLA	4	610	X	-	-	-
17	CLA	4	611	X	-	-	-
17	CLA	4	612	X	-	-	-
17	CLA	4	613	X	-	-	-
17	CLA	4	614	X	-	-	-
17	CLA	6	304	X	-	-	-
17	CLA	6	305	X	-	-	-
17	CLA	6	306	X	-	-	-
17	CLA	6	307	X	-	-	-
17	CLA	6	309	X	-	-	-
17	CLA	6	310	X	-	-	-
17	CLA	6	311	X	-	-	X
17	CLA	6	312	X	-	-	-
17	CLA	6	313	X	-	-	-
17	CLA	6	314	X	-	-	-
17	CLA	6	315	X	-	-	-
17	CLA	6	316	X	-	-	X
17	CLA	7	602	X	-	-	-
17	CLA	7	603	X	-	-	-
17	CLA	7	604	X	-	-	-
17	CLA	7	608	X	-	-	-
17	CLA	7	609	X	-	-	-
17	CLA	7	610	X	-	-	-
17	CLA	7	611	X	-	-	-
17	CLA	7	612	X	-	-	-
17	CLA	7	613	X	-	-	-
17	CLA	8	301	X	-	-	-
17	CLA	8	302	X	-	-	-
17	CLA	8	303	X	-	-	-
17	CLA	8	304	X	-	-	-
17	CLA	8	305	X	-	-	-
17	CLA	8	307	X	-	-	-
17	CLA	8	308	X	-	-	-
17	CLA	8	309	X	-	-	-
17	CLA	8	310	X	-	-	-
17	CLA	8	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	8	312	X	-	-	-
17	CLA	8	313	X	-	-	-
17	CLA	9	601	X	-	-	-
17	CLA	9	602	X	-	-	-
17	CLA	9	603	X	-	-	-
17	CLA	9	604	X	-	-	-
17	CLA	9	608	X	-	-	-
17	CLA	9	609	X	-	-	X
17	CLA	9	610	X	-	-	-
17	CLA	9	611	X	-	-	-
17	CLA	9	612	X	-	-	-
17	CLA	9	613	X	-	-	-
17	CLA	9	614	X	-	-	-
17	CLA	A	801	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	X
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	A	845	X	-	-	X
17	CLA	A	854	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	X
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	F	301	X	-	-	-
17	CLA	F	303	X	-	-	-
17	CLA	F	304	X	-	-	-
17	CLA	G	101	X	-	-	-
17	CLA	G	103	X	-	-	-
17	CLA	G	104	X	-	-	-
17	CLA	J	3002	X	-	-	-
17	CLA	K	4002	X	-	-	X
17	CLA	K	4003	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
17	CLA	L	204	X	-	-	-
17	CLA	a	801	X	-	-	-
17	CLA	a	802	X	-	-	-
17	CLA	a	803	X	-	-	-
17	CLA	a	804	X	-	-	-
17	CLA	a	805	X	-	-	-
17	CLA	a	806	X	-	-	-
17	CLA	a	807	X	-	-	-
17	CLA	a	808	X	-	-	-
17	CLA	a	809	X	-	-	-
17	CLA	a	810	X	-	-	-
17	CLA	a	811	X	-	-	X
17	CLA	a	812	X	-	-	-
17	CLA	a	813	X	-	-	-
17	CLA	a	814	X	-	-	-
17	CLA	a	815	X	-	-	-
17	CLA	a	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	a	817	X	-	-	-
17	CLA	a	818	X	-	-	-
17	CLA	a	819	X	-	-	-
17	CLA	a	820	X	-	-	-
17	CLA	a	821	X	-	-	-
17	CLA	a	822	X	-	-	-
17	CLA	a	823	X	-	-	-
17	CLA	a	824	X	-	-	X
17	CLA	a	825	X	-	-	-
17	CLA	a	826	X	-	-	-
17	CLA	a	827	X	-	-	-
17	CLA	a	828	X	-	-	-
17	CLA	a	829	X	-	-	-
17	CLA	a	830	X	-	-	-
17	CLA	a	831	X	-	-	-
17	CLA	a	832	X	-	-	-
17	CLA	a	833	X	-	-	-
17	CLA	a	834	X	-	-	-
17	CLA	a	835	X	-	-	-
17	CLA	a	836	X	-	-	-
17	CLA	a	837	X	-	-	-
17	CLA	a	838	X	-	-	-
17	CLA	a	839	X	-	-	-
17	CLA	a	840	X	-	-	-
17	CLA	a	841	X	-	-	-
17	CLA	a	842	X	-	-	-
17	CLA	a	843	X	-	-	-
17	CLA	a	844	X	-	-	-
17	CLA	a	846	X	-	-	-
17	CLA	a	856	X	-	-	-
17	CLA	b	802	X	-	-	-
17	CLA	b	803	X	-	-	-
17	CLA	b	804	X	-	-	-
17	CLA	b	805	X	-	-	-
17	CLA	b	806	X	-	-	-
17	CLA	b	807	X	-	-	-
17	CLA	b	808	X	-	-	-
17	CLA	b	809	X	-	-	-
17	CLA	b	810	X	-	-	-
17	CLA	b	811	X	-	-	-
17	CLA	b	812	X	-	-	-
17	CLA	b	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	b	814	X	-	-	-
17	CLA	b	815	X	-	-	-
17	CLA	b	816	X	-	-	-
17	CLA	b	817	X	-	-	-
17	CLA	b	818	X	-	-	-
17	CLA	b	819	X	-	-	-
17	CLA	b	820	X	-	-	-
17	CLA	b	821	X	-	-	-
17	CLA	b	822	X	-	-	-
17	CLA	b	823	X	-	-	-
17	CLA	b	824	X	-	-	-
17	CLA	b	825	X	-	-	-
17	CLA	b	826	X	-	-	-
17	CLA	b	827	X	-	-	-
17	CLA	b	828	X	-	-	-
17	CLA	b	829	X	-	-	-
17	CLA	b	830	X	-	-	-
17	CLA	b	831	X	-	-	-
17	CLA	b	832	X	-	-	-
17	CLA	b	833	X	-	-	-
17	CLA	b	834	X	-	-	-
17	CLA	b	835	X	-	-	-
17	CLA	b	836	X	-	-	-
17	CLA	b	837	X	-	-	-
17	CLA	b	838	X	-	-	-
17	CLA	b	839	X	-	-	-
17	CLA	b	840	X	-	-	-
17	CLA	b	841	X	-	-	-
17	CLA	f	7002	X	-	-	-
17	CLA	f	7003	X	-	-	-
17	CLA	g	101	X	-	-	-
17	CLA	g	102	X	-	-	X
17	CLA	g	103	X	-	-	-
17	CLA	j	3002	X	-	-	-
17	CLA	k	1401	X	-	-	-
17	CLA	k	1402	X	-	-	-
17	CLA	k	1403	X	-	-	-
17	CLA	l	202	X	-	-	X
17	CLA	l	203	X	-	-	-
17	CLA	l	204	X	-	-	-
18	PQN	B	842	-	-	-	X
19	LHG	1	319	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	LHG	6	320	-	-	-	X
20	BCR	1	318	-	-	-	X
20	BCR	2	617	-	-	-	X
20	BCR	4	618	-	-	-	X
20	BCR	6	319	-	-	-	X
20	BCR	7	617	-	-	-	X
20	BCR	9	618	-	-	-	X
20	BCR	A	849	-	-	-	X
20	BCR	A	850	-	-	-	X
20	BCR	B	844	-	-	-	X
20	BCR	K	4001	-	-	-	X
20	BCR	K	4004	-	-	-	X
20	BCR	L	206	-	-	-	X
20	BCR	a	852	-	-	-	X
20	BCR	g	104	-	-	-	X
20	BCR	l	205	-	-	-	X
20	BCR	l	206	-	-	-	X
22	HTG	f	7001	-	-	-	X
25	LMG	4	620	-	-	-	X
26	CHL	1	302	X	-	-	-
26	CHL	2	601	X	-	-	-
26	CHL	2	606	-	-	-	X
26	CHL	4	605	X	-	-	-
26	CHL	6	303	X	-	-	-
26	CHL	7	601	X	-	-	-
26	CHL	9	605	X	-	-	-
27	LUT	6	317	-	-	-	X
27	LUT	6	321	-	-	-	X
27	LUT	7	615	-	-	-	X

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 71157 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	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			
1	a	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5863	3853	1002	994	14			
2	b	733	Total	C	N	O	S	0	0	0
			5863	3853	1002	994	14			

- 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
			611	379	107	114	11			
3	c	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1114	716	193	202	3			
4	d	140	Total	C	N	O	S	0	0	0
			1107	712	192	200	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	63	Total	C	N	O	0	0	0
			507	321	90	96			
5	e	63	Total	C	N	O	0	0	0
			506	322	90	94			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	151	Total	C	N	O	S	0	0	0
			1193	776	204	210	3			
6	f	151	Total	C	N	O	S	0	0	0
			1193	776	204	210	3			

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			741	480	121	140			
7	g	95	Total	C	N	O	0	0	0
			737	478	121	138			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	90	Total	C	N	O	0	0	0
			678	439	110	129			
8	h	90	Total	C	N	O	0	0	0
			682	442	111	129			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			221	153	33	34	1			
9	i	30	Total	C	N	O	S	0	0	0
			226	156	34	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total	C	N	O	S	0	0	0
			311	211	48	51	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	j	39	Total	C	N	O	S	0	0	0
			311	211	48	51	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	45	Total	C	N	O	S	0	0	0
			311	204	48	56	3			
11	k	46	Total	C	N	O	S	0	0	0
			316	207	49	57	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	153	Total	C	N	O	S	0	0	0
			1136	746	183	206	1			
12	l	151	Total	C	N	O	S	0	0	0
			1122	738	180	203	1			

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1	195	Total	C	N	O	S	0	0	0
			1491	969	249	268	5			
13	6	195	Total	C	N	O	S	0	0	0
			1483	963	247	268	5			

- Molecule 14 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			
14	7	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			

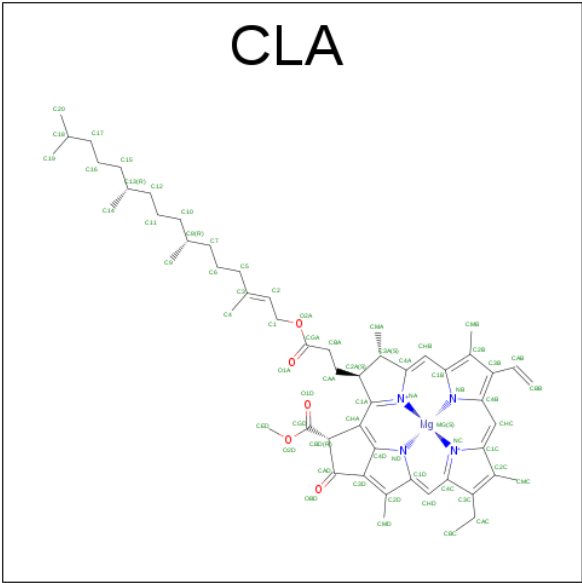
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	218	Total	C	N	O	S	0	0	0
			1680	1100	273	302	5			
15	8	217	Total	C	N	O	S	0	0	0
			1672	1094	272	301	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	4	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			
16	9	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
17	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	f	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	f	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	g	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
17	g	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	g	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	j	1	Total 42	C 34	Mg 1	N 4	O 3	0	0
17	k	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	k	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	k	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	7	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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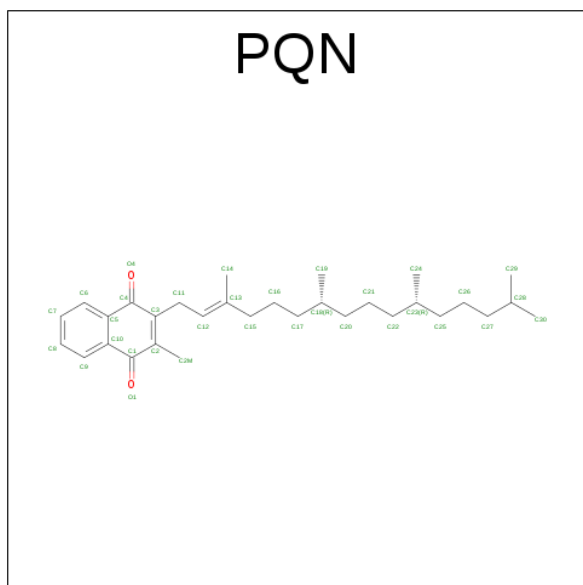
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	7	1	Total 43	C 35	Mg 1	N 4	O 3	0	0
17	8	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	8	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	8	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	8	1	Total 42	C 34	Mg 1	N 4	O 3	0	0
17	8	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
17	8	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	8	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	8	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	8	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	8	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	8	1	Total 25	C 20	Mg 1	N 4		0	0
17	9	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	9	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	9	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	9	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	9	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	9	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	9	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
17	9	1	Total 52	C 42	Mg 1	N 4	O 5	0	0

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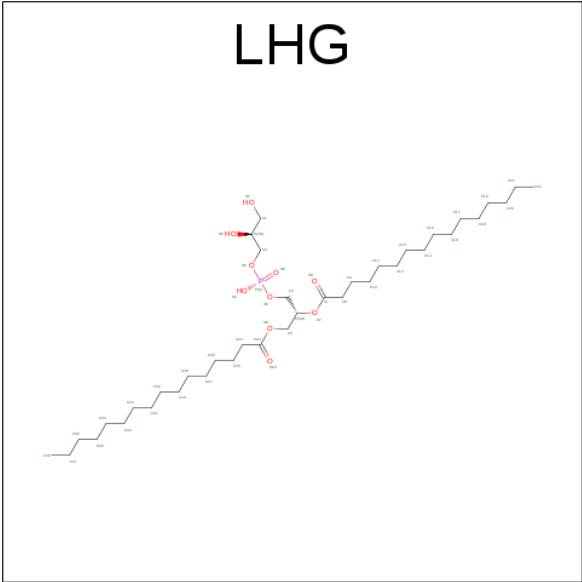
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	9	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



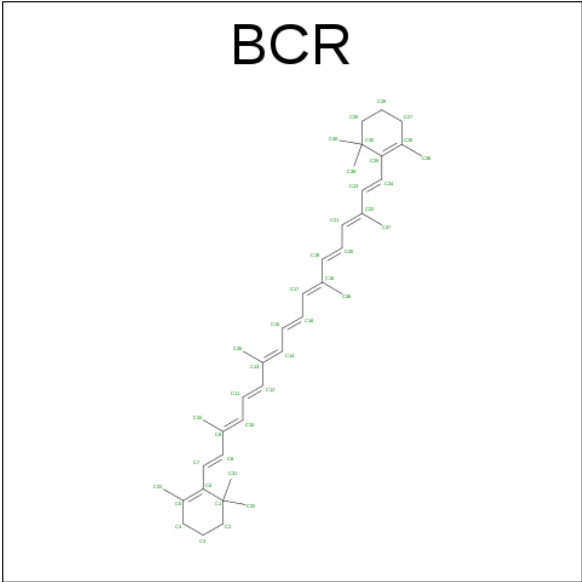
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			33	31	2		
18	B	1	Total	C	O	0	0
			33	31	2		
18	a	1	Total	C	O	0	0
			33	31	2		
18	b	1	Total	C	O	0	0
			33	31	2		

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			49	38	10	1		
19	A	1	Total	C	O	P	0	0
			27	16	10	1		
19	1	1	Total	C	O	P	0	0
			23	12	10	1		
19	1	1	Total	C	O	P	0	0
			49	38	10	1		
19	2	1	Total	C	O	P	0	0
			37	26	10	1		
19	3	1	Total	C	O	P	0	0
			20	10	9	1		
19	a	1	Total	C	O	P	0	0
			49	38	10	1		
19	a	1	Total	C	O	P	0	0
			27	16	10	1		
19	6	1	Total	C	O	P	0	0
			23	12	10	1		
19	6	1	Total	C	O	P	0	0
			49	38	10	1		
19	7	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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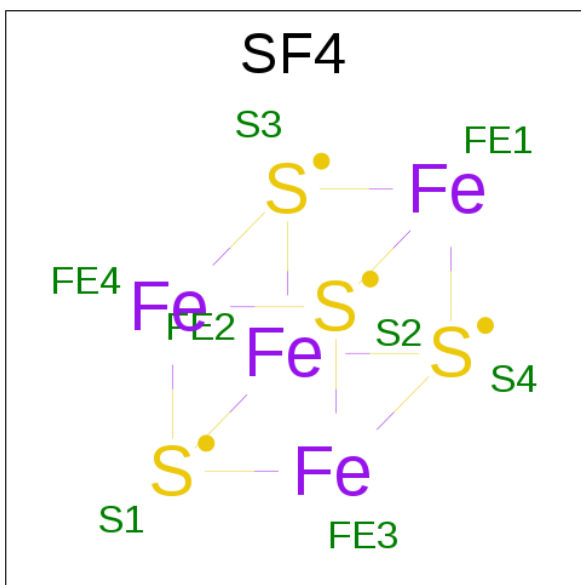
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C 40 40	0	0
20	I	1	Total C 40 40	0	0
20	J	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	1	1	Total C 40 40	0	0
20	2	1	Total C 40 40	0	0
20	3	1	Total C 40 40	0	0
20	4	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0

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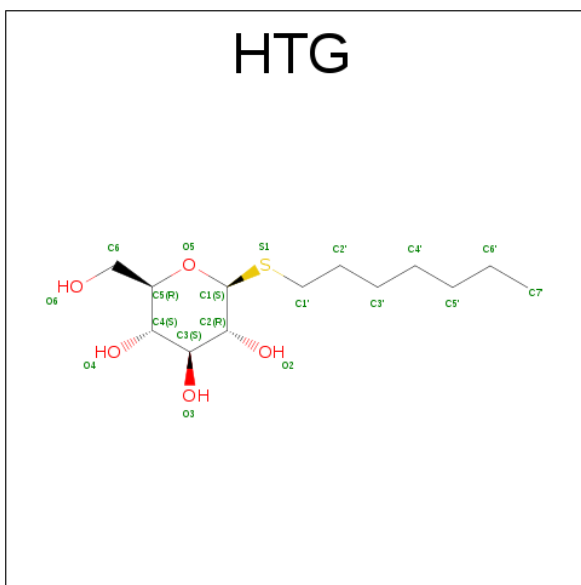
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	f	1	Total C 40 40	0	0
20	g	1	Total C 40 40	0	0
20	i	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	k	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	6	1	Total C 40 40	0	0
20	7	1	Total C 40 40	0	0
20	8	1	Total C 40 40	0	0
20	9	1	Total C 40 40	0	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



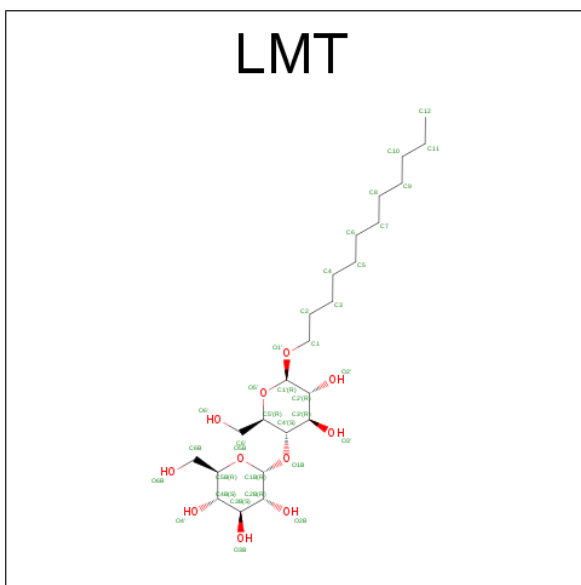
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	a	1	Total	Fe	S	0	0
			8	4	4		
21	c	1	Total	Fe	S	0	0
			8	4	4		
21	c	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 22 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



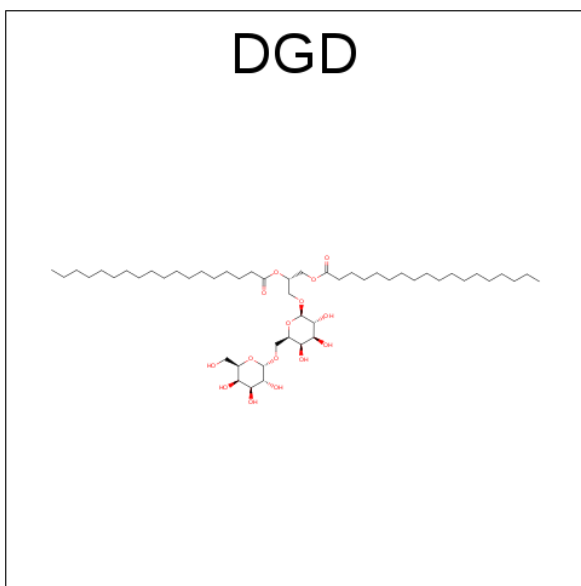
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	S	0	0
			19	13	5	1		
22	F	1	Total	C	O	S	0	0
			19	13	5	1		
22	J	1	Total	C	O	S	0	0
			19	13	5	1		
22	a	1	Total	C	O	S	0	0
			19	13	5	1		
22	f	1	Total	C	O	S	0	0
			19	13	5	1		
22	j	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



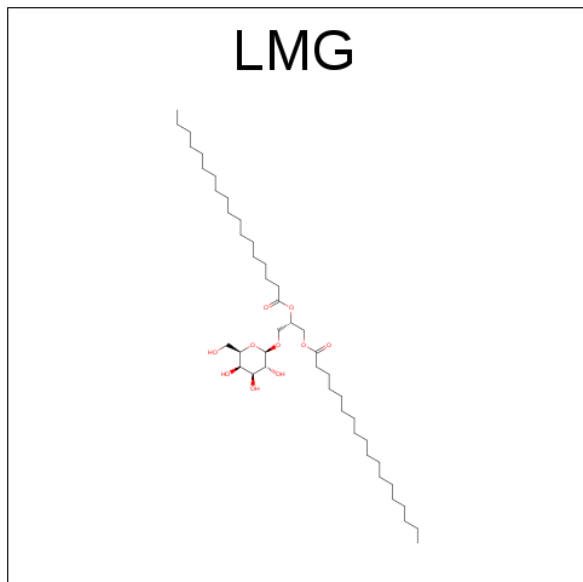
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



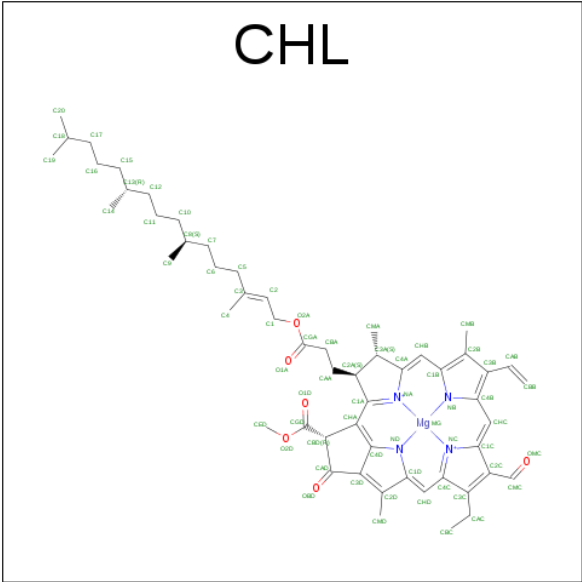
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total 66	C 51	O 15	0	0
24	b	1	Total 66	C 51	O 15	0	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	G	1	Total	C	O	0	0
			44	34	10		
25	4	1	Total	C	O	0	0
			44	34	10		
25	4	1	Total	C	O	0	0
			44	34	10		
25	6	1	Total	C	O	0	0
			40	30	10		
25	9	1	Total	C	O	0	0
			50	40	10		

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



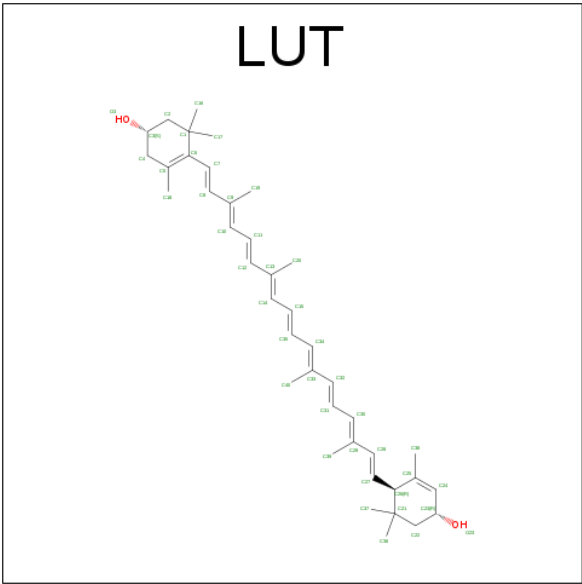
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	1	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	1	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
26	2	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	2	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
26	2	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	3	1	Total 47	C 36	Mg 1	N 4	O 6	0	0
26	4	1	Total 56	C 45	Mg 1	N 4	O 6	0	0
26	4	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	4	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	4	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	6	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	6	1	Total 47	C 36	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	7	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	7	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

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



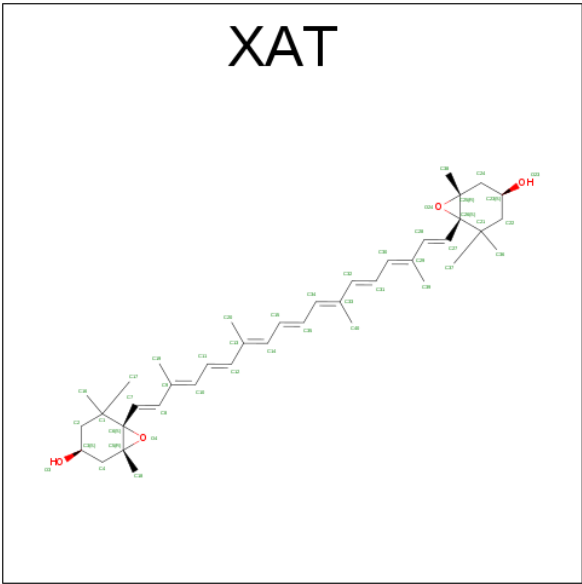
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		
27	2	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	6	1	Total	C	O	0	0
			42	40	2		
27	6	1	Total	C	O	0	0
			42	40	2		
27	7	1	Total	C	O	0	0
			42	40	2		
27	8	1	Total	C	O	0	0
			42	40	2		
27	9	1	Total	C	O	0	0
			42	40	2		

- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	1	1	Total	C	O	0	0
			44	40	4		
28	2	1	Total	C	O	0	0
			44	40	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	3	1	Total	C	O	0	0
			44	40	4		
28	4	1	Total	C	O	0	0
			44	40	4		
28	6	1	Total	C	O	0	0
			44	40	4		
28	7	1	Total	C	O	0	0
			44	40	4		
28	8	1	Total	C	O	0	0
			44	40	4		
28	9	1	Total	C	O	0	0
			44	40	4		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	29	Total	O	0	0
			29	29		
29	B	42	Total	O	0	0
			42	42		
29	C	1	Total	O	0	0
			1	1		
29	D	2	Total	O	0	0
			2	2		
29	F	5	Total	O	0	0
			5	5		
29	I	1	Total	O	0	0
			1	1		
29	L	1	Total	O	0	0
			1	1		
29	1	3	Total	O	0	0
			3	3		
29	2	4	Total	O	0	0
			4	4		
29	3	3	Total	O	0	0
			3	3		
29	4	6	Total	O	0	0
			6	6		
29	a	30	Total	O	0	0
			30	30		
29	b	32	Total	O	0	0
			32	32		

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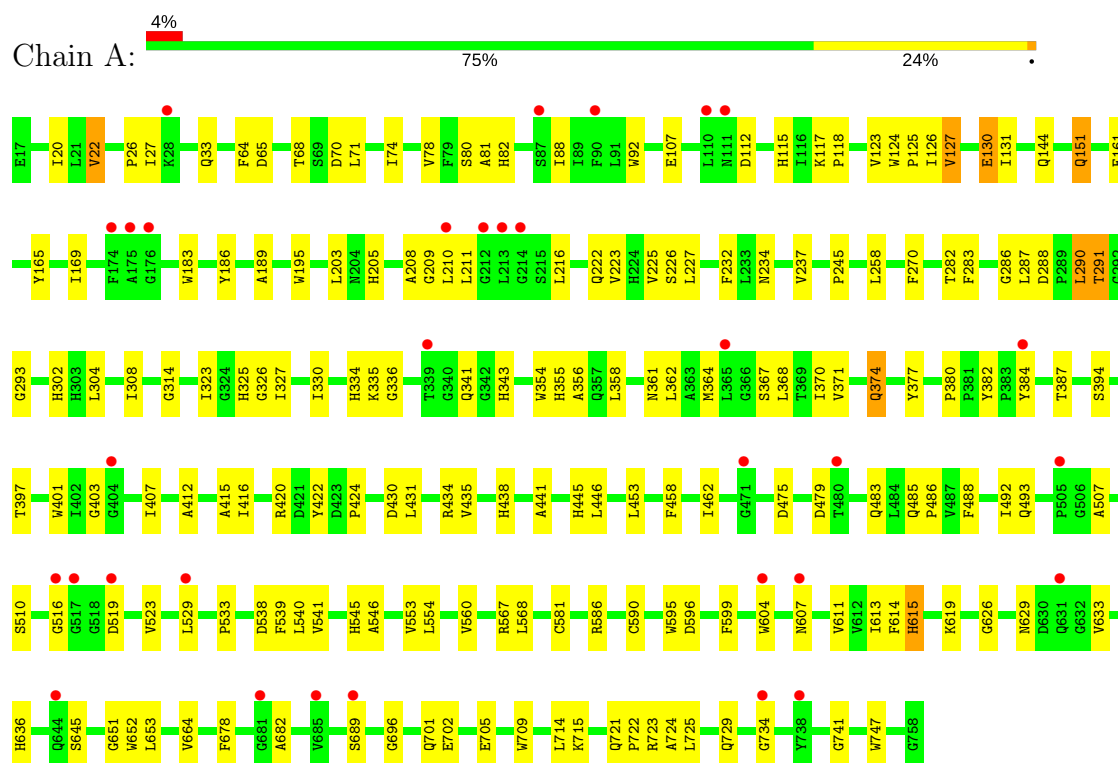
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	d	1	Total 1	O 1	0	0
29	f	4	Total 4	O 4	0	0
29	h	1	Total 1	O 1	0	0
29	l	3	Total 3	O 3	0	0
29	6	3	Total 3	O 3	0	0
29	7	6	Total 6	O 6	0	0
29	8	3	Total 3	O 3	0	0
29	9	5	Total 5	O 5	0	0

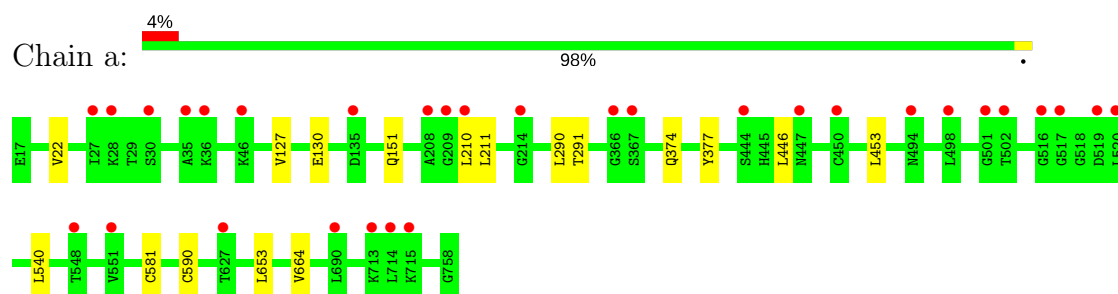
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

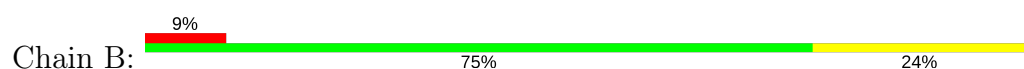
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

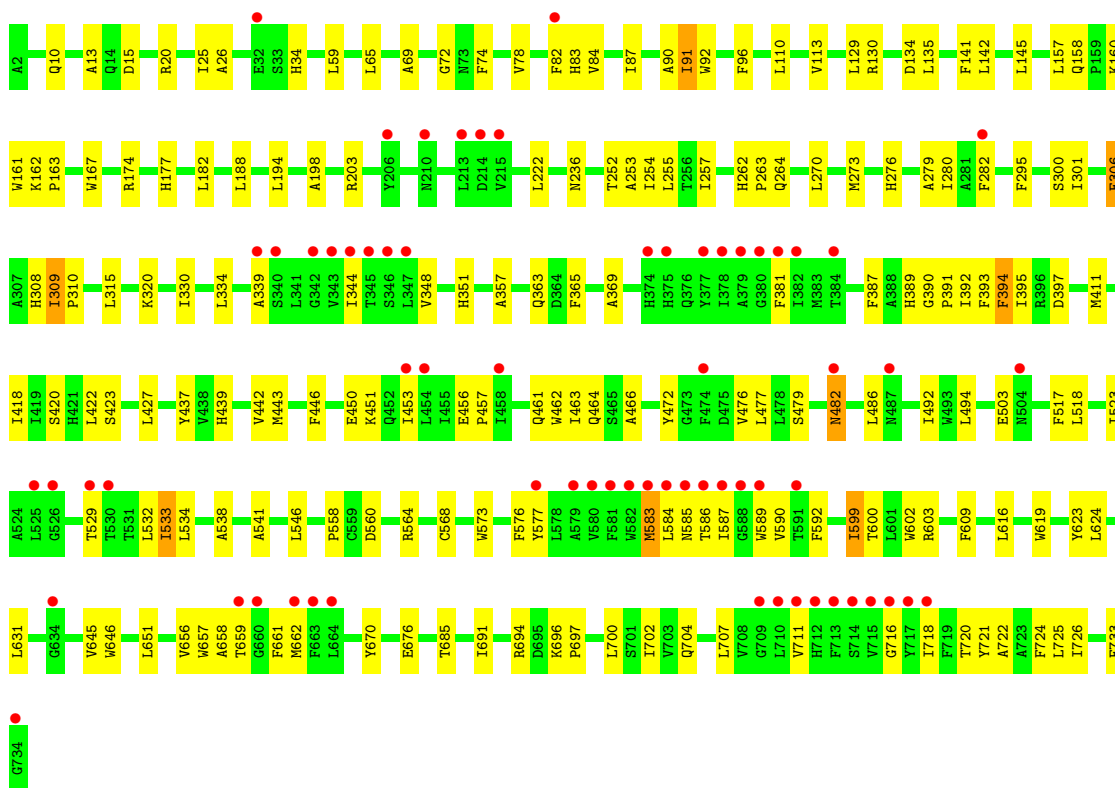


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

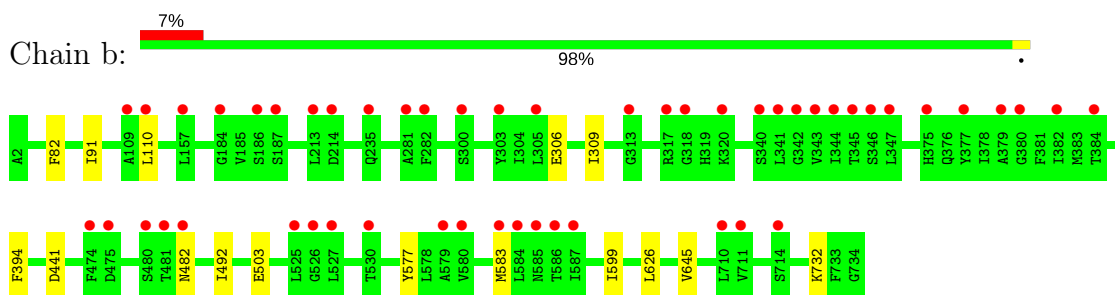


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

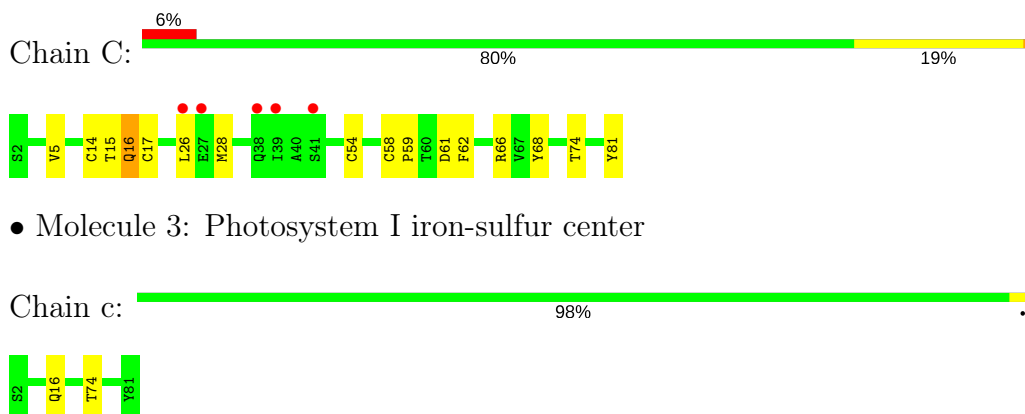




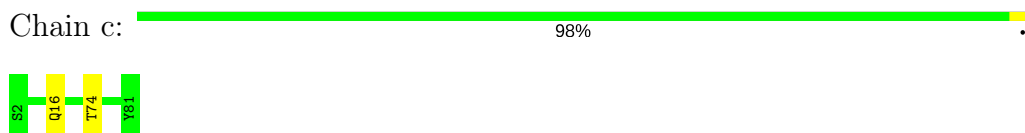
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



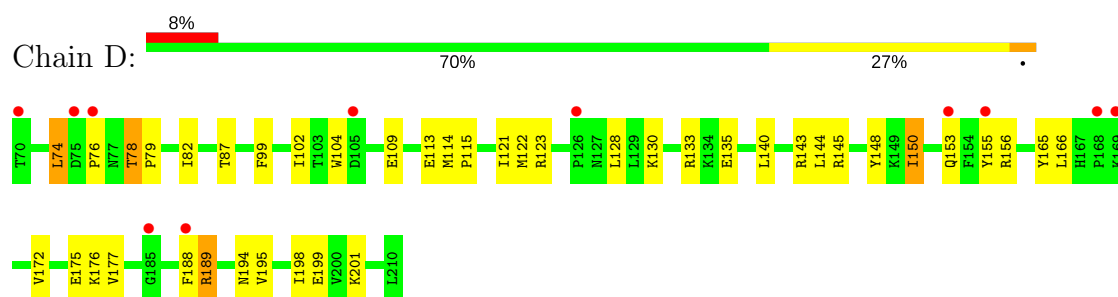
- Molecule 3: Photosystem I iron-sulfur center



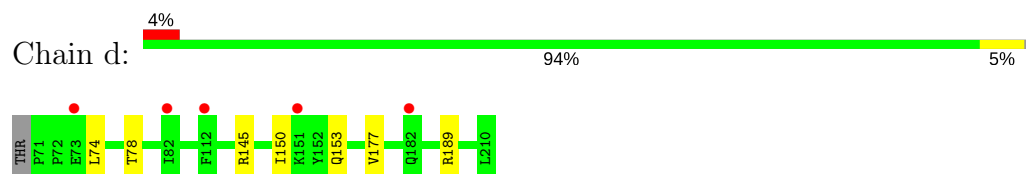
- Molecule 3: Photosystem I iron-sulfur center



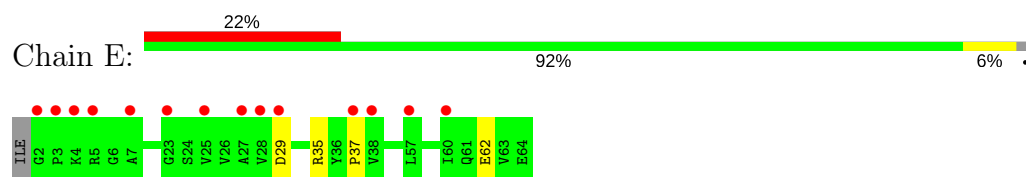
- Molecule 4: Uncharacterized protein



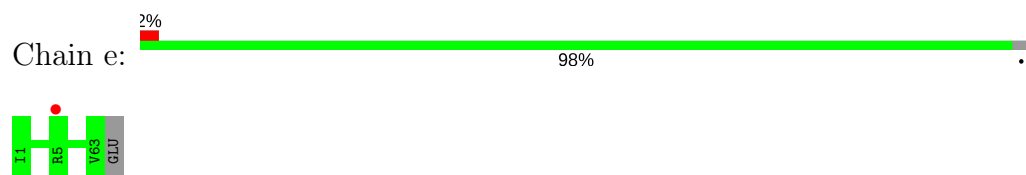
- Molecule 4: Uncharacterized protein



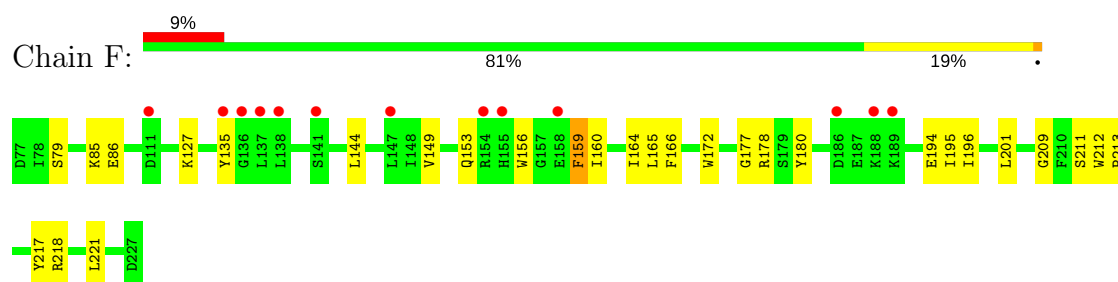
- Molecule 5: Putative uncharacterized protein



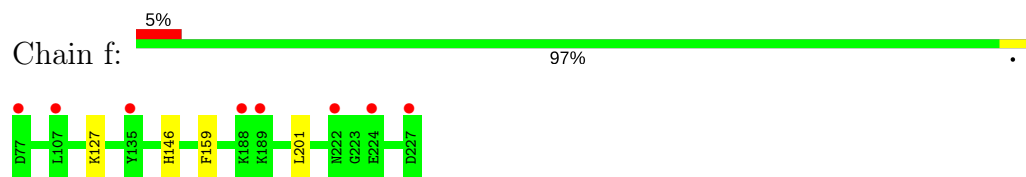
- Molecule 5: Putative uncharacterized protein



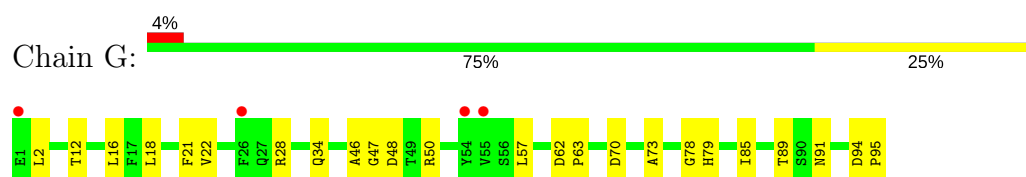
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



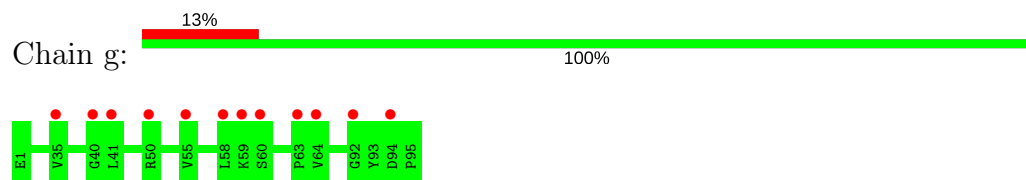
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



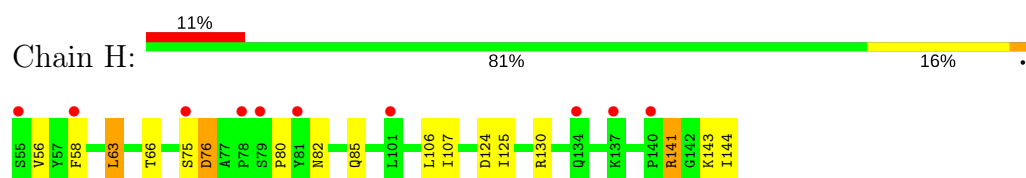
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



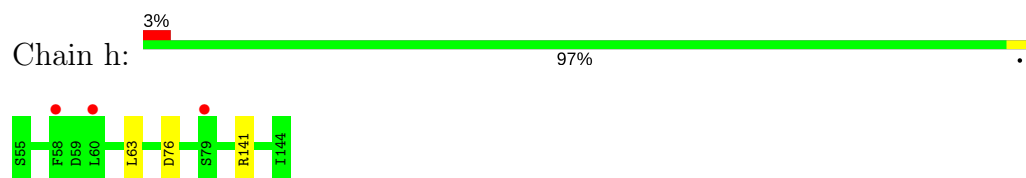
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



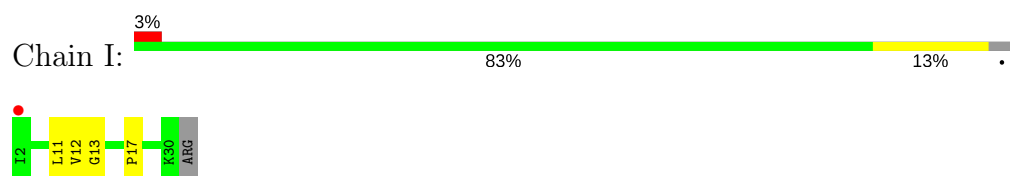
- Molecule 8: Putative uncharacterized protein



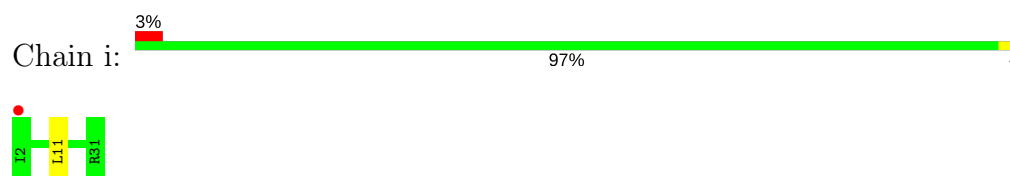
- Molecule 8: Putative uncharacterized protein



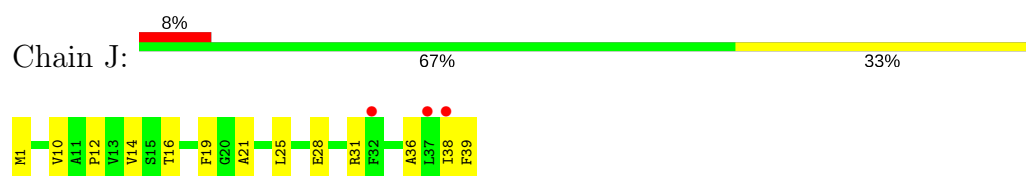
- Molecule 9: Photosystem I reaction center subunit VIII



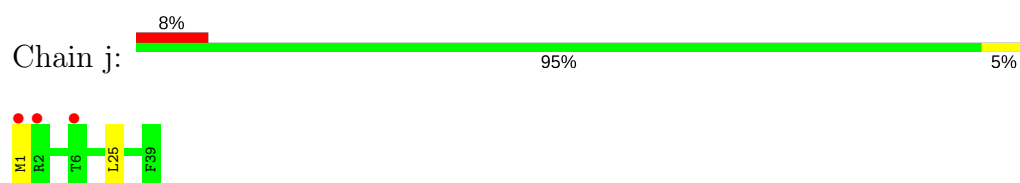
- Molecule 9: Photosystem I reaction center subunit VIII



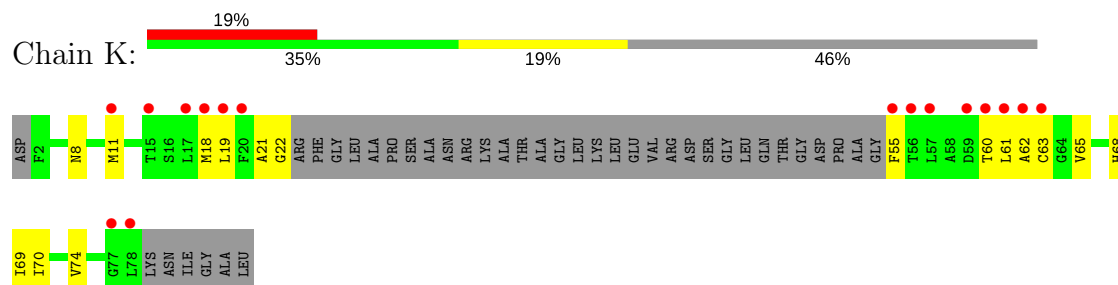
- Molecule 10: Photosystem I reaction center subunit IX



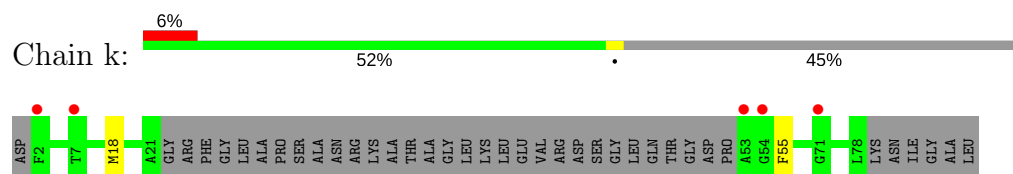
- Molecule 10: Photosystem I reaction center subunit IX



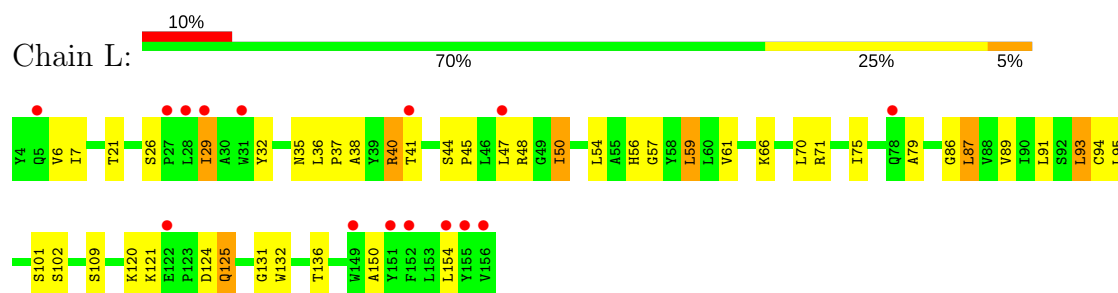
- Molecule 11: Photosystem I reaction center subunit X psaK



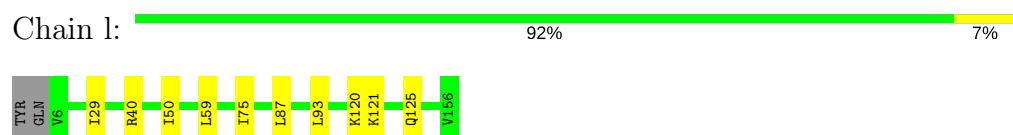
- Molecule 11: Photosystem I reaction center subunit X psaK



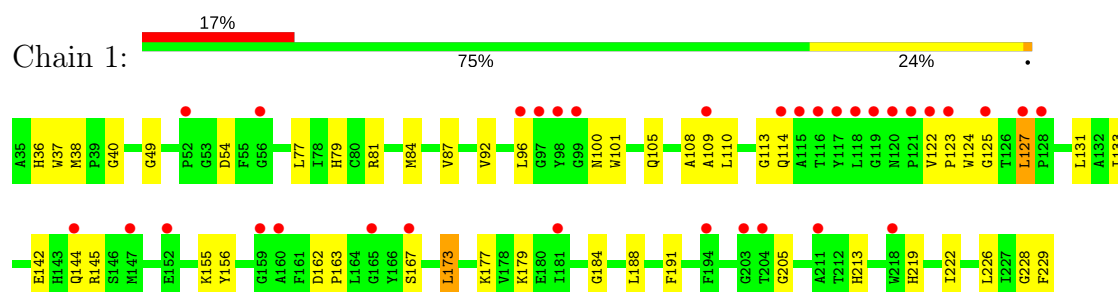
- Molecule 12: Putative uncharacterized protein



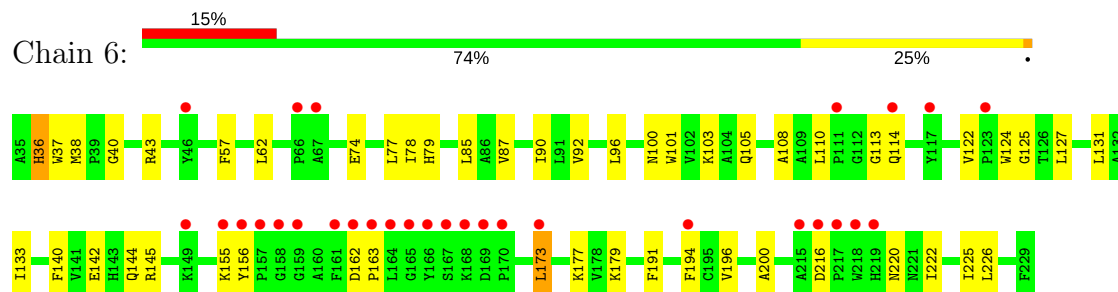
- Molecule 12: Putative uncharacterized protein



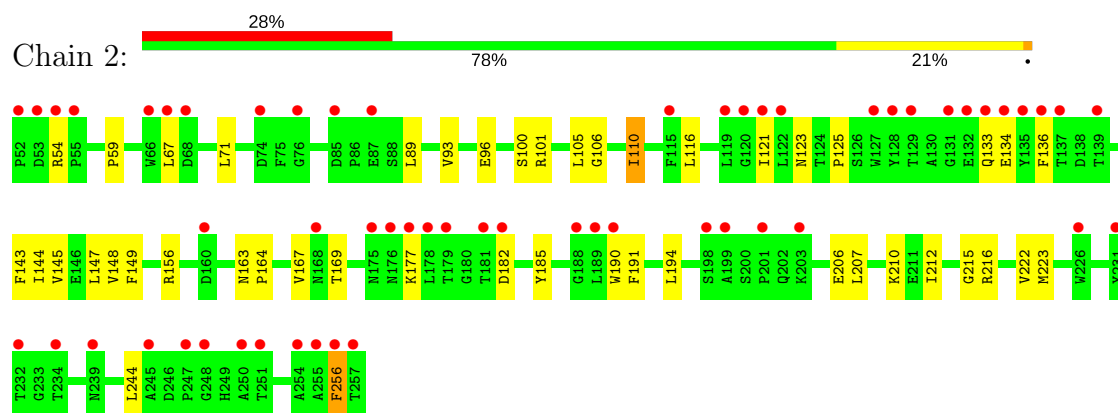
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



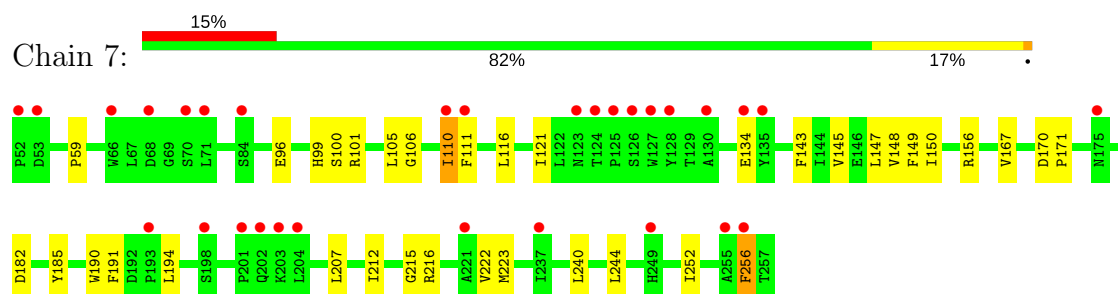
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



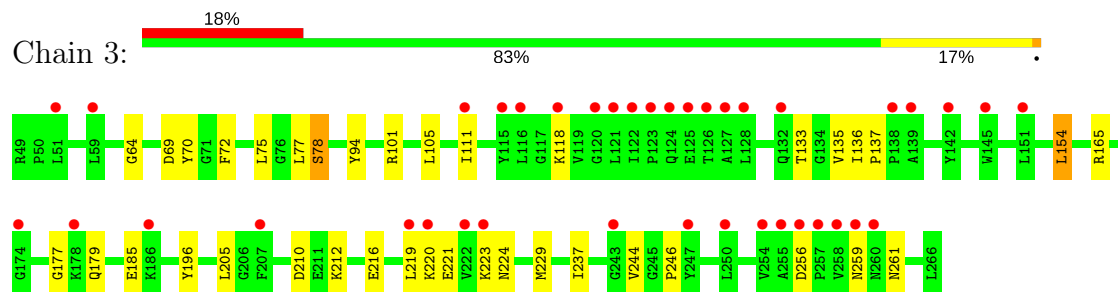
- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I



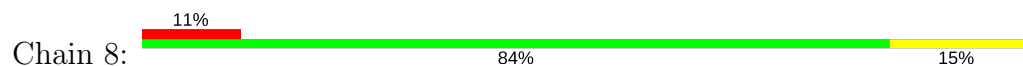
- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I

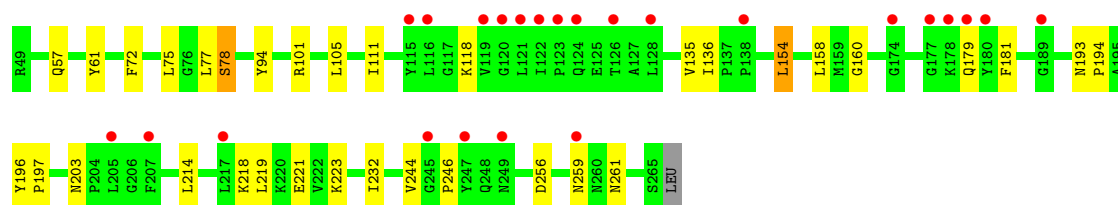


- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

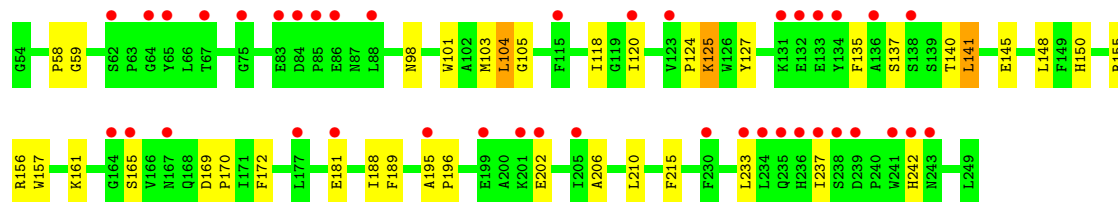
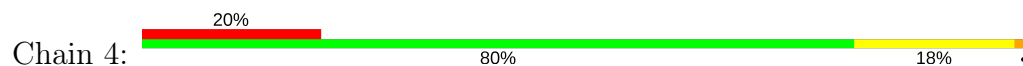


- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

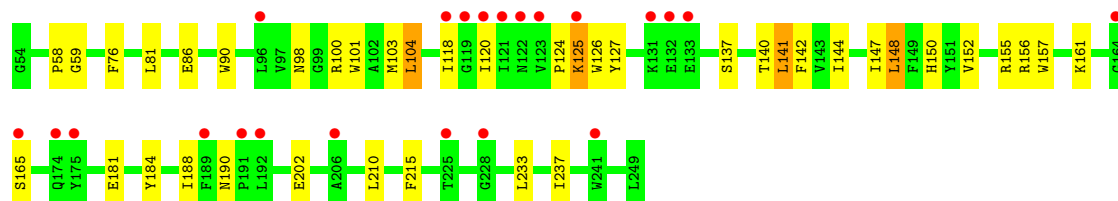
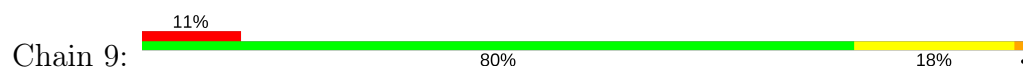




- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	165.62Å 192.22Å 175.09Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	49.15 – 2.80 49.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.80) 99.8 (49.15-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.210 , 0.248 0.211 , 0.249	Depositor DCC
R_{free} test set	13491 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	71157	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, HTG, LUT, DGD, CHL, SF4, XAT, CLA, PQN, LMT, 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	0.25	0/6043	0.41	0/8245
1	a	0.26	0/6043	0.42	0/8245
2	B	0.25	0/6077	0.42	0/8299
2	b	0.25	0/6077	0.42	0/8299
3	C	0.22	0/624	0.41	0/846
3	c	0.23	0/624	0.43	0/846
4	D	0.23	0/1143	0.42	0/1545
4	d	0.24	0/1136	0.43	0/1534
5	E	0.21	0/517	0.39	0/701
5	e	0.21	0/516	0.39	0/700
6	F	0.23	0/1221	0.40	0/1648
6	f	0.24	0/1221	0.40	0/1648
7	G	0.24	0/759	0.39	0/1033
7	g	0.24	0/755	0.40	0/1028
8	H	0.22	0/697	0.39	0/950
8	h	0.22	0/701	0.40	0/954
9	I	0.26	0/227	0.44	0/310
9	i	0.26	0/232	0.44	0/317
10	J	0.24	0/319	0.40	0/434
10	j	0.24	0/319	0.41	0/434
11	K	0.22	0/314	0.37	0/426
11	k	0.24	0/319	0.38	0/433
12	L	0.23	0/1167	0.43	0/1596
12	l	0.25	0/1153	0.44	0/1577
13	1	0.24	0/1539	0.40	0/2099
13	6	0.23	0/1531	0.38	0/2091
14	2	0.23	0/1670	0.40	0/2288
14	7	0.23	0/1670	0.39	0/2288
15	3	0.25	0/1732	0.39	0/2352
15	8	0.25	0/1724	0.39	0/2341
16	4	0.24	0/1589	0.40	0/2168
16	9	0.23	0/1589	0.39	0/2168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.24	0/51248	0.41	0/69843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5846	0	5708	155	0
1	a	5846	0	5708	0	0
2	B	5863	0	5654	168	0
2	b	5863	0	5654	0	0
3	C	611	0	591	8	0
3	c	611	0	591	0	0
4	D	1114	0	1119	27	0
4	d	1107	0	1113	0	0
5	E	507	0	504	3	0
5	e	506	0	512	0	0
6	F	1193	0	1219	23	0
6	f	1193	0	1219	0	0
7	G	741	0	728	23	0
7	g	737	0	724	0	0
8	H	678	0	670	19	0
8	h	682	0	681	0	0
9	I	221	0	240	3	0
9	i	226	0	242	0	0
10	J	311	0	326	16	0
10	j	311	0	326	0	0
11	K	311	0	324	15	0
11	k	316	0	329	0	0
12	L	1136	0	1147	38	0
12	l	1122	0	1137	0	0
13	1	1491	0	1456	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	6	1483	0	1434	45	0
14	2	1610	0	1547	33	0
14	7	1610	0	1547	32	0
15	3	1680	0	1643	27	0
15	8	1672	0	1632	24	0
16	4	1540	0	1502	35	0
16	9	1540	0	1502	40	0
17	1	683	0	659	39	0
17	2	501	0	478	35	0
17	3	650	0	494	40	0
17	4	570	0	477	35	0
17	6	648	0	593	33	0
17	7	487	0	447	33	0
17	8	567	0	436	30	0
17	9	553	0	453	37	0
17	A	2712	0	2791	277	0
17	B	2403	0	2449	240	0
17	F	165	0	154	11	0
17	G	141	0	105	12	0
17	J	42	0	31	2	0
17	K	91	0	66	6	0
17	L	180	0	183	18	0
17	a	2777	0	2862	0	0
17	b	2398	0	2439	0	0
17	f	100	0	82	0	0
17	g	137	0	101	0	0
17	j	42	0	31	0	0
17	k	137	0	99	0	0
17	l	180	0	183	0	0
18	A	33	0	46	5	0
18	B	33	0	46	2	0
18	a	33	0	46	0	0
18	b	33	0	46	0	0
19	1	72	0	90	3	0
19	2	37	0	44	3	0
19	3	20	0	14	1	0
19	6	72	0	90	5	0
19	7	37	0	44	2	0
19	A	76	0	98	7	0
19	a	76	0	98	0	0
20	1	40	0	56	4	0
20	2	40	0	56	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	3	40	0	56	3	0
20	4	40	0	56	9	0
20	6	40	0	56	7	0
20	7	40	0	56	14	0
20	8	40	0	56	7	0
20	9	40	0	56	7	0
20	A	240	0	336	38	0
20	B	280	0	392	50	0
20	F	40	0	56	6	0
20	G	40	0	56	5	0
20	I	40	0	56	7	0
20	J	40	0	56	6	0
20	K	80	0	112	6	0
20	L	120	0	168	14	0
20	a	240	0	336	0	0
20	b	280	0	392	0	0
20	f	40	0	56	0	0
20	g	40	0	56	0	0
20	i	40	0	56	0	0
20	j	80	0	112	0	0
20	k	40	0	56	0	0
20	l	120	0	168	0	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
21	a	8	0	0	0	0
21	c	16	0	0	0	0
22	A	19	0	26	0	0
22	F	19	0	26	2	0
22	J	19	0	26	0	0
22	a	19	0	26	0	0
22	f	19	0	26	0	0
22	j	19	0	26	0	0
23	B	35	0	46	2	0
24	B	66	0	96	2	0
24	b	66	0	96	0	0
25	4	88	0	122	8	0
25	6	40	0	53	3	0
25	9	50	0	73	2	0
25	G	44	0	61	2	0
26	1	109	0	90	13	0
26	2	246	0	185	16	0
26	3	47	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	4	201	0	150	11	0
26	6	108	0	88	12	0
26	7	246	0	185	19	0
26	8	47	0	31	3	0
26	9	201	0	150	12	0
27	1	84	0	112	11	0
27	2	42	0	56	6	0
27	3	42	0	56	7	0
27	4	42	0	56	5	0
27	6	84	0	112	14	0
27	7	42	0	56	9	0
27	8	42	0	56	7	0
27	9	42	0	56	5	0
28	1	44	0	56	7	0
28	2	44	0	56	6	0
28	3	44	0	56	5	0
28	4	44	0	56	5	0
28	6	44	0	56	8	0
28	7	44	0	56	6	0
28	8	44	0	56	7	0
28	9	44	0	56	8	0
29	1	3	0	0	0	0
29	2	4	0	0	0	0
29	3	3	0	0	0	0
29	4	6	0	0	0	0
29	6	3	0	0	0	0
29	7	6	0	0	0	0
29	8	3	0	0	0	0
29	9	5	0	0	0	0
29	A	29	0	0	1	0
29	B	42	0	0	0	0
29	C	1	0	0	0	0
29	D	2	0	0	0	0
29	F	5	0	0	0	0
29	I	1	0	0	0	0
29	L	1	0	0	0	0
29	a	30	0	0	0	0
29	b	32	0	0	0	0
29	d	1	0	0	0	0
29	f	4	0	0	0	0
29	h	1	0	0	0	0
29	l	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	71157	0	70537	1415	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1415) 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)
17:4:609:CLA:HBB1	27:4:616:LUT:H32	1.51	0.92
17:2:609:CLA:HBB1	27:2:615:LUT:H32	1.53	0.88
2:B:334:LEU:HD11	17:B:829:CLA:HBB1	1.54	0.88
17:3:309:CLA:HBB1	27:3:316:LUT:H32	1.55	0.87
13:1:179:LYS:HD3	17:1:312:CLA:HBA1	1.60	0.84
2:B:177:HIS:HB3	17:B:813:CLA:HBB1	1.58	0.83
17:B:806:CLA:HBB1	17:B:829:CLA:HAB	1.57	0.83
17:8:308:CLA:HBB1	27:8:314:LUT:H32	1.60	0.82
17:A:842:CLA:HHC	17:A:842:CLA:HBB1	1.87	0.82
26:7:607:CHL:HMB3	20:7:617:BCR:H16C	1.61	0.82
2:B:391:PRO:HB3	2:B:538:ALA:HA	1.68	0.80
17:F:301:CLA:HHC	17:F:301:CLA:HBB1	1.63	0.80
17:A:813:CLA:HBB1	17:A:813:CLA:HHC	1.72	0.80
17:7:608:CLA:HHC	17:7:608:CLA:HBB1	1.62	0.79
17:F:304:CLA:HMB2	20:F:305:BCR:H24C	1.63	0.79
17:8:305:CLA:HHC	17:8:305:CLA:HBB1	1.64	0.79
17:F:303:CLA:HHC	17:F:303:CLA:HBB1	1.64	0.78
17:6:313:CLA:HHC	17:6:313:CLA:HBB1	1.65	0.78
17:B:805:CLA:HBB1	17:B:805:CLA:HHC	1.90	0.77
17:1:304:CLA:HHC	17:1:304:CLA:HBB1	1.65	0.77
17:A:817:CLA:HHC	17:A:817:CLA:HBB1	1.75	0.77
17:2:608:CLA:HBB1	17:2:608:CLA:HHC	1.66	0.77
20:A:852:BCR:H362	17:A:854:CLA:H42	1.67	0.76
17:A:804:CLA:HBB2	17:A:812:CLA:H72	1.66	0.76
17:A:837:CLA:HBB1	17:A:837:CLA:HHC	1.68	0.76
17:6:311:CLA:HBB1	27:6:317:LUT:H32	1.66	0.76
17:A:806:CLA:H61	20:A:851:BCR:HC8	23.57	0.76
17:B:803:CLA:H143	20:B:848:BCR:H362	1.68	0.75
17:A:802:CLA:H122	20:A:852:BCR:H23C	1.66	0.75
20:A:848:BCR:H362	20:A:849:BCR:H21C	1.68	0.75
12:L:95:LEU:HB3	12:L:136:THR:HG22	1.69	0.75
17:B:806:CLA:HED3	17:B:806:CLA:H2	3.38	0.74
17:3:303:CLA:H2	17:3:303:CLA:HED3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:PHE:HB3	17:A:838:CLA:H11	2.14	0.74
17:A:811:CLA:H12	17:A:813:CLA:H43	1.69	0.74
17:A:806:CLA:H61	20:A:849:BCR:HC8	1.70	0.73
2:B:560:ASP:OD2	2:B:564:ARG:NH2	2.25	0.73
1:A:546:ALA:HB1	17:A:839:CLA:HMB3	1.71	0.73
17:A:819:CLA:H102	17:A:837:CLA:HBA1	1.71	0.72
2:B:282:PHE:CZ	17:B:816:CLA:HBB2	2.25	0.72
17:B:820:CLA:HBB1	17:B:820:CLA:HHC	1.96	0.72
1:A:358:LEU:HD11	17:A:831:CLA:HBB1	1.85	0.72
1:A:288:ASP:HB3	1:A:291:THR:HG22	1.71	0.72
17:A:854:CLA:H11	2:B:616:LEU:HD12	1.72	0.72
17:B:830:CLA:HBB1	17:B:841:CLA:H121	2.82	0.72
20:B:801:BCR:H323	17:B:832:CLA:HBB1	1.71	0.71
17:9:603:CLA:HHC	17:9:603:CLA:HBB1	1.72	0.71
1:A:604:TRP:CH2	17:A:803:CLA:HAB	2.26	0.71
17:A:826:CLA:HBA1	17:A:830:CLA:H193	2.13	0.71
17:A:841:CLA:HBB1	17:A:841:CLA:HHC	1.71	0.71
17:B:818:CLA:HHC	17:B:818:CLA:HBB1	1.70	0.71
12:L:94:CYS:HB3	20:L:205:BCR:H19C	1.72	0.71
17:A:828:CLA:HBB1	17:A:828:CLA:HHC	2.41	0.71
14:7:185:TYR:HB3	17:7:609:CLA:HED2	1.72	0.71
2:B:546:LEU:O	2:B:564:ARG:NH1	4.91	0.71
17:2:613:CLA:HBB1	17:2:613:CLA:HHC	1.73	0.70
2:B:707:LEU:HD22	24:B:850:DGD:HB22	1.72	0.70
1:A:714:LEU:O	6:F:178:ARG:NH1	2.27	0.70
1:A:26:PRO:HB2	1:A:27:ILE:HD12	1.81	0.70
17:A:822:CLA:HMB2	17:A:826:CLA:HMA3	1.74	0.70
18:A:844:PQN:H172	20:B:801:BCR:H382	1.72	0.70
17:B:827:CLA:HHC	17:B:827:CLA:HBB1	1.74	0.70
14:7:105:LEU:HB3	17:7:604:CLA:HBB2	1.73	0.69
17:A:808:CLA:HMB3	17:A:809:CLA:HHB	1.99	0.69
2:B:721:TYR:HB2	17:B:802:CLA:HED2	1.74	0.69
26:2:601:CHL:H2	19:2:618:LHG:H132	1.74	0.68
17:4:601:CLA:HAA1	25:4:619:LMG:H332	1.74	0.68
17:A:805:CLA:HBA2	17:A:812:CLA:H2	1.75	0.68
17:B:825:CLA:HMA1	20:B:847:BCR:H14C	1.76	0.68
1:A:747:TRP:HB2	17:A:829:CLA:HBB1	1.76	0.67
17:A:801:CLA:HBB1	17:A:854:CLA:HED1	1.76	0.67
17:A:811:CLA:HBB1	17:A:811:CLA:HHC	2.00	0.67
13:6:222:ILE:HB	17:6:314:CLA:H12	1.77	0.67
12:L:38:ALA:HB2	17:L:203:CLA:HMD1	1.86	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:PHE:CE2	17:B:816:CLA:HBB2	2.30	0.67
17:G:104:CLA:HBB1	17:G:104:CLA:HHC	1.76	0.67
17:A:836:CLA:HHC	17:A:836:CLA:HBB1	1.85	0.67
1:A:446:LEU:HD13	1:A:554:LEU:HA	5.25	0.67
17:A:842:CLA:HAC1	18:A:844:PQN:H171	1.77	0.67
13:1:133:ILE:HG21	17:1:306:CLA:HED3	1.77	0.66
26:1:302:CHL:HBB1	17:1:303:CLA:HMD2	1.76	0.66
17:A:841:CLA:H72	17:B:832:CLA:H11	5.33	0.66
4:D:189:ARG:NH1	4:D:194:ASN:OD1	2.41	0.66
17:2:604:CLA:H62	20:2:617:BCR:H402	1.78	0.66
17:B:819:CLA:HMB2	17:B:824:CLA:HMA3	1.78	0.66
17:A:804:CLA:H12	17:A:843:CLA:H52	53.95	0.66
26:2:601:CHL:HMD2	20:3:318:BCR:HC21	1.77	0.66
13:6:133:ILE:HG21	17:6:307:CLA:HED3	1.76	0.66
1:A:714:LEU:HD21	17:B:831:CLA:HBA1	1.96	0.66
26:2:614:CHL:HBB1	26:2:614:CHL:HHC	1.77	0.66
17:3:304:CLA:HBB1	20:3:318:BCR:H393	1.77	0.66
17:8:302:CLA:H2	17:8:302:CLA:HED3	1.78	0.66
17:B:836:CLA:H43	17:F:304:CLA:HBB2	1.78	0.66
12:L:35:ASN:HB3	17:L:202:CLA:HAC1	1.77	0.66
13:1:79:HIS:HD2	28:1:317:XAT:H15	1.60	0.65
1:A:343:HIS:HE1	19:A:847:LHG:HC11	1.60	0.65
17:B:828:CLA:HHC	17:B:828:CLA:HBB1	2.05	0.65
16:4:202:GLU:HG3	17:4:610:CLA:HED2	1.79	0.65
13:6:156:TYR:HB3	17:6:311:CLA:HED2	1.79	0.65
1:A:65:ASP:OD2	1:A:355:HIS:NE2	2.28	0.65
17:A:822:CLA:HBC3	17:A:828:CLA:H172	1.78	0.65
17:A:834:CLA:HMC2	17:L:204:CLA:HBB2	3.05	0.65
26:2:607:CHL:HMA1	20:2:617:BCR:H361	1.79	0.65
26:2:601:CHL:HHC	26:2:601:CHL:HBB1	1.79	0.64
17:A:805:CLA:HAB	17:A:812:CLA:H142	1.79	0.64
4:D:188:PHE:HB3	5:E:35:ARG:HH12	1.61	0.64
17:2:613:CLA:HAA2	15:3:154:LEU:HG	1.79	0.64
17:6:311:CLA:CBB	27:6:317:LUT:H32	2.27	0.64
17:8:309:CLA:H2	17:8:309:CLA:HMA2	1.78	0.64
20:A:856:BCR:H401	10:J:12:PRO:HB2	1.79	0.64
13:1:219:HIS:NE2	16:4:135:PHE:O	2.30	0.64
17:A:813:CLA:H2	15:3:75:LEU:HD13	1.80	0.64
17:A:807:CLA:H151	17:A:830:CLA:HBB2	1.79	0.64
16:4:124:PRO:HG2	17:4:604:CLA:HED3	1.79	0.64
17:B:836:CLA:HMB1	17:B:836:CLA:HBB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:6:303:CHL:HED1	16:9:155:ARG:HA	1.80	0.64
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.78	0.64
17:B:806:CLA:HMC2	20:B:844:BCR:H401	2.07	0.64
17:4:602:CLA:H61	28:4:617:XAT:H28	1.79	0.64
17:A:813:CLA:H2	15:8:75:LEU:HD13	91.67	0.63
17:A:827:CLA:H52	17:A:836:CLA:HBB2	1.80	0.63
13:1:173:LEU:HD22	13:1:177:LYS:HE3	1.80	0.63
15:3:196:TYR:HB3	17:3:309:CLA:HED2	1.81	0.63
13:6:87:VAL:HG11	27:6:317:LUT:H10	1.79	0.63
17:A:802:CLA:H191	17:A:809:CLA:H193	1.81	0.63
17:A:804:CLA:HBB1	17:A:804:CLA:HMB1	4.73	0.63
6:F:194:GLU:HA	17:F:301:CLA:HED3	1.80	0.63
17:B:807:CLA:H12	9:I:12:VAL:HG21	1.79	0.63
26:2:607:CHL:HBB2	26:2:614:CHL:C2C	2.29	0.62
26:4:605:CHL:HBA2	20:4:618:BCR:H19C	1.80	0.62
17:4:602:CLA:CBB	28:4:617:XAT:H32	2.28	0.62
17:6:314:CLA:HHC	17:6:314:CLA:HBB1	1.79	0.62
2:B:463:ILE:HD11	17:B:836:CLA:H2	1.79	0.62
17:B:841:CLA:HMB3	17:6:305:CLA:H92	124.75	0.62
4:D:156:ARG:HB2	4:D:166:LEU:HD11	1.81	0.62
17:A:841:CLA:H121	17:F:303:CLA:HAC1	1.81	0.62
13:1:87:VAL:HG11	27:1:316:LUT:H10	1.82	0.62
17:A:831:CLA:H143	19:A:846:LHG:H372	1.80	0.62
2:B:177:HIS:CG	17:B:813:CLA:HMC2	2.36	0.62
26:6:303:CHL:HBB1	17:6:304:CLA:HMD2	1.81	0.62
2:B:254:ILE:HG13	2:B:255:LEU:HG	1.81	0.62
13:1:156:TYR:HB3	17:1:310:CLA:HED2	1.81	0.62
16:4:118:ILE:HG13	16:4:120:ILE:HG12	1.81	0.62
17:9:609:CLA:CBB	27:9:616:LUT:H32	2.30	0.62
17:B:804:CLA:HBC3	17:B:829:CLA:H41	5.37	0.62
17:G:103:CLA:HHC	17:G:103:CLA:HBB1	1.81	0.62
17:A:806:CLA:H11	17:A:807:CLA:HBB1	1.80	0.62
1:A:539:PHE:HA	17:A:839:CLA:HED1	1.95	0.62
17:3:314:CLA:HBB1	17:3:314:CLA:HHC	1.80	0.62
1:A:401:TRP:HB3	17:A:829:CLA:HMC3	1.92	0.62
16:4:104:LEU:HB3	17:4:604:CLA:HBB2	1.82	0.61
12:L:32:TYR:OH	17:L:202:CLA:HBB2	1.99	0.61
17:6:314:CLA:HMB3	27:6:317:LUT:H162	1.81	0.61
17:B:840:CLA:HBB1	17:B:840:CLA:HHC	1.81	0.61
15:3:229:MET:SD	17:3:302:CLA:HBB1	2.40	0.61
17:A:807:CLA:HHB	17:A:831:CLA:HAB	1.95	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:7:602:CLA:CBB	28:7:616:XAT:H32	2.30	0.61
17:A:806:CLA:H51	17:A:814:CLA:H12	1.82	0.61
26:1:302:CHL:HED1	16:4:155:ARG:HA	1.82	0.61
17:9:602:CLA:CBB	28:9:617:XAT:H32	2.31	0.61
17:A:803:CLA:HED2	17:B:802:CLA:HBB1	1.83	0.61
17:A:833:CLA:HMB1	17:A:843:CLA:HAA2	1.82	0.61
17:B:810:CLA:HBD	17:B:810:CLA:HBA2	1.82	0.61
13:1:145:ARG:NH1	17:1:309:CLA:O1D	2.33	0.61
13:6:131:LEU:HD23	25:6:302:LMG:H121	1.83	0.61
4:D:82:ILE:HB	4:D:121:ILE:HB	1.83	0.61
17:A:809:CLA:H71	17:A:831:CLA:H171	1.82	0.61
26:7:601:CHL:HBB1	17:7:602:CLA:HMD2	1.83	0.60
2:B:26:ALA:HA	17:B:829:CLA:H43	1.82	0.60
17:B:822:CLA:HHC	17:B:841:CLA:HED1	1.83	0.60
17:B:810:CLA:HAB	9:I:13:GLY:HA3	1.93	0.60
17:A:820:CLA:H8	17:A:820:CLA:HAB	1.84	0.60
17:1:308:CLA:H11	27:1:316:LUT:H383	1.83	0.60
7:G:63:PRO:HG2	17:G:103:CLA:HBC2	28.84	0.60
14:7:149:PHE:CD2	20:7:617:BCR:H15C	2.35	0.60
1:A:415:ALA:HB2	1:A:560:VAL:HG12	1.82	0.60
15:3:261:ASN:ND2	17:3:313:CLA:O1D	2.32	0.60
17:A:843:CLA:HAB	2:B:691:ILE:HG21	1.83	0.60
4:D:113:GLU:O	4:D:143:ARG:NH1	2.35	0.60
15:3:101:ARG:NH1	15:3:221:GLU:OE2	2.35	0.60
16:9:184:TYR:HB3	17:9:609:CLA:HED2	1.82	0.60
2:B:158:GLN:HB2	2:B:161:TRP:HD1	1.69	0.60
7:G:21:PHE:HZ	17:G:103:CLA:HMC2	23.84	0.60
14:2:105:LEU:HB3	17:2:604:CLA:HBB2	1.84	0.60
6:F:135:TYR:HB3	10:J:38:ILE:HD12	1.84	0.60
17:1:310:CLA:CBB	27:1:316:LUT:H32	2.32	0.59
17:A:843:CLA:H111	17:B:839:CLA:H52	1.83	0.59
17:2:604:CLA:H2	20:2:617:BCR:H272	1.84	0.59
1:A:394:SER:HB3	17:A:829:CLA:HMA1	1.83	0.59
20:7:617:BCR:H312	25:9:619:LMG:H301	1.82	0.59
17:B:814:CLA:HMA1	20:B:845:BCR:H323	18.93	0.59
6:F:195:ILE:HG13	6:F:196:ILE:HG13	1.90	0.59
26:1:302:CHL:H8	17:1:314:CLA:H62	1.84	0.59
17:A:834:CLA:HAB	17:A:835:CLA:HHB	1.83	0.59
17:A:806:CLA:H42	20:A:851:BCR:HC31	21.86	0.59
2:B:517:PHE:HA	17:B:837:CLA:HED1	1.84	0.59
1:A:209:GLY:HA2	17:A:821:CLA:HBC1	1.97	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:LEU:HD13	17:B:814:CLA:HED3	1.94	0.59
17:2:604:CLA:HBB1	20:2:617:BCR:H393	1.85	0.59
17:3:305:CLA:HMB1	17:3:308:CLA:HBC2	1.85	0.59
26:4:606:CHL:H2	25:4:620:LMG:H322	1.84	0.59
2:B:280:ILE:HD12	17:B:818:CLA:HBB1	2.17	0.59
2:B:306:GLU:HG3	2:B:320:LYS:HG2	1.85	0.59
2:B:422:LEU:HG	17:B:838:CLA:HBB1	1.83	0.59
17:B:831:CLA:HBB1	17:B:831:CLA:HHC	1.84	0.59
17:A:841:CLA:HED2	2:B:420:SER:HB2	2.21	0.58
17:B:837:CLA:H152	20:F:305:BCR:H23C	1.85	0.58
15:3:205:LEU:HD22	27:3:316:LUT:H222	1.85	0.58
17:B:825:CLA:H42	17:B:837:CLA:HBA1	1.98	0.58
17:6:315:CLA:H42	16:9:148:LEU:HD11	1.84	0.58
17:8:301:CLA:HBB1	17:8:301:CLA:HHC	1.84	0.58
26:7:601:CHL:HMD2	20:8:316:BCR:HC21	1.85	0.58
2:B:486:LEU:HD12	2:B:494:LEU:HD13	1.85	0.58
26:2:601:CHL:HBB1	17:2:602:CLA:HMD2	1.84	0.58
17:3:302:CLA:HAC2	19:3:319:LHG:H242	1.85	0.58
14:7:212:ILE:O	14:7:216:ARG:HG2	2.04	0.58
2:B:694:ARG:NH2	12:L:101:SER:O	2.36	0.58
17:1:303:CLA:CBB	28:1:317:XAT:H32	2.34	0.58
17:3:312:CLA:HHC	17:3:312:CLA:HBB1	1.84	0.58
8:H:82:ASN:HB3	8:H:85:GLN:HB2	1.84	0.58
17:2:602:CLA:CBB	28:2:616:XAT:H32	2.34	0.58
17:B:831:CLA:HAC1	17:B:838:CLA:HBC3	1.96	0.58
17:A:830:CLA:H61	20:A:851:BCR:H342	22.61	0.58
17:B:810:CLA:H143	12:L:86:GLY:HA2	2.39	0.58
2:B:72:GLY:HA2	2:B:87:ILE:HB	1.86	0.58
14:2:191:PHE:HB3	17:2:609:CLA:HMD1	1.86	0.58
13:6:77:LEU:HD12	13:6:155:LYS:HB2	1.85	0.57
10:J:10:VAL:HG13	10:J:12:PRO:HD2	1.93	0.57
10:J:31:ARG:NH2	17:J:3002:CLA:O1D	3.77	0.57
16:9:118:ILE:HG13	16:9:120:ILE:HG12	1.85	0.57
1:A:327:ILE:HG21	17:A:826:CLA:HAC1	1.94	0.57
17:B:836:CLA:HMB2	17:B:838:CLA:HED1	1.85	0.57
2:B:83:HIS:HA	8:H:143:LYS:HG2	1.86	0.57
2:B:222:LEU:HB3	23:B:849:LMT:H4B	1.86	0.57
17:1:306:CLA:HAA1	20:1:318:BCR:H383	1.85	0.57
17:8:301:CLA:HBB2	28:8:315:XAT:H34	1.86	0.57
14:2:169:THR:HG22	14:2:177:LYS:HG2	1.85	0.57
14:7:194:LEU:HD12	27:7:615:LUT:H222	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:834:CLA:HBA2	17:B:835:CLA:HMB3	2.33	0.57
17:A:843:CLA:H161	12:L:91:LEU:HD21	1.87	0.57
2:B:282:PHE:CD2	17:B:816:CLA:HBB2	2.76	0.57
17:F:301:CLA:H42	10:J:14:VAL:HG12	1.86	0.57
13:1:222:ILE:HD12	17:1:313:CLA:H43	1.86	0.57
14:2:212:ILE:O	14:2:216:ARG:HG2	2.05	0.57
14:7:147:LEU:HA	17:7:608:CLA:HBB2	1.86	0.57
26:9:607:CHL:H12	27:9:616:LUT:H383	1.87	0.57
15:3:216:GLU:HG2	15:3:220:LYS:HE3	1.85	0.57
26:1:302:CHL:OBD	16:4:155:ARG:NH1	2.37	0.57
13:6:173:LEU:HD22	13:6:177:LYS:HE3	1.87	0.57
26:9:605:CHL:HBA2	20:9:618:BCR:H21C	1.85	0.57
16:9:190:ASN:OD1	27:9:616:LUT:O23	2.22	0.56
2:B:662:MET:HB2	17:B:803:CLA:C1C	2.35	0.56
1:A:397:THR:HG23	1:A:613:ILE:HG21	1.91	0.56
17:A:808:CLA:H102	17:A:810:CLA:H92	1.88	0.56
17:A:805:CLA:H42	17:A:812:CLA:HMC2	1.85	0.56
2:B:339:ALA:HB2	20:B:847:BCR:H372	1.87	0.56
17:2:611:CLA:HHC	17:2:611:CLA:HBB1	1.87	0.56
14:2:101:ARG:NH1	26:2:607:CHL:OBD	2.37	0.56
23:B:849:LMT:H61	17:G:103:CLA:HMC3	1.87	0.56
17:3:302:CLA:HBB2	28:3:317:XAT:H34	1.87	0.56
1:A:701:GLN:HE21	1:A:724:ALA:H	1.58	0.56
17:A:833:CLA:H2	17:L:203:CLA:H43	1.87	0.56
17:7:611:CLA:H2	17:7:611:CLA:HMA2	1.87	0.56
17:B:823:CLA:H51	17:B:824:CLA:H142	1.88	0.56
1:A:354:TRP:HB3	17:A:806:CLA:HAC1	1.87	0.56
17:A:807:CLA:HAB	17:A:830:CLA:HMC2	1.88	0.56
17:B:823:CLA:HBA1	20:B:846:BCR:H16C	2.34	0.56
14:2:54:ARG:NH2	14:2:67:LEU:O	2.39	0.56
17:4:604:CLA:HBB1	20:4:618:BCR:H393	1.87	0.56
1:A:567:ARG:NH1	4:D:87:THR:O	2.39	0.56
17:A:806:CLA:H151	20:A:848:BCR:H323	1.87	0.56
17:A:818:CLA:CHD	17:A:819:CLA:HBB2	2.46	0.56
17:3:303:CLA:HBB1	17:3:303:CLA:HHC	1.88	0.56
13:6:108:ALA:HB3	26:6:308:CHL:HMD3	1.88	0.56
13:6:85:LEU:HB3	17:6:306:CLA:HBB2	1.88	0.56
14:7:101:ARG:NH1	26:7:607:CHL:OBD	2.35	0.56
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.48	0.56
17:A:802:CLA:H122	17:A:843:CLA:H101	54.21	0.56
17:B:823:CLA:HBA1	20:B:846:BCR:H14C	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:145:ARG:NH1	17:6:310:CLA:O1D	2.40	0.55
15:8:101:ARG:NH1	15:8:221:GLU:OE2	2.38	0.55
16:9:104:LEU:HD13	17:9:609:CLA:HMC1	1.87	0.55
16:4:157:TRP:CE2	16:4:161:LYS:HD2	2.41	0.55
16:4:105:GLY:HA2	28:4:617:XAT:H181	1.86	0.55
14:7:143:PHE:HB2	26:7:606:CHL:HBC1	1.89	0.55
17:A:821:CLA:HMB2	11:K:61:LEU:HD22	1.89	0.55
4:D:133:ARG:NH2	4:D:135:GLU:OE1	2.37	0.55
11:K:62:ALA:HB1	20:K:4001:BCR:H403	1.89	0.55
17:3:311:CLA:HBB1	17:3:311:CLA:HHC	1.88	0.55
17:4:613:CLA:HHC	17:4:613:CLA:HBB1	1.87	0.55
13:6:37:TRP:O	26:6:303:CHL:ND	2.39	0.55
17:8:312:CLA:HHC	17:8:312:CLA:HBB1	1.88	0.55
17:A:832:CLA:CBB	17:A:840:CLA:HAB	3.59	0.55
2:B:387:PHE:HB3	2:B:534:LEU:HB3	2.02	0.55
1:A:127:VAL:HB	17:B:833:CLA:HMD1	1.88	0.55
14:2:194:LEU:HD12	27:2:615:LUT:H222	1.89	0.55
14:7:156:ARG:NH1	17:9:601:CLA:OBD	2.39	0.55
11:K:60:THR:HG21	17:3:301:CLA:H3A	1.89	0.55
17:A:804:CLA:H8	10:J:16:THR:HG22	2.02	0.55
26:2:607:CHL:HBB2	26:2:614:CHL:CMC	2.37	0.55
15:8:57:GLN:HG2	15:8:61:TYR:HE2	1.71	0.55
17:B:831:CLA:HBC3	20:F:305:BCR:H362	1.87	0.55
15:8:105:LEU:HB3	17:8:303:CLA:HBB2	1.89	0.55
17:A:804:CLA:HBB1	17:A:804:CLA:HHC	1.89	0.55
1:A:462:ILE:HG22	17:A:835:CLA:HBC2	5.06	0.55
17:B:818:CLA:HAB	17:B:818:CLA:H8	2.40	0.55
14:2:185:TYR:HB3	17:2:609:CLA:HED2	1.89	0.55
1:A:604:TRP:HH2	17:A:803:CLA:HAB	1.72	0.55
17:A:842:CLA:H112	10:J:14:VAL:HG13	13.76	0.55
17:B:826:CLA:H122	20:B:846:BCR:H373	2.14	0.55
13:1:81:ARG:NH1	17:1:308:CLA:OBD	2.35	0.55
17:2:604:CLA:HMB3	28:2:616:XAT:H162	1.88	0.55
13:6:124:TRP:NE1	17:6:307:CLA:OBD	2.22	0.55
26:6:303:CHL:OBD	16:9:155:ARG:NH1	2.40	0.55
2:B:411:MET:HE2	20:B:846:BCR:H292	2.34	0.55
17:B:808:CLA:O1A	17:B:827:CLA:HBD	2.12	0.55
17:1:313:CLA:HMB3	27:1:316:LUT:H162	1.89	0.54
16:4:101:TRP:CE2	26:4:607:CHL:HED2	2.42	0.54
1:A:533:PRO:O	1:A:619:LYS:NZ	2.60	0.54
17:A:804:CLA:HBC3	10:J:10:VAL:HG21	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:832:CLA:H18	20:F:305:BCR:H17C	1.89	0.54
17:1:315:CLA:HBA2	27:1:320:LUT:H41	1.88	0.54
26:4:606:CHL:HBC2	25:4:620:LMG:H171	1.90	0.54
7:G:63:PRO:HG2	17:G:104:CLA:HBC2	1.89	0.54
2:B:466:ALA:HB1	2:B:477:LEU:HD12	2.03	0.54
17:B:834:CLA:HBB1	17:B:834:CLA:HHC	1.88	0.54
17:6:306:CLA:H52	17:6:307:CLA:HAA2	1.89	0.54
16:9:101:TRP:CE2	26:9:607:CHL:HED2	2.43	0.54
17:A:831:CLA:H193	17:A:842:CLA:H3A	1.88	0.54
25:4:620:LMG:H332	25:4:620:LMG:H172	1.89	0.54
14:7:100:SER:HB3	14:7:215:GLY:HA3	1.90	0.54
15:8:196:TYR:HB3	17:8:308:CLA:HED2	1.88	0.54
17:8:308:CLA:HBB2	27:8:314:LUT:H34	1.89	0.54
1:A:151:GLN:NE2	1:A:384:TYR:O	2.46	0.54
2:B:203:ARG:NH2	2:B:253:ALA:O	2.41	0.54
17:9:602:CLA:H72	28:9:617:XAT:H28	1.89	0.54
2:B:92:TRP:H	17:B:809:CLA:HED2	1.99	0.54
13:6:40:GLY:HA2	16:9:165:SER:HB2	1.90	0.54
16:9:157:TRP:CE2	16:9:161:LYS:HD2	2.42	0.54
20:B:843:BCR:H321	7:G:73:ALA:HB1	1.99	0.54
17:7:604:CLA:H121	20:7:617:BCR:H372	1.89	0.54
17:8:304:CLA:HMB1	17:8:307:CLA:HBC2	1.89	0.54
1:A:125:PRO:HA	1:A:130:GLU:HG2	1.92	0.54
2:B:142:LEU:HD23	2:B:145:LEU:HD12	1.92	0.54
26:7:607:CHL:HMA1	20:7:617:BCR:H361	1.89	0.53
2:B:167:TRP:CZ2	17:B:811:CLA:HMA1	2.43	0.53
17:B:830:CLA:CBB	17:B:838:CLA:HAB	2.37	0.53
17:B:838:CLA:HBB1	17:B:838:CLA:HMB1	2.56	0.53
1:A:446:LEU:HD22	1:A:554:LEU:HB2	4.80	0.53
2:B:694:ARG:HD2	12:L:102:SER:HA	1.89	0.53
2:B:59:LEU:HD21	17:B:807:CLA:H101	3.09	0.53
1:A:222:GLN:HA	1:A:226:SER:HB2	1.96	0.53
13:1:77:LEU:HD12	13:1:155:LYS:HB2	1.90	0.53
7:G:21:PHE:HB3	20:6:319:BCR:HC42	130.55	0.53
26:7:614:CHL:HHC	26:7:614:CHL:HBB1	1.91	0.53
2:B:34:HIS:CE1	17:B:804:CLA:HED1	3.23	0.53
14:2:156:ARG:NH1	17:4:601:CLA:OBD	2.42	0.53
17:A:822:CLA:H12	17:A:825:CLA:HBA2	1.91	0.53
17:A:842:CLA:H42	10:J:14:VAL:HG12	16.11	0.53
2:B:34:HIS:HE1	17:B:804:CLA:HED1	2.42	0.53
17:8:301:CLA:HBB1	28:8:315:XAT:H32	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:8:310:CLA:HHC	17:8:310:CLA:HBB1	1.90	0.53
1:A:216:LEU:HG	17:A:816:CLA:HBB2	1.90	0.53
2:B:443:MET:SD	2:B:451:LYS:HE3	2.57	0.53
12:L:44:SER:HB3	12:L:47:LEU:HD13	5.34	0.53
17:4:609:CLA:HBB2	27:4:616:LUT:H34	1.91	0.53
17:A:839:CLA:H102	17:A:839:CLA:HMC2	1.91	0.53
2:B:129:LEU:HD12	2:B:134:ASP:HB3	1.90	0.53
17:A:808:CLA:HHB	17:A:809:CLA:HMB3	2.28	0.52
17:A:809:CLA:HAB	17:A:829:CLA:H102	1.90	0.52
12:L:154:LEU:HG	17:L:204:CLA:HED3	1.96	0.52
14:7:244:LEU:HD21	17:7:613:CLA:HMC3	1.91	0.52
17:A:801:CLA:CGD	17:A:801:CLA:HAA2	2.42	0.52
17:B:805:CLA:H93	17:B:813:CLA:H2	1.91	0.52
17:B:839:CLA:H8	17:B:840:CLA:H121	1.91	0.52
16:4:237:ILE:HD11	17:4:613:CLA:HMC3	1.92	0.52
13:6:216:ASP:OD1	13:6:220:ASN:ND2	2.42	0.52
17:A:818:CLA:H93	20:K:4004:BCR:HC22	1.92	0.52
2:B:351:HIS:ND1	17:B:817:CLA:OBD	2.41	0.52
17:B:816:CLA:O1A	7:G:91:ASN:ND2	2.32	0.52
2:B:257:ILE:HG12	17:B:817:CLA:HMB1	1.92	0.52
17:B:839:CLA:H93	20:I:101:BCR:H382	1.92	0.52
17:3:308:CLA:H2	17:3:314:CLA:HBB2	1.91	0.52
15:3:105:LEU:HB3	17:3:304:CLA:HBB2	1.91	0.52
1:A:401:TRP:CD1	17:A:829:CLA:HAB	2.44	0.52
17:B:826:CLA:H102	20:B:847:BCR:H17C	1.92	0.52
8:H:125:ILE:HG23	12:L:70:LEU:HD11	1.91	0.52
16:9:126:TRP:HB2	28:9:617:XAT:H3	1.91	0.52
2:B:308:HIS:HA	17:B:841:CLA:HMD1	1.92	0.52
17:6:304:CLA:H62	17:6:305:CLA:HMA1	1.91	0.52
27:6:321:LUT:H392	17:9:608:CLA:H2	1.90	0.52
17:A:803:CLA:O2A	2:B:651:LEU:HB3	2.10	0.52
17:A:809:CLA:HAB	17:A:829:CLA:H13	1.92	0.52
17:A:833:CLA:H43	12:L:29:ILE:HG13	2.08	0.52
17:B:815:CLA:H43	20:B:845:BCR:HC22	1.92	0.52
14:2:106:GLY:HA2	28:2:616:XAT:H181	1.91	0.52
17:B:813:CLA:H11	20:B:844:BCR:H21C	2.23	0.52
17:8:301:CLA:CBB	28:8:315:XAT:H32	2.40	0.52
1:A:595:TRP:NE1	17:A:831:CLA:HMD1	2.25	0.52
13:1:222:ILE:HG12	13:1:226:LEU:HG	1.92	0.52
26:7:605:CHL:H3A	20:7:617:BCR:H21C	1.92	0.52
17:7:609:CLA:CBB	27:7:615:LUT:H32	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TRP:CD2	17:A:810:CLA:HED3	2.45	0.52
2:B:174:ARG:HB2	17:B:813:CLA:HBC2	1.92	0.52
13:6:222:ILE:HG12	13:6:226:LEU:HG	1.92	0.51
26:9:605:CHL:HBA2	20:9:618:BCR:H19C	1.92	0.51
17:9:601:CLA:HHC	17:9:601:CLA:HBB1	1.93	0.51
1:A:225:VAL:HG13	1:A:245:PRO:HB3	2.06	0.51
1:A:629:ASN:HB3	1:A:633:VAL:HB	1.92	0.51
17:A:816:CLA:H11	20:A:849:BCR:HC41	33.49	0.51
17:B:813:CLA:H43	20:B:844:BCR:H19C	1.95	0.51
7:G:21:PHE:HZ	17:G:104:CLA:HMC2	1.76	0.51
12:L:48:ARG:NH2	12:L:124:ASP:OD1	2.52	0.51
1:A:232:PHE:HE1	1:A:258:LEU:HD11	1.75	0.51
17:A:836:CLA:HBA2	17:A:837:CLA:HMB3	2.07	0.51
17:B:819:CLA:CMB	17:B:824:CLA:HMA3	2.46	0.51
17:A:842:CLA:H201	10:J:21:ALA:HB2	9.32	0.51
13:6:162:ASP:OD1	27:6:317:LUT:O23	2.28	0.51
1:A:364:MET:HG3	17:A:826:CLA:HMB2	1.92	0.51
3:C:66:ARG:HG2	3:C:68:TYR:CZ	2.45	0.51
17:A:811:CLA:HBB2	17:A:814:CLA:HMA3	1.93	0.51
4:D:198:ILE:HD12	4:D:201:LYS:HG3	2.05	0.51
17:A:833:CLA:HBB1	17:A:839:CLA:H192	1.91	0.51
15:3:224:ASN:HD22	17:3:309:CLA:HAB	1.76	0.51
17:7:612:CLA:HBB1	17:7:612:CLA:HHC	1.92	0.51
2:B:657:TRP:CE3	17:B:802:CLA:HMA1	2.54	0.51
17:B:839:CLA:H152	17:B:840:CLA:H13	2.06	0.51
17:B:839:CLA:H193	20:I:101:BCR:H362	1.98	0.51
4:D:144:LEU:HB3	4:D:150:ILE:HG23	1.92	0.51
2:B:282:PHE:HE2	20:G:105:BCR:HC22	1.76	0.51
17:3:308:CLA:H2	17:3:314:CLA:CBB	2.41	0.51
16:9:202:GLU:HG3	17:9:610:CLA:HED2	1.93	0.51
2:B:658:ALA:O	2:B:661:PHE:HB2	2.16	0.51
2:B:694:ARG:HG3	17:B:839:CLA:HED2	1.92	0.51
17:2:609:CLA:CBB	27:2:615:LUT:H34	2.41	0.51
14:2:222:VAL:HG11	28:2:616:XAT:H12	1.93	0.51
13:6:179:LYS:HD3	17:6:313:CLA:HBA1	1.92	0.51
17:6:315:CLA:HBA1	16:9:144:ILE:HG12	1.93	0.51
16:9:156:ARG:NH1	17:9:608:CLA:O1D	2.44	0.51
17:A:827:CLA:H111	17:A:840:CLA:H71	1.93	0.51
17:A:834:CLA:C3B	17:A:835:CLA:HMB2	2.46	0.51
17:A:841:CLA:HBC1	18:A:844:PQN:H201	1.93	0.51
16:4:104:LEU:HD13	17:4:609:CLA:HMC1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:142:GLU:OE1	13:6:145:ARG:NH2	2.43	0.51
1:A:323:ILE:HB	17:A:823:CLA:HMD1	2.30	0.51
26:2:607:CHL:HMB3	20:2:617:BCR:H362	1.93	0.50
14:7:106:GLY:HA2	28:7:616:XAT:H181	1.93	0.50
14:7:148:VAL:HG23	14:7:149:PHE:HD1	1.75	0.50
1:A:232:PHE:HD2	1:A:237:VAL:HG11	1.76	0.50
1:A:596:ASP:HA	1:A:599:PHE:HB3	2.07	0.50
2:B:182:LEU:HD13	17:B:813:CLA:HBB	2.01	0.50
2:B:659:THR:N	17:B:803:CLA:HAB	2.30	0.50
17:B:818:CLA:HBB2	17:B:824:CLA:H201	2.56	0.50
16:4:169:ASP:OD2	26:4:615:CHL:NB	2.44	0.50
13:6:191:PHE:CE1	28:6:318:XAT:H10	2.46	0.50
1:A:64:PHE:CD2	17:A:806:CLA:HMC2	2.46	0.50
1:A:205:HIS:CG	17:A:814:CLA:HMC2	2.45	0.50
2:B:174:ARG:HG2	17:B:824:CLA:HMD1	2.07	0.50
17:A:803:CLA:H122	20:B:848:BCR:H12C	1.97	0.50
7:G:28:ARG:NH2	7:G:70:ASP:OD2	2.44	0.50
15:8:135:VAL:HG13	15:8:136:ILE:HG13	1.93	0.50
2:B:523:ILE:HG12	2:B:590:VAL:HG12	1.93	0.50
17:B:833:CLA:H122	6:F:165:LEU:HD11	2.24	0.50
17:9:611:CLA:HED3	17:9:611:CLA:H12	1.92	0.50
2:B:583:MET:HE1	2:B:584:LEU:HD23	1.95	0.50
4:D:130:LYS:NZ	8:H:66:THR:O	2.42	0.50
17:A:814:CLA:HBB1	17:A:814:CLA:HHC	1.92	0.50
19:1:319:LHG:HC92	20:4:618:BCR:HC32	1.92	0.50
15:8:160:GLY:HA2	17:8:307:CLA:HAB	1.93	0.50
1:A:68:THR:HG22	1:A:70:ASP:H	1.77	0.50
17:9:612:CLA:HBB1	17:9:612:CLA:HHC	1.93	0.50
1:A:20:ILE:HD13	17:A:811:CLA:HAA2	1.93	0.50
1:A:538:ASP:OD1	1:A:619:LYS:HE3	2.17	0.50
17:B:819:CLA:O1A	17:B:824:CLA:HAB	4.56	0.50
15:8:261:ASN:ND2	17:8:311:CLA:O1D	2.38	0.50
1:A:80:SER:OG	1:A:186:TYR:HB2	2.12	0.50
1:A:325:HIS:HB3	1:A:330:ILE:HD11	1.94	0.50
1:A:343:HIS:CD2	17:A:825:CLA:ND	2.80	0.50
17:B:822:CLA:HAB	20:B:846:BCR:H321	1.94	0.50
4:D:128:LEU:HD21	8:H:58:PHE:HD2	1.80	0.50
14:2:147:LEU:HA	17:2:608:CLA:HBB2	1.94	0.50
13:6:216:ASP:OD1	13:6:216:ASP:N	2.42	0.50
17:8:303:CLA:HBB1	20:8:316:BCR:H393	1.94	0.50
11:K:74:VAL:HG22	17:K:4002:CLA:HBB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:125:PRO:HD2	17:2:604:CLA:HED2	1.94	0.49
17:3:309:CLA:CBB	27:3:316:LUT:H32	2.37	0.49
1:A:291:THR:HG23	1:A:293:GLY:H	1.77	0.49
17:A:820:CLA:HMB2	17:A:820:CLA:H43	2.04	0.49
2:B:301:ILE:HG21	17:B:824:CLA:HAC1	1.93	0.49
17:B:841:CLA:HMC3	17:1:304:CLA:H12	1.94	0.49
1:A:475:ASP:OD1	12:L:71:ARG:NH2	2.45	0.49
17:7:611:CLA:H12	17:7:611:CLA:HED3	1.93	0.49
1:A:126:ILE:HG23	20:A:856:BCR:H322	1.93	0.49
17:A:841:CLA:HBC3	17:F:301:CLA:C1C	2.41	0.49
13:1:222:ILE:HB	17:1:313:CLA:H12	1.93	0.49
13:1:105:GLN:NE2	28:1:317:XAT:H21	2.27	0.49
14:7:105:LEU:HB3	17:7:604:CLA:CBB	2.40	0.49
1:A:493:GLN:HB3	1:A:516:GLY:H	1.92	0.49
17:B:827:CLA:H122	17:B:829:CLA:H192	6.43	0.49
17:1:313:CLA:HBB1	17:1:313:CLA:HHC	1.94	0.49
13:6:36:HIS:HB3	13:6:43:ARG:HH11	1.76	0.49
12:L:50:ILE:O	12:L:54:LEU:HB2	2.16	0.49
17:3:303:CLA:HMD2	17:3:308:CLA:C1D	2.42	0.49
2:B:381:PHE:HB3	17:B:806:CLA:H112	1.95	0.49
17:B:839:CLA:HAA1	20:L:205:BCR:H362	2.08	0.49
7:G:16:LEU:HB3	17:G:103:CLA:HMB1	10.90	0.49
17:2:611:CLA:H12	17:2:611:CLA:HED3	1.94	0.49
20:2:617:BCR:H312	17:4:610:CLA:HMC3	1.94	0.49
2:B:365:PHE:HB3	2:B:602:TRP:CZ3	2.47	0.49
14:2:206:GLU:HG3	14:2:210:LYS:HE3	1.95	0.49
26:6:303:CHL:H2	26:6:303:CHL:H62	1.56	0.49
17:A:843:CLA:HBB1	17:A:843:CLA:HHC	2.59	0.49
2:B:457:PRO:HG3	2:B:517:PHE:HB2	1.95	0.49
6:F:172:TRP:CD1	6:F:209:GLY:HA3	2.50	0.49
14:2:100:SER:HB3	14:2:215:GLY:HA3	1.95	0.49
15:8:219:LEU:HG	15:8:223:LYS:HE3	1.93	0.49
17:A:803:CLA:OBD	17:B:802:CLA:HMB3	2.12	0.49
17:A:807:CLA:HMD1	17:A:812:CLA:H141	1.94	0.49
2:B:558:PRO:HB3	2:B:702:ILE:HD12	1.95	0.49
4:D:74:LEU:HD23	4:D:74:LEU:H	1.77	0.49
17:1:308:CLA:H18	17:1:308:CLA:H141	1.94	0.49
13:1:144:GLN:HG3	17:1:308:CLA:HMC3	1.94	0.49
14:2:207:LEU:HB3	17:2:609:CLA:HMA1	1.94	0.49
17:3:306:CLA:HBA2	17:3:306:CLA:H3A	1.52	0.49
17:B:817:CLA:HED2	17:B:818:CLA:H12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:7:618:LHG:H262	19:7:618:LHG:HC62	1.94	0.49
6:F:211:SER:HB3	16:9:81:LEU:HD22	113.69	0.49
17:A:806:CLA:H11	17:A:807:CLA:CBB	2.43	0.49
17:A:841:CLA:HMC3	17:A:842:CLA:C4D	15.38	0.49
17:B:825:CLA:H142	17:B:836:CLA:H13	2.74	0.49
4:D:99:PHE:HE1	8:H:63:LEU:HD11	1.78	0.49
16:4:150:HIS:CD2	17:4:608:CLA:HMB1	2.47	0.48
17:B:827:CLA:O1D	17:B:828:CLA:HMA1	2.13	0.48
12:L:54:LEU:HB3	17:L:202:CLA:HMA2	1.94	0.48
17:6:306:CLA:HBB1	20:6:319:BCR:H393	1.94	0.48
17:7:613:CLA:HAA2	15:8:154:LEU:HG	1.94	0.48
2:B:348:VAL:HG21	17:B:828:CLA:HHD	1.93	0.48
2:B:733:PHE:HB3	8:H:141:ARG:HE	1.78	0.48
17:A:824:CLA:NA	17:A:824:CLA:H12	2.50	0.48
17:A:807:CLA:HED3	17:A:831:CLA:H71	2.65	0.48
2:B:188:LEU:HG	17:B:815:CLA:CBB	2.45	0.48
13:1:162:ASP:OD1	27:1:316:LUT:O23	2.31	0.48
14:2:59:PRO:HD2	26:2:601:CHL:O1D	2.13	0.48
17:4:609:CLA:CBB	27:4:616:LUT:H32	2.36	0.48
26:7:605:CHL:HHC	26:7:605:CHL:HBB1	1.95	0.48
17:8:308:CLA:CBB	27:8:314:LUT:H32	2.36	0.48
16:9:124:PRO:HG2	17:9:604:CLA:HED3	1.96	0.48
1:A:270:PHE:HA	17:K:4003:CLA:HBC3	1.94	0.48
17:A:808:CLA:H61	17:A:808:CLA:H41	1.59	0.48
17:A:829:CLA:HBD	17:A:829:CLA:HAA1	2.01	0.48
7:G:2:LEU:HD22	7:G:89:THR:HG21	2.66	0.48
12:L:94:CYS:HB3	20:L:205:BCR:C19	2.42	0.48
13:1:108:ALA:HB3	26:1:307:CHL:HMD3	1.94	0.48
13:1:122:VAL:HG23	13:1:125:GLY:HA3	1.95	0.48
14:2:148:VAL:HG23	14:2:149:PHE:HD1	1.78	0.48
17:9:609:CLA:HBB1	27:9:616:LUT:H32	1.95	0.48
17:B:806:CLA:HED1	17:B:829:CLA:H2	1.94	0.48
17:B:825:CLA:H161	17:B:831:CLA:HBC1	2.47	0.48
17:B:836:CLA:H41	17:B:836:CLA:H62	1.63	0.48
13:1:123:PRO:HG2	13:1:124:TRP:CE3	2.49	0.48
14:7:59:PRO:HD2	26:7:601:CHL:O1D	2.13	0.48
17:7:604:CLA:HBB1	20:7:617:BCR:H393	1.94	0.48
16:9:81:LEU:HD13	17:9:602:CLA:H42	1.96	0.48
1:A:397:THR:HG22	17:A:829:CLA:HAB	2.03	0.48
17:A:815:CLA:HBB1	20:A:848:BCR:C12	2.43	0.48
17:A:819:CLA:HHC	17:A:819:CLA:HBB1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:834:CLA:H161	17:B:839:CLA:HMB2	2.23	0.48
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.57	0.48
2:B:391:PRO:HA	2:B:394:PHE:HB2	1.95	0.48
2:B:315:LEU:HD21	17:B:841:CLA:H2	2.09	0.48
6:F:85:LYS:HG3	6:F:86:GLU:HG3	1.95	0.48
16:9:150:HIS:HA	17:9:608:CLA:HAB	1.96	0.48
1:A:208:ALA:HB2	1:A:314:GLY:HA3	1.95	0.48
1:A:696:GLY:HA3	2:B:568:CYS:HB2	2.01	0.48
17:A:806:CLA:HMB3	17:A:807:CLA:HAA2	2.16	0.48
17:A:818:CLA:H91	11:K:69:ILE:HG23	1.95	0.48
2:B:141:PHE:CG	17:B:814:CLA:H12	2.49	0.48
17:A:833:CLA:H151	17:L:203:CLA:H203	1.96	0.48
15:3:237:ILE:HD12	17:3:312:CLA:HAC2	1.95	0.48
14:7:96:GLU:HG2	14:7:212:ILE:HD11	1.95	0.48
17:A:843:CLA:H61	17:A:843:CLA:H41	3.07	0.48
20:A:849:BCR:H15C	20:A:849:BCR:H351	1.80	0.48
11:K:21:ALA:HA	11:K:22:GLY:HA3	1.56	0.48
13:1:101:TRP:HE3	28:1:317:XAT:H173	1.79	0.48
14:2:244:LEU:HD21	17:2:613:CLA:HMC3	1.94	0.48
14:7:145:VAL:HG11	26:7:605:CHL:HED2	1.96	0.48
20:7:617:BCR:H15C	20:7:617:BCR:H351	1.66	0.48
1:A:287:LEU:HD21	1:A:380:PRO:HD2	2.05	0.48
1:A:595:TRP:CD1	17:A:831:CLA:HMD1	2.49	0.48
17:A:829:CLA:H161	17:A:829:CLA:H193	1.82	0.48
1:A:492:ILE:HD11	17:A:838:CLA:H12	2.42	0.48
2:B:482:ASN:O	2:B:482:ASN:ND2	2.46	0.48
2:B:276:HIS:HB2	17:B:817:CLA:C1B	2.44	0.48
17:B:825:CLA:H92	17:B:836:CLA:H41	1.97	0.48
1:A:446:LEU:HB3	1:A:554:LEU:HD13	1.99	0.48
1:A:492:ILE:HD13	17:A:836:CLA:HBB1	1.96	0.48
17:A:843:CLA:H62	17:A:843:CLA:H41	1.57	0.48
17:B:805:CLA:H3A	17:B:805:CLA:HBA1	1.58	0.48
17:B:808:CLA:HMC3	17:B:809:CLA:C3D	2.60	0.48
15:3:64:GLY:HA2	15:3:69:ASP:HB3	1.96	0.47
16:9:233:LEU:O	16:9:237:ILE:HG12	2.14	0.47
2:B:90:ALA:HA	2:B:113:VAL:HG12	1.96	0.47
8:H:107:ILE:HD11	12:L:93:LEU:HD21	1.95	0.47
17:2:609:CLA:HBB2	27:2:615:LUT:H34	1.95	0.47
16:4:58:PRO:HA	16:4:59:GLY:HA2	1.51	0.47
17:4:610:CLA:C1D	17:4:611:CLA:HMD2	2.44	0.47
17:A:834:CLA:H61	17:A:834:CLA:H41	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:802:CLA:CMD	2:B:533:ILE:HD12	2.45	0.47
17:B:825:CLA:H112	17:B:825:CLA:H142	1.81	0.47
17:B:830:CLA:HMB2	17:B:831:CLA:C2D	2.59	0.47
19:2:618:LHG:HC12	20:3:318:BCR:HC22	1.95	0.47
15:3:219:LEU:HG	15:3:223:LYS:HE3	1.96	0.47
14:7:150:ILE:HG13	26:7:605:CHL:HMB3	1.96	0.47
17:7:609:CLA:HBB1	27:7:615:LUT:H32	1.95	0.47
16:9:100:ARG:NH2	26:9:607:CHL:OBD	2.46	0.47
17:9:611:CLA:HMA2	17:9:611:CLA:H2	1.95	0.47
2:B:279:ALA:HA	17:B:816:CLA:HMC3	1.95	0.47
2:B:427:LEU:HB3	17:B:832:CLA:CED	2.55	0.47
17:B:809:CLA:H121	17:B:827:CLA:H193	1.96	0.47
20:A:856:BCR:H312	10:J:31:ARG:HD3	1.96	0.47
11:K:19:LEU:HD23	11:K:63:CYS:HB2	1.97	0.47
13:1:228:GLY:HA2	13:1:229:PHE:HA	1.71	0.47
17:3:309:CLA:H11	27:3:316:LUT:H373	1.95	0.47
2:B:576:PHE:CE1	17:B:829:CLA:HAC2	2.50	0.47
17:8:308:CLA:CBB	27:8:314:LUT:H34	2.44	0.47
26:9:605:CHL:HBA2	20:9:618:BCR:C21	2.44	0.47
1:A:117:LYS:HD3	1:A:144:GLN:OE1	2.14	0.47
17:A:854:CLA:HHB	17:B:802:CLA:H202	1.95	0.47
2:B:91:ILE:HD11	2:B:96:PHE:CZ	2.58	0.47
13:1:110:LEU:HD12	13:1:113:GLY:H	1.79	0.47
13:1:87:VAL:HG11	27:1:316:LUT:H12	1.96	0.47
13:6:100:ASN:HB3	13:6:103:LYS:HB2	1.96	0.47
17:8:305:CLA:H3A	17:8:305:CLA:HBA2	1.35	0.47
17:A:831:CLA:H61	17:A:831:CLA:H41	1.61	0.47
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.96	0.47
2:B:270:LEU:HD23	2:B:273:MET:HE3	2.18	0.47
2:B:461:GLN:HG2	2:B:472:TYR:CZ	2.72	0.47
3:C:58:CYS:HA	3:C:59:PRO:HD3	1.74	0.47
17:F:304:CLA:HED3	17:F:304:CLA:H2	1.95	0.47
14:2:96:GLU:HG2	14:2:212:ILE:HD11	1.96	0.47
16:9:215:PHE:CE1	28:9:617:XAT:H10	2.50	0.47
17:A:802:CLA:CGA	17:A:802:CLA:H3A	2.43	0.47
17:A:807:CLA:HED2	17:A:807:CLA:H61	2.22	0.47
17:A:809:CLA:HBA2	17:A:809:CLA:H3A	1.51	0.47
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.96	0.47
2:B:422:LEU:HG	17:B:838:CLA:CBB	2.44	0.47
13:1:142:GLU:OE1	13:1:145:ARG:NH2	2.48	0.47
14:7:156:ARG:HD3	26:7:607:CHL:HBB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:9:606:CHL:HHC	26:9:606:CHL:HBB1	1.96	0.47
6:F:218:ARG:NH2	16:9:86:GLU:OE1	114.97	0.47
1:A:446:LEU:HD11	1:A:553:VAL:HG12	3.86	0.47
1:A:287:LEU:HD11	1:A:529:LEU:HD12	1.97	0.47
17:A:807:CLA:HBA2	17:A:807:CLA:O1D	2.15	0.47
17:A:842:CLA:H61	17:A:842:CLA:H102	1.57	0.47
2:B:369:ALA:HB1	2:B:725:LEU:HD11	2.01	0.47
17:B:823:CLA:HMA1	17:B:841:CLA:CGD	2.45	0.47
17:2:603:CLA:H61	17:2:603:CLA:H41	1.75	0.47
15:3:135:VAL:HG13	15:3:136:ILE:HG13	1.97	0.47
20:4:618:BCR:H15C	20:4:618:BCR:H351	1.76	0.47
17:7:602:CLA:HMC2	28:7:616:XAT:C31	2.45	0.47
15:8:158:LEU:HB3	20:8:316:BCR:C16	2.44	0.47
16:9:142:PHE:HB2	26:9:606:CHL:HBC1	1.97	0.47
17:A:832:CLA:HMB2	17:A:833:CLA:C1D	2.56	0.47
2:B:599:ILE:HG23	2:B:603:ARG:HD3	2.06	0.47
17:L:202:CLA:HBA2	17:L:202:CLA:H3A	1.58	0.47
13:1:49:GLY:HA2	13:1:54:ASP:HB3	1.97	0.47
17:2:611:CLA:H2	17:2:611:CLA:HMA2	1.96	0.47
7:G:85:ILE:HG12	25:6:302:LMG:H111	133.17	0.47
15:8:232:ILE:HG21	28:8:315:XAT:H12	1.97	0.47
16:9:141:LEU:HD21	26:9:605:CHL:HMD3	1.97	0.47
17:B:809:CLA:H101	17:B:827:CLA:H171	5.14	0.47
25:G:102:LMG:H132	13:1:131:LEU:HD23	1.97	0.47
17:2:603:CLA:HMD2	17:2:608:CLA:C1D	2.44	0.47
17:8:307:CLA:H3A	17:8:307:CLA:HBA1	1.70	0.47
17:A:818:CLA:H41	17:A:818:CLA:H62	1.56	0.47
17:A:843:CLA:H12	17:A:843:CLA:C4D	4.90	0.47
17:A:802:CLA:H91	20:A:852:BCR:C22	2.45	0.47
2:B:236:ASN:OD1	2:B:252:THR:OG1	2.32	0.47
14:2:116:LEU:HD22	14:2:121:ILE:HD12	1.97	0.46
26:7:614:CHL:HBB2	20:7:617:BCR:H10C	1.97	0.46
16:9:104:LEU:HB3	17:9:604:CLA:HBB2	1.97	0.46
26:9:615:CHL:HBB2	20:9:618:BCR:HC8	1.97	0.46
1:A:130:GLU:HG3	1:A:130:GLU:H	1.40	0.46
1:A:611:VAL:HG13	29:A:906:HOH:O	45.48	0.46
17:A:813:CLA:H72	17:3:302:CLA:H102	1.97	0.46
17:A:843:CLA:H102	20:B:801:BCR:H363	55.71	0.46
2:B:670:TYR:OH	17:B:803:CLA:OBD	2.38	0.46
20:K:4001:BCR:H15C	20:K:4001:BCR:H351	1.67	0.46
17:1:314:CLA:HED3	16:4:140:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:136:PHE:O	16:4:242:HIS:NE2	2.48	0.46
20:2:617:BCR:H333	25:4:619:LMG:H301	1.95	0.46
1:A:80:SER:HB3	17:A:812:CLA:HHD	1.97	0.46
2:B:182:LEU:HD11	17:B:813:CLA:H12	2.26	0.46
2:B:587:ILE:HA	2:B:590:VAL:HG22	1.96	0.46
17:B:818:CLA:HBA2	17:B:818:CLA:H3A	1.62	0.46
17:B:827:CLA:H93	17:B:827:CLA:H111	1.79	0.46
6:F:217:TYR:CZ	6:F:221:LEU:HD11	2.72	0.46
19:2:618:LHG:H142	19:2:618:LHG:H111	1.78	0.46
17:4:608:CLA:HMB2	17:4:614:CLA:C2C	2.46	0.46
17:A:820:CLA:H92	17:A:830:CLA:H91	2.13	0.46
20:A:856:BCR:H403	10:J:16:THR:HG21	1.97	0.46
2:B:65:LEU:HD11	20:B:845:BCR:H271	1.96	0.46
17:G:101:CLA:HHC	17:G:101:CLA:HBB1	1.98	0.46
14:2:71:LEU:HD11	14:2:93:VAL:HG21	1.97	0.46
19:6:320:LHG:HC91	19:6:320:LHG:H272	1.97	0.46
14:7:149:PHE:HD2	20:7:617:BCR:H17C	1.81	0.46
14:7:191:PHE:HB3	17:7:609:CLA:HMD1	1.98	0.46
17:A:810:CLA:H122	20:J:3003:BCR:HC41	2.32	0.46
17:A:842:CLA:H41	17:A:842:CLA:H62	1.59	0.46
2:B:718:ILE:HG23	17:B:827:CLA:CBB	2.49	0.46
2:B:397:ASP:HA	4:D:198:ILE:HD13	2.04	0.46
20:1:318:BCR:H15C	20:1:318:BCR:H351	1.78	0.46
16:4:156:ARG:NH1	17:4:608:CLA:O1D	2.48	0.46
14:7:106:GLY:O	14:7:110:ILE:HG23	2.16	0.46
1:A:302:HIS:HE1	17:A:819:CLA:ND	2.14	0.46
1:A:81:ALA:HB1	17:A:806:CLA:HBB1	2.04	0.46
2:B:65:LEU:HD11	20:B:845:BCR:HC42	25.93	0.46
26:1:302:CHL:C7	20:4:618:BCR:HC7	2.45	0.46
15:8:78:SER:HB2	17:8:301:CLA:O1A	2.15	0.46
17:A:803:CLA:HBD	17:A:803:CLA:HAA2	1.99	0.46
17:B:802:CLA:HBA2	17:B:802:CLA:H3A	1.66	0.46
17:B:822:CLA:H41	17:B:822:CLA:H62	1.62	0.46
17:4:611:CLA:HMA2	17:4:611:CLA:H2	1.97	0.46
1:A:330:ILE:O	1:A:334:HIS:ND1	2.45	0.46
1:A:519:ASP:OD1	1:A:519:ASP:N	2.47	0.46
1:A:652:TRP:CE2	17:A:801:CLA:H142	2.94	0.46
12:L:66:LYS:HB2	17:L:204:CLA:HMB3	2.12	0.46
13:6:105:GLN:NE2	28:6:318:XAT:H21	2.30	0.46
17:A:803:CLA:H191	17:B:809:CLA:H2	2.30	0.46
17:A:806:CLA:HBA1	17:A:806:CLA:H3A	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:809:CLA:HMC3	17:A:810:CLA:HMD2	1.97	0.46
17:A:839:CLA:H141	17:A:839:CLA:H161	1.77	0.46
17:A:841:CLA:H193	6:F:180:TYR:HB2	2.12	0.46
17:B:816:CLA:H41	17:B:816:CLA:H62	1.81	0.46
17:G:101:CLA:HBC1	26:6:308:CHL:HMD2	134.04	0.46
13:1:191:PHE:CE1	28:1:317:XAT:H10	2.51	0.46
17:6:315:CLA:HED1	16:9:140:THR:HG23	1.98	0.46
20:6:319:BCR:H351	20:6:319:BCR:H15C	1.76	0.46
17:7:609:CLA:CBB	27:7:615:LUT:H34	2.46	0.46
2:B:74:PHE:O	2:B:78:VAL:HG13	2.19	0.46
4:D:79:PRO:HA	8:H:56:VAL:HG12	2.41	0.46
20:J:3003:BCR:H351	20:J:3003:BCR:H15C	1.77	0.46
11:K:68:HIS:CD2	20:K:4004:BCR:H12C	2.51	0.46
8:H:106:LEU:HD22	12:L:89:VAL:HG13	1.98	0.46
12:L:95:LEU:HB3	12:L:136:THR:CG2	2.53	0.46
13:6:92:VAL:HG13	13:6:96:LEU:HD23	1.98	0.46
17:A:834:CLA:H93	17:B:839:CLA:H92	2.38	0.46
17:A:839:CLA:HBB1	17:A:839:CLA:HHC	2.25	0.46
3:C:14:CYS:SG	3:C:16:GLN:HB2	2.56	0.46
7:G:89:THR:HA	25:G:102:LMG:HC62	1.97	0.46
26:1:302:CHL:H143	17:1:314:CLA:H71	1.99	0.45
17:4:608:CLA:HHC	17:4:608:CLA:HBB1	1.97	0.45
27:6:321:LUT:H15	27:6:321:LUT:H201	1.72	0.45
1:A:645:SER:O	1:A:651:GLY:HA3	2.28	0.45
17:A:804:CLA:H41	17:A:804:CLA:H61	4.30	0.45
2:B:10:GLN:HA	2:B:13:ALA:HB3	1.98	0.45
17:B:827:CLA:CGA	17:B:827:CLA:H3A	2.43	0.45
17:1:312:CLA:H62	17:1:312:CLA:H41	1.64	0.45
16:4:215:PHE:CE1	28:4:617:XAT:H10	2.51	0.45
16:4:98:ASN:ND2	17:4:608:CLA:HMD1	2.31	0.45
13:6:225:ILE:HD12	17:6:314:CLA:HMD1	1.98	0.45
17:8:308:CLA:H11	27:8:314:LUT:H373	1.98	0.45
16:9:152:VAL:HG21	20:9:618:BCR:H16C	1.98	0.45
1:A:165:TYR:O	1:A:169:ILE:HG12	2.19	0.45
17:A:839:CLA:HAA1	17:A:839:CLA:HBD	2.03	0.45
12:L:37:PRO:O	12:L:48:ARG:HD3	2.16	0.45
15:8:111:ILE:HD12	15:8:246:PRO:HG2	1.98	0.45
17:9:610:CLA:C1D	17:9:611:CLA:HMD2	2.47	0.45
1:A:286:GLY:N	1:A:510:SER:O	2.59	0.45
17:A:833:CLA:HMB2	2:B:685:THR:HG21	2.03	0.45
1:A:124:TRP:HB3	20:A:856:BCR:H323	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:LEU:HG	17:B:815:CLA:HBB2	2.00	0.45
17:A:841:CLA:H172	6:F:177:GLY:HA2	1.99	0.45
17:A:809:CLA:HAB	20:J:3003:BCR:H352	2.68	0.45
13:6:144:GLN:HG3	17:6:309:CLA:HMC3	1.98	0.45
1:A:341:GLN:HB2	1:A:430:ASP:HB2	1.98	0.45
17:A:843:CLA:NC	17:A:843:CLA:H43	3.55	0.45
17:B:832:CLA:HAA1	17:B:832:CLA:HBD	1.98	0.45
17:B:815:CLA:H143	20:B:844:BCR:HC42	1.99	0.45
25:9:619:LMG:H171	25:9:619:LMG:H142	1.76	0.45
1:A:131:ILE:HG21	2:B:446:PHE:HA	1.99	0.45
1:A:234:ASN:HB3	1:A:290:LEU:HD11	2.17	0.45
17:B:804:CLA:H3A	17:B:804:CLA:HBA2	1.64	0.45
17:B:830:CLA:HMB2	17:B:831:CLA:C3D	2.46	0.45
2:B:472:TYR:HB3	6:F:79:SER:HA	2.00	0.45
14:2:144:ILE:HG21	17:4:613:CLA:HED1	1.98	0.45
13:6:87:VAL:HG11	27:6:317:LUT:H12	1.98	0.45
16:9:58:PRO:HA	16:9:59:GLY:HA2	1.52	0.45
1:A:112:ASP:OD2	1:A:115:HIS:HB2	2.29	0.45
1:A:441:ALA:O	1:A:445:HIS:ND1	2.42	0.45
17:A:804:CLA:H111	17:A:804:CLA:H72	1.81	0.45
1:A:195:TRP:CZ2	17:A:811:CLA:HMA1	2.53	0.45
7:G:18:LEU:HA	7:G:22:VAL:HG22	1.99	0.45
17:B:833:CLA:HBA1	10:J:36:ALA:HB3	1.98	0.45
17:B:810:CLA:H42	12:L:79:ALA:HB1	4.02	0.45
17:8:309:CLA:HBB1	17:8:309:CLA:HHC	1.98	0.45
17:8:301:CLA:H72	28:8:315:XAT:H28	1.99	0.45
20:B:848:BCR:H24C	20:B:848:BCR:H371	1.86	0.45
4:D:128:LEU:HD21	8:H:58:PHE:CD2	2.54	0.45
6:F:153:GLN:HA	6:F:156:TRP:CD1	2.51	0.45
13:1:213:HIS:CG	17:1:313:CLA:HAA2	2.52	0.45
17:1:311:CLA:NB	19:1:319:LHG:O4	2.50	0.45
17:3:309:CLA:HBB2	27:3:316:LUT:H34	1.98	0.45
14:7:116:LEU:HD22	14:7:121:ILE:HD12	1.98	0.45
15:8:105:LEU:HB3	17:8:303:CLA:CBB	2.46	0.45
15:8:203:ASN:OD1	27:8:314:LUT:O23	2.32	0.45
17:A:818:CLA:H11	17:A:818:CLA:H51	2.44	0.45
17:A:829:CLA:H3A	17:A:829:CLA:HBA2	1.65	0.45
17:A:829:CLA:O1D	17:A:830:CLA:HMA1	2.16	0.45
17:A:834:CLA:HMD3	17:A:839:CLA:H13	2.25	0.45
2:B:300:SER:HB3	7:G:34:GLN:HB3	2.12	0.45
17:B:808:CLA:CGA	17:B:808:CLA:C1A	2.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:825:CLA:H3A	17:B:825:CLA:HBA2	1.67	0.45
20:G:105:BCR:H351	20:G:105:BCR:H15C	1.84	0.45
13:1:188:LEU:HD13	17:1:303:CLA:HMC3	1.98	0.45
14:2:145:VAL:HG11	26:2:605:CHL:HED2	1.98	0.45
15:3:72:PHE:HE2	28:3:317:XAT:H383	1.82	0.45
16:4:141:LEU:HD21	26:4:605:CHL:HMD3	1.99	0.45
1:A:74:ILE:O	1:A:78:VAL:HG13	2.16	0.45
17:A:819:CLA:HBA2	17:A:819:CLA:H3A	1.59	0.45
17:A:827:CLA:HMB2	17:A:840:CLA:HBA1	2.08	0.45
17:A:834:CLA:H112	18:B:842:PQN:H201	1.98	0.45
17:B:815:CLA:H3A	17:B:815:CLA:HBA1	1.84	0.45
2:B:676:GLU:HG2	3:C:81:TYR:HE1	1.82	0.45
15:3:105:LEU:HB3	17:3:304:CLA:CBB	2.47	0.45
26:7:606:CHL:HHC	26:7:606:CHL:HBB1	1.98	0.45
15:8:72:PHE:HE2	28:8:315:XAT:H383	1.81	0.45
16:9:76:PHE:HE2	28:9:617:XAT:H383	1.82	0.45
1:A:367:SER:O	1:A:371:VAL:HG13	2.17	0.45
1:A:701:GLN:NE2	1:A:723:ARG:HA	2.41	0.45
17:A:807:CLA:H93	17:A:807:CLA:H61	1.80	0.45
17:A:833:CLA:H41	17:A:833:CLA:H61	1.53	0.45
20:A:852:BCR:H20C	20:A:852:BCR:H361	1.73	0.45
2:B:631:LEU:HD22	2:B:724:PHE:HA	2.05	0.45
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.46	0.45
17:4:609:CLA:CBB	27:4:616:LUT:H34	2.47	0.44
26:7:601:CHL:HMD2	20:8:316:BCR:H323	1.99	0.44
17:A:805:CLA:H43	17:A:812:CLA:HBB1	5.12	0.44
17:A:816:CLA:HBA2	17:A:816:CLA:H3A	3.40	0.44
17:A:832:CLA:HMA2	12:L:21:THR:HG21	2.01	0.44
17:B:817:CLA:H52	17:B:817:CLA:H8	1.71	0.44
17:B:812:CLA:HED1	7:G:48:ASP:OD2	2.18	0.44
14:2:163:ASN:HA	14:2:164:PRO:HD2	1.72	0.44
17:2:610:CLA:C1D	17:2:611:CLA:HMD2	2.47	0.44
17:6:307:CLA:HMC3	26:6:308:CHL:C2C	2.47	0.44
14:7:207:LEU:HB3	17:7:609:CLA:HMA1	1.99	0.44
17:A:804:CLA:H18	17:A:842:CLA:H172	1.99	0.44
2:B:330:ILE:HG22	17:B:805:CLA:HHH	1.99	0.44
17:B:837:CLA:C1A	17:B:837:CLA:CGA	2.96	0.44
11:K:69:ILE:HG22	17:K:4002:CLA:HBC1	1.98	0.44
11:K:70:ILE:HA	17:K:4002:CLA:HBC2	1.99	0.44
16:9:125:LYS:HD3	16:9:127:TYR:CZ	2.52	0.44
16:9:98:ASN:ND2	17:9:608:CLA:OBD	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:VAL:HA	1:A:227:LEU:HD12	2.08	0.44
1:A:729:GLN:HB2	19:A:847:LHG:HC42	43.68	0.44
17:A:801:CLA:H3A	17:A:801:CLA:HBA2	1.62	0.44
17:A:827:CLA:H51	17:A:838:CLA:H51	2.83	0.44
17:A:839:CLA:H41	17:A:839:CLA:H62	1.63	0.44
17:B:824:CLA:H161	17:B:824:CLA:H122	2.37	0.44
17:B:823:CLA:HMD1	17:B:824:CLA:HMC2	1.99	0.44
4:D:172:VAL:HG13	4:D:176:LYS:HE3	1.99	0.44
6:F:149:VAL:HG12	6:F:159:PHE:HB2	2.09	0.44
27:1:320:LUT:H191	27:1:320:LUT:H11	1.86	0.44
17:6:305:CLA:HED2	17:6:305:CLA:H43	1.99	0.44
17:6:310:CLA:H3A	17:6:310:CLA:HBA1	1.71	0.44
14:7:99:HIS:CE1	17:7:608:CLA:HMD1	2.51	0.44
17:8:302:CLA:HMD2	17:8:307:CLA:C1D	2.47	0.44
20:8:316:BCR:H11C	20:8:316:BCR:H341	1.83	0.44
1:A:183:TRP:HB2	17:A:812:CLA:HMC3	1.99	0.44
17:A:820:CLA:H12	17:A:820:CLA:CHB	2.48	0.44
1:A:725:LEU:HD11	17:A:842:CLA:HMD3	1.99	0.44
1:A:335:LYS:O	17:A:845:CLA:HBC3	2.16	0.44
17:B:832:CLA:H162	17:B:832:CLA:H121	2.01	0.44
20:B:846:BCR:H341	20:B:846:BCR:H11C	1.89	0.44
8:H:76:ASP:N	8:H:76:ASP:OD1	2.53	0.44
17:A:834:CLA:CAD	20:L:201:BCR:H10C	2.47	0.44
14:2:106:GLY:O	14:2:110:ILE:HG23	2.18	0.44
17:3:302:CLA:H41	17:3:302:CLA:H61	1.58	0.44
20:2:617:BCR:H313	17:4:610:CLA:CBB	2.47	0.44
26:7:601:CHL:CBB	17:7:602:CLA:HMD2	2.46	0.44
1:A:22:VAL:HG11	1:A:189:ALA:HB1	2.16	0.44
1:A:302:HIS:CE1	17:A:819:CLA:ND	2.85	0.44
17:B:817:CLA:H3A	17:B:817:CLA:HBA2	1.71	0.44
20:B:845:BCR:H24C	20:B:845:BCR:H371	1.57	0.44
14:2:105:LEU:HB3	17:2:604:CLA:CBB	2.48	0.44
17:2:612:CLA:HBB1	17:2:612:CLA:HHC	2.00	0.44
26:4:606:CHL:H3A	26:4:606:CHL:HBA2	1.39	0.44
16:4:150:HIS:HA	17:4:608:CLA:HAB	2.00	0.44
13:6:87:VAL:HG22	13:6:194:PHE:HE2	1.83	0.44
17:8:309:CLA:H41	17:8:309:CLA:H62	1.73	0.44
16:9:150:HIS:CD2	17:9:608:CLA:HMB1	2.53	0.44
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.99	0.44
17:B:822:CLA:H41	17:B:822:CLA:H61	2.99	0.44
17:B:821:CLA:CAD	20:B:843:BCR:H312	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:124:ASP:OD1	8:H:130:ARG:NH2	2.73	0.44
20:1:318:BCR:H24C	20:1:318:BCR:H371	1.87	0.44
16:4:145:GLU:OE1	26:4:606:CHL:HMC	2.17	0.44
13:6:79:HIS:HD2	28:6:318:XAT:H15	1.82	0.44
17:7:612:CLA:HBB1	17:7:612:CLA:H91	2.00	0.44
14:7:111:PHE:CE2	27:7:615:LUT:H8	2.53	0.44
17:A:827:CLA:CHB	17:A:840:CLA:HAA2	2.48	0.44
2:B:389:HIS:HA	2:B:392:ILE:HD12	2.00	0.44
2:B:456:GLU:HA	2:B:457:PRO:HD3	1.88	0.44
2:B:257:ILE:HG13	17:B:816:CLA:O1D	2.18	0.44
13:1:100:ASN:HD21	13:1:205:GLY:N	2.16	0.44
17:1:309:CLA:H111	17:1:309:CLA:H142	1.82	0.44
17:1:315:CLA:HBC3	25:4:620:LMG:H181	1.99	0.44
20:2:617:BCR:H371	20:2:617:BCR:H24C	1.78	0.44
15:3:77:LEU:HG	17:3:302:CLA:H42	2.00	0.44
13:6:140:PHE:CZ	20:6:319:BCR:H10C	2.52	0.44
26:6:303:CHL:CBB	17:6:304:CLA:HMD2	2.47	0.44
1:A:485:GLN:HA	1:A:486:PRO:HD3	1.88	0.44
17:A:832:CLA:H2	17:A:833:CLA:HMD2	2.32	0.44
2:B:573:TRP:CD1	17:B:829:CLA:HMD1	2.55	0.44
17:B:811:CLA:C3D	17:B:811:CLA:H52	2.47	0.44
3:C:61:ASP:HA	3:C:62:PHE:HA	1.80	0.44
4:D:195:VAL:HB	4:D:199:GLU:HG3	2.00	0.44
20:L:201:BCR:H351	20:L:201:BCR:H15C	1.80	0.44
26:1:302:CHL:H143	26:1:302:CHL:H111	1.77	0.44
17:1:306:CLA:HMC2	28:1:317:XAT:H163	1.99	0.44
14:2:143:PHE:HB2	26:2:606:CHL:HBC1	1.99	0.44
17:3:308:CLA:HBA2	17:3:308:CLA:H3A	1.37	0.44
13:6:196:VAL:HG13	27:6:321:LUT:H3	1.99	0.44
26:9:607:CHL:CGA	17:9:609:CLA:HMD2	2.47	0.44
17:9:604:CLA:HMB2	20:9:618:BCR:H382	1.99	0.44
1:A:232:PHE:CE1	1:A:258:LEU:HD11	2.52	0.44
17:A:810:CLA:H102	20:J:3003:BCR:H332	2.37	0.44
20:A:851:BCR:H15C	20:A:851:BCR:H351	1.80	0.44
17:B:812:CLA:H92	17:B:812:CLA:H62	1.86	0.44
20:B:846:BCR:H24C	20:B:846:BCR:H371	1.79	0.44
8:H:75:SER:O	12:L:41:THR:HG22	2.18	0.44
16:9:58:PRO:O	17:9:601:CLA:HED1	2.18	0.43
17:B:813:CLA:H102	17:B:813:CLA:H62	2.19	0.43
17:B:806:CLA:HMB2	17:B:829:CLA:HBB2	2.00	0.43
13:6:163:PRO:HD2	27:6:317:LUT:H23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:9:616:LUT:H201	27:9:616:LUT:H15	1.88	0.43
17:B:808:CLA:HBD	17:B:808:CLA:HAA1	2.00	0.43
17:B:829:CLA:H93	17:B:840:CLA:HED1	2.00	0.43
17:L:202:CLA:H43	20:L:206:BCR:H19C	3.70	0.43
13:1:92:VAL:HG13	13:1:96:LEU:HD23	2.00	0.43
17:6:312:CLA:NB	19:6:320:LHG:O4	2.51	0.43
16:9:90:TRP:HZ2	17:9:608:CLA:HAA2	1.83	0.43
1:A:370:ILE:HD13	17:A:827:CLA:C2D	2.48	0.43
1:A:689:SER:HB2	1:A:734:GLY:O	2.19	0.43
17:A:804:CLA:HMB2	19:A:846:LHG:H162	2.00	0.43
17:A:820:CLA:H3A	17:A:820:CLA:HBA2	1.76	0.43
2:B:82:PHE:O	8:H:143:LYS:HE2	2.18	0.43
26:2:601:CHL:HED1	15:3:165:ARG:HA	1.99	0.43
17:4:601:CLA:HBB2	17:4:602:CLA:HHD	2.00	0.43
17:6:316:CLA:HHC	17:6:316:CLA:HBB1	1.98	0.43
26:6:303:CHL:H12	19:6:320:LHG:H172	2.00	0.43
17:7:608:CLA:HBA1	17:7:608:CLA:H3A	1.65	0.43
12:L:36:LEU:HD11	17:L:202:CLA:HBB1	2.01	0.43
14:2:256:PHE:HA	14:2:256:PHE:HD1	1.70	0.43
17:3:302:CLA:H62	17:3:303:CLA:HMA1	1.99	0.43
16:4:169:ASP:HB3	16:4:172:PHE:O	2.19	0.43
27:8:314:LUT:H201	27:8:314:LUT:H15	1.90	0.43
1:A:71:LEU:HD21	17:A:826:CLA:H201	1.99	0.43
1:A:682:ALA:HB1	1:A:741:GLY:O	2.19	0.43
17:A:820:CLA:CAD	17:A:830:CLA:H41	2.52	0.43
17:B:807:CLA:H3A	17:B:808:CLA:HMB3	2.01	0.43
17:B:812:CLA:H3A	17:B:812:CLA:HBA2	1.67	0.43
2:B:451:LYS:HB3	17:B:833:CLA:HED3	2.23	0.43
20:2:617:BCR:H322	17:4:610:CLA:HAB	2.00	0.43
17:4:608:CLA:HBA1	17:4:608:CLA:H3A	1.84	0.43
13:6:105:GLN:HE22	28:6:318:XAT:H21	1.83	0.43
14:7:216:ARG:HB2	19:7:618:LHG:H241	2.01	0.43
17:9:611:CLA:HBB1	17:9:611:CLA:HHC	1.99	0.43
16:9:98:ASN:ND2	17:9:608:CLA:HMD1	2.33	0.43
1:A:151:GLN:HB2	1:A:382:TYR:HB3	2.06	0.43
1:A:33:GLN:HB2	17:A:812:CLA:HAA2	2.04	0.43
1:A:362:LEU:HD21	17:A:831:CLA:CBB	2.48	0.43
1:A:368:LEU:O	1:A:371:VAL:HG22	2.24	0.43
1:A:430:ASP:O	1:A:434:ARG:HG3	2.26	0.43
1:A:479:ASP:HA	1:A:483:GLN:HG2	2.00	0.43
1:A:387:THR:HG21	1:A:523:VAL:HB	2.04	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:841:CLA:C1B	17:B:832:CLA:H41	2.99	0.43
1:A:725:LEU:HD11	17:A:843:CLA:HMD3	33.88	0.43
2:B:423:SER:O	2:B:427:LEU:HB2	2.23	0.43
2:B:476:VAL:HG12	2:B:477:LEU:HG	2.03	0.43
6:F:212:TRP:CD1	6:F:213:PRO:HD3	2.53	0.43
7:G:62:ASP:OD2	17:G:104:CLA:ND	2.51	0.43
12:L:61:VAL:HG21	12:L:150:ALA:HB3	2.00	0.43
26:1:302:CHL:H91	17:1:313:CLA:H121	1.99	0.43
17:1:311:CLA:HBB2	20:4:618:BCR:H322	2.00	0.43
17:6:313:CLA:H41	17:6:313:CLA:H62	1.67	0.43
1:A:304:LEU:O	1:A:308:ILE:HG12	2.19	0.43
1:A:325:HIS:NE2	17:A:823:CLA:ND	2.67	0.43
17:A:810:CLA:H112	17:A:810:CLA:H142	2.06	0.43
17:A:818:CLA:H111	17:A:818:CLA:H152	1.71	0.43
2:B:619:TRP:O	2:B:623:TYR:HB3	2.19	0.43
17:B:802:CLA:H142	17:B:802:CLA:H112	3.85	0.43
17:B:825:CLA:O1A	17:B:836:CLA:HMA1	2.29	0.43
17:B:828:CLA:H61	20:B:845:BCR:H311	24.86	0.43
1:A:709:TRP:CH2	17:B:831:CLA:HED3	2.54	0.43
3:C:15:THR:HG22	3:C:28:MET:HG3	2.02	0.43
11:K:11:MET:HG3	17:K:4003:CLA:HMD2	2.00	0.43
20:8:316:BCR:H24C	20:8:316:BCR:H371	1.88	0.43
17:A:813:CLA:H12	15:8:77:LEU:HD11	89.68	0.43
1:A:545:HIS:NE2	1:A:615:HIS:HD2	2.17	0.43
17:A:811:CLA:H111	17:A:811:CLA:H152	1.81	0.43
17:A:843:CLA:H111	17:A:843:CLA:H143	4.77	0.43
20:A:849:BCR:H371	20:A:849:BCR:H24C	1.71	0.43
17:B:803:CLA:H3A	17:B:803:CLA:CGA	2.50	0.43
17:B:808:CLA:H2	17:B:808:CLA:H111	2.01	0.43
12:L:132:TRP:O	12:L:136:THR:HG23	2.18	0.43
13:1:84:MET:HG3	13:1:184:GLY:HA2	2.01	0.43
13:6:140:PHE:CE2	20:6:319:BCR:H10C	2.54	0.43
28:6:318:XAT:H35	28:6:318:XAT:H401	1.87	0.43
13:6:57:PHE:HE2	28:6:318:XAT:H383	1.83	0.43
17:7:602:CLA:HBB1	28:7:616:XAT:H32	1.99	0.43
1:A:435:VAL:HA	1:A:438:HIS:HE1	1.83	0.43
17:A:854:CLA:HMB1	17:A:854:CLA:HBB1	2.01	0.43
2:B:439:HIS:CD2	2:B:453:ILE:HG22	2.55	0.43
17:B:837:CLA:H91	17:B:837:CLA:H111	1.86	0.43
12:L:109:SER:OG	12:L:124:ASP:O	2.56	0.43
13:1:37:TRP:O	26:1:302:CHL:ND	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:601:CHL:H61	26:2:601:CHL:H92	1.68	0.43
28:3:317:XAT:H401	28:3:317:XAT:H35	1.80	0.43
26:7:605:CHL:H3A	20:7:617:BCR:H19C	2.00	0.43
1:A:117:LYS:HA	1:A:118:PRO:HD3	1.85	0.43
17:A:803:CLA:NB	17:B:803:CLA:HBB1	2.33	0.43
17:A:815:CLA:HBA1	17:A:815:CLA:H3A	1.87	0.43
17:A:829:CLA:H112	17:A:829:CLA:H71	3.95	0.43
20:A:851:BCR:H20C	20:A:851:BCR:H361	1.79	0.43
2:B:476:VAL:H	2:B:479:SER:HB3	1.83	0.43
20:B:801:BCR:H24C	20:B:801:BCR:H371	1.88	0.43
17:A:801:CLA:HAB	17:B:802:CLA:C1A	2.49	0.43
2:B:427:LEU:HB3	17:B:832:CLA:HED3	2.49	0.43
4:D:109:GLU:HA	4:D:122:MET:O	2.27	0.43
5:E:62:GLU:OE2	8:H:82:ASN:ND2	104.35	0.43
20:1:318:BCR:H11C	20:1:318:BCR:H341	1.85	0.42
16:4:155:ARG:NH2	16:4:170:PRO:HD3	2.33	0.42
15:8:197:PRO:HG3	26:8:306:CHL:HMD2	2.01	0.42
1:A:65:ASP:HB2	1:A:420:ARG:NH1	2.55	0.42
17:A:842:CLA:NC	17:A:842:CLA:H43	2.33	0.42
2:B:273:MET:SD	2:B:357:ALA:HB1	2.58	0.42
2:B:658:ALA:HB3	17:B:803:CLA:HBB2	2.01	0.42
17:B:811:CLA:H3A	17:B:811:CLA:HBA1	1.89	0.42
17:B:817:CLA:H41	17:B:817:CLA:H61	1.72	0.42
20:A:852:BCR:H292	17:B:832:CLA:HMB3	2.01	0.42
17:B:841:CLA:C2B	17:1:304:CLA:H71	2.48	0.42
7:G:28:ARG:HD3	7:G:28:ARG:HA	1.87	0.42
17:1:313:CLA:HBC3	19:1:319:LHG:H352	2.01	0.42
15:3:111:ILE:HD12	15:3:246:PRO:HG2	2.01	0.42
13:6:200:ALA:HB1	13:6:225:ILE:HD13	2.01	0.42
17:9:611:CLA:H62	17:9:611:CLA:H41	1.71	0.42
17:A:814:CLA:H61	17:A:814:CLA:H41	1.69	0.42
2:B:659:THR:O	2:B:662:MET:HB3	2.26	0.42
17:B:828:CLA:HBA2	17:B:828:CLA:H3A	1.39	0.42
17:B:833:CLA:H61	17:B:833:CLA:H41	1.66	0.42
20:B:844:BCR:H351	20:B:844:BCR:H15C	1.79	0.42
17:B:813:CLA:H42	20:B:844:BCR:H21C	2.00	0.42
20:B:847:BCR:H15C	20:B:847:BCR:H351	1.75	0.42
17:L:203:CLA:HMB3	17:L:204:CLA:HBC2	2.05	0.42
12:L:44:SER:HA	12:L:45:PRO:HD3	1.87	0.42
15:3:137:PRO:HD2	17:3:306:CLA:C2B	2.49	0.42
20:A:852:BCR:H15C	20:A:852:BCR:H351	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:815:CLA:HBB1	20:B:843:BCR:H382	2.01	0.42
17:2:602:CLA:H71	28:2:616:XAT:H28	2.00	0.42
16:4:233:LEU:O	16:4:237:ILE:HG12	2.18	0.42
15:8:256:ASP:OD2	15:8:259:ASN:ND2	2.48	0.42
17:A:805:CLA:HBB1	17:A:806:CLA:CMB	2.49	0.42
1:A:361:ASN:CG	17:A:826:CLA:HAA1	2.41	0.42
20:A:850:BCR:H11C	20:A:850:BCR:H341	1.78	0.42
2:B:262:HIS:HE1	2:B:264:GLN:HB3	1.91	0.42
2:B:529:THR:O	2:B:533:ILE:HG12	2.26	0.42
3:C:5:VAL:HG11	3:C:26:LEU:HD21	2.00	0.42
17:L:202:CLA:H122	17:L:202:CLA:H161	1.75	0.42
27:6:321:LUT:H31	27:6:321:LUT:H391	1.94	0.42
14:7:222:VAL:HG11	28:7:616:XAT:H12	2.00	0.42
1:A:702:GLU:O	1:A:705:GLU:HB2	2.27	0.42
17:A:801:CLA:H203	17:A:801:CLA:H162	1.82	0.42
17:A:807:CLA:HBA2	17:A:807:CLA:HBD	2.30	0.42
17:A:812:CLA:H161	17:A:812:CLA:H143	2.09	0.42
17:A:824:CLA:H3A	17:A:824:CLA:HBA2	1.68	0.42
17:A:829:CLA:H62	17:A:829:CLA:H41	1.80	0.42
17:A:839:CLA:HMB2	17:A:840:CLA:C3D	2.50	0.42
2:B:387:PHE:HZ	17:B:825:CLA:HAB	2.02	0.42
2:B:722:ALA:O	2:B:726:ILE:HG12	2.30	0.42
17:B:807:CLA:H162	17:B:807:CLA:H203	1.90	0.42
17:B:809:CLA:H161	17:B:809:CLA:H143	1.87	0.42
4:D:114:MET:HA	4:D:115:PRO:HD3	1.95	0.42
17:1:309:CLA:HBA2	17:1:309:CLA:H3A	1.65	0.42
15:8:181:PHE:CZ	26:8:306:CHL:HBB2	2.55	0.42
17:9:608:CLA:HMB2	17:9:614:CLA:C2C	2.49	0.42
28:9:617:XAT:H401	28:9:617:XAT:H35	1.79	0.42
1:A:232:PHE:O	1:A:237:VAL:HG12	2.25	0.42
1:A:607:ASN:O	1:A:611:VAL:HG12	2.20	0.42
17:A:802:CLA:O2A	17:A:802:CLA:H3A	2.93	0.42
2:B:450:GLU:HA	6:F:144:LEU:HD22	2.09	0.42
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.02	0.42
17:B:806:CLA:HED1	17:B:829:CLA:C2	2.85	0.42
4:D:148:TYR:HB2	4:D:150:ILE:HG22	2.02	0.42
20:L:206:BCR:H24C	20:L:206:BCR:H371	1.64	0.42
26:2:601:CHL:CBB	17:2:602:CLA:HMD2	2.49	0.42
20:2:617:BCR:H313	17:4:610:CLA:HHC	2.01	0.42
28:3:317:XAT:H15	28:3:317:XAT:H201	1.91	0.42
17:6:311:CLA:H41	17:6:311:CLA:H62	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:216:ARG:HD2	17:7:602:CLA:C4C	2.49	0.42
1:A:701:GLN:O	1:A:705:GLU:HG3	2.26	0.42
17:A:810:CLA:H41	17:A:810:CLA:H61	1.86	0.42
17:A:840:CLA:H121	17:A:840:CLA:H161	2.10	0.42
20:B:843:BCR:H351	20:B:843:BCR:H15C	1.71	0.42
20:F:305:BCR:H11C	20:F:305:BCR:H341	1.81	0.42
17:A:835:CLA:H111	17:L:203:CLA:HMB1	2.01	0.42
14:2:133:GLN:HE22	17:2:604:CLA:HED1	1.85	0.42
15:3:136:ILE:HG12	17:3:306:CLA:C1C	2.50	0.42
15:3:256:ASP:OD2	15:3:259:ASN:ND2	2.49	0.42
17:3:302:CLA:HMC2	28:3:317:XAT:C31	2.49	0.42
17:7:609:CLA:H61	27:7:615:LUT:C30	2.50	0.42
17:A:807:CLA:H71	17:A:831:CLA:HBC3	2.37	0.42
17:A:809:CLA:H152	17:A:809:CLA:H112	1.63	0.42
17:A:828:CLA:O1A	20:A:851:BCR:H17C	2.20	0.42
20:A:848:BCR:H11C	20:A:848:BCR:H341	1.89	0.42
2:B:589:TRP:CZ2	17:B:802:CLA:H172	2.55	0.42
17:B:808:CLA:H92	20:B:848:BCR:HC7	2.26	0.42
3:C:17:CYS:HB2	3:C:54:CYS:HB2	2.02	0.42
20:K:4001:BCR:H361	20:K:4001:BCR:H20C	1.72	0.42
17:1:306:CLA:HMC3	26:1:307:CHL:C1C	2.49	0.42
15:3:78:SER:HB2	17:3:302:CLA:O1A	2.19	0.42
20:6:319:BCR:H11C	20:6:319:BCR:H341	1.88	0.42
13:6:74:GLU:O	13:6:78:ILE:HG12	2.20	0.42
17:7:608:CLA:HBB1	17:7:608:CLA:CHC	2.42	0.42
17:A:809:CLA:C4D	17:A:829:CLA:H12	2.50	0.42
1:A:368:LEU:HD11	17:A:820:CLA:H71	2.09	0.42
17:A:822:CLA:H152	17:A:822:CLA:H111	1.79	0.42
20:A:850:BCR:H351	20:A:850:BCR:H15C	1.79	0.42
2:B:222:LEU:HA	2:B:222:LEU:HD12	1.84	0.42
17:B:818:CLA:CAB	17:B:818:CLA:H8	2.53	0.42
17:B:825:CLA:HAA2	17:B:836:CLA:HMB3	2.23	0.42
2:B:418:ILE:HG23	17:B:838:CLA:HBB2	2.24	0.42
7:G:46:ALA:N	7:G:47:GLY:HA2	2.36	0.42
20:I:101:BCR:H372	20:L:201:BCR:H403	2.01	0.42
20:L:206:BCR:H11C	20:L:206:BCR:H341	1.79	0.42
14:2:89:LEU:O	14:2:93:VAL:HG23	2.20	0.42
16:4:125:LYS:H	16:4:125:LYS:HG2	1.52	0.42
20:7:617:BCR:H20C	20:7:617:BCR:H361	1.76	0.42
1:A:434:ARG:O	1:A:438:HIS:ND1	2.51	0.42
1:A:626:GLY:HA3	1:A:636:HIS:HA	2.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:824:CLA:HAA1	17:A:824:CLA:HBD	2.02	0.42
17:A:835:CLA:H122	17:L:203:CLA:HAB	2.02	0.42
18:A:844:PQN:H2M1	18:A:844:PQN:H111	1.88	0.42
2:B:295:PHE:HE2	17:B:812:CLA:HMA1	2.16	0.42
17:A:843:CLA:HMC3	17:B:839:CLA:ND	2.35	0.42
4:D:155:TYR:CE2	4:D:165:TYR:HD1	2.38	0.42
12:L:56:HIS:HA	12:L:59:LEU:HD23	2.08	0.42
12:L:57:GLY:O	12:L:61:VAL:HG23	2.20	0.42
13:1:163:PRO:HD2	27:1:316:LUT:H23	2.02	0.41
27:2:615:LUT:H15	27:2:615:LUT:H201	1.86	0.41
27:3:316:LUT:H31	27:3:316:LUT:H391	1.87	0.41
16:4:189:PHE:HB3	17:4:609:CLA:HMD1	2.02	0.41
1:A:458:PHE:CZ	1:A:462:ILE:HD11	2.61	0.41
17:A:809:CLA:HHC	17:A:809:CLA:HBB1	3.86	0.41
1:A:216:LEU:HG	17:A:816:CLA:CBB	2.50	0.41
17:A:822:CLA:H62	17:A:825:CLA:H51	2.02	0.41
17:A:835:CLA:H142	17:A:835:CLA:H112	1.91	0.41
1:A:336:GLY:N	19:A:847:LHG:HC32	2.35	0.41
20:A:851:BCR:H371	20:A:851:BCR:H24C	2.37	0.41
2:B:129:LEU:O	2:B:130:ARG:HD2	2.26	0.41
2:B:59:LEU:HG	17:B:807:CLA:HBB2	2.02	0.41
17:B:811:CLA:HAA1	17:B:811:CLA:HBD	2.02	0.41
18:B:842:PQN:H162	18:B:842:PQN:H192	1.92	0.41
20:B:844:BCR:H361	20:B:844:BCR:H20C	1.92	0.41
4:D:115:PRO:HG3	4:D:140:LEU:HB2	2.19	0.41
17:G:101:CLA:HAC2	13:1:109:ALA:HB2	2.02	0.41
13:1:40:GLY:HA2	16:4:165:SER:HB2	2.02	0.41
14:2:216:ARG:HD2	17:2:602:CLA:C4C	2.50	0.41
15:3:210:ASP:OD2	15:3:212:LYS:HG2	2.19	0.41
17:3:311:CLA:H41	17:3:311:CLA:H62	1.74	0.41
16:4:103:MET:HE3	17:4:609:CLA:HMC3	2.02	0.41
17:4:611:CLA:H41	17:4:611:CLA:H62	1.75	0.41
17:9:602:CLA:HMC2	28:9:617:XAT:C31	2.50	0.41
1:A:701:GLN:NE2	1:A:724:ALA:H	2.18	0.41
20:A:852:BCR:H371	20:A:852:BCR:H24C	1.97	0.41
17:A:854:CLA:HBC2	2:B:585:ASN:HB2	2.02	0.41
2:B:162:LYS:HA	2:B:163:PRO:HD3	1.93	0.41
2:B:82:PHE:HE1	2:B:363:GLN:HG3	1.85	0.41
2:B:25:ILE:HA	17:B:804:CLA:HMD3	2.00	0.41
17:B:806:CLA:H92	17:B:806:CLA:H61	2.15	0.41
17:B:825:CLA:H151	17:B:825:CLA:H18	4.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:833:CLA:HHB	22:F:302:HTG:H62	2.02	0.41
17:B:837:CLA:HAA1	17:B:837:CLA:HBD	2.05	0.41
8:H:141:ARG:HB3	8:H:143:LYS:HE3	2.41	0.41
1:A:88:ILE:HG23	20:J:3003:BCR:HC22	2.02	0.41
17:A:835:CLA:H92	17:L:204:CLA:HBB2	2.02	0.41
20:L:205:BCR:H11C	20:L:205:BCR:H341	1.97	0.41
17:2:602:CLA:H41	17:2:602:CLA:H61	1.77	0.41
28:2:616:XAT:H201	28:2:616:XAT:H15	1.87	0.41
20:2:617:BCR:H11C	20:2:617:BCR:H341	1.87	0.41
26:4:607:CHL:HMB3	20:4:618:BCR:C16	2.50	0.41
13:6:62:LEU:HD13	17:6:304:CLA:H42	2.02	0.41
17:6:314:CLA:H61	17:6:314:CLA:H41	1.64	0.41
27:7:615:LUT:H15	27:7:615:LUT:H201	1.89	0.41
1:A:195:TRP:HH2	17:A:811:CLA:HMB3	1.95	0.41
1:A:403:GLY:O	1:A:407:ILE:HG13	2.20	0.41
1:A:538:ASP:HA	1:A:541:VAL:HG22	2.02	0.41
17:A:825:CLA:HMA1	17:A:845:CLA:HBB2	2.02	0.41
20:A:851:BCR:H341	20:A:851:BCR:H11C	1.92	0.41
2:B:464:GLN:NE2	17:B:836:CLA:HMD1	2.35	0.41
2:B:696:LYS:HA	2:B:697:PRO:HD3	1.84	0.41
1:A:709:TRP:HH2	17:B:831:CLA:HED3	1.85	0.41
17:B:841:CLA:H13	17:B:841:CLA:H172	3.74	0.41
20:B:843:BCR:H20C	20:B:843:BCR:H361	1.91	0.41
17:F:303:CLA:HBC2	10:J:19:PHE:CZ	2.55	0.41
15:3:177:GLY:HA2	15:3:185:GLU:HB2	2.03	0.41
16:4:125:LYS:HD3	16:4:127:TYR:CZ	2.56	0.41
16:9:103:MET:HE3	17:9:609:CLA:HMC3	2.01	0.41
1:A:208:ALA:HB1	17:A:821:CLA:HBC3	2.01	0.41
18:A:844:PQN:H161	18:A:844:PQN:H141	1.78	0.41
17:A:845:CLA:HBA2	17:A:845:CLA:H12	1.92	0.41
2:B:160:LYS:HD3	2:B:161:TRP:CZ2	2.55	0.41
17:B:806:CLA:HED3	17:B:829:CLA:H61	2.03	0.41
17:B:830:CLA:H2	17:B:831:CLA:HMD2	3.46	0.41
2:B:656:VAL:HG22	17:B:840:CLA:HMB3	2.02	0.41
20:B:843:BCR:H371	20:B:843:BCR:H24C	1.76	0.41
20:L:206:BCR:H351	20:L:206:BCR:H15C	1.86	0.41
27:1:316:LUT:H35	27:1:316:LUT:H401	1.83	0.41
13:1:105:GLN:HE22	28:1:317:XAT:H21	1.83	0.41
17:2:603:CLA:H162	17:2:603:CLA:H192	1.86	0.41
16:4:206:ALA:HB2	25:4:619:LMG:HC5	2.01	0.41
20:4:618:BCR:H11C	20:4:618:BCR:H341	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:6:303:CHL:HMB2	17:9:614:CLA:O2D	2.20	0.41
20:7:617:BCR:H341	20:7:617:BCR:H11C	1.68	0.41
15:8:57:GLN:HG2	15:8:61:TYR:CE2	2.54	0.41
1:A:446:LEU:HD21	1:A:553:VAL:HG12	2.01	0.41
1:A:282:THR:HA	17:A:818:CLA:HED1	2.11	0.41
17:A:824:CLA:H12	17:A:824:CLA:C4A	2.52	0.41
17:A:834:CLA:H62	17:A:834:CLA:H92	1.96	0.41
17:B:804:CLA:HMC1	24:B:850:DGD:HAH1	2.03	0.41
17:B:814:CLA:CMA	20:B:845:BCR:H282	2.49	0.41
17:B:820:CLA:HBC3	20:B:844:BCR:H332	2.02	0.41
17:B:837:CLA:HBC2	22:F:302:HTG:H5'2	2.03	0.41
20:J:3003:BCR:H371	20:J:3003:BCR:H24C	1.79	0.41
26:1:302:CHL:H72	20:4:618:BCR:H342	2.03	0.41
17:1:304:CLA:H111	17:1:304:CLA:H91	1.79	0.41
26:1:302:CHL:HED1	16:4:155:ARG:HD2	2.02	0.41
26:7:607:CHL:HBB2	26:7:614:CHL:OMC	2.20	0.41
26:9:606:CHL:H3A	26:9:606:CHL:HBA2	1.43	0.41
1:A:568:LEU:HD11	1:A:586:ARG:HB3	2.17	0.41
17:A:803:CLA:HBB1	17:A:803:CLA:HMB1	2.21	0.41
20:A:852:BCR:H341	20:A:852:BCR:H11C	4.54	0.41
2:B:344:ILE:HD11	17:B:828:CLA:HBC1	2.09	0.41
2:B:334:LEU:HD23	2:B:389:HIS:CE1	2.58	0.41
17:B:840:CLA:H111	17:B:840:CLA:H152	1.90	0.41
4:D:145:ARG:NH2	4:D:175:GLU:OE1	2.54	0.41
20:G:105:BCR:H361	20:G:105:BCR:H20C	1.89	0.41
20:I:101:BCR:H341	20:I:101:BCR:H11C	1.90	0.41
11:K:61:LEU:O	11:K:65:VAL:HG23	2.28	0.41
12:L:6:VAL:HB	12:L:7:ILE:HD12	2.02	0.41
17:1:313:CLA:H142	17:1:313:CLA:H112	1.84	0.41
17:3:312:CLA:HMB3	27:3:316:LUT:H162	2.03	0.41
17:7:609:CLA:HBB2	27:7:615:LUT:H34	2.02	0.41
17:7:612:CLA:HMC2	17:7:612:CLA:H92	2.02	0.41
14:7:252:ILE:HA	17:7:612:CLA:OBD	2.20	0.41
1:A:721:GLN:HA	1:A:722:PRO:HD3	1.94	0.41
1:A:729:GLN:HB2	19:A:846:LHG:HC42	2.02	0.41
2:B:411:MET:HG2	20:B:846:BCR:H292	2.03	0.41
2:B:387:PHE:CZ	17:B:825:CLA:HAB	2.70	0.41
17:B:810:CLA:HMC3	20:I:101:BCR:C18	2.52	0.41
10:J:28:GLU:OE2	17:J:3002:CLA:NA	2.53	0.41
15:3:133:THR:HG22	17:3:304:CLA:HED2	2.03	0.41
25:4:619:LMG:H232	25:4:619:LMG:H262	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:6:319:BCR:H371	20:6:319:BCR:H24C	1.84	0.41
27:6:321:LUT:H28	17:9:614:CLA:HBC3	2.02	0.41
17:8:307:CLA:HBD	17:8:307:CLA:HAA1	2.03	0.41
28:8:315:XAT:H35	28:8:315:XAT:H401	1.78	0.41
16:9:76:PHE:HB3	17:9:602:CLA:CAD	2.50	0.41
1:A:326:GLY:O	1:A:330:ILE:HG13	2.21	0.41
1:A:422:TYR:CE1	1:A:424:PRO:HD3	2.55	0.41
1:A:678:PHE:HZ	17:A:829:CLA:H111	1.85	0.41
17:A:804:CLA:H61	17:A:804:CLA:H102	4.56	0.41
17:A:843:CLA:H101	17:A:843:CLA:H13	1.66	0.41
2:B:344:ILE:O	2:B:348:VAL:HG23	2.21	0.41
17:B:813:CLA:H92	17:B:824:CLA:H42	2.27	0.41
17:B:839:CLA:H152	17:B:839:CLA:H111	1.90	0.41
2:B:84:VAL:HG22	8:H:144:ILE:HD12	2.08	0.41
4:D:76:PRO:HG2	4:D:78:THR:HG22	2.18	0.41
6:F:156:TRP:CZ2	17:F:304:CLA:HBA1	2.55	0.41
20:B:801:BCR:H321	6:F:166:PHE:HB2	2.03	0.41
11:K:19:LEU:HB3	17:3:301:CLA:HMB1	2.02	0.41
1:A:304:LEU:HD13	17:A:816:CLA:HMC1	2.31	0.41
1:A:614:PHE:HB3	1:A:652:TRP:HZ3	1.88	0.41
17:A:835:CLA:H72	20:L:201:BCR:H14C	2.01	0.41
17:A:830:CLA:H61	20:A:849:BCR:H342	2.02	0.41
20:A:850:BCR:H24C	20:A:850:BCR:H371	1.79	0.41
2:B:390:GLY:O	2:B:393:PHE:HB3	2.21	0.41
2:B:600:THR:HG21	2:B:609:PHE:HB2	2.03	0.41
17:B:806:CLA:H111	17:B:806:CLA:H72	1.90	0.41
17:B:807:CLA:H72	20:I:101:BCR:HC32	4.18	0.41
17:B:815:CLA:C1B	20:B:843:BCR:H271	2.61	0.41
17:B:815:CLA:H11	17:B:815:CLA:H51	1.85	0.41
17:B:837:CLA:H72	17:B:837:CLA:HBB1	2.05	0.41
2:B:411:MET:HG2	20:B:846:BCR:H401	2.11	0.41
1:A:715:LYS:HB2	6:F:178:ARG:HH12	1.85	0.41
6:F:212:TRP:CG	6:F:213:PRO:HD3	2.56	0.41
17:2:612:CLA:H122	17:2:612:CLA:H162	1.77	0.41
17:3:306:CLA:HHC	17:3:306:CLA:HBB1	2.02	0.41
16:4:101:TRP:CD2	26:4:607:CHL:HED2	2.56	0.41
26:4:607:CHL:CGA	17:4:609:CLA:HMD2	2.51	0.41
19:6:320:LHG:H191	19:6:320:LHG:H162	1.91	0.41
16:9:215:PHE:CD2	28:9:617:XAT:H14	2.56	0.41
1:A:374:GLN:HB3	1:A:374:GLN:HE21	1.59	0.41
1:A:123:VAL:HA	17:A:810:CLA:HED2	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:825:CLA:H42	20:A:851:BCR:H363	2.03	0.41
2:B:157:LEU:HA	2:B:157:LEU:HD23	1.94	0.41
2:B:437:TYR:CZ	2:B:518:LEU:HB3	2.69	0.41
2:B:586:THR:O	2:B:590:VAL:HG13	2.21	0.41
17:B:811:CLA:HAA2	7:G:50:ARG:NE	2.69	0.41
17:B:819:CLA:H61	17:B:819:CLA:H41	1.81	0.41
17:B:826:CLA:H102	20:B:847:BCR:C17	2.51	0.41
17:B:830:CLA:HBB2	17:B:838:CLA:HAB	2.02	0.41
17:1:304:CLA:OBD	17:1:309:CLA:HAA1	2.21	0.41
13:6:90:ILE:HG23	13:6:101:TRP:CG	2.56	0.41
13:6:191:PHE:HA	13:6:194:PHE:CD2	2.56	0.41
17:6:305:CLA:H51	17:6:305:CLA:H11	1.82	0.41
27:6:317:LUT:H391	27:6:317:LUT:H31	1.99	0.41
14:7:256:PHE:HA	14:7:256:PHE:HD1	1.71	0.41
15:8:214:LEU:HG	15:8:218:LYS:HE3	2.03	0.41
26:8:306:CHL:HMB3	20:8:316:BCR:C16	2.51	0.41
16:9:125:LYS:HG2	16:9:125:LYS:H	1.58	0.41
17:9:614:CLA:HHC	17:9:614:CLA:HBB1	2.02	0.41
1:A:431:LEU:HD13	17:A:825:CLA:C1C	2.51	0.41
17:A:818:CLA:HAC2	17:A:818:CLA:H143	2.03	0.41
17:A:825:CLA:H12	20:A:852:BCR:H14C	44.20	0.41
17:A:843:CLA:HMC3	17:B:839:CLA:C4D	2.51	0.41
1:A:92:TRP:CZ2	17:A:829:CLA:HED2	2.62	0.41
2:B:646:TRP:CZ2	2:B:726:ILE:HG21	2.61	0.41
2:B:716:GLY:O	2:B:720:THR:OG1	2.31	0.41
17:B:832:CLA:H122	20:F:305:BCR:HC8	2.02	0.41
17:B:810:CLA:HMD3	20:I:101:BCR:H403	2.04	0.41
9:I:12:VAL:O	9:I:17:PRO:HD3	2.21	0.41
13:1:127:LEU:O	13:1:131:LEU:HB2	2.20	0.40
7:G:89:THR:HA	25:6:302:LMG:HC62	136.08	0.40
26:6:303:CHL:H43	16:9:147:ILE:HG22	2.03	0.40
19:6:320:LHG:H282	19:6:320:LHG:H111	2.03	0.40
27:7:615:LUT:H31	27:7:615:LUT:H391	1.99	0.40
1:A:356:ALA:HB1	20:A:850:BCR:H393	2.03	0.40
1:A:453:LEU:HD12	1:A:453:LEU:HA	4.42	0.40
1:A:203:LEU:HG	17:A:826:CLA:HMD3	2.02	0.40
17:A:839:CLA:CGA	17:A:839:CLA:C1A	2.98	0.40
17:A:801:CLA:HMB3	17:A:854:CLA:HMD1	2.03	0.40
2:B:592:PHE:CE2	2:B:624:LEU:HD21	2.62	0.40
2:B:174:ARG:NH1	17:B:805:CLA:H141	2.36	0.40
17:B:806:CLA:HED1	17:B:829:CLA:C3	3.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:697:PRO:HB3	17:B:839:CLA:C2C	2.50	0.40
20:B:843:BCR:H341	20:B:843:BCR:H11C	1.92	0.40
5:E:29:ASP:HB3	5:E:37:PRO:HB3	2.22	0.40
2:B:282:PHE:CE2	20:G:105:BCR:HC22	2.56	0.40
7:G:79:HIS:CE1	20:G:105:BCR:H14C	2.57	0.40
10:J:38:ILE:HG22	10:J:39:PHE:CD2	2.56	0.40
17:A:816:CLA:C3B	20:K:4001:BCR:H333	2.51	0.40
12:L:26:SER:OG	12:L:29:ILE:HG22	2.20	0.40
8:H:80:PRO:HG3	12:L:40:ARG:NH1	2.55	0.40
16:4:195:ALA:HA	16:4:196:PRO:HD3	1.89	0.40
17:4:603:CLA:HMC2	28:4:617:XAT:C12	2.51	0.40
27:6:317:LUT:H35	27:6:317:LUT:H401	1.78	0.40
17:7:604:CLA:HBB1	20:7:617:BCR:C39	2.52	0.40
17:A:814:CLA:H111	17:A:814:CLA:H93	1.93	0.40
17:A:815:CLA:HBB1	20:A:850:BCR:C19	34.62	0.40
17:A:822:CLA:CMB	17:A:826:CLA:HMA3	2.49	0.40
17:A:843:CLA:H142	17:B:839:CLA:H122	2.03	0.40
2:B:700:LEU:HD11	17:B:840:CLA:HMD3	2.11	0.40
2:B:718:ILE:HD12	17:B:827:CLA:CBB	2.51	0.40
17:B:807:CLA:H42	17:B:807:CLA:C1D	4.26	0.40
2:B:442:VAL:HG21	17:B:833:CLA:HAC2	2.03	0.40
2:B:711:VAL:HG11	17:B:840:CLA:HED3	2.03	0.40
2:B:411:MET:HE2	20:B:846:BCR:H282	2.02	0.40
11:K:8:ASN:ND2	17:K:4003:CLA:OBD	2.42	0.40
17:L:203:CLA:C4C	20:L:205:BCR:H281	2.73	0.40
12:L:87:LEU:HD22	12:L:91:LEU:HG	2.11	0.40
17:1:308:CLA:H142	17:1:308:CLA:H112	1.78	0.40
27:1:320:LUT:H35	27:1:320:LUT:H401	1.89	0.40
13:6:191:PHE:CE2	28:6:318:XAT:H12	2.56	0.40
13:6:191:PHE:CD2	28:6:318:XAT:H14	2.57	0.40
17:8:307:CLA:HMB2	17:8:312:CLA:C4B	2.52	0.40
1:A:107:GLU:OE2	1:A:161:GLU:HG3	2.29	0.40
1:A:283:PHE:O	1:A:507:ALA:HA	2.40	0.40
17:A:818:CLA:HBB1	17:A:818:CLA:HHC	2.04	0.40
17:A:820:CLA:O1A	17:A:830:CLA:HMD1	2.22	0.40
17:A:829:CLA:H62	17:A:829:CLA:H92	1.84	0.40
2:B:142:LEU:HG	20:B:845:BCR:H382	2.03	0.40
17:B:808:CLA:H141	17:B:808:CLA:H161	2.37	0.40
20:B:848:BCR:H351	20:B:848:BCR:H15C	1.89	0.40
4:D:102:ILE:HG23	4:D:104:TRP:HZ3	1.89	0.40
4:D:109:GLU:HG2	4:D:123:ARG:HA	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:94:ASP:HA	7:G:95:PRO:HD3	1.92	0.40
17:2:611:CLA:HMC2	27:2:615:LUT:C11	2.52	0.40
15:3:70:TYR:OH	15:3:223:LYS:HE2	2.21	0.40
27:4:616:LUT:H401	27:4:616:LUT:H35	1.84	0.40
13:6:110:LEU:HD12	13:6:113:GLY:H	1.86	0.40
17:7:604:CLA:C3B	28:7:616:XAT:H183	2.51	0.40
1:A:82:HIS:ND1	17:A:814:CLA:OBD	2.64	0.40
17:A:841:CLA:H51	17:A:841:CLA:C3C	2.52	0.40
2:B:462:TRP:NE1	2:B:476:VAL:HG21	2.37	0.40
6:F:160:ILE:O	6:F:164:ILE:HG13	2.22	0.40
7:G:12:THR:HA	7:G:78:GLY:HA3	2.27	0.40
12:L:125:GLN:O	12:L:131:GLY:HA3	2.21	0.40
20:L:206:BCR:H20C	20:L:206:BCR:H361	1.90	0.40
13:1:167:SER:HA	13:1:173:LEU:HG	2.03	0.40
17:3:302:CLA:H93	17:3:303:CLA:HMB3	2.02	0.40
13:6:122:VAL:HG23	13:6:125:GLY:HA3	2.03	0.40
13:6:87:VAL:HG13	13:6:194:PHE:CZ	2.57	0.40
14:7:170:ASP:HA	14:7:171:PRO:HD2	1.91	0.40
15:8:193:ASN:HA	15:8:194:PRO:HD2	1.96	0.40
17:9:604:CLA:HBB1	20:9:618:BCR:H393	2.04	0.40
1:A:412:ALA:O	1:A:416:ILE:HG13	2.22	0.40
17:A:811:CLA:H72	17:A:811:CLA:H112	1.93	0.40
19:A:846:LHG:H312	19:A:846:LHG:H281	1.91	0.40
20:A:849:BCR:H403	11:K:62:ALA:HB1	18.11	0.40
2:B:262:HIS:HA	2:B:263:PRO:HD2	1.92	0.40
2:B:309:ILE:HA	2:B:310:PRO:HD3	2.00	0.40
17:B:811:CLA:HBA1	17:B:812:CLA:OBD	2.52	0.40
17:B:840:CLA:CBB	17:B:840:CLA:HHC	2.54	0.40
20:B:801:BCR:C32	6:F:166:PHE:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/742 (100%)	710 (96%)	28 (4%)	2 (0%)	44	77
1	a	740/742 (100%)	709 (96%)	29 (4%)	2 (0%)	44	77
2	B	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	55	86
2	b	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	55	86
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
3	c	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
4	d	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
5	E	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
5	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
6	F	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	25	59
6	f	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	25	59
7	G	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
7	g	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
8	H	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
8	h	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
9	I	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
9	i	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
10	J	37/39 (95%)	37 (100%)	0	0	100	100
10	j	37/39 (95%)	37 (100%)	0	0	100	100
11	K	41/84 (49%)	41 (100%)	0	0	100	100
11	k	42/84 (50%)	42 (100%)	0	0	100	100
12	L	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
12	l	149/153 (97%)	143 (96%)	6 (4%)	0	100	100
13	1	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
13	6	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
14	2	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
14	7	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
15	3	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
15	8	215/218 (99%)	204 (95%)	11 (5%)	0	100	100
16	4	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	32	67
16	9	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	32	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6282/6434 (98%)	6041 (96%)	231 (4%)	10 (0%)	51 83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	159	PHE
6	f	159	PHE
1	A	581	CYS
16	9	137	SER
16	4	137	SER
1	a	581	CYS
1	A	127	VAL
1	a	127	VAL
2	B	492	ILE
2	b	492	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	602/602 (100%)	588 (98%)	14 (2%)	56 86
1	a	602/602 (100%)	587 (98%)	15 (2%)	53 84
2	B	597/597 (100%)	585 (98%)	12 (2%)	60 88
2	b	597/597 (100%)	582 (98%)	15 (2%)	53 84
3	C	69/69 (100%)	67 (97%)	2 (3%)	48 81
3	c	69/69 (100%)	67 (97%)	2 (3%)	48 81
4	D	119/120 (99%)	113 (95%)	6 (5%)	28 62
4	d	118/120 (98%)	111 (94%)	7 (6%)	23 54
5	E	55/56 (98%)	55 (100%)	0	100 100
5	e	55/56 (98%)	55 (100%)	0	100 100
6	F	123/125 (98%)	121 (98%)	2 (2%)	68 91
6	f	123/125 (98%)	120 (98%)	3 (2%)	54 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	81/81 (100%)	80 (99%)	1 (1%)	75	94
7	g	80/81 (99%)	80 (100%)	0	100	100
8	H	72/73 (99%)	69 (96%)	3 (4%)	34	68
8	h	73/73 (100%)	70 (96%)	3 (4%)	35	69
9	I	25/26 (96%)	24 (96%)	1 (4%)	36	70
9	i	25/26 (96%)	24 (96%)	1 (4%)	36	70
10	J	33/33 (100%)	31 (94%)	2 (6%)	22	53
10	j	33/33 (100%)	31 (94%)	2 (6%)	22	53
11	K	34/62 (55%)	32 (94%)	2 (6%)	23	54
11	k	34/62 (55%)	32 (94%)	2 (6%)	23	54
12	L	118/119 (99%)	108 (92%)	10 (8%)	12	35
12	l	117/119 (98%)	107 (92%)	10 (8%)	12	35
13	1	149/153 (97%)	144 (97%)	5 (3%)	42	76
13	6	147/153 (96%)	142 (97%)	5 (3%)	42	76
14	2	166/166 (100%)	158 (95%)	8 (5%)	30	63
14	7	166/166 (100%)	158 (95%)	8 (5%)	30	63
15	3	169/169 (100%)	163 (96%)	6 (4%)	40	74
15	8	168/169 (99%)	162 (96%)	6 (4%)	40	74
16	4	161/161 (100%)	154 (96%)	7 (4%)	33	67
16	9	161/161 (100%)	154 (96%)	7 (4%)	33	67
All	All	5141/5224 (98%)	4974 (97%)	167 (3%)	44	78

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	130	GLU
1	A	151	GLN
1	A	210	LEU
1	A	211	LEU
1	A	290	LEU
1	A	291	THR
1	A	374	GLN
1	A	377	TYR
1	A	540	LEU

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Mol	Chain	Res	Type
1	A	590	CYS
1	A	615	HIS
1	A	653	LEU
1	A	664	VAL
2	B	91	ILE
2	B	110	LEU
2	B	306	GLU
2	B	309	ILE
2	B	394	PHE
2	B	482	ASN
2	B	503	GLU
2	B	533	ILE
2	B	577	TYR
2	B	583	MET
2	B	599	ILE
2	B	645	VAL
3	C	16	GLN
3	C	74	THR
4	D	74	LEU
4	D	78	THR
4	D	150	ILE
4	D	153	GLN
4	D	177	VAL
4	D	189	ARG
6	F	127	LYS
6	F	201	LEU
7	G	57	LEU
8	H	63	LEU
8	H	76	ASP
8	H	141	ARG
9	I	11	LEU
10	J	1	MET
10	J	25	LEU
11	K	18	MET
11	K	55	PHE
12	L	29	ILE
12	L	40	ARG
12	L	50	ILE
12	L	59	LEU
12	L	75	ILE
12	L	87	LEU
12	L	93	LEU

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Mol	Chain	Res	Type
12	L	120	LYS
12	L	121	LYS
12	L	125	GLN
13	1	36	HIS
13	1	38	MET
13	1	114	GLN
13	1	127	LEU
13	1	173	LEU
14	2	110	ILE
14	2	123	ASN
14	2	134	GLU
14	2	167	VAL
14	2	182	ASP
14	2	190	TRP
14	2	223	MET
14	2	256	PHE
15	3	78	SER
15	3	94	TYR
15	3	118	LYS
15	3	154	LEU
15	3	179	GLN
15	3	244	VAL
16	4	104	LEU
16	4	125	LYS
16	4	141	LEU
16	4	148	LEU
16	4	181	GLU
16	4	188	ILE
16	4	210	LEU
1	a	22	VAL
1	a	130	GLU
1	a	151	GLN
1	a	210	LEU
1	a	211	LEU
1	a	290	LEU
1	a	291	THR
1	a	374	GLN
1	a	377	TYR
1	a	446	LEU
1	a	453	LEU
1	a	540	LEU
1	a	590	CYS

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Mol	Chain	Res	Type
1	a	653	LEU
1	a	664	VAL
2	b	82	PHE
2	b	91	ILE
2	b	110	LEU
2	b	306	GLU
2	b	309	ILE
2	b	394	PHE
2	b	441	ASP
2	b	482	ASN
2	b	503	GLU
2	b	577	TYR
2	b	583	MET
2	b	599	ILE
2	b	626	LEU
2	b	645	VAL
2	b	732	LYS
3	c	16	GLN
3	c	74	THR
4	d	74	LEU
4	d	78	THR
4	d	145	ARG
4	d	150	ILE
4	d	153	GLN
4	d	177	VAL
4	d	189	ARG
6	f	127	LYS
6	f	146	HIS
6	f	201	LEU
8	h	63	LEU
8	h	76	ASP
8	h	141	ARG
9	i	11	LEU
10	j	1	MET
10	j	25	LEU
11	k	18	MET
11	k	55	PHE
12	l	29	ILE
12	l	40	ARG
12	l	50	ILE
12	l	59	LEU
12	l	75	ILE

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Mol	Chain	Res	Type
12	1	87	LEU
12	1	93	LEU
12	1	120	LYS
12	1	121	LYS
12	1	125	GLN
13	6	36	HIS
13	6	38	MET
13	6	114	GLN
13	6	127	LEU
13	6	173	LEU
14	7	110	ILE
14	7	134	GLU
14	7	167	VAL
14	7	182	ASP
14	7	190	TRP
14	7	223	MET
14	7	240	LEU
14	7	256	PHE
15	8	78	SER
15	8	94	TYR
15	8	118	LYS
15	8	154	LEU
15	8	179	GLN
15	8	244	VAL
16	9	104	LEU
16	9	125	LYS
16	9	141	LEU
16	9	148	LEU
16	9	181	GLU
16	9	188	ILE
16	9	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	343	HIS
1	A	374	GLN
1	A	398	HIS
1	A	615	HIS
1	A	701	GLN
2	B	439	HIS

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Mol	Chain	Res	Type
3	C	71	HIS
4	D	110	GLN
4	D	153	GLN
12	L	5	GLN
13	1	105	GLN
13	1	114	GLN
14	2	123	ASN
15	3	99	ASN
16	4	98	ASN
16	4	150	HIS
16	4	168	GLN
1	a	151	GLN
1	a	374	GLN
1	a	701	GLN
3	c	71	HIS
4	d	153	GLN
13	6	105	GLN
13	6	114	GLN
15	8	99	ASN
16	9	98	ASN
16	9	150	HIS
16	9	168	GLN
16	9	232	ASN

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](#)

414 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
19	LHG	1	301	17	22,22,48	1.15	2 (9%)	23,28,54	1.36	2 (8%)
26	CHL	1	302	13	59,69,74	3.72	24 (40%)	45,108,114	2.77	17 (37%)
17	CLA	1	303	13	56,73,73	1.94	12 (21%)	65,113,113	2.09	21 (32%)
17	CLA	1	304	13	56,73,73	1.97	12 (21%)	65,113,113	2.15	20 (30%)
17	CLA	1	305	29	43,60,73	2.24	12 (27%)	49,97,113	2.39	22 (44%)
17	CLA	1	306	-	43,60,73	2.23	12 (27%)	49,97,113	2.35	22 (44%)
26	CHL	1	307	13	46,56,74	4.24	25 (54%)	30,92,114	3.27	16 (53%)
17	CLA	1	308	29	56,73,73	1.96	12 (21%)	65,113,113	2.08	19 (29%)
17	CLA	1	309	13	56,73,73	1.97	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	1	310	13	51,68,73	2.06	12 (23%)	59,107,113	2.15	22 (37%)
17	CLA	1	311	19	32,49,73	2.52	12 (37%)	37,84,113	2.73	18 (48%)
17	CLA	1	312	13	43,60,73	2.24	12 (27%)	49,97,113	2.46	19 (38%)
17	CLA	1	313	13	56,73,73	1.97	12 (21%)	65,113,113	2.10	20 (30%)
17	CLA	1	314	13	46,63,73	2.17	12 (26%)	53,101,113	2.34	21 (39%)
17	CLA	1	315	13	37,54,73	2.41	12 (32%)	43,90,113	2.46	17 (39%)
27	LUT	1	316	-	41,43,43	0.74	0	50,60,60	1.54	12 (24%)
28	XAT	1	317	-	39,47,47	0.84	0	54,74,74	2.70	21 (38%)
20	BCR	1	318	-	41,41,41	1.05	1 (2%)	56,56,56	1.88	16 (28%)
19	LHG	1	319	17	48,48,48	0.92	2 (4%)	49,54,54	1.07	3 (6%)
27	LUT	1	320	-	41,43,43	0.73	0	50,60,60	1.69	12 (24%)
26	CHL	2	601	14	59,69,74	3.73	23 (38%)	45,108,114	2.80	18 (40%)
17	CLA	2	602	14	56,73,73	1.97	12 (21%)	65,113,113	2.05	22 (33%)
17	CLA	2	603	14	56,73,73	1.94	12 (21%)	65,113,113	2.09	18 (27%)
17	CLA	2	604	29	51,68,73	2.06	12 (23%)	59,107,113	2.17	21 (35%)
26	CHL	2	605	29	41,51,74	4.42	22 (53%)	24,86,114	3.51	13 (54%)
26	CHL	2	606	-	46,56,74	4.22	24 (52%)	30,92,114	3.29	15 (50%)
26	CHL	2	607	29	49,59,74	4.14	26 (53%)	33,96,114	3.19	16 (48%)
17	CLA	2	608	14	41,58,73	2.30	12 (29%)	47,95,113	2.48	22 (46%)
17	CLA	2	609	14	51,68,73	2.07	12 (23%)	59,107,113	2.14	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	2	610	19	32,49,73	2.49	12 (37%)	37,84,113	2.79	19 (51%)
17	CLA	2	611	14	43,60,73	2.25	12 (27%)	49,97,113	2.43	20 (40%)
17	CLA	2	612	14	56,73,73	1.97	12 (21%)	65,113,113	2.09	18 (27%)
17	CLA	2	613	14	34,51,73	2.41	11 (32%)	39,86,113	2.52	16 (41%)
26	CHL	2	614	14	41,51,74	4.43	23 (56%)	24,86,114	3.46	13 (54%)
27	LUT	2	615	-	41,43,43	0.74	0	50,60,60	1.61	11 (22%)
28	XAT	2	616	-	39,47,47	0.85	0	54,74,74	2.62	19 (35%)
20	BCR	2	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.85	18 (32%)
19	LHG	2	618	17	36,36,48	1.06	2 (5%)	37,42,54	1.21	4 (10%)
17	CLA	3	301	-	37,54,73	2.41	12 (32%)	43,90,113	2.47	17 (39%)
17	CLA	3	302	15	51,68,73	2.04	12 (23%)	59,107,113	2.17	22 (37%)
17	CLA	3	303	15	41,58,73	2.29	12 (29%)	47,95,113	2.49	19 (40%)
17	CLA	3	304	29	33,53,73	2.42	11 (33%)	37,89,113	2.58	18 (48%)
17	CLA	3	305	29	33,50,73	2.43	11 (33%)	38,85,113	2.61	18 (47%)
17	CLA	3	306	15	38,55,73	2.41	12 (31%)	44,91,113	2.44	18 (40%)
26	CHL	3	307	29	45,55,74	4.29	24 (53%)	29,91,114	3.29	12 (41%)
17	CLA	3	308	15	41,58,73	2.29	12 (29%)	47,95,113	2.41	20 (42%)
17	CLA	3	309	15	41,58,73	2.30	12 (29%)	47,95,113	2.37	22 (46%)
17	CLA	3	310	19	29,45,73	2.46	11 (37%)	33,78,113	2.71	16 (48%)
17	CLA	3	311	-	43,60,73	2.26	12 (27%)	49,97,113	2.43	21 (42%)
17	CLA	3	312	15	46,63,73	2.18	12 (26%)	53,101,113	2.29	20 (37%)
17	CLA	3	313	15	33,53,73	2.47	11 (33%)	37,89,113	2.61	18 (48%)
17	CLA	3	314	15	37,54,73	2.40	12 (32%)	43,90,113	2.53	17 (39%)
17	CLA	3	315	-	17,32,73	2.99	10 (58%)	24,54,113	4.44	19 (79%)
27	LUT	3	316	-	41,43,43	0.74	0	50,60,60	1.62	13 (26%)
28	XAT	3	317	-	39,47,47	0.86	0	54,74,74	2.69	19 (35%)
20	BCR	3	318	-	41,41,41	1.04	1 (2%)	56,56,56	1.88	14 (25%)
19	LHG	3	319	17	19,19,48	1.09	1 (5%)	19,24,54	1.04	1 (5%)
17	CLA	4	601	16	37,54,73	2.39	12 (32%)	43,90,113	2.51	17 (39%)
17	CLA	4	602	16	51,68,73	2.06	12 (23%)	59,107,113	2.15	23 (38%)
17	CLA	4	603	16	37,54,73	2.34	12 (32%)	43,90,113	2.57	18 (41%)
17	CLA	4	604	29	41,58,73	2.28	12 (29%)	47,95,113	2.45	22 (46%)
26	CHL	4	605	29	54,64,74	3.94	24 (44%)	39,102,114	3.06	18 (46%)
26	CHL	4	606	29	49,59,74	4.11	24 (48%)	33,96,114	3.10	18 (54%)
26	CHL	4	607	29	49,59,74	4.11	24 (48%)	33,96,114	3.12	15 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	4	608	16	41,58,73	2.30	12 (29%)	47,95,113	2.46	20 (42%)
17	CLA	4	609	16	51,68,73	2.04	12 (23%)	59,107,113	2.14	22 (37%)
17	CLA	4	610	29	46,63,73	2.17	12 (26%)	53,101,113	2.26	21 (39%)
17	CLA	4	611	16	43,60,73	2.22	12 (27%)	49,97,113	2.42	19 (38%)
17	CLA	4	612	16	47,64,73	2.16	12 (25%)	54,102,113	2.30	20 (37%)
17	CLA	4	613	16	33,53,73	2.44	11 (33%)	37,89,113	2.62	18 (48%)
17	CLA	4	614	16	41,58,73	2.29	12 (29%)	47,95,113	2.48	21 (44%)
26	CHL	4	615	16	41,51,74	4.41	23 (56%)	24,86,114	3.47	13 (54%)
27	LUT	4	616	-	41,43,43	0.75	0	50,60,60	1.65	14 (28%)
28	XAT	4	617	-	39,47,47	0.86	0	54,74,74	2.60	18 (33%)
20	BCR	4	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.79	15 (26%)
25	LMG	4	619	-	44,44,55	0.99	2 (4%)	52,52,63	1.03	3 (5%)
25	LMG	4	620	-	44,44,55	1.01	3 (6%)	52,52,63	1.21	5 (9%)
19	LHG	6	301	17	22,22,48	1.15	2 (9%)	23,28,54	1.28	2 (8%)
25	LMG	6	302	-	40,40,55	1.04	2 (5%)	48,48,63	1.12	3 (6%)
26	CHL	6	303	13	59,69,74	3.73	24 (40%)	45,108,114	2.77	17 (37%)
17	CLA	6	304	13	56,73,73	1.96	12 (21%)	65,113,113	2.08	20 (30%)
17	CLA	6	305	13	56,73,73	1.95	12 (21%)	65,113,113	2.14	20 (30%)
17	CLA	6	306	29	42,59,73	2.27	12 (28%)	48,96,113	2.46	21 (43%)
17	CLA	6	307	-	33,50,73	2.44	11 (33%)	38,85,113	2.54	17 (44%)
26	CHL	6	308	13	45,55,74	4.26	24 (53%)	29,91,114	3.31	15 (51%)
17	CLA	6	309	29	37,54,73	2.41	12 (32%)	43,90,113	2.41	15 (34%)
17	CLA	6	310	13	56,73,73	1.97	12 (21%)	65,113,113	2.10	18 (27%)
17	CLA	6	311	13	51,68,73	2.06	12 (23%)	59,107,113	2.13	23 (38%)
17	CLA	6	312	19	32,49,73	2.50	12 (37%)	37,84,113	2.80	19 (51%)
17	CLA	6	313	13	43,60,73	2.25	12 (27%)	49,97,113	2.43	20 (40%)
17	CLA	6	314	13	51,68,73	2.05	12 (23%)	59,107,113	2.20	19 (32%)
17	CLA	6	315	13	46,63,73	2.17	12 (26%)	53,101,113	2.34	21 (39%)
17	CLA	6	316	13	37,54,73	2.41	12 (32%)	43,90,113	2.44	17 (39%)
27	LUT	6	317	-	41,43,43	0.75	0	50,60,60	1.66	13 (26%)
28	XAT	6	318	-	39,47,47	0.88	0	54,74,74	2.62	19 (35%)
20	BCR	6	319	-	41,41,41	1.05	1 (2%)	56,56,56	1.88	15 (26%)
19	LHG	6	320	17	48,48,48	0.93	2 (4%)	49,54,54	1.12	4 (8%)
27	LUT	6	321	-	41,43,43	0.73	0	50,60,60	1.74	10 (20%)
26	CHL	7	601	14	59,69,74	3.74	25 (42%)	45,108,114	2.91	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	7	602	14	56,73,73	1.94	12 (21%)	65,113,113	2.06	20 (30%)
17	CLA	7	603	14	42,59,73	2.24	12 (28%)	48,96,113	2.45	20 (41%)
17	CLA	7	604	29	51,68,73	2.05	12 (23%)	59,107,113	2.19	22 (37%)
26	CHL	7	605	29	41,51,74	4.40	23 (56%)	24,86,114	3.53	13 (54%)
26	CHL	7	606	-	46,56,74	4.22	25 (54%)	30,92,114	3.30	15 (50%)
26	CHL	7	607	29	49,59,74	4.09	24 (48%)	33,96,114	3.13	16 (48%)
17	CLA	7	608	14	41,58,73	2.28	12 (29%)	47,95,113	2.42	22 (46%)
17	CLA	7	609	14	51,68,73	2.06	12 (23%)	59,107,113	2.12	22 (37%)
17	CLA	7	610	19	32,49,73	2.50	12 (37%)	37,84,113	2.79	18 (48%)
17	CLA	7	611	14	43,60,73	2.24	12 (27%)	49,97,113	2.45	21 (42%)
17	CLA	7	612	14	56,73,73	1.97	12 (21%)	65,113,113	2.11	19 (29%)
17	CLA	7	613	14	34,51,73	2.39	11 (32%)	39,86,113	2.50	17 (43%)
26	CHL	7	614	14	41,51,74	4.42	23 (56%)	24,86,114	3.57	15 (62%)
27	LUT	7	615	-	41,43,43	0.74	0	50,60,60	1.56	11 (22%)
28	XAT	7	616	-	39,47,47	0.84	0	54,74,74	2.60	19 (35%)
20	BCR	7	617	-	41,41,41	1.07	1 (2%)	56,56,56	2.08	13 (23%)
19	LHG	7	618	17	36,36,48	1.06	2 (5%)	37,42,54	1.22	3 (8%)
17	CLA	8	301	15	51,68,73	2.07	12 (23%)	59,107,113	2.14	22 (37%)
17	CLA	8	302	15	41,58,73	2.27	12 (29%)	47,95,113	2.52	20 (42%)
17	CLA	8	303	29	33,53,73	2.42	11 (33%)	37,89,113	2.61	17 (45%)
17	CLA	8	304	29	33,50,73	2.44	11 (33%)	38,85,113	2.51	18 (47%)
17	CLA	8	305	15	38,55,73	2.40	12 (31%)	44,91,113	2.43	18 (40%)
26	CHL	8	306	29	45,55,74	4.26	24 (53%)	29,91,114	3.25	16 (55%)
17	CLA	8	307	15	41,58,73	2.29	12 (29%)	47,95,113	2.34	20 (42%)
17	CLA	8	308	15	41,58,73	2.31	12 (29%)	47,95,113	2.35	21 (44%)
17	CLA	8	309	-	43,60,73	2.27	12 (27%)	49,97,113	2.40	19 (38%)
17	CLA	8	310	15	46,63,73	2.17	12 (26%)	53,101,113	2.29	19 (35%)
17	CLA	8	311	15	33,53,73	2.46	11 (33%)	37,89,113	2.63	19 (51%)
17	CLA	8	312	15	37,54,73	2.39	12 (32%)	43,90,113	2.51	18 (41%)
17	CLA	8	313	-	17,32,73	3.00	10 (58%)	24,54,113	4.44	19 (79%)
27	LUT	8	314	-	41,43,43	0.73	0	50,60,60	1.52	11 (22%)
28	XAT	8	315	-	39,47,47	0.86	0	54,74,74	2.72	21 (38%)
20	BCR	8	316	-	41,41,41	1.05	1 (2%)	56,56,56	1.92	15 (26%)
17	CLA	9	601	16	37,54,73	2.38	12 (32%)	43,90,113	2.49	19 (44%)
17	CLA	9	602	16	51,68,73	2.04	12 (23%)	59,107,113	2.20	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	9	603	16	37,54,73	2.35	12 (32%)	43,90,113	2.53	18 (41%)
17	CLA	9	604	29	41,58,73	2.28	12 (29%)	47,95,113	2.43	21 (44%)
26	CHL	9	605	29	54,64,74	3.91	24 (44%)	39,102,114	3.08	19 (48%)
26	CHL	9	606	29	49,59,74	4.09	24 (48%)	33,96,114	3.21	16 (48%)
26	CHL	9	607	29	49,59,74	4.09	25 (51%)	33,96,114	3.16	14 (42%)
17	CLA	9	608	16	41,58,73	2.28	12 (29%)	47,95,113	2.50	20 (42%)
17	CLA	9	609	16	51,68,73	2.05	12 (23%)	59,107,113	2.14	22 (37%)
17	CLA	9	610	29	32,49,73	2.50	12 (37%)	37,84,113	2.72	18 (48%)
17	CLA	9	611	16	43,60,73	2.25	12 (27%)	49,97,113	2.47	20 (40%)
17	CLA	9	612	16	47,64,73	2.16	12 (25%)	54,102,113	2.25	19 (35%)
17	CLA	9	613	16	33,53,73	2.44	11 (33%)	37,89,113	2.61	18 (48%)
17	CLA	9	614	16	38,55,73	2.36	12 (31%)	44,91,113	2.47	19 (43%)
26	CHL	9	615	16	41,51,74	4.44	23 (56%)	24,86,114	3.58	14 (58%)
27	LUT	9	616	-	41,43,43	0.74	0	50,60,60	1.61	11 (22%)
28	XAT	9	617	-	39,47,47	0.84	0	54,74,74	2.62	17 (31%)
20	BCR	9	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.80	16 (28%)
25	LMG	9	619	-	50,50,55	0.92	2 (4%)	58,58,63	1.01	3 (5%)
17	CLA	A	801	1	56,73,73	1.93	12 (21%)	65,113,113	2.24	23 (35%)
17	CLA	A	802	1	56,73,73	1.97	12 (21%)	65,113,113	2.00	18 (27%)
17	CLA	A	803	29	56,73,73	1.92	12 (21%)	65,113,113	2.22	22 (33%)
17	CLA	A	804	1	56,73,73	1.93	12 (21%)	65,113,113	2.18	21 (32%)
17	CLA	A	805	1	46,63,73	2.16	12 (26%)	53,101,113	2.43	22 (41%)
17	CLA	A	806	1	56,73,73	1.96	12 (21%)	65,113,113	2.05	21 (32%)
17	CLA	A	807	1	56,73,73	1.95	12 (21%)	65,113,113	2.14	19 (29%)
17	CLA	A	808	1	56,73,73	1.99	12 (21%)	65,113,113	2.14	19 (29%)
17	CLA	A	809	1	56,73,73	1.96	12 (21%)	65,113,113	2.16	20 (30%)
17	CLA	A	810	1	56,73,73	1.94	12 (21%)	65,113,113	2.18	19 (29%)
17	CLA	A	811	1	56,73,73	1.95	12 (21%)	65,113,113	2.08	20 (30%)
17	CLA	A	812	1	56,73,73	1.95	12 (21%)	65,113,113	2.10	21 (32%)
17	CLA	A	813	1	45,62,73	2.19	12 (26%)	51,99,113	2.27	20 (39%)
17	CLA	A	814	1	56,73,73	1.95	12 (21%)	65,113,113	2.16	20 (30%)
17	CLA	A	815	1	33,53,73	2.42	11 (33%)	37,89,113	2.54	17 (45%)
17	CLA	A	816	1	41,58,73	2.29	12 (29%)	47,95,113	2.44	19 (40%)
17	CLA	A	817	29	33,53,73	2.43	11 (33%)	37,89,113	2.57	15 (40%)
17	CLA	A	818	1	56,73,73	1.97	12 (21%)	65,113,113	2.17	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	819	1	56,73,73	1.95	12 (21%)	65,113,113	2.12	21 (32%)
17	CLA	A	820	1	56,73,73	1.95	12 (21%)	65,113,113	2.07	20 (30%)
17	CLA	A	821	1	33,53,73	2.42	11 (33%)	37,89,113	2.82	18 (48%)
17	CLA	A	822	29	56,73,73	1.95	12 (21%)	65,113,113	2.04	20 (30%)
17	CLA	A	823	1	40,57,73	2.33	12 (30%)	46,93,113	2.45	18 (39%)
17	CLA	A	824	1	42,59,73	2.27	12 (28%)	48,96,113	2.47	20 (41%)
17	CLA	A	825	1	46,63,73	2.19	12 (26%)	53,101,113	2.34	19 (35%)
17	CLA	A	826	29	56,73,73	1.93	12 (21%)	65,113,113	2.18	17 (26%)
17	CLA	A	827	29	56,73,73	1.97	12 (21%)	65,113,113	2.02	19 (29%)
17	CLA	A	828	1	56,73,73	1.93	12 (21%)	65,113,113	2.13	19 (29%)
17	CLA	A	829	1	56,73,73	1.91	12 (21%)	65,113,113	2.11	20 (30%)
17	CLA	A	830	1	56,73,73	1.99	12 (21%)	65,113,113	2.16	20 (30%)
17	CLA	A	831	1	56,73,73	1.93	12 (21%)	65,113,113	2.21	19 (29%)
17	CLA	A	832	1	41,58,73	2.28	12 (29%)	47,95,113	2.53	21 (44%)
17	CLA	A	833	1	56,73,73	1.95	12 (21%)	65,113,113	2.08	20 (30%)
17	CLA	A	834	1	56,73,73	1.94	12 (21%)	65,113,113	2.21	19 (29%)
17	CLA	A	835	1	56,73,73	1.95	12 (21%)	65,113,113	2.20	22 (33%)
17	CLA	A	836	1	41,58,73	2.28	12 (29%)	47,95,113	2.55	20 (42%)
17	CLA	A	837	1	33,53,73	2.46	11 (33%)	37,89,113	2.63	18 (48%)
17	CLA	A	838	1	42,59,73	2.24	12 (28%)	48,96,113	2.43	19 (39%)
17	CLA	A	839	1	56,73,73	1.93	12 (21%)	65,113,113	2.17	19 (29%)
17	CLA	A	840	1	56,73,73	1.96	12 (21%)	65,113,113	2.16	20 (30%)
17	CLA	A	841	1	56,73,73	1.99	11 (19%)	65,113,113	2.05	16 (24%)
17	CLA	A	842	1	56,73,73	1.96	12 (21%)	65,113,113	2.09	20 (30%)
17	CLA	A	843	29	56,73,73	1.92	12 (21%)	65,113,113	2.11	19 (29%)
18	PQN	A	844	-	34,34,34	1.41	2 (5%)	43,45,45	1.16	4 (9%)
17	CLA	A	845	19	43,60,73	2.26	12 (27%)	49,97,113	2.41	18 (36%)
19	LHG	A	846	-	48,48,48	0.92	2 (4%)	49,54,54	1.11	3 (6%)
19	LHG	A	847	17	26,26,48	1.26	2 (7%)	27,32,54	1.33	3 (11%)
20	BCR	A	848	-	41,41,41	1.01	1 (2%)	56,56,56	1.81	14 (25%)
20	BCR	A	849	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	13 (23%)
20	BCR	A	850	-	41,41,41	1.03	1 (2%)	56,56,56	1.94	15 (26%)
20	BCR	A	851	-	41,41,41	1.04	1 (2%)	56,56,56	2.02	14 (25%)
20	BCR	A	852	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	14 (25%)
21	SF4	A	853	1,2	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	854	29	56,73,73	1.94	12 (21%)	65,113,113	2.41	24 (36%)
22	HTG	A	855	-	19,19,19	1.01	2 (10%)	23,24,24	0.73	0
20	BCR	A	856	-	41,41,41	1.01	1 (2%)	56,56,56	2.03	16 (28%)
20	BCR	B	801	-	41,41,41	1.03	1 (2%)	56,56,56	1.47	8 (14%)
17	CLA	B	802	2	56,73,73	1.95	12 (21%)	65,113,113	2.14	22 (33%)
17	CLA	B	803	2	56,73,73	1.96	12 (21%)	65,113,113	1.92	21 (32%)
17	CLA	B	804	2	33,53,73	2.41	11 (33%)	37,89,113	2.69	18 (48%)
17	CLA	B	805	2	56,73,73	1.93	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	B	806	2	56,73,73	1.95	12 (21%)	65,113,113	2.04	19 (29%)
17	CLA	B	807	2	56,73,73	1.98	12 (21%)	65,113,113	2.15	23 (35%)
17	CLA	B	808	2	56,73,73	1.96	12 (21%)	65,113,113	2.22	23 (35%)
17	CLA	B	809	2	56,73,73	1.91	12 (21%)	65,113,113	2.11	18 (27%)
17	CLA	B	810	2	56,73,73	1.95	12 (21%)	65,113,113	2.14	22 (33%)
17	CLA	B	811	2	45,62,73	2.02	12 (26%)	56,100,113	2.38	21 (37%)
17	CLA	B	812	2	46,63,73	2.18	12 (26%)	53,101,113	2.24	18 (33%)
17	CLA	B	813	2	56,73,73	1.94	12 (21%)	65,113,113	2.11	20 (30%)
17	CLA	B	814	2	56,73,73	1.93	12 (21%)	65,113,113	2.06	22 (33%)
17	CLA	B	815	2	51,68,73	2.06	12 (23%)	59,107,113	2.21	20 (33%)
17	CLA	B	816	2	46,63,73	2.15	12 (26%)	53,101,113	2.33	21 (39%)
17	CLA	B	817	2	50,67,73	2.05	12 (24%)	57,105,113	2.26	22 (38%)
17	CLA	B	818	2	51,68,73	2.05	12 (23%)	59,107,113	2.24	19 (32%)
17	CLA	B	819	29	56,73,73	1.95	12 (21%)	65,113,113	2.13	23 (35%)
17	CLA	B	820	2	41,58,73	2.31	12 (29%)	47,95,113	2.41	19 (40%)
17	CLA	B	821	2	37,54,73	2.40	12 (32%)	43,90,113	2.57	17 (39%)
17	CLA	B	822	2	46,63,73	2.18	12 (26%)	53,101,113	2.24	20 (37%)
17	CLA	B	823	2	51,68,73	2.06	12 (23%)	59,107,113	2.19	22 (37%)
17	CLA	B	824	29	56,73,73	1.93	12 (21%)	65,113,113	2.11	20 (30%)
17	CLA	B	825	29	56,73,73	1.95	12 (21%)	65,113,113	2.13	23 (35%)
17	CLA	B	826	2	56,73,73	1.94	12 (21%)	65,113,113	2.18	19 (29%)
17	CLA	B	827	2	56,73,73	1.94	12 (21%)	65,113,113	2.15	21 (32%)
17	CLA	B	828	2	56,73,73	1.97	12 (21%)	65,113,113	2.08	19 (29%)
17	CLA	B	829	2	56,73,73	1.94	12 (21%)	65,113,113	2.25	21 (32%)
17	CLA	B	830	2	41,58,73	2.27	12 (29%)	47,95,113	2.44	19 (40%)
17	CLA	B	831	2	40,57,73	2.30	12 (30%)	46,93,113	2.35	18 (39%)
17	CLA	B	832	2	56,73,73	1.95	12 (21%)	65,113,113	2.03	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	833	2	49,66,73	2.08	12 (24%)	56,104,113	2.28	18 (32%)
17	CLA	B	834	2	56,73,73	1.98	12 (21%)	65,113,113	2.04	19 (29%)
17	CLA	B	835	29	33,53,73	2.42	11 (33%)	37,89,113	2.52	18 (48%)
17	CLA	B	836	2	51,68,73	2.08	12 (23%)	59,107,113	2.27	18 (30%)
17	CLA	B	837	2	56,73,73	1.95	12 (21%)	65,113,113	2.13	22 (33%)
17	CLA	B	838	2	38,55,73	2.34	12 (31%)	44,91,113	2.53	18 (40%)
17	CLA	B	839	29	56,73,73	1.96	12 (21%)	65,113,113	2.13	18 (27%)
17	CLA	B	840	2	56,73,73	1.96	12 (21%)	65,113,113	2.10	19 (29%)
17	CLA	B	841	19	56,73,73	1.96	12 (21%)	65,113,113	2.15	20 (30%)
18	PQN	B	842	-	34,34,34	1.40	2 (5%)	43,45,45	1.08	2 (4%)
20	BCR	B	843	-	41,41,41	1.03	1 (2%)	56,56,56	1.87	13 (23%)
20	BCR	B	844	-	41,41,41	1.02	1 (2%)	56,56,56	1.97	13 (23%)
20	BCR	B	845	-	41,41,41	0.99	1 (2%)	56,56,56	2.01	17 (30%)
20	BCR	B	846	-	41,41,41	1.02	1 (2%)	56,56,56	1.75	18 (32%)
20	BCR	B	847	-	41,41,41	1.04	1 (2%)	56,56,56	1.73	15 (26%)
20	BCR	B	848	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	13 (23%)
23	LMT	B	849	-	36,36,36	0.48	0	47,47,47	0.99	3 (6%)
24	DGD	B	850	-	67,67,67	0.85	2 (2%)	81,81,81	0.96	5 (6%)
21	SF4	C	101	3	0,12,12	0.00	-	0,24,24	0.00	-
21	SF4	C	102	3	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	F	301	29	56,73,73	1.97	12 (21%)	65,113,113	2.12	18 (27%)
22	HTG	F	302	-	19,19,19	0.99	2 (10%)	23,24,24	0.63	0
17	CLA	F	303	29	33,53,73	2.42	11 (33%)	37,89,113	2.60	16 (43%)
17	CLA	F	304	6	46,63,73	2.17	12 (26%)	53,101,113	2.26	22 (41%)
20	BCR	F	305	-	41,41,41	1.02	1 (2%)	56,56,56	1.73	17 (30%)
17	CLA	G	101	29	33,53,73	2.42	11 (33%)	37,89,113	2.60	16 (43%)
25	LMG	G	102	-	44,44,55	0.99	2 (4%)	52,52,63	1.01	3 (5%)
17	CLA	G	103	7	41,58,73	2.30	12 (29%)	47,95,113	2.42	19 (40%)
17	CLA	G	104	7	37,54,73	2.40	12 (32%)	43,90,113	2.41	17 (39%)
20	BCR	G	105	-	41,41,41	1.03	1 (2%)	56,56,56	1.85	16 (28%)
20	BCR	I	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.92	16 (28%)
22	HTG	J	3001	-	19,19,19	1.04	2 (10%)	23,24,24	0.54	0
17	CLA	J	3002	10	33,50,73	2.47	11 (33%)	38,85,113	2.61	18 (47%)
20	BCR	J	3003	-	41,41,41	1.01	1 (2%)	56,56,56	1.76	14 (25%)
20	BCR	K	4001	-	41,41,41	1.03	1 (2%)	56,56,56	1.79	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	K	4002	-	33,53,73	2.45	11 (33%)	37,89,113	2.61	17 (45%)
17	CLA	K	4003	11	37,54,73	2.42	12 (32%)	43,90,113	2.53	18 (41%)
20	BCR	K	4004	-	41,41,41	1.02	1 (2%)	56,56,56	1.81	13 (23%)
20	BCR	L	201	-	41,41,41	1.04	1 (2%)	56,56,56	1.87	14 (25%)
17	CLA	L	202	12	56,73,73	1.95	12 (21%)	65,113,113	2.09	20 (30%)
17	CLA	L	203	12	56,73,73	1.96	12 (21%)	65,113,113	2.06	22 (33%)
17	CLA	L	204	29	41,58,73	2.29	12 (29%)	47,95,113	2.42	20 (42%)
20	BCR	L	205	-	41,41,41	1.01	1 (2%)	56,56,56	1.66	11 (19%)
20	BCR	L	206	-	41,41,41	1.04	1 (2%)	56,56,56	1.84	12 (21%)
17	CLA	a	801	1	56,73,73	1.95	12 (21%)	65,113,113	2.28	22 (33%)
17	CLA	a	802	1	56,73,73	1.97	12 (21%)	65,113,113	2.03	24 (36%)
17	CLA	a	803	29	56,73,73	1.91	12 (21%)	65,113,113	2.24	20 (30%)
17	CLA	a	804	1	56,73,73	1.97	12 (21%)	65,113,113	2.15	21 (32%)
17	CLA	a	805	1	46,63,73	2.15	12 (26%)	53,101,113	2.32	20 (37%)
17	CLA	a	806	1	56,73,73	1.96	12 (21%)	65,113,113	2.18	22 (33%)
17	CLA	a	807	1	56,73,73	1.95	12 (21%)	65,113,113	2.18	22 (33%)
17	CLA	a	808	1	56,73,73	1.96	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	a	809	1	56,73,73	1.96	11 (19%)	65,113,113	2.14	19 (29%)
17	CLA	a	810	1	56,73,73	1.96	12 (21%)	65,113,113	2.15	20 (30%)
17	CLA	a	811	1	56,73,73	1.96	12 (21%)	65,113,113	2.11	22 (33%)
17	CLA	a	812	1	56,73,73	1.96	12 (21%)	65,113,113	2.08	21 (32%)
17	CLA	a	813	1	45,62,73	2.23	12 (26%)	51,99,113	2.32	19 (37%)
17	CLA	a	814	1	56,73,73	1.96	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	a	815	1	33,53,73	2.45	11 (33%)	37,89,113	2.51	16 (43%)
17	CLA	a	816	1	41,58,73	2.30	12 (29%)	47,95,113	2.40	19 (40%)
17	CLA	a	817	29	33,53,73	2.42	11 (33%)	37,89,113	2.67	16 (43%)
17	CLA	a	818	1	56,73,73	1.98	12 (21%)	65,113,113	2.20	21 (32%)
17	CLA	a	819	1	56,73,73	1.99	12 (21%)	65,113,113	2.01	19 (29%)
17	CLA	a	820	1	56,73,73	1.98	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	a	821	1	33,53,73	2.40	10 (30%)	37,89,113	2.86	17 (45%)
17	CLA	a	822	29	56,73,73	1.95	12 (21%)	65,113,113	2.06	20 (30%)
17	CLA	a	823	1	40,57,73	2.33	12 (30%)	46,93,113	2.44	18 (39%)
17	CLA	a	824	1	42,59,73	2.26	12 (28%)	48,96,113	2.48	18 (37%)
17	CLA	a	825	1	46,63,73	2.18	12 (26%)	53,101,113	2.28	19 (35%)
17	CLA	a	826	29	56,73,73	1.94	12 (21%)	65,113,113	2.17	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	a	827	29	56,73,73	1.96	12 (21%)	65,113,113	2.03	19 (29%)
17	CLA	a	828	1	56,73,73	1.92	12 (21%)	65,113,113	2.17	19 (29%)
17	CLA	a	829	1	56,73,73	1.93	12 (21%)	65,113,113	2.14	19 (29%)
17	CLA	a	830	1	56,73,73	1.99	12 (21%)	65,113,113	2.16	19 (29%)
17	CLA	a	831	1	56,73,73	1.92	12 (21%)	65,113,113	2.21	21 (32%)
17	CLA	a	832	1	41,58,73	2.29	12 (29%)	47,95,113	2.56	21 (44%)
17	CLA	a	833	1	56,73,73	1.96	12 (21%)	65,113,113	2.06	19 (29%)
17	CLA	a	834	1	56,73,73	1.94	12 (21%)	65,113,113	2.13	20 (30%)
17	CLA	a	835	1	56,73,73	1.95	12 (21%)	65,113,113	2.19	22 (33%)
17	CLA	a	836	1	41,58,73	2.27	12 (29%)	47,95,113	2.53	20 (42%)
17	CLA	a	837	1	33,53,73	2.44	11 (33%)	37,89,113	2.71	18 (48%)
17	CLA	a	838	1	42,59,73	2.25	11 (26%)	48,96,113	2.43	22 (45%)
17	CLA	a	839	1	56,73,73	1.95	12 (21%)	65,113,113	2.14	18 (27%)
17	CLA	a	840	1	56,73,73	1.96	12 (21%)	65,113,113	2.19	20 (30%)
17	CLA	a	841	1	56,73,73	1.96	12 (21%)	65,113,113	2.06	20 (30%)
17	CLA	a	842	29	56,73,73	1.97	12 (21%)	65,113,113	2.10	19 (29%)
17	CLA	a	843	1	56,73,73	1.93	12 (21%)	65,113,113	2.10	21 (32%)
17	CLA	a	844	29	56,73,73	1.91	12 (21%)	65,113,113	2.15	18 (27%)
18	PQN	a	845	-	34,34,34	1.43	2 (5%)	43,45,45	1.04	4 (9%)
17	CLA	a	846	19	43,60,73	2.26	12 (27%)	49,97,113	2.40	18 (36%)
19	LHG	a	847	-	48,48,48	0.92	2 (4%)	49,54,54	1.11	3 (6%)
19	LHG	a	848	17	26,26,48	1.24	2 (7%)	27,32,54	1.38	3 (11%)
20	BCR	a	849	-	41,41,41	1.03	1 (2%)	56,56,56	1.95	12 (21%)
20	BCR	a	850	-	41,41,41	0.99	1 (2%)	56,56,56	1.86	15 (26%)
20	BCR	a	851	-	41,41,41	1.01	1 (2%)	56,56,56	1.72	16 (28%)
20	BCR	a	852	-	41,41,41	1.02	1 (2%)	56,56,56	1.93	17 (30%)
20	BCR	a	853	-	41,41,41	1.03	1 (2%)	56,56,56	1.93	14 (25%)
20	BCR	a	854	-	41,41,41	1.02	1 (2%)	56,56,56	1.73	12 (21%)
21	SF4	a	855	1,2	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	a	856	29	56,73,73	1.92	12 (21%)	65,113,113	2.38	23 (35%)
22	HTG	a	857	-	19,19,19	1.03	2 (10%)	23,24,24	0.56	0
20	BCR	b	801	-	41,41,41	1.01	1 (2%)	56,56,56	1.42	6 (10%)
17	CLA	b	802	2	56,73,73	1.94	12 (21%)	65,113,113	2.13	22 (33%)
17	CLA	b	803	2	56,73,73	1.96	12 (21%)	65,113,113	1.92	19 (29%)
17	CLA	b	804	2	33,53,73	2.40	11 (33%)	37,89,113	2.75	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	b	805	2	56,73,73	1.93	12 (21%)	65,113,113	2.14	20 (30%)
17	CLA	b	806	2	56,73,73	1.95	12 (21%)	65,113,113	2.01	19 (29%)
17	CLA	b	807	2	56,73,73	1.98	12 (21%)	65,113,113	2.12	19 (29%)
17	CLA	b	808	2	56,73,73	1.94	12 (21%)	65,113,113	2.26	23 (35%)
17	CLA	b	809	2	56,73,73	1.88	12 (21%)	65,113,113	2.14	19 (29%)
17	CLA	b	810	2	56,73,73	1.96	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	b	811	2	45,62,73	2.01	12 (26%)	56,100,113	2.44	22 (39%)
17	CLA	b	812	2	46,63,73	2.18	12 (26%)	53,101,113	2.29	20 (37%)
17	CLA	b	813	2	56,73,73	1.94	12 (21%)	65,113,113	2.12	18 (27%)
17	CLA	b	814	2	56,73,73	1.95	12 (21%)	65,113,113	2.07	20 (30%)
17	CLA	b	815	2	46,63,73	2.15	12 (26%)	53,101,113	2.39	21 (39%)
17	CLA	b	816	2	46,63,73	2.15	12 (26%)	53,101,113	2.33	21 (39%)
17	CLA	b	817	2	50,67,73	2.07	12 (24%)	57,105,113	2.23	22 (38%)
17	CLA	b	818	2	51,68,73	2.03	12 (23%)	59,107,113	2.27	19 (32%)
17	CLA	b	819	29	56,73,73	1.95	12 (21%)	65,113,113	2.11	19 (29%)
17	CLA	b	820	2	41,58,73	2.29	12 (29%)	47,95,113	2.48	21 (44%)
17	CLA	b	821	2	37,54,73	2.39	12 (32%)	43,90,113	2.53	16 (37%)
17	CLA	b	822	2	46,63,73	2.17	12 (26%)	53,101,113	2.25	19 (35%)
17	CLA	b	823	2	51,68,73	2.05	12 (23%)	59,107,113	2.14	18 (30%)
17	CLA	b	824	29	56,73,73	1.95	12 (21%)	65,113,113	2.16	21 (32%)
17	CLA	b	825	29	56,73,73	1.95	12 (21%)	65,113,113	2.07	21 (32%)
17	CLA	b	826	2	56,73,73	1.93	12 (21%)	65,113,113	2.14	20 (30%)
17	CLA	b	827	2	56,73,73	1.94	12 (21%)	65,113,113	2.13	19 (29%)
17	CLA	b	828	2	56,73,73	1.96	12 (21%)	65,113,113	2.07	19 (29%)
17	CLA	b	829	2	56,73,73	1.89	12 (21%)	65,113,113	2.30	20 (30%)
17	CLA	b	830	2	41,58,73	2.29	12 (29%)	47,95,113	2.45	22 (46%)
17	CLA	b	831	2	40,57,73	2.30	12 (30%)	46,93,113	2.38	17 (36%)
17	CLA	b	832	2	56,73,73	1.94	12 (21%)	65,113,113	2.08	21 (32%)
17	CLA	b	833	2	49,66,73	2.10	12 (24%)	56,104,113	2.34	19 (33%)
17	CLA	b	834	2	56,73,73	1.97	12 (21%)	65,113,113	2.17	20 (30%)
17	CLA	b	835	29	33,53,73	2.42	11 (33%)	37,89,113	2.57	18 (48%)
17	CLA	b	836	2	51,68,73	2.06	12 (23%)	59,107,113	2.32	19 (32%)
17	CLA	b	837	2	56,73,73	1.95	12 (21%)	65,113,113	2.11	23 (35%)
17	CLA	b	838	2	38,55,73	2.41	12 (31%)	44,91,113	2.50	19 (43%)
17	CLA	b	839	29	56,73,73	1.98	12 (21%)	65,113,113	2.13	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	b	840	2	56,73,73	1.96	12 (21%)	65,113,113	2.16	18 (27%)
17	CLA	b	841	19	56,73,73	1.96	12 (21%)	65,113,113	2.15	21 (32%)
18	PQN	b	842	-	34,34,34	1.42	2 (5%)	43,45,45	1.02	2 (4%)
20	BCR	b	843	-	41,41,41	1.04	1 (2%)	56,56,56	1.92	14 (25%)
20	BCR	b	844	-	41,41,41	1.01	1 (2%)	56,56,56	2.07	14 (25%)
20	BCR	b	845	-	41,41,41	1.03	1 (2%)	56,56,56	1.94	14 (25%)
20	BCR	b	846	-	41,41,41	1.06	1 (2%)	56,56,56	1.65	13 (23%)
20	BCR	b	847	-	41,41,41	1.03	1 (2%)	56,56,56	1.82	15 (26%)
20	BCR	b	848	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	10 (17%)
24	DGD	b	849	-	67,67,67	0.85	2 (2%)	81,81,81	1.03	4 (4%)
21	SF4	c	101	3	0,12,12	0.00	-	0,24,24	0.00	-
21	SF4	c	102	3	0,12,12	0.00	-	0,24,24	0.00	-
22	HTG	f	7001	-	19,19,19	1.03	2 (10%)	23,24,24	0.59	0
17	CLA	f	7002	29	33,53,73	2.41	11 (33%)	37,89,113	2.60	18 (48%)
17	CLA	f	7003	6	46,63,73	2.18	12 (26%)	53,101,113	2.32	21 (39%)
20	BCR	f	7004	-	41,41,41	1.01	1 (2%)	56,56,56	1.74	17 (30%)
17	CLA	g	101	-	32,49,73	2.47	12 (37%)	37,84,113	2.75	17 (45%)
17	CLA	g	102	7	41,58,73	2.30	12 (29%)	47,95,113	2.49	21 (44%)
17	CLA	g	103	7	37,54,73	2.39	12 (32%)	43,90,113	2.47	17 (39%)
20	BCR	g	104	-	41,41,41	1.03	1 (2%)	56,56,56	1.89	16 (28%)
20	BCR	i	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.59	11 (19%)
22	HTG	j	3001	-	19,19,19	1.09	2 (10%)	23,24,24	0.60	0
17	CLA	j	3002	10	33,50,73	2.47	11 (33%)	38,85,113	2.60	18 (47%)
20	BCR	j	3003	-	41,41,41	1.00	1 (2%)	56,56,56	1.71	15 (26%)
20	BCR	j	3004	-	41,41,41	1.03	1 (2%)	56,56,56	2.15	18 (32%)
17	CLA	k	1401	-	33,53,73	2.44	11 (33%)	37,89,113	2.58	17 (45%)
17	CLA	k	1402	11	37,54,73	2.39	12 (32%)	43,90,113	2.44	16 (37%)
17	CLA	k	1403	-	37,54,73	2.42	12 (32%)	43,90,113	2.50	18 (41%)
20	BCR	k	1404	-	41,41,41	1.02	1 (2%)	56,56,56	1.78	12 (21%)
20	BCR	l	201	-	41,41,41	1.02	1 (2%)	56,56,56	1.84	15 (26%)
17	CLA	l	202	12	56,73,73	1.96	12 (21%)	65,113,113	2.10	20 (30%)
17	CLA	l	203	12	56,73,73	1.96	12 (21%)	65,113,113	2.09	22 (33%)
17	CLA	l	204	29	41,58,73	2.28	12 (29%)	47,95,113	2.43	22 (46%)
20	BCR	l	205	-	41,41,41	1.00	1 (2%)	56,56,56	1.59	10 (17%)
20	BCR	l	206	-	41,41,41	1.04	1 (2%)	56,56,56	1.79	11 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	1	301	17	-	0/26/26/53	0/0/0/0
26	CHL	1	302	13	1/1/29/36	0/35/171/177	0/0/9/9
17	CLA	1	303	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	1	304	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	1	305	29	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	1	306	-	3/3/17/25	0/22/120/135	0/0/9/9
26	CHL	1	307	13	-	0/20/156/177	0/0/9/9
17	CLA	1	308	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	1	309	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	1	310	13	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	1	311	19	3/3/15/25	0/8/106/135	0/0/9/9
17	CLA	1	312	13	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	1	313	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	1	314	13	2/2/18/25	0/25/123/135	0/0/9/9
17	CLA	1	315	13	3/3/16/25	0/15/113/135	0/0/9/9
27	LUT	1	316	-	-	0/29/67/67	0/2/2/2
28	XAT	1	317	-	-	0/31/93/93	0/2/4/4
20	BCR	1	318	-	-	0/29/63/63	0/2/2/2
19	LHG	1	319	17	-	0/53/53/53	0/0/0/0
27	LUT	1	320	-	-	0/29/67/67	0/2/2/2
26	CHL	2	601	14	1/1/29/36	0/35/171/177	0/0/9/9
17	CLA	2	602	14	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	2	603	14	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	2	604	29	3/3/19/25	0/31/129/135	0/0/9/9
26	CHL	2	605	29	-	0/14/150/177	0/0/9/9
26	CHL	2	606	-	-	0/20/156/177	0/0/9/9
26	CHL	2	607	29	-	0/23/159/177	0/0/9/9
17	CLA	2	608	14	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	2	609	14	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	2	610	19	2/2/15/25	0/8/106/135	0/0/9/9
17	CLA	2	611	14	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	2	612	14	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	2	613	14	3/3/15/25	0/11/109/135	0/0/9/9
26	CHL	2	614	14	-	0/14/150/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LUT	2	615	-	-	0/29/67/67	0/2/2/2
28	XAT	2	616	-	-	0/31/93/93	0/2/4/4
20	BCR	2	617	-	-	0/29/63/63	0/2/2/2
19	LHG	2	618	17	-	0/41/41/53	0/0/0/0
17	CLA	3	301	-	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	3	302	15	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	3	303	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	3	304	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	3	305	29	3/3/15/25	0/10/108/135	0/0/9/9
17	CLA	3	306	15	3/3/16/25	0/16/114/135	0/0/9/9
26	CHL	3	307	29	-	0/19/155/177	0/0/9/9
17	CLA	3	308	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	3	309	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	3	310	19	3/3/13/25	0/2/96/135	0/0/9/9
17	CLA	3	311	-	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	3	312	15	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	3	313	15	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	3	314	15	2/2/16/25	0/15/113/135	0/0/9/9
17	CLA	3	315	-	3/3/7/25	0/0/66/135	0/0/8/9
27	LUT	3	316	-	-	0/29/67/67	0/2/2/2
28	XAT	3	317	-	-	0/31/93/93	0/2/4/4
20	BCR	3	318	-	-	0/29/63/63	0/2/2/2
19	LHG	3	319	17	-	0/23/23/53	0/0/0/0
17	CLA	4	601	16	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	4	602	16	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	4	603	16	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	4	604	29	3/3/17/25	0/19/117/135	0/0/9/9
26	CHL	4	605	29	1/1/28/36	0/29/165/177	0/0/9/9
26	CHL	4	606	29	-	0/23/159/177	0/0/9/9
26	CHL	4	607	29	-	0/23/159/177	0/0/9/9
17	CLA	4	608	16	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	4	609	16	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	4	610	29	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	4	611	16	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	4	612	16	3/3/18/25	0/27/125/135	0/0/9/9
17	CLA	4	613	16	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	614	16	3/3/17/25	0/19/117/135	0/0/9/9
26	CHL	4	615	16	-	0/14/150/177	0/0/9/9
27	LUT	4	616	-	-	0/29/67/67	0/2/2/2
28	XAT	4	617	-	-	0/31/93/93	0/2/4/4
20	BCR	4	618	-	-	0/29/63/63	0/2/2/2
25	LMG	4	619	-	-	0/39/59/70	0/1/1/1
25	LMG	4	620	-	-	0/39/59/70	0/1/1/1
19	LHG	6	301	17	-	0/26/26/53	0/0/0/0
25	LMG	6	302	-	-	0/35/55/70	0/1/1/1
26	CHL	6	303	13	1/1/29/36	1/35/171/177	0/0/9/9
17	CLA	6	304	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	6	305	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	6	306	29	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	6	307	-	3/3/15/25	0/10/108/135	0/0/9/9
26	CHL	6	308	13	-	0/19/155/177	0/0/9/9
17	CLA	6	309	29	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	6	310	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	6	311	13	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	6	312	19	3/3/15/25	0/8/106/135	0/0/9/9
17	CLA	6	313	13	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	6	314	13	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	6	315	13	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	6	316	13	3/3/16/25	0/15/113/135	0/0/9/9
27	LUT	6	317	-	-	0/29/67/67	0/2/2/2
28	XAT	6	318	-	-	0/31/93/93	0/2/4/4
20	BCR	6	319	-	-	0/29/63/63	0/2/2/2
19	LHG	6	320	17	-	0/53/53/53	0/0/0/0
27	LUT	6	321	-	-	0/29/67/67	0/2/2/2
26	CHL	7	601	14	1/1/29/36	1/35/171/177	0/0/9/9
17	CLA	7	602	14	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	7	603	14	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	7	604	29	3/3/19/25	0/31/129/135	0/0/9/9
26	CHL	7	605	29	-	0/14/150/177	0/0/9/9
26	CHL	7	606	-	-	0/20/156/177	0/0/9/9
26	CHL	7	607	29	-	0/23/159/177	0/0/9/9
17	CLA	7	608	14	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	7	609	14	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	7	610	19	3/3/15/25	0/8/106/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	7	611	14	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	7	612	14	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	7	613	14	2/2/15/25	0/11/109/135	0/0/9/9
26	CHL	7	614	14	-	0/14/150/177	0/0/9/9
27	LUT	7	615	-	-	0/29/67/67	0/2/2/2
28	XAT	7	616	-	-	0/31/93/93	0/2/4/4
20	BCR	7	617	-	-	0/29/63/63	0/2/2/2
19	LHG	7	618	17	-	0/41/41/53	0/0/0/0
17	CLA	8	301	15	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	8	302	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	8	303	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	8	304	29	3/3/15/25	0/10/108/135	0/0/9/9
17	CLA	8	305	15	3/3/16/25	0/16/114/135	0/0/9/9
26	CHL	8	306	29	-	0/19/155/177	0/0/9/9
17	CLA	8	307	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	8	308	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	8	309	-	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	8	310	15	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	8	311	15	2/2/16/25	0/11/111/135	0/0/9/9
17	CLA	8	312	15	2/2/16/25	0/15/113/135	0/0/9/9
17	CLA	8	313	-	3/3/7/25	0/0/66/135	0/0/8/9
27	LUT	8	314	-	-	0/29/67/67	0/2/2/2
28	XAT	8	315	-	-	0/31/93/93	0/2/4/4
20	BCR	8	316	-	-	0/29/63/63	0/2/2/2
17	CLA	9	601	16	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	9	602	16	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	9	603	16	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	9	604	29	3/3/17/25	0/19/117/135	0/0/9/9
26	CHL	9	605	29	1/1/28/36	0/29/165/177	0/0/9/9
26	CHL	9	606	29	-	0/23/159/177	0/0/9/9
26	CHL	9	607	29	-	0/23/159/177	0/0/9/9
17	CLA	9	608	16	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	9	609	16	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	9	610	29	3/3/15/25	0/8/106/135	0/0/9/9
17	CLA	9	611	16	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	9	612	16	3/3/18/25	0/27/125/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	9	613	16	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	9	614	16	3/3/16/25	0/16/114/135	0/0/9/9
26	CHL	9	615	16	-	0/14/150/177	0/0/9/9
27	LUT	9	616	-	-	0/29/67/67	0/2/2/2
28	XAT	9	617	-	-	0/31/93/93	0/2/4/4
20	BCR	9	618	-	-	0/29/63/63	0/2/2/2
25	LMG	9	619	-	-	0/45/65/70	0/1/1/1
17	CLA	A	801	1	4/4/20/25	0/37/135/135	0/0/9/9
17	CLA	A	802	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	803	29	1/1/20/25	0/37/135/135	0/0/9/9
17	CLA	A	804	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	805	1	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	A	806	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	807	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	808	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	809	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	810	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	811	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	812	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	813	1	3/3/17/25	0/24/122/135	0/0/9/9
17	CLA	A	814	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	815	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	A	816	1	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	A	817	29	2/2/16/25	0/11/111/135	0/0/9/9
17	CLA	A	818	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	819	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	820	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	821	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	A	822	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	823	1	3/3/16/25	0/18/116/135	0/0/9/9
17	CLA	A	824	1	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	A	825	1	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	A	826	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	827	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	828	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
17	CLA	A	829	1	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	A	830	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	831	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	832	1	2/2/17/25	0/19/117/135	0/0/9/9
17	CLA	A	833	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	834	1	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	A	835	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	836	1	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	A	837	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	A	838	1	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	A	839	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	840	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	841	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	842	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	843	29	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	A	844	-	-	0/23/43/43	0/2/2/2
17	CLA	A	845	19	3/3/17/25	0/22/120/135	0/0/9/9
19	LHG	A	846	-	-	0/53/53/53	0/0/0/0
19	LHG	A	847	17	-	0/31/31/53	0/0/0/0
20	BCR	A	848	-	-	0/29/63/63	0/2/2/2
20	BCR	A	849	-	-	0/29/63/63	0/2/2/2
20	BCR	A	850	-	-	0/29/63/63	0/2/2/2
20	BCR	A	851	-	-	0/29/63/63	0/2/2/2
20	BCR	A	852	-	-	0/29/63/63	0/2/2/2
21	SF4	A	853	1,2	-	0/0/48/48	0/6/5/5
17	CLA	A	854	29	1/1/20/25	0/37/135/135	0/0/9/9
22	HTG	A	855	-	-	0/10/30/30	0/1/1/1
20	BCR	A	856	-	-	0/29/63/63	0/2/2/2
20	BCR	B	801	-	-	0/29/63/63	0/2/2/2
17	CLA	B	802	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	803	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	804	2	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	B	805	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	806	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	807	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	808	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	809	2	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	810	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	811	2	3/3/18/25	0/25/121/135	0/0/9/9
17	CLA	B	812	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	B	813	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	814	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	815	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	B	816	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	B	817	2	3/3/18/25	0/30/128/135	0/0/9/9
17	CLA	B	818	2	2/2/19/25	0/31/129/135	0/0/9/9
17	CLA	B	819	29	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	820	2	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	B	821	2	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	B	822	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	B	823	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	B	824	29	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	825	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	826	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	827	2	1/1/20/25	0/37/135/135	0/0/9/9
17	CLA	B	828	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	829	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	830	2	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	B	831	2	3/3/16/25	0/18/116/135	0/0/9/9
17	CLA	B	832	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	833	2	3/3/18/25	0/29/127/135	0/0/9/9
17	CLA	B	834	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	835	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	B	836	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	B	837	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	838	2	2/2/16/25	0/16/114/135	0/0/9/9
17	CLA	B	839	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	840	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	841	19	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	B	842	-	-	0/23/43/43	0/2/2/2
20	BCR	B	843	-	-	0/29/63/63	0/2/2/2
20	BCR	B	844	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	B	845	-	-	0/29/63/63	0/2/2/2
20	BCR	B	846	-	-	0/29/63/63	0/2/2/2
20	BCR	B	847	-	-	0/29/63/63	0/2/2/2
20	BCR	B	848	-	-	0/29/63/63	0/2/2/2
23	LMT	B	849	-	-	0/21/61/61	0/2/2/2
24	DGD	B	850	-	-	0/55/95/95	0/2/2/2
21	SF4	C	101	3	-	0/0/48/48	0/6/5/5
21	SF4	C	102	3	-	0/0/48/48	0/6/5/5
17	CLA	F	301	29	3/3/20/25	0/37/135/135	0/0/9/9
22	HTG	F	302	-	-	0/10/30/30	0/1/1/1
17	CLA	F	303	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	F	304	6	3/3/18/25	0/25/123/135	0/0/9/9
20	BCR	F	305	-	-	0/29/63/63	0/2/2/2
17	CLA	G	101	29	3/3/16/25	0/11/111/135	0/0/9/9
25	LMG	G	102	-	-	0/39/59/70	0/1/1/1
17	CLA	G	103	7	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	G	104	7	3/3/16/25	0/15/113/135	0/0/9/9
20	BCR	G	105	-	-	0/29/63/63	0/2/2/2
20	BCR	I	101	-	-	0/29/63/63	0/2/2/2
22	HTG	J	3001	-	-	0/10/30/30	0/1/1/1
17	CLA	J	3002	10	3/3/15/25	0/10/108/135	0/0/9/9
20	BCR	J	3003	-	-	0/29/63/63	0/2/2/2
20	BCR	K	4001	-	-	0/29/63/63	0/2/2/2
17	CLA	K	4002	-	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	K	4003	11	3/3/16/25	0/15/113/135	0/0/9/9
20	BCR	K	4004	-	-	0/29/63/63	0/2/2/2
20	BCR	L	201	-	-	0/29/63/63	0/2/2/2
17	CLA	L	202	12	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	L	203	12	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	L	204	29	3/3/17/25	0/19/117/135	0/0/9/9
20	BCR	L	205	-	-	0/29/63/63	0/2/2/2
20	BCR	L	206	-	-	0/29/63/63	0/2/2/2
17	CLA	a	801	1	4/4/20/25	0/37/135/135	0/0/9/9
17	CLA	a	802	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	803	29	1/1/20/25	0/37/135/135	0/0/9/9
17	CLA	a	804	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	805	1	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	a	806	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
17	CLA	a	807	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	808	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	809	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	810	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	811	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	812	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	813	1	3/3/17/25	0/24/122/135	0/0/9/9
17	CLA	a	814	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	815	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	a	816	1	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	a	817	29	2/2/16/25	0/11/111/135	0/0/9/9
17	CLA	a	818	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	819	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	820	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	821	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	a	822	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	823	1	3/3/16/25	0/18/116/135	0/0/9/9
17	CLA	a	824	1	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	a	825	1	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	a	826	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	827	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	828	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	829	1	1/1/20/25	0/37/135/135	0/0/9/9
17	CLA	a	830	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	831	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	832	1	2/2/17/25	0/19/117/135	0/0/9/9
17	CLA	a	833	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	834	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	835	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	836	1	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	a	837	1	2/2/16/25	0/11/111/135	0/0/9/9
17	CLA	a	838	1	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	a	839	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	840	1	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	841	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	842	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	843	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	844	29	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	a	845	-	-	0/23/43/43	0/2/2/2
17	CLA	a	846	19	3/3/17/25	0/22/120/135	0/0/9/9
19	LHG	a	847	-	-	0/53/53/53	0/0/0/0
19	LHG	a	848	17	-	0/31/31/53	0/0/0/0
20	BCR	a	849	-	-	0/29/63/63	0/2/2/2
20	BCR	a	850	-	-	0/29/63/63	0/2/2/2
20	BCR	a	851	-	-	0/29/63/63	0/2/2/2
20	BCR	a	852	-	-	0/29/63/63	0/2/2/2
20	BCR	a	853	-	-	0/29/63/63	0/2/2/2
20	BCR	a	854	-	-	0/29/63/63	0/2/2/2
21	SF4	a	855	1,2	-	0/0/48/48	0/6/5/5
17	CLA	a	856	29	1/1/20/25	0/37/135/135	0/0/9/9
22	HTG	a	857	-	-	0/10/30/30	0/1/1/1
20	BCR	b	801	-	-	0/29/63/63	0/2/2/2
17	CLA	b	802	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	b	803	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	804	2	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	b	805	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	806	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	807	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	808	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	809	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	810	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	811	2	3/3/18/25	0/25/121/135	0/0/9/9
17	CLA	b	812	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	b	813	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	814	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	815	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	b	816	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	b	817	2	3/3/18/25	0/30/128/135	0/0/9/9
17	CLA	b	818	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	b	819	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	820	2	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	821	2	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	b	822	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	b	823	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	b	824	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	825	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	826	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	827	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	b	828	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	829	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	830	2	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	b	831	2	2/2/16/25	0/18/116/135	0/0/9/9
17	CLA	b	832	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	833	2	3/3/18/25	0/29/127/135	0/0/9/9
17	CLA	b	834	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	835	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	b	836	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	b	837	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	838	2	3/3/16/25	0/16/114/135	0/0/9/9
17	CLA	b	839	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	840	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	841	19	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	b	842	-	-	0/23/43/43	0/2/2/2
20	BCR	b	843	-	-	0/29/63/63	0/2/2/2
20	BCR	b	844	-	-	0/29/63/63	0/2/2/2
20	BCR	b	845	-	-	0/29/63/63	0/2/2/2
20	BCR	b	846	-	-	0/29/63/63	0/2/2/2
20	BCR	b	847	-	-	0/29/63/63	0/2/2/2
20	BCR	b	848	-	-	0/29/63/63	0/2/2/2
24	DGD	b	849	-	-	0/55/95/95	0/2/2/2
21	SF4	c	101	3	-	0/0/48/48	0/6/5/5
21	SF4	c	102	3	-	0/0/48/48	0/6/5/5
22	HTG	f	7001	-	-	0/10/30/30	0/1/1/1
17	CLA	f	7002	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	f	7003	6	1/1/18/25	0/25/123/135	0/0/9/9
20	BCR	f	7004	-	-	0/29/63/63	0/2/2/2
17	CLA	g	101	-	2/2/15/25	0/8/106/135	0/0/9/9
17	CLA	g	102	7	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	g	103	7	3/3/16/25	0/15/113/135	0/0/9/9
20	BCR	g	104	-	-	0/29/63/63	0/2/2/2
20	BCR	i	101	-	-	0/29/63/63	0/2/2/2
22	HTG	j	3001	-	-	0/10/30/30	0/1/1/1
17	CLA	j	3002	10	3/3/15/25	0/10/108/135	0/0/9/9
20	BCR	j	3003	-	-	0/29/63/63	0/2/2/2
20	BCR	j	3004	-	-	0/29/63/63	0/2/2/2
17	CLA	k	1401	-	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	k	1402	11	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	k	1403	-	3/3/16/25	0/15/113/135	0/0/9/9
20	BCR	k	1404	-	-	0/29/63/63	0/2/2/2
20	BCR	l	201	-	-	0/29/63/63	0/2/2/2
17	CLA	l	202	12	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	l	203	12	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	l	204	29	3/3/17/25	0/19/117/135	0/0/9/9
20	BCR	l	205	-	-	0/29/63/63	0/2/2/2
20	BCR	l	206	-	-	0/29/63/63	0/2/2/2

All (4063) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	601	CHL	C3D-C4D	-14.22	1.38	1.54
26	4	606	CHL	C3D-C4D	-14.18	1.38	1.54
26	1	307	CHL	C3D-C4D	-14.09	1.38	1.54
26	2	601	CHL	C3D-C4D	-14.07	1.38	1.54
26	9	615	CHL	C3D-C4D	-14.03	1.38	1.54
26	4	605	CHL	C3D-C4D	-14.03	1.38	1.54
26	2	607	CHL	C3D-C4D	-14.03	1.38	1.54
26	2	614	CHL	C3D-C4D	-14.03	1.38	1.54
26	7	614	CHL	C3D-C4D	-14.02	1.38	1.54
26	8	306	CHL	C3D-C4D	-14.02	1.38	1.54
26	6	308	CHL	C3D-C4D	-14.02	1.38	1.54
26	2	606	CHL	C3D-C4D	-13.98	1.38	1.54
26	2	605	CHL	C3D-C4D	-13.96	1.38	1.54
26	6	303	CHL	C3D-C4D	-13.96	1.38	1.54
26	4	615	CHL	C3D-C4D	-13.96	1.38	1.54
26	9	606	CHL	C3D-C4D	-13.91	1.38	1.54
26	4	607	CHL	C3D-C4D	-13.89	1.38	1.54
26	3	307	CHL	C3D-C4D	-13.89	1.38	1.54
26	9	605	CHL	C3D-C4D	-13.89	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	605	CHL	C3D-C4D	-13.88	1.38	1.54
26	7	606	CHL	C3D-C4D	-13.88	1.38	1.54
26	7	607	CHL	C3D-C4D	-13.87	1.38	1.54
26	1	302	CHL	C3D-C4D	-13.85	1.38	1.54
26	9	607	CHL	C3D-C4D	-13.84	1.38	1.54
26	6	303	CHL	CHB-C4A	-8.15	1.33	1.52
26	4	605	CHL	CHB-C4A	-8.11	1.33	1.52
26	7	601	CHL	CHB-C4A	-8.11	1.33	1.52
26	1	302	CHL	CHB-C4A	-8.09	1.33	1.52
26	2	607	CHL	CHB-C4A	-8.07	1.33	1.52
26	2	605	CHL	CHB-C4A	-8.07	1.33	1.52
26	9	605	CHL	CHB-C4A	-8.07	1.33	1.52
26	3	307	CHL	CHB-C4A	-8.06	1.33	1.52
26	9	615	CHL	CHB-C4A	-8.05	1.33	1.52
26	4	606	CHL	CHB-C4A	-8.05	1.33	1.52
26	9	606	CHL	CHB-C4A	-8.05	1.33	1.52
26	4	607	CHL	CHB-C4A	-8.05	1.33	1.52
26	9	607	CHL	CHB-C4A	-8.05	1.33	1.52
26	2	601	CHL	CHB-C4A	-8.05	1.33	1.52
26	2	614	CHL	CHB-C4A	-8.03	1.33	1.52
26	7	607	CHL	CHB-C4A	-8.01	1.33	1.52
26	1	307	CHL	CHB-C4A	-8.01	1.33	1.52
26	2	606	CHL	CHB-C4A	-8.01	1.33	1.52
26	7	605	CHL	CHB-C4A	-8.01	1.33	1.52
26	7	606	CHL	CHB-C4A	-7.97	1.33	1.52
26	6	308	CHL	CHB-C4A	-7.96	1.33	1.52
26	4	615	CHL	CHB-C4A	-7.94	1.33	1.52
26	8	306	CHL	CHB-C4A	-7.92	1.33	1.52
26	3	307	CHL	C1B-NB	-7.91	1.33	1.50
26	7	614	CHL	CHB-C4A	-7.88	1.33	1.52
26	8	306	CHL	C1B-NB	-7.86	1.33	1.50
26	1	307	CHL	C1B-NB	-7.79	1.33	1.50
26	6	308	CHL	C1B-NB	-7.77	1.33	1.50
26	4	607	CHL	C1B-NB	-7.77	1.33	1.50
26	4	606	CHL	C1B-NB	-7.76	1.33	1.50
26	2	607	CHL	C1B-NB	-7.75	1.33	1.50
26	2	614	CHL	C1B-NB	-7.74	1.33	1.50
26	4	605	CHL	C1B-NB	-7.73	1.33	1.50
26	1	302	CHL	C1B-NB	-7.73	1.33	1.50
26	2	606	CHL	C1B-NB	-7.73	1.33	1.50
26	9	606	CHL	C1B-NB	-7.73	1.33	1.50
26	9	607	CHL	C1B-NB	-7.73	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	606	CHL	C1B-NB	-7.73	1.33	1.50
26	7	614	CHL	C1B-NB	-7.72	1.33	1.50
26	2	601	CHL	C1B-NB	-7.72	1.33	1.50
26	9	605	CHL	C1B-NB	-7.72	1.33	1.50
26	7	607	CHL	C1B-NB	-7.70	1.33	1.50
26	6	303	CHL	C1B-NB	-7.69	1.33	1.50
26	1	307	CHL	C1D-ND	-7.69	1.33	1.50
26	9	607	CHL	C1D-ND	-7.69	1.33	1.50
26	4	607	CHL	C1D-ND	-7.68	1.33	1.50
26	9	615	CHL	C1B-NB	-7.67	1.33	1.50
26	4	615	CHL	C1B-NB	-7.67	1.33	1.50
26	7	614	CHL	C1D-ND	-7.66	1.33	1.50
26	9	615	CHL	C1D-ND	-7.66	1.33	1.50
26	7	605	CHL	C1B-NB	-7.66	1.33	1.50
26	6	308	CHL	C1D-ND	-7.66	1.33	1.50
26	1	302	CHL	C1D-ND	-7.65	1.33	1.50
26	2	605	CHL	C1B-NB	-7.65	1.33	1.50
26	7	605	CHL	C1D-ND	-7.64	1.33	1.50
26	2	607	CHL	C4B-NB	-7.64	1.33	1.50
26	2	607	CHL	C1D-ND	-7.64	1.33	1.50
26	8	306	CHL	C1D-ND	-7.63	1.33	1.50
26	7	601	CHL	C1D-ND	-7.63	1.33	1.50
26	7	606	CHL	C1D-ND	-7.63	1.33	1.50
26	9	615	CHL	C4B-NB	-7.62	1.33	1.50
26	4	615	CHL	C1D-ND	-7.62	1.33	1.50
26	9	606	CHL	C1D-ND	-7.62	1.33	1.50
26	4	605	CHL	C1D-ND	-7.62	1.34	1.50
26	7	601	CHL	C1B-NB	-7.61	1.34	1.50
26	2	606	CHL	C1D-ND	-7.61	1.34	1.50
26	4	606	CHL	C1D-ND	-7.60	1.34	1.50
26	7	607	CHL	C1D-ND	-7.60	1.34	1.50
26	9	605	CHL	C1D-ND	-7.59	1.34	1.50
26	2	614	CHL	C1D-ND	-7.59	1.34	1.50
26	6	303	CHL	C1D-ND	-7.58	1.34	1.50
26	3	307	CHL	C1D-ND	-7.56	1.34	1.50
26	4	606	CHL	C4B-NB	-7.56	1.34	1.50
26	2	601	CHL	C1D-ND	-7.56	1.34	1.50
26	7	614	CHL	C4B-NB	-7.54	1.34	1.50
26	3	307	CHL	C4B-NB	-7.54	1.34	1.50
26	6	308	CHL	C4B-NB	-7.54	1.34	1.50
26	2	605	CHL	C1D-ND	-7.52	1.34	1.50
26	9	606	CHL	C4B-NB	-7.49	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	605	CHL	C4B-NB	-7.49	1.34	1.50
26	9	607	CHL	C4B-NB	-7.48	1.34	1.50
26	7	607	CHL	C4B-NB	-7.47	1.34	1.50
26	7	601	CHL	C4B-NB	-7.47	1.34	1.50
26	8	306	CHL	C4B-NB	-7.47	1.34	1.50
26	1	307	CHL	C4B-NB	-7.47	1.34	1.50
26	2	614	CHL	C4B-NB	-7.46	1.34	1.50
26	6	303	CHL	C4B-NB	-7.46	1.34	1.50
26	7	606	CHL	C4B-NB	-7.45	1.34	1.50
26	4	615	CHL	C4B-NB	-7.45	1.34	1.50
26	4	605	CHL	C4B-NB	-7.45	1.34	1.50
26	2	605	CHL	C4B-NB	-7.43	1.34	1.50
26	2	606	CHL	C4B-NB	-7.43	1.34	1.50
26	4	607	CHL	C4B-NB	-7.42	1.34	1.50
26	2	601	CHL	C4B-NB	-7.39	1.34	1.50
26	7	605	CHL	C4B-NB	-7.36	1.34	1.50
26	1	302	CHL	C4B-NB	-7.35	1.34	1.50
26	6	303	CHL	C3B-C2B	-6.12	1.47	1.55
26	7	607	CHL	C3B-C2B	-5.92	1.48	1.55
26	4	605	CHL	C3B-C2B	-5.92	1.48	1.55
26	4	607	CHL	C3B-C2B	-5.90	1.48	1.55
26	2	607	CHL	C3B-C2B	-5.86	1.48	1.55
26	1	302	CHL	C3B-C2B	-5.85	1.48	1.55
26	9	605	CHL	C3B-C2B	-5.84	1.48	1.55
26	9	607	CHL	C3B-C2B	-5.78	1.48	1.55
26	3	307	CHL	C3B-C2B	-5.77	1.48	1.55
26	2	605	CHL	C3B-C2B	-5.72	1.48	1.55
26	2	601	CHL	C3B-C2B	-5.70	1.48	1.55
26	7	601	CHL	C3B-C2B	-5.64	1.48	1.55
26	8	306	CHL	C3B-C2B	-5.62	1.48	1.55
26	9	606	CHL	C3B-C2B	-5.61	1.48	1.55
26	7	605	CHL	C3B-C2B	-5.60	1.48	1.55
26	1	307	CHL	C3B-C2B	-5.60	1.48	1.55
26	2	614	CHL	C3B-C2B	-5.57	1.48	1.55
26	4	615	CHL	C3B-C2B	-5.56	1.48	1.55
26	2	607	CHL	C4D-ND	-5.55	1.38	1.50
26	1	307	CHL	C4D-ND	-5.53	1.38	1.50
26	7	606	CHL	C3B-C2B	-5.53	1.48	1.55
26	9	607	CHL	C4D-ND	-5.51	1.38	1.50
26	7	607	CHL	C4D-ND	-5.51	1.38	1.50
26	9	615	CHL	C3B-C2B	-5.51	1.48	1.55
26	4	607	CHL	C4D-ND	-5.50	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	614	CHL	C3B-C2B	-5.50	1.48	1.55
26	2	606	CHL	C3B-C2B	-5.49	1.48	1.55
26	2	601	CHL	C4D-ND	-5.49	1.38	1.50
26	6	308	CHL	C3B-C2B	-5.48	1.48	1.55
26	6	308	CHL	C4D-ND	-5.48	1.38	1.50
26	8	306	CHL	C4D-ND	-5.47	1.38	1.50
26	7	614	CHL	C4D-ND	-5.47	1.38	1.50
26	7	606	CHL	C4D-ND	-5.46	1.38	1.50
26	1	302	CHL	C4D-ND	-5.45	1.38	1.50
26	4	615	CHL	C4D-ND	-5.45	1.38	1.50
26	2	606	CHL	C4D-ND	-5.45	1.38	1.50
26	9	615	CHL	C4D-ND	-5.44	1.38	1.50
26	4	605	CHL	C4D-ND	-5.44	1.38	1.50
26	2	614	CHL	C4D-ND	-5.43	1.38	1.50
26	3	307	CHL	C4D-ND	-5.43	1.38	1.50
26	7	601	CHL	C4D-ND	-5.42	1.38	1.50
26	6	303	CHL	C4D-ND	-5.42	1.38	1.50
26	2	605	CHL	C4D-ND	-5.42	1.38	1.50
26	9	606	CHL	C4D-ND	-5.41	1.38	1.50
26	7	605	CHL	C4D-ND	-5.40	1.38	1.50
26	4	606	CHL	C4D-ND	-5.40	1.38	1.50
26	9	605	CHL	C4D-ND	-5.39	1.38	1.50
20	A	849	BCR	C23-C22	-5.39	1.34	1.45
20	b	843	BCR	C23-C22	-5.33	1.34	1.45
20	B	843	BCR	C23-C22	-5.33	1.34	1.45
26	4	606	CHL	C3B-C2B	-5.30	1.49	1.55
20	8	316	BCR	C23-C22	-5.29	1.34	1.45
20	3	318	BCR	C23-C22	-5.28	1.34	1.45
20	G	105	BCR	C23-C22	-5.27	1.34	1.45
20	A	851	BCR	C23-C22	-5.26	1.34	1.45
20	l	206	BCR	C23-C22	-5.26	1.34	1.45
20	6	319	BCR	C23-C22	-5.26	1.34	1.45
20	7	617	BCR	C23-C22	-5.24	1.34	1.45
20	b	846	BCR	C23-C22	-5.24	1.34	1.45
20	A	850	BCR	C23-C22	-5.23	1.34	1.45
20	L	206	BCR	C23-C22	-5.23	1.34	1.45
20	g	104	BCR	C23-C22	-5.23	1.34	1.45
20	B	847	BCR	C23-C22	-5.23	1.34	1.45
20	k	1404	BCR	C23-C22	-5.22	1.34	1.45
20	A	852	BCR	C23-C22	-5.22	1.34	1.45
20	K	4001	BCR	C23-C22	-5.21	1.34	1.45
20	b	845	BCR	C23-C22	-5.21	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	318	BCR	C23-C22	-5.21	1.34	1.45
20	L	201	BCR	C23-C22	-5.20	1.34	1.45
20	4	618	BCR	C23-C22	-5.20	1.34	1.45
20	K	4004	BCR	C23-C22	-5.20	1.34	1.45
20	a	852	BCR	C23-C22	-5.19	1.34	1.45
20	b	847	BCR	C23-C22	-5.19	1.34	1.45
20	a	851	BCR	C23-C22	-5.19	1.34	1.45
20	F	305	BCR	C23-C22	-5.18	1.34	1.45
20	a	854	BCR	C23-C22	-5.17	1.34	1.45
20	B	848	BCR	C23-C22	-5.17	1.34	1.45
20	f	7004	BCR	C23-C22	-5.16	1.34	1.45
20	a	853	BCR	C23-C22	-5.15	1.34	1.45
20	a	849	BCR	C23-C22	-5.15	1.34	1.45
20	9	618	BCR	C23-C22	-5.13	1.34	1.45
20	A	856	BCR	C23-C22	-5.12	1.34	1.45
20	I	101	BCR	C23-C22	-5.10	1.34	1.45
20	2	617	BCR	C23-C22	-5.10	1.34	1.45
20	B	844	BCR	C23-C22	-5.09	1.34	1.45
20	A	848	BCR	C23-C22	-5.07	1.34	1.45
20	B	801	BCR	C23-C22	-5.06	1.34	1.45
20	J	3003	BCR	C23-C22	-5.06	1.34	1.45
20	b	848	BCR	C23-C22	-5.05	1.34	1.45
20	l	201	BCR	C23-C22	-5.05	1.34	1.45
20	a	850	BCR	C23-C22	-5.03	1.35	1.45
20	b	844	BCR	C23-C22	-5.03	1.35	1.45
20	i	101	BCR	C23-C22	-5.02	1.35	1.45
20	j	3004	BCR	C23-C22	-5.01	1.35	1.45
20	b	801	BCR	C23-C22	-4.99	1.35	1.45
20	B	846	BCR	C23-C22	-4.99	1.35	1.45
20	B	845	BCR	C23-C22	-4.98	1.35	1.45
20	l	205	BCR	C23-C22	-4.98	1.35	1.45
20	j	3003	BCR	C23-C22	-4.97	1.35	1.45
20	L	205	BCR	C23-C22	-4.96	1.35	1.45
26	2	607	CHL	C3B-C4B	-4.52	1.49	1.54
26	4	607	CHL	CHD-C1D	-4.48	1.46	1.53
26	4	607	CHL	C3B-C4B	-4.44	1.49	1.54
26	1	302	CHL	CHD-C1D	-4.39	1.46	1.53
26	7	606	CHL	CHD-C1D	-4.37	1.46	1.53
26	1	307	CHL	CHD-C1D	-4.34	1.46	1.53
26	8	306	CHL	CHD-C1D	-4.34	1.46	1.53
26	7	607	CHL	CHD-C1D	-4.33	1.46	1.53
26	2	606	CHL	CHD-C1D	-4.33	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	601	CHL	CHD-C1D	-4.32	1.46	1.53
26	3	307	CHL	CHD-C1D	-4.32	1.46	1.53
26	2	607	CHL	CHD-C1D	-4.32	1.46	1.53
26	9	606	CHL	CHD-C1D	-4.30	1.46	1.53
26	4	605	CHL	CHB-C1B	-4.29	1.46	1.53
26	7	601	CHL	CHD-C1D	-4.29	1.46	1.53
26	2	614	CHL	CHD-C1D	-4.29	1.46	1.53
26	9	606	CHL	CHB-C1B	-4.29	1.46	1.53
26	3	307	CHL	C3B-C4B	-4.28	1.49	1.54
26	6	303	CHL	CHB-C1B	-4.26	1.46	1.53
26	9	605	CHL	CHB-C1B	-4.25	1.46	1.53
26	2	607	CHL	CHB-C1B	-4.24	1.46	1.53
26	4	605	CHL	C3B-C4B	-4.24	1.49	1.54
26	9	605	CHL	CHD-C1D	-4.24	1.46	1.53
26	4	606	CHL	CHB-C1B	-4.22	1.46	1.53
26	9	615	CHL	CHB-C1B	-4.21	1.46	1.53
26	9	607	CHL	CHD-C1D	-4.21	1.46	1.53
26	6	308	CHL	CHD-C1D	-4.21	1.46	1.53
26	9	607	CHL	C3B-C4B	-4.20	1.49	1.54
26	2	605	CHL	CHB-C1B	-4.20	1.46	1.53
26	7	605	CHL	CHD-C1D	-4.19	1.46	1.53
26	4	615	CHL	CHD-C1D	-4.19	1.46	1.53
26	7	614	CHL	CHD-C1D	-4.18	1.47	1.53
26	3	307	CHL	CHC-C4B	-4.17	1.47	1.53
26	1	302	CHL	CHB-C1B	-4.17	1.47	1.53
26	7	607	CHL	C3B-C4B	-4.17	1.49	1.54
26	4	605	CHL	CHD-C1D	-4.16	1.47	1.53
26	9	615	CHL	CHD-C1D	-4.16	1.47	1.53
26	9	607	CHL	CHB-C1B	-4.16	1.47	1.53
26	6	303	CHL	CHD-C1D	-4.16	1.47	1.53
26	2	614	CHL	CHB-C1B	-4.16	1.47	1.53
26	2	606	CHL	CHB-C1B	-4.16	1.47	1.53
26	8	306	CHL	C3B-C4B	-4.16	1.49	1.54
26	9	615	CHL	C3B-C4B	-4.15	1.49	1.54
26	7	606	CHL	CHB-C1B	-4.14	1.47	1.53
26	2	601	CHL	CHB-C1B	-4.14	1.47	1.53
26	3	307	CHL	CHB-C1B	-4.14	1.47	1.53
26	7	614	CHL	C3B-C4B	-4.14	1.49	1.54
26	4	607	CHL	CHB-C1B	-4.13	1.47	1.53
26	2	605	CHL	CHD-C1D	-4.12	1.47	1.53
26	6	308	CHL	CHB-C1B	-4.08	1.47	1.53
26	4	606	CHL	CHD-C1D	-4.08	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	308	CHL	C3B-C4B	-4.08	1.49	1.54
26	1	307	CHL	CHB-C1B	-4.05	1.47	1.53
26	6	303	CHL	C3B-C4B	-4.05	1.49	1.54
26	8	306	CHL	CHB-C1B	-4.05	1.47	1.53
26	7	605	CHL	CHB-C1B	-4.02	1.47	1.53
26	4	605	CHL	CHC-C4B	-4.01	1.47	1.53
26	4	615	CHL	CHB-C1B	-4.01	1.47	1.53
26	7	601	CHL	CHB-C1B	-4.01	1.47	1.53
26	4	606	CHL	C3B-C4B	-3.99	1.49	1.54
26	7	607	CHL	CHB-C1B	-3.99	1.47	1.53
26	1	307	CHL	C3B-C4B	-3.97	1.49	1.54
26	9	605	CHL	C3B-C4B	-3.96	1.49	1.54
26	7	614	CHL	CHB-C1B	-3.96	1.47	1.53
26	7	614	CHL	CHC-C4B	-3.94	1.47	1.53
26	9	615	CHL	CHC-C4B	-3.93	1.47	1.53
26	7	606	CHL	C3B-C4B	-3.92	1.49	1.54
26	2	606	CHL	C3B-C4B	-3.91	1.49	1.54
26	8	306	CHL	CHC-C4B	-3.91	1.47	1.53
26	4	615	CHL	C3B-C4B	-3.91	1.49	1.54
26	2	614	CHL	CHC-C4B	-3.90	1.47	1.53
26	2	614	CHL	C3B-C4B	-3.90	1.49	1.54
26	9	607	CHL	CHC-C4B	-3.90	1.47	1.53
26	4	607	CHL	CHC-C4B	-3.89	1.47	1.53
26	1	307	CHL	CHC-C4B	-3.89	1.47	1.53
26	9	606	CHL	CHC-C4B	-3.88	1.47	1.53
26	2	607	CHL	CHC-C4B	-3.88	1.47	1.53
26	2	605	CHL	C3B-C4B	-3.88	1.49	1.54
26	4	606	CHL	CHC-C4B	-3.88	1.47	1.53
26	6	308	CHL	CHC-C4B	-3.87	1.47	1.53
26	7	607	CHL	CHC-C4B	-3.84	1.47	1.53
26	2	601	CHL	CHC-C4B	-3.84	1.47	1.53
26	9	605	CHL	CHC-C4B	-3.84	1.47	1.53
26	2	606	CHL	CHC-C4B	-3.84	1.47	1.53
22	j	3001	HTG	C1'-S1	-3.84	1.76	1.81
26	6	303	CHL	CHC-C4B	-3.83	1.47	1.53
26	7	605	CHL	CHC-C4B	-3.82	1.47	1.53
26	7	606	CHL	CHC-C4B	-3.80	1.47	1.53
26	4	615	CHL	CHC-C4B	-3.78	1.47	1.53
26	2	605	CHL	CHC-C4B	-3.77	1.47	1.53
26	1	302	CHL	CHC-C4B	-3.73	1.47	1.53
26	9	606	CHL	C3B-C4B	-3.73	1.50	1.54
26	7	601	CHL	C3B-C4B	-3.73	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	f	7001	HTG	C1'-S1	-3.72	1.76	1.81
26	2	601	CHL	C3B-C4B	-3.67	1.50	1.54
26	1	302	CHL	C3B-C4B	-3.65	1.50	1.54
22	J	3001	HTG	C1'-S1	-3.64	1.76	1.81
26	7	605	CHL	C3B-C4B	-3.62	1.50	1.54
22	a	857	HTG	C1'-S1	-3.60	1.76	1.81
26	7	601	CHL	CHC-C4B	-3.56	1.48	1.53
22	A	855	HTG	C1'-S1	-3.56	1.76	1.81
22	F	302	HTG	C1'-S1	-3.48	1.76	1.81
26	7	601	CHL	C1A-CHA	-3.34	1.48	1.53
26	3	307	CHL	CHC-C1C	-3.19	1.47	1.53
26	2	614	CHL	C1A-CHA	-3.12	1.48	1.53
26	7	606	CHL	CHD-C4C	-3.12	1.47	1.53
26	8	306	CHL	CHD-C4C	-3.10	1.47	1.53
26	7	601	CHL	C1A-C2A	-3.10	1.50	1.53
26	4	615	CHL	C1A-CHA	-3.10	1.48	1.53
26	9	606	CHL	CHD-C4C	-3.09	1.47	1.53
26	4	607	CHL	CHD-C4C	-3.08	1.47	1.53
26	9	607	CHL	CHC-C1C	-3.07	1.47	1.53
26	2	607	CHL	CHC-C1C	-3.07	1.47	1.53
26	7	614	CHL	CHC-C1C	-3.07	1.47	1.53
26	2	606	CHL	CHD-C4C	-3.06	1.47	1.53
26	9	606	CHL	CHC-C1C	-3.05	1.47	1.53
26	2	607	CHL	CHD-C4C	-3.04	1.47	1.53
26	1	302	CHL	CHD-C4C	-3.04	1.47	1.53
26	7	607	CHL	CHC-C1C	-3.04	1.47	1.53
26	8	306	CHL	C1A-CHA	-3.04	1.49	1.53
26	4	607	CHL	CHC-C1C	-3.04	1.47	1.53
26	3	307	CHL	CHD-C4C	-3.04	1.47	1.53
26	7	607	CHL	CHD-C4C	-3.03	1.47	1.53
26	3	307	CHL	C1A-CHA	-3.03	1.49	1.53
26	9	615	CHL	C1A-CHA	-3.02	1.49	1.53
26	7	601	CHL	CHD-C4C	-3.02	1.47	1.53
26	9	615	CHL	CHC-C1C	-3.02	1.47	1.53
26	7	605	CHL	C1A-CHA	-3.02	1.49	1.53
26	7	605	CHL	CHD-C4C	-3.01	1.47	1.53
26	2	601	CHL	CHD-C4C	-3.01	1.47	1.53
26	2	601	CHL	CHC-C1C	-3.01	1.47	1.53
26	4	605	CHL	CHC-C1C	-3.00	1.47	1.53
26	2	614	CHL	CHC-C1C	-2.99	1.47	1.53
26	2	614	CHL	CHD-C4C	-2.99	1.47	1.53
26	6	308	CHL	CHD-C4C	-2.99	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	606	CHL	C4A-C3A	-2.99	1.50	1.53
26	9	607	CHL	CBD-CAD	-2.99	1.48	1.53
26	9	605	CHL	C1A-CHA	-2.99	1.49	1.53
26	9	607	CHL	C1A-CHA	-2.99	1.49	1.53
26	7	614	CHL	CHD-C4C	-2.98	1.47	1.53
26	9	605	CHL	CHD-C4C	-2.98	1.47	1.53
26	4	607	CHL	C1A-CHA	-2.96	1.49	1.53
26	1	307	CHL	CHD-C4C	-2.95	1.47	1.53
26	7	606	CHL	CHC-C1C	-2.95	1.47	1.53
26	3	307	CHL	C4A-C3A	-2.95	1.50	1.53
26	6	308	CHL	CHC-C1C	-2.94	1.47	1.53
26	2	607	CHL	CBD-CAD	-2.93	1.48	1.53
26	7	607	CHL	C1A-CHA	-2.93	1.49	1.53
26	9	607	CHL	CHD-C4C	-2.92	1.47	1.53
26	7	605	CHL	CHC-C1C	-2.92	1.47	1.53
26	1	302	CHL	C1A-CHA	-2.92	1.49	1.53
26	8	306	CHL	CHC-C1C	-2.92	1.47	1.53
26	9	605	CHL	C4A-C3A	-2.92	1.50	1.53
26	1	307	CHL	CHC-C1C	-2.91	1.47	1.53
26	4	605	CHL	C4A-C3A	-2.90	1.50	1.53
26	9	615	CHL	CHD-C4C	-2.90	1.48	1.53
26	4	615	CHL	CHC-C1C	-2.90	1.48	1.53
26	4	606	CHL	C4A-C3A	-2.90	1.50	1.53
26	2	607	CHL	C1A-CHA	-2.90	1.49	1.53
26	2	605	CHL	CHC-C1C	-2.89	1.48	1.53
26	6	303	CHL	CHD-C4C	-2.88	1.48	1.53
26	7	606	CHL	CBD-CAD	-2.88	1.48	1.53
26	2	606	CHL	CHC-C1C	-2.88	1.48	1.53
26	2	605	CHL	CHD-C4C	-2.88	1.48	1.53
26	6	308	CHL	C4A-C3A	-2.87	1.50	1.53
26	2	601	CHL	CBD-CAD	-2.87	1.48	1.53
26	4	606	CHL	CHD-C4C	-2.87	1.48	1.53
26	1	307	CHL	C1A-CHA	-2.87	1.49	1.53
26	6	303	CHL	CHC-C1C	-2.86	1.48	1.53
26	9	605	CHL	CHC-C1C	-2.86	1.48	1.53
26	3	307	CHL	CBD-CAD	-2.86	1.48	1.53
26	4	615	CHL	CHD-C4C	-2.86	1.48	1.53
26	2	601	CHL	C1A-CHA	-2.86	1.49	1.53
26	7	614	CHL	C1A-CHA	-2.86	1.49	1.53
26	4	605	CHL	CHD-C4C	-2.85	1.48	1.53
26	4	606	CHL	C1A-CHA	-2.85	1.49	1.53
26	7	606	CHL	C1A-CHA	-2.84	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	303	CHL	C1A-CHA	-2.84	1.49	1.53
26	4	605	CHL	CBD-CAD	-2.84	1.48	1.53
26	2	606	CHL	CBD-CAD	-2.84	1.48	1.53
26	6	303	CHL	CBD-CAD	-2.83	1.48	1.53
26	2	605	CHL	C1A-CHA	-2.83	1.49	1.53
26	2	606	CHL	C1A-CHA	-2.83	1.49	1.53
26	1	302	CHL	CBD-CAD	-2.82	1.48	1.53
26	4	607	CHL	CBD-CAD	-2.82	1.48	1.53
26	6	303	CHL	C4A-C3A	-2.82	1.50	1.53
26	9	607	CHL	C4A-C3A	-2.82	1.50	1.53
26	4	605	CHL	C1A-CHA	-2.81	1.49	1.53
26	1	302	CHL	CHC-C1C	-2.81	1.48	1.53
26	1	307	CHL	C4A-C3A	-2.80	1.50	1.53
26	9	606	CHL	CBD-CAD	-2.80	1.48	1.53
26	6	308	CHL	CBD-CAD	-2.80	1.48	1.53
26	9	605	CHL	CBD-CAD	-2.80	1.48	1.53
26	1	307	CHL	CBD-CAD	-2.79	1.48	1.53
26	2	601	CHL	C4A-C3A	-2.79	1.50	1.53
26	2	607	CHL	C4A-C3A	-2.78	1.50	1.53
26	4	607	CHL	C4A-C3A	-2.78	1.50	1.53
26	4	615	CHL	CBD-CAD	-2.76	1.48	1.53
26	2	606	CHL	C4A-C3A	-2.75	1.50	1.53
26	8	306	CHL	CBD-CAD	-2.73	1.49	1.53
26	2	605	CHL	C4A-C3A	-2.72	1.50	1.53
26	7	614	CHL	CBD-CAD	-2.71	1.49	1.53
26	2	614	CHL	CBD-CAD	-2.71	1.49	1.53
26	6	308	CHL	C1A-CHA	-2.71	1.49	1.53
26	7	605	CHL	CBD-CAD	-2.71	1.49	1.53
26	9	606	CHL	C1A-CHA	-2.71	1.49	1.53
26	7	601	CHL	CBD-CAD	-2.70	1.49	1.53
26	8	306	CHL	C4A-C3A	-2.70	1.50	1.53
26	2	605	CHL	CBD-CAD	-2.70	1.49	1.53
26	7	607	CHL	CBD-CAD	-2.70	1.49	1.53
26	4	606	CHL	CBD-CAD	-2.69	1.49	1.53
26	7	606	CHL	C4A-C3A	-2.68	1.50	1.53
26	4	606	CHL	CHC-C1C	-2.67	1.48	1.53
26	4	606	CHL	C3D-C2D	-2.66	1.48	1.55
26	7	605	CHL	C4A-C3A	-2.66	1.50	1.53
26	1	302	CHL	C4A-C3A	-2.66	1.50	1.53
26	4	615	CHL	C4A-C3A	-2.65	1.50	1.53
26	9	615	CHL	CBD-CAD	-2.64	1.49	1.53
26	7	601	CHL	CHC-C1C	-2.64	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	601	CHL	C4A-C3A	-2.63	1.50	1.53
26	2	614	CHL	C4A-C3A	-2.63	1.50	1.53
26	4	615	CHL	C3D-C2D	-2.62	1.48	1.55
26	9	606	CHL	C3D-C2D	-2.61	1.48	1.55
26	2	606	CHL	C3D-C2D	-2.61	1.48	1.55
26	9	615	CHL	C4A-C3A	-2.61	1.50	1.53
26	7	601	CHL	C3D-C2D	-2.60	1.48	1.55
26	9	607	CHL	C3D-C2D	-2.59	1.48	1.55
26	2	601	CHL	C3D-C2D	-2.59	1.48	1.55
22	j	3001	HTG	C1-S1	-2.59	1.76	1.80
26	8	306	CHL	C3D-C2D	-2.59	1.48	1.55
26	7	606	CHL	C3D-C2D	-2.58	1.48	1.55
26	2	607	CHL	C3D-C2D	-2.57	1.48	1.55
26	1	307	CHL	C3D-C2D	-2.57	1.48	1.55
26	3	307	CHL	C3D-C2D	-2.55	1.48	1.55
26	2	614	CHL	C3D-C2D	-2.55	1.48	1.55
26	4	607	CHL	C3D-C2D	-2.55	1.48	1.55
26	6	308	CHL	C3D-C2D	-2.54	1.48	1.55
26	7	614	CHL	C3D-C2D	-2.54	1.48	1.55
26	9	615	CHL	C3D-C2D	-2.54	1.48	1.55
26	9	605	CHL	C3D-C2D	-2.53	1.48	1.55
26	1	302	CHL	C3D-C2D	-2.52	1.48	1.55
26	4	605	CHL	C3D-C2D	-2.52	1.48	1.55
26	2	605	CHL	C3D-C2D	-2.51	1.48	1.55
17	7	610	CLA	C3A-C2A	-2.50	1.52	1.54
26	6	303	CHL	C3D-C2D	-2.49	1.48	1.55
22	a	857	HTG	C1-S1	-2.48	1.76	1.80
26	9	615	CHL	C1A-C2A	-2.47	1.50	1.53
17	2	610	CLA	C3A-C2A	-2.47	1.52	1.54
26	7	605	CHL	C3D-C2D	-2.47	1.48	1.55
26	7	607	CHL	C4A-C3A	-2.47	1.50	1.53
26	7	607	CHL	C3D-C2D	-2.47	1.48	1.55
26	7	614	CHL	C4A-C3A	-2.45	1.50	1.53
26	2	607	CHL	C3B-CAB	-2.45	1.48	1.50
22	J	3001	HTG	C1-S1	-2.43	1.76	1.80
17	9	610	CLA	C3A-C2A	-2.41	1.52	1.54
26	4	605	CHL	C1A-C2A	-2.39	1.50	1.53
22	A	855	HTG	C1-S1	-2.36	1.77	1.80
26	4	615	CHL	C1A-C2A	-2.35	1.50	1.53
26	9	605	CHL	C1A-C2A	-2.32	1.50	1.53
22	F	302	HTG	C1-S1	-2.30	1.77	1.80
17	6	312	CLA	C3A-C2A	-2.29	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	f	7001	HTG	C1-S1	-2.28	1.77	1.80
17	1	311	CLA	C3A-C2A	-2.27	1.52	1.54
26	4	606	CHL	C1A-C2A	-2.27	1.51	1.53
17	g	101	CLA	C3A-C2A	-2.26	1.52	1.54
26	7	605	CHL	C1A-C2A	-2.24	1.51	1.53
26	2	614	CHL	C1A-C2A	-2.21	1.51	1.53
26	6	308	CHL	C1A-C2A	-2.21	1.51	1.53
26	7	606	CHL	C1A-C2A	-2.21	1.51	1.53
26	9	607	CHL	C1A-C2A	-2.20	1.51	1.53
26	2	607	CHL	C2D-C1D	-2.19	1.48	1.53
26	8	306	CHL	C2B-C1B	-2.16	1.48	1.53
17	3	310	CLA	C3A-C2A	-2.16	1.52	1.54
26	4	607	CHL	C2D-C1D	-2.16	1.48	1.53
26	7	614	CHL	C1A-C2A	-2.15	1.51	1.53
26	6	303	CHL	C3B-CAB	-2.14	1.48	1.50
26	7	601	CHL	C2B-C1B	-2.14	1.49	1.53
26	1	302	CHL	C2D-C1D	-2.14	1.49	1.53
26	7	605	CHL	C2B-C1B	-2.13	1.49	1.53
26	9	606	CHL	C2D-C1D	-2.13	1.49	1.53
26	2	607	CHL	C2B-C1B	-2.13	1.49	1.53
26	2	606	CHL	C1A-C2A	-2.13	1.51	1.53
26	2	605	CHL	C2B-C1B	-2.12	1.49	1.53
26	7	607	CHL	C1A-C2A	-2.12	1.51	1.53
26	1	307	CHL	C2D-C1D	-2.11	1.49	1.53
26	2	605	CHL	C1A-C2A	-2.11	1.51	1.53
26	2	607	CHL	C1A-C2A	-2.10	1.51	1.53
26	2	606	CHL	C2D-C1D	-2.10	1.49	1.53
26	1	307	CHL	C2B-C1B	-2.10	1.49	1.53
26	3	307	CHL	C1A-C2A	-2.10	1.51	1.53
26	7	606	CHL	C2D-C1D	-2.10	1.49	1.53
26	2	601	CHL	C2B-C1B	-2.10	1.49	1.53
26	9	605	CHL	C2B-C1B	-2.07	1.49	1.53
26	1	302	CHL	C2B-C1B	-2.07	1.49	1.53
26	4	615	CHL	C2D-C1D	-2.06	1.49	1.53
26	9	607	CHL	C2D-C1D	-2.06	1.49	1.53
26	9	607	CHL	C2B-C1B	-2.05	1.49	1.53
26	8	306	CHL	C2D-C1D	-2.05	1.49	1.53
26	6	303	CHL	C2B-C1B	-2.05	1.49	1.53
26	2	601	CHL	C2D-C1D	-2.05	1.49	1.53
26	4	605	CHL	C2B-C1B	-2.05	1.49	1.53
26	1	307	CHL	C1A-C2A	-2.04	1.51	1.53
26	7	607	CHL	C2D-C1D	-2.04	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	601	CHL	C2D-C1D	-2.04	1.49	1.53
26	7	606	CHL	C2B-C1B	-2.03	1.49	1.53
26	9	615	CHL	C2B-C1B	-2.03	1.49	1.53
26	3	307	CHL	C2D-C1D	-2.03	1.49	1.53
26	7	614	CHL	C2D-C1D	-2.03	1.49	1.53
26	4	606	CHL	C2B-C1B	-2.03	1.49	1.53
26	7	601	CHL	CHA-CBD	-2.02	1.48	1.53
26	6	308	CHL	C2D-C1D	-2.02	1.49	1.53
26	2	614	CHL	C2D-C1D	-2.02	1.49	1.53
26	9	606	CHL	C2B-C1B	-2.01	1.49	1.53
26	7	605	CHL	C2D-C1D	-2.01	1.49	1.53
26	4	607	CHL	C3B-CAB	-2.00	1.48	1.50
17	3	315	CLA	C3B-C2B	2.01	1.49	1.39
25	4	620	LMG	O1-C1	2.01	1.43	1.40
17	b	809	CLA	C4C-C3C	2.01	1.48	1.45
26	1	302	CHL	CMC-C2C	2.02	1.48	1.45
17	B	826	CLA	C4C-C3C	2.03	1.48	1.45
26	4	605	CHL	CMC-C2C	2.04	1.48	1.45
17	8	313	CLA	C1B-CHB	2.04	1.47	1.43
17	A	805	CLA	C4C-C3C	2.04	1.48	1.45
17	B	829	CLA	C1C-C2C	2.05	1.48	1.44
26	9	606	CHL	CMC-C2C	2.05	1.48	1.45
26	4	606	CHL	CMC-C2C	2.05	1.48	1.45
26	6	303	CHL	CMC-C2C	2.06	1.48	1.45
17	A	828	CLA	C4C-C3C	2.06	1.48	1.45
26	8	306	CHL	CMC-C2C	2.06	1.48	1.45
26	9	605	CHL	CMC-C2C	2.06	1.48	1.45
17	f	7002	CLA	C4C-C3C	2.07	1.48	1.45
17	b	828	CLA	C4C-C3C	2.07	1.48	1.45
26	6	308	CHL	CMC-C2C	2.07	1.48	1.45
17	a	833	CLA	C4C-C3C	2.08	1.48	1.45
17	A	810	CLA	C4C-C3C	2.08	1.48	1.45
26	4	615	CHL	CMC-C2C	2.08	1.48	1.45
26	3	307	CHL	CMC-C2C	2.09	1.48	1.45
26	9	615	CHL	CMC-C2C	2.09	1.48	1.45
17	b	804	CLA	C4C-C3C	2.10	1.48	1.45
17	a	828	CLA	C4C-C3C	2.11	1.48	1.45
17	4	603	CLA	C4C-C3C	2.11	1.48	1.45
17	b	803	CLA	C4C-C3C	2.11	1.48	1.45
17	B	837	CLA	C4C-C3C	2.11	1.48	1.45
26	1	307	CHL	CMC-C2C	2.11	1.48	1.45
26	7	614	CHL	CMC-C2C	2.12	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	825	CLA	C4C-C3C	2.12	1.48	1.45
17	B	814	CLA	C4C-C3C	2.12	1.48	1.45
17	a	830	CLA	C4C-C3C	2.13	1.48	1.45
17	a	804	CLA	C4C-C3C	2.13	1.48	1.45
17	8	313	CLA	C3D-C2D	2.13	1.49	1.39
26	4	607	CHL	CMC-C2C	2.13	1.49	1.45
17	b	822	CLA	C4C-C3C	2.13	1.48	1.45
17	B	833	CLA	C1C-C2C	2.13	1.48	1.44
17	A	819	CLA	C4C-C3C	2.14	1.48	1.45
17	B	836	CLA	C4C-C3C	2.14	1.48	1.45
17	1	203	CLA	C4C-C3C	2.14	1.48	1.45
17	2	608	CLA	C1C-C2C	2.14	1.48	1.44
17	B	833	CLA	C4C-C3C	2.14	1.48	1.45
17	b	827	CLA	C4C-C3C	2.15	1.48	1.45
26	2	606	CHL	CMC-C2C	2.15	1.49	1.45
17	b	840	CLA	C4C-C3C	2.15	1.48	1.45
17	B	811	CLA	C3B-C2B	2.15	1.48	1.41
17	b	825	CLA	C4C-C3C	2.15	1.48	1.45
17	A	812	CLA	C4C-C3C	2.15	1.48	1.45
17	4	609	CLA	C4C-C3C	2.15	1.48	1.45
17	b	829	CLA	C1C-C2C	2.15	1.48	1.44
17	A	829	CLA	C4C-C3C	2.16	1.48	1.45
26	7	606	CHL	CMC-C2C	2.16	1.49	1.45
26	9	607	CHL	CMC-C2C	2.16	1.49	1.45
17	A	854	CLA	C4C-C3C	2.16	1.48	1.45
17	3	315	CLA	C3D-C2D	2.16	1.49	1.39
17	A	821	CLA	C4C-C3C	2.16	1.48	1.45
17	b	808	CLA	C4C-C3C	2.16	1.48	1.45
17	L	203	CLA	C4C-C3C	2.17	1.48	1.45
17	A	835	CLA	C1C-C2C	2.17	1.48	1.44
17	B	802	CLA	C4C-C3C	2.17	1.48	1.45
17	b	808	CLA	C1C-C2C	2.17	1.48	1.44
17	b	802	CLA	C1C-C2C	2.18	1.48	1.44
26	2	607	CHL	CMC-C2C	2.18	1.49	1.45
17	b	806	CLA	C4C-C3C	2.18	1.48	1.45
26	2	614	CHL	CMC-C2C	2.18	1.49	1.45
17	B	841	CLA	C4C-C3C	2.18	1.48	1.45
17	A	818	CLA	C4C-C3C	2.19	1.48	1.45
17	b	811	CLA	C3B-C2B	2.19	1.48	1.41
17	A	806	CLA	C1C-C2C	2.19	1.48	1.44
17	b	805	CLA	C1C-C2C	2.19	1.48	1.44
17	3	309	CLA	C4C-C3C	2.19	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	836	CLA	C4C-C3C	2.20	1.48	1.45
17	a	823	CLA	C4C-C3C	2.20	1.48	1.45
17	b	820	CLA	C4C-C3C	2.20	1.48	1.45
17	a	803	CLA	C1C-C2C	2.20	1.48	1.44
17	B	818	CLA	C4C-C3C	2.20	1.48	1.45
26	7	607	CHL	CMC-C2C	2.20	1.49	1.45
17	b	814	CLA	C4C-C3C	2.21	1.48	1.45
17	k	1402	CLA	C1C-C2C	2.21	1.48	1.44
17	l	304	CLA	C1C-C2C	2.21	1.48	1.44
17	a	835	CLA	C4C-C3C	2.21	1.48	1.45
17	A	834	CLA	C1C-C2C	2.21	1.48	1.44
17	a	834	CLA	C4C-C3C	2.21	1.48	1.45
17	B	834	CLA	C1C-C2C	2.21	1.48	1.44
17	b	831	CLA	C1C-C2C	2.22	1.48	1.44
17	a	814	CLA	C4C-C3C	2.22	1.49	1.45
17	a	843	CLA	C4C-C3C	2.22	1.49	1.45
17	a	818	CLA	C1C-C2C	2.22	1.48	1.44
17	b	819	CLA	C1C-C2C	2.22	1.48	1.44
17	B	828	CLA	C4C-C3C	2.22	1.49	1.45
17	B	835	CLA	C4C-C3C	2.22	1.49	1.45
17	6	311	CLA	C4C-C3C	2.22	1.49	1.45
17	a	801	CLA	C4C-C3C	2.23	1.49	1.45
17	a	808	CLA	C4C-C3C	2.23	1.49	1.45
17	8	307	CLA	C4C-C3C	2.23	1.49	1.45
17	L	202	CLA	C1C-C2C	2.23	1.48	1.44
17	a	856	CLA	C1C-C2C	2.23	1.48	1.44
17	a	825	CLA	C4C-C3C	2.23	1.49	1.45
17	A	831	CLA	C1C-C2C	2.23	1.48	1.44
17	A	843	CLA	C1C-C2C	2.23	1.48	1.44
17	k	1403	CLA	C1C-C2C	2.24	1.48	1.44
17	a	816	CLA	C4C-C3C	2.24	1.49	1.45
17	4	612	CLA	C1C-C2C	2.24	1.48	1.44
17	G	101	CLA	C4C-C3C	2.24	1.49	1.45
17	7	604	CLA	C1C-C2C	2.24	1.48	1.44
17	6	312	CLA	C4C-C3C	2.24	1.49	1.45
17	b	831	CLA	C4C-C3C	2.24	1.49	1.45
17	B	840	CLA	C4C-C3C	2.24	1.49	1.45
17	1	314	CLA	C1C-C2C	2.24	1.48	1.44
17	a	817	CLA	C1C-C2C	2.24	1.48	1.44
17	B	819	CLA	C1C-C2C	2.25	1.48	1.44
17	B	806	CLA	C4C-C3C	2.25	1.49	1.45
17	2	609	CLA	C4C-C3C	2.25	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	837	CLA	C4C-C3C	2.25	1.49	1.45
17	F	303	CLA	C4C-C3C	2.25	1.49	1.45
17	B	838	CLA	C4C-C3C	2.25	1.49	1.45
17	a	842	CLA	C4C-C3C	2.25	1.49	1.45
17	7	609	CLA	C4C-C3C	2.25	1.49	1.45
17	a	806	CLA	C4C-C3C	2.25	1.49	1.45
17	a	828	CLA	CHD-C4C	2.25	1.47	1.41
17	B	805	CLA	C1C-C2C	2.25	1.48	1.44
17	9	602	CLA	C4C-C3C	2.25	1.49	1.45
17	6	304	CLA	C1C-C2C	2.26	1.48	1.44
17	A	842	CLA	C1C-C2C	2.26	1.48	1.44
17	A	839	CLA	C1C-C2C	2.26	1.48	1.44
17	A	830	CLA	C4C-C3C	2.26	1.49	1.45
17	a	805	CLA	C4C-C3C	2.26	1.49	1.45
17	a	844	CLA	C4C-C3C	2.26	1.49	1.45
17	9	603	CLA	C4C-C3C	2.26	1.49	1.45
17	A	839	CLA	C4C-C3C	2.26	1.49	1.45
17	7	610	CLA	C1C-C2C	2.26	1.48	1.44
17	A	801	CLA	C4C-C3C	2.27	1.49	1.45
17	b	838	CLA	C4C-C3C	2.27	1.49	1.45
17	a	813	CLA	C1C-C2C	2.27	1.48	1.44
17	3	312	CLA	C1C-C2C	2.27	1.48	1.44
17	B	809	CLA	C1C-C2C	2.27	1.48	1.44
17	A	826	CLA	C4C-C3C	2.27	1.49	1.45
17	b	811	CLA	C4C-C3C	2.27	1.49	1.45
17	A	802	CLA	C4C-C3C	2.28	1.49	1.45
17	1	309	CLA	C1C-C2C	2.28	1.48	1.44
17	2	610	CLA	C1C-C2C	2.28	1.48	1.44
17	1	204	CLA	C4C-C3C	2.28	1.49	1.45
17	A	803	CLA	C4C-C3C	2.28	1.49	1.45
17	1	306	CLA	C1C-C2C	2.28	1.48	1.44
17	6	315	CLA	C1C-C2C	2.28	1.48	1.44
17	8	303	CLA	C1C-C2C	2.28	1.48	1.44
17	A	827	CLA	C4C-C3C	2.28	1.49	1.45
17	A	821	CLA	C1C-C2C	2.28	1.48	1.44
17	A	825	CLA	C1C-C2C	2.28	1.48	1.44
17	A	854	CLA	CHD-C4C	2.28	1.48	1.41
17	1	313	CLA	C1C-C2C	2.29	1.49	1.44
17	A	811	CLA	C1C-C2C	2.29	1.49	1.44
17	3	305	CLA	C1C-C2C	2.29	1.49	1.44
17	9	613	CLA	C1C-C2C	2.29	1.49	1.44
17	K	4003	CLA	C1C-C2C	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	833	CLA	C4C-C3C	2.29	1.49	1.45
17	7	608	CLA	C4C-C3C	2.29	1.49	1.45
17	B	827	CLA	C4C-C3C	2.29	1.49	1.45
17	1	305	CLA	C1C-C2C	2.29	1.49	1.44
17	a	811	CLA	C1C-C2C	2.29	1.49	1.44
17	a	822	CLA	C4C-C3C	2.29	1.49	1.45
17	a	802	CLA	C4C-C3C	2.29	1.49	1.45
17	4	614	CLA	C4C-C3C	2.29	1.49	1.45
17	A	826	CLA	CHD-C4C	2.29	1.48	1.41
17	A	810	CLA	CHD-C4C	2.29	1.48	1.41
17	b	813	CLA	C1C-C2C	2.29	1.49	1.44
17	4	613	CLA	C1C-C2C	2.29	1.49	1.44
17	a	815	CLA	C4C-C3C	2.30	1.49	1.45
17	g	101	CLA	C4C-C3C	2.30	1.49	1.45
17	A	819	CLA	C1C-C2C	2.30	1.49	1.44
17	b	837	CLA	C1C-C2C	2.30	1.49	1.44
17	b	815	CLA	C4C-C3C	2.30	1.49	1.45
17	3	303	CLA	C1C-C2C	2.30	1.49	1.44
17	4	603	CLA	C1C-C2C	2.30	1.49	1.44
17	a	824	CLA	C1C-C2C	2.30	1.49	1.44
17	9	612	CLA	C1C-C2C	2.30	1.49	1.44
17	9	610	CLA	C4C-C3C	2.30	1.49	1.45
17	8	312	CLA	C4C-C3C	2.30	1.49	1.45
17	4	602	CLA	C4C-C3C	2.30	1.49	1.45
17	3	306	CLA	C4C-C3C	2.30	1.49	1.45
17	8	304	CLA	C1C-C2C	2.30	1.49	1.44
17	A	822	CLA	C1C-C2C	2.30	1.49	1.44
17	7	613	CLA	C1C-C2C	2.30	1.49	1.44
17	b	817	CLA	C1C-C2C	2.30	1.49	1.44
17	8	311	CLA	C1C-C2C	2.30	1.49	1.44
17	B	805	CLA	C4C-C3C	2.30	1.49	1.45
17	a	819	CLA	C4C-C3C	2.31	1.49	1.45
17	4	604	CLA	C1C-C2C	2.31	1.49	1.44
17	B	810	CLA	C4C-C3C	2.31	1.49	1.45
17	8	302	CLA	C1C-C2C	2.31	1.49	1.44
17	9	608	CLA	C4C-C3C	2.31	1.49	1.45
17	7	603	CLA	C4C-C3C	2.31	1.49	1.45
17	B	815	CLA	C4C-C3C	2.31	1.49	1.45
17	b	816	CLA	C1C-C2C	2.31	1.49	1.44
17	a	802	CLA	C1C-C2C	2.31	1.49	1.44
17	A	804	CLA	C4C-C3C	2.31	1.49	1.45
17	2	612	CLA	C1C-C2C	2.31	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	836	CLA	C4C-C3C	2.31	1.49	1.45
17	A	816	CLA	C4C-C3C	2.31	1.49	1.45
17	6	305	CLA	C1C-C2C	2.31	1.49	1.44
17	B	838	CLA	C1C-C2C	2.31	1.49	1.44
17	3	304	CLA	C1C-C2C	2.31	1.49	1.44
17	A	836	CLA	C1C-C2C	2.31	1.49	1.44
17	4	611	CLA	C1C-C2C	2.31	1.49	1.44
17	9	608	CLA	C1C-C2C	2.31	1.49	1.44
17	a	841	CLA	C4C-C3C	2.31	1.49	1.45
17	a	843	CLA	C1C-C2C	2.31	1.49	1.44
17	b	807	CLA	C4C-C3C	2.32	1.49	1.45
17	a	807	CLA	C4C-C3C	2.32	1.49	1.45
17	a	812	CLA	C4C-C3C	2.32	1.49	1.45
17	b	810	CLA	C4C-C3C	2.32	1.49	1.45
17	7	608	CLA	C1C-C2C	2.32	1.49	1.44
17	a	827	CLA	C4C-C3C	2.32	1.49	1.45
17	A	832	CLA	C4C-C3C	2.32	1.49	1.45
17	6	306	CLA	C1C-C2C	2.32	1.49	1.44
17	7	602	CLA	C4C-C3C	2.32	1.49	1.45
17	A	817	CLA	C1C-C2C	2.32	1.49	1.44
17	A	805	CLA	C1C-C2C	2.32	1.49	1.44
17	g	101	CLA	C1C-C2C	2.32	1.49	1.44
17	b	826	CLA	C4C-C3C	2.32	1.49	1.45
17	1	315	CLA	C1C-C2C	2.32	1.49	1.44
17	a	820	CLA	C1C-C2C	2.32	1.49	1.44
17	B	811	CLA	C1C-C2C	2.32	1.49	1.44
17	1	305	CLA	C4C-C3C	2.32	1.49	1.45
17	A	816	CLA	C1C-C2C	2.33	1.49	1.44
17	B	811	CLA	C4C-C3C	2.33	1.49	1.45
17	1	315	CLA	C4C-C3C	2.33	1.49	1.45
17	4	610	CLA	C4C-C3C	2.33	1.49	1.45
17	A	832	CLA	C1C-C2C	2.33	1.49	1.44
17	8	301	CLA	C4C-C3C	2.33	1.49	1.45
17	6	313	CLA	C1C-C2C	2.33	1.49	1.44
17	3	313	CLA	C1C-C2C	2.33	1.49	1.44
17	A	813	CLA	C1C-C2C	2.33	1.49	1.44
17	l	204	CLA	C1C-C2C	2.33	1.49	1.44
17	g	103	CLA	C1C-C2C	2.33	1.49	1.44
17	1	306	CLA	C4C-C3C	2.33	1.49	1.45
17	G	101	CLA	C1C-C2C	2.33	1.49	1.44
17	2	604	CLA	C1C-C2C	2.33	1.49	1.44
17	b	809	CLA	C1C-C2C	2.33	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	601	CLA	C1C-C2C	2.33	1.49	1.44
17	a	836	CLA	C1C-C2C	2.33	1.49	1.44
17	a	844	CLA	C1C-C2C	2.33	1.49	1.44
17	6	316	CLA	C1C-C2C	2.34	1.49	1.44
17	7	612	CLA	C1C-C2C	2.34	1.49	1.44
17	A	840	CLA	C4C-C3C	2.34	1.49	1.45
17	B	809	CLA	C4C-C3C	2.34	1.49	1.45
17	6	310	CLA	C4C-C3C	2.34	1.49	1.45
17	8	309	CLA	C1C-C2C	2.34	1.49	1.44
17	A	807	CLA	C4C-C3C	2.34	1.49	1.45
17	B	831	CLA	C1C-C2C	2.34	1.49	1.44
17	A	837	CLA	C1C-C2C	2.34	1.49	1.44
17	a	816	CLA	CHD-C4C	2.34	1.48	1.41
17	B	826	CLA	CHD-C4C	2.34	1.48	1.41
17	l	202	CLA	C4C-C3C	2.34	1.49	1.45
17	A	802	CLA	C1B-CHB	2.34	1.46	1.40
17	b	834	CLA	C1C-C2C	2.34	1.49	1.44
17	B	818	CLA	C1C-C2C	2.34	1.49	1.44
17	1	309	CLA	C4C-C3C	2.34	1.49	1.45
17	A	828	CLA	CHD-C4C	2.34	1.48	1.41
17	B	824	CLA	C4C-C3C	2.34	1.49	1.45
17	L	204	CLA	C4C-C3C	2.34	1.49	1.45
17	9	604	CLA	C4C-C3C	2.34	1.49	1.45
17	b	802	CLA	C4C-C3C	2.34	1.49	1.45
17	3	314	CLA	C1C-C2C	2.34	1.49	1.44
17	7	611	CLA	C1C-C2C	2.35	1.49	1.44
17	2	613	CLA	C1C-C2C	2.35	1.49	1.44
17	9	604	CLA	C1C-C2C	2.35	1.49	1.44
17	f	7002	CLA	CHD-C4C	2.35	1.48	1.41
17	8	305	CLA	C1C-C2C	2.35	1.49	1.44
17	l	202	CLA	C1C-C2C	2.35	1.49	1.44
17	B	836	CLA	CHD-C4C	2.35	1.48	1.41
17	A	809	CLA	C4C-C3C	2.35	1.49	1.45
17	a	826	CLA	C4C-C3C	2.35	1.49	1.45
17	b	833	CLA	C1C-C2C	2.35	1.49	1.44
17	G	103	CLA	C4C-C3C	2.35	1.49	1.45
17	B	810	CLA	C1C-C2C	2.35	1.49	1.44
17	b	811	CLA	CHD-C4C	2.35	1.48	1.41
17	1	311	CLA	C1C-C2C	2.35	1.49	1.44
17	B	840	CLA	C1C-C2C	2.35	1.49	1.44
17	b	812	CLA	C1C-C2C	2.35	1.49	1.44
17	a	837	CLA	C1C-C2C	2.35	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	830	CLA	C1C-C2C	2.35	1.49	1.44
17	4	614	CLA	C1C-C2C	2.35	1.49	1.44
17	a	831	CLA	C4C-C3C	2.35	1.49	1.45
17	8	308	CLA	C4C-C3C	2.35	1.49	1.45
17	9	614	CLA	C1C-C2C	2.35	1.49	1.44
17	b	840	CLA	CHD-C4C	2.35	1.48	1.41
17	b	815	CLA	CHD-C4C	2.35	1.48	1.41
17	f	7003	CLA	C1C-C2C	2.35	1.49	1.44
17	9	611	CLA	C1C-C2C	2.35	1.49	1.44
17	3	310	CLA	C1C-C2C	2.35	1.49	1.44
17	b	839	CLA	CHD-C4C	2.36	1.48	1.41
17	2	611	CLA	C4C-C3C	2.36	1.49	1.45
17	G	103	CLA	C1C-C2C	2.36	1.49	1.44
17	A	842	CLA	C4C-C3C	2.36	1.49	1.45
17	2	602	CLA	C4C-C3C	2.36	1.49	1.45
17	A	815	CLA	C4C-C3C	2.36	1.49	1.45
17	a	839	CLA	C4C-C3C	2.36	1.49	1.45
17	3	301	CLA	C1C-C2C	2.36	1.49	1.44
17	8	304	CLA	C4C-C3C	2.36	1.49	1.45
17	B	820	CLA	C1C-C2C	2.36	1.49	1.44
17	b	803	CLA	C1C-C2C	2.36	1.49	1.44
17	8	310	CLA	C1C-C2C	2.36	1.49	1.44
17	F	301	CLA	C4C-C3C	2.36	1.49	1.45
17	1	312	CLA	C1C-C2C	2.36	1.49	1.44
17	a	806	CLA	C1C-C2C	2.36	1.49	1.44
17	a	821	CLA	C1C-C2C	2.36	1.49	1.44
17	3	302	CLA	C4C-C3C	2.36	1.49	1.45
17	b	809	CLA	CHD-C4C	2.36	1.48	1.41
17	4	612	CLA	C4C-C3C	2.36	1.49	1.45
17	9	609	CLA	C4C-C3C	2.37	1.49	1.45
17	4	602	CLA	C1C-C2C	2.37	1.49	1.44
17	a	835	CLA	C1C-C2C	2.37	1.49	1.44
17	6	307	CLA	C1C-C2C	2.37	1.49	1.44
17	2	602	CLA	C1C-C2C	2.37	1.49	1.44
17	B	835	CLA	C1C-C2C	2.37	1.49	1.44
17	9	608	CLA	CHD-C4C	2.37	1.48	1.41
17	k	1401	CLA	C4C-C3C	2.37	1.49	1.45
17	a	833	CLA	CHD-C4C	2.37	1.48	1.41
17	A	824	CLA	C1C-C2C	2.37	1.49	1.44
17	6	310	CLA	C1C-C2C	2.37	1.49	1.44
17	a	841	CLA	C1C-C2C	2.37	1.49	1.44
17	B	812	CLA	C1C-C2C	2.37	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	803	CLA	C4C-C3C	2.37	1.49	1.45
17	b	827	CLA	CHD-C4C	2.37	1.48	1.41
17	4	603	CLA	CHD-C4C	2.37	1.48	1.41
17	J	3002	CLA	C1C-C2C	2.37	1.49	1.44
17	1	310	CLA	C4C-C3C	2.37	1.49	1.45
17	B	839	CLA	C4C-C3C	2.37	1.49	1.45
17	A	818	CLA	C1C-C2C	2.37	1.49	1.44
17	a	844	CLA	CHD-C4C	2.37	1.48	1.41
17	A	845	CLA	C1C-C2C	2.37	1.49	1.44
17	6	312	CLA	C1C-C2C	2.37	1.49	1.44
17	a	805	CLA	C1C-C2C	2.37	1.49	1.44
17	A	806	CLA	C4C-C3C	2.37	1.49	1.45
17	3	308	CLA	C4C-C3C	2.37	1.49	1.45
17	2	603	CLA	C4C-C3C	2.37	1.49	1.45
17	7	611	CLA	C4C-C3C	2.37	1.49	1.45
17	a	821	CLA	CHD-C4C	2.38	1.48	1.41
17	A	836	CLA	C4C-C3C	2.38	1.49	1.45
17	4	608	CLA	CHD-C4C	2.38	1.48	1.41
17	2	603	CLA	C1C-C2C	2.38	1.49	1.44
17	B	817	CLA	C1C-C2C	2.38	1.49	1.44
17	a	817	CLA	C4C-C3C	2.38	1.49	1.45
17	4	611	CLA	C4C-C3C	2.38	1.49	1.45
17	A	854	CLA	C1C-C2C	2.38	1.49	1.44
17	b	815	CLA	C1C-C2C	2.38	1.49	1.44
17	a	802	CLA	C1B-CHB	2.38	1.46	1.40
17	b	835	CLA	C1C-C2C	2.38	1.49	1.44
17	B	816	CLA	C1C-C2C	2.38	1.49	1.44
17	L	204	CLA	C1C-C2C	2.38	1.49	1.44
17	b	839	CLA	C4C-C3C	2.38	1.49	1.45
17	F	303	CLA	CHD-C4C	2.38	1.48	1.41
17	a	831	CLA	C1C-C2C	2.38	1.49	1.44
17	b	824	CLA	C4C-C3C	2.38	1.49	1.45
17	9	614	CLA	C4C-C3C	2.38	1.49	1.45
17	a	810	CLA	C1C-C2C	2.38	1.49	1.44
17	b	836	CLA	CHD-C4C	2.38	1.48	1.41
17	6	316	CLA	C4C-C3C	2.38	1.49	1.45
17	k	1402	CLA	C4C-C3C	2.38	1.49	1.45
17	6	314	CLA	C1C-C2C	2.38	1.49	1.44
17	b	821	CLA	C1C-C2C	2.39	1.49	1.44
17	6	313	CLA	C4C-C3C	2.39	1.49	1.45
17	a	808	CLA	CHD-C4C	2.39	1.48	1.41
17	B	820	CLA	C4C-C3C	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	820	CLA	CHD-C4C	2.39	1.48	1.41
17	3	305	CLA	C4C-C3C	2.39	1.49	1.45
17	B	838	CLA	CHD-C4C	2.39	1.48	1.41
17	a	801	CLA	CHD-C4C	2.39	1.48	1.41
17	a	822	CLA	C1C-C2C	2.39	1.49	1.44
17	B	823	CLA	CHD-C4C	2.39	1.48	1.41
17	A	829	CLA	CHD-C4C	2.39	1.48	1.41
17	B	824	CLA	C1C-C2C	2.39	1.49	1.44
17	4	601	CLA	C4C-C3C	2.39	1.49	1.45
17	1	310	CLA	C1C-C2C	2.39	1.49	1.44
17	a	809	CLA	CHD-C4C	2.39	1.48	1.41
17	b	826	CLA	CHD-C4C	2.39	1.48	1.41
17	A	841	CLA	CHD-C4C	2.39	1.48	1.41
17	9	610	CLA	C1C-C2C	2.39	1.49	1.44
17	A	805	CLA	CHD-C4C	2.39	1.48	1.41
17	A	838	CLA	C4C-C3C	2.39	1.49	1.45
17	b	841	CLA	C4C-C3C	2.39	1.49	1.45
17	A	819	CLA	CHD-C4C	2.39	1.48	1.41
17	6	309	CLA	C4C-C3C	2.39	1.49	1.45
17	b	821	CLA	C4C-C3C	2.39	1.49	1.45
17	B	807	CLA	C4C-C3C	2.39	1.49	1.45
17	4	608	CLA	C4C-C3C	2.39	1.49	1.45
17	3	306	CLA	C1C-C2C	2.39	1.49	1.44
17	f	7003	CLA	C4C-C3C	2.39	1.49	1.45
17	j	3002	CLA	C1C-C2C	2.39	1.49	1.44
17	a	824	CLA	C4C-C3C	2.40	1.49	1.45
17	b	818	CLA	C1C-C2C	2.40	1.49	1.44
17	3	314	CLA	C4C-C3C	2.40	1.49	1.45
17	b	810	CLA	CHD-C4C	2.40	1.48	1.41
17	B	821	CLA	C4C-C3C	2.40	1.49	1.45
17	a	801	CLA	C1C-C2C	2.40	1.49	1.44
17	a	826	CLA	CHD-C4C	2.40	1.48	1.41
17	a	830	CLA	CHD-C4C	2.40	1.48	1.41
17	B	809	CLA	CHD-C4C	2.40	1.48	1.41
17	b	834	CLA	C4C-C3C	2.40	1.49	1.45
17	b	833	CLA	C4C-C3C	2.40	1.49	1.45
17	1	311	CLA	C4C-C3C	2.40	1.49	1.45
17	3	308	CLA	C1C-C2C	2.40	1.49	1.44
17	a	829	CLA	C4C-C3C	2.40	1.49	1.45
17	A	808	CLA	C4C-C3C	2.40	1.49	1.45
17	B	823	CLA	C4C-C3C	2.40	1.49	1.45
17	1	303	CLA	C1C-C2C	2.40	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	833	CLA	CHD-C4C	2.40	1.48	1.41
17	3	304	CLA	C4C-C3C	2.40	1.49	1.45
17	8	310	CLA	C4C-C3C	2.40	1.49	1.45
17	a	812	CLA	C1C-C2C	2.40	1.49	1.44
17	a	846	CLA	C1C-C2C	2.40	1.49	1.44
17	b	804	CLA	CHD-C4C	2.40	1.48	1.41
17	A	814	CLA	C1C-C2C	2.40	1.49	1.44
17	B	822	CLA	C1C-C2C	2.40	1.49	1.44
17	8	305	CLA	C4C-C3C	2.40	1.49	1.45
17	4	613	CLA	C4C-C3C	2.40	1.49	1.45
17	g	102	CLA	C4C-C3C	2.40	1.49	1.45
17	9	609	CLA	C1C-C2C	2.41	1.49	1.44
17	a	806	CLA	CHD-C4C	2.41	1.48	1.41
17	B	839	CLA	C1C-C2C	2.41	1.49	1.44
17	A	834	CLA	C4C-C3C	2.41	1.49	1.45
17	B	814	CLA	CHD-C4C	2.41	1.48	1.41
17	b	807	CLA	C1C-C2C	2.41	1.49	1.44
17	B	837	CLA	C1C-C2C	2.41	1.49	1.44
17	9	603	CLA	C1C-C2C	2.41	1.49	1.44
17	4	601	CLA	C1C-C2C	2.41	1.49	1.44
17	9	611	CLA	CHD-C4C	2.41	1.48	1.41
17	A	839	CLA	CHD-C4C	2.41	1.48	1.41
17	b	812	CLA	C4C-C3C	2.41	1.49	1.45
17	a	831	CLA	CHD-C4C	2.41	1.48	1.41
17	B	818	CLA	CHD-C4C	2.41	1.48	1.41
17	g	102	CLA	C1C-C2C	2.41	1.49	1.44
17	A	843	CLA	C4C-C3C	2.41	1.49	1.45
17	1	303	CLA	C4C-C3C	2.41	1.49	1.45
17	A	815	CLA	C1C-C2C	2.41	1.49	1.44
17	a	818	CLA	C4C-C3C	2.41	1.49	1.45
17	8	311	CLA	C4C-C3C	2.41	1.49	1.45
17	A	820	CLA	C1C-C2C	2.41	1.49	1.44
17	B	815	CLA	CHD-C4C	2.41	1.48	1.41
17	B	827	CLA	CHD-C4C	2.41	1.48	1.41
17	G	104	CLA	C4C-C3C	2.41	1.49	1.45
17	a	840	CLA	C1C-C2C	2.42	1.49	1.44
17	B	817	CLA	C4C-C3C	2.42	1.49	1.45
17	1	308	CLA	C4C-C3C	2.42	1.49	1.45
17	B	825	CLA	CHD-C4C	2.42	1.48	1.41
17	6	307	CLA	C4C-C3C	2.42	1.49	1.45
17	7	604	CLA	C4C-C3C	2.42	1.49	1.45
17	B	802	CLA	CHD-C4C	2.42	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	309	CLA	C1C-C2C	2.42	1.49	1.44
17	6	311	CLA	C1C-C2C	2.42	1.49	1.44
17	4	610	CLA	C1C-C2C	2.42	1.49	1.44
17	a	811	CLA	C4C-C3C	2.42	1.49	1.45
17	B	808	CLA	C1C-C2C	2.42	1.49	1.44
17	b	835	CLA	C4C-C3C	2.42	1.49	1.45
17	b	840	CLA	C1C-C2C	2.42	1.49	1.44
17	8	312	CLA	C1C-C2C	2.42	1.49	1.44
17	B	814	CLA	C1C-C2C	2.42	1.49	1.44
17	a	842	CLA	CHD-C4C	2.42	1.48	1.41
17	2	608	CLA	C4C-C3C	2.42	1.49	1.45
17	A	829	CLA	C1C-C2C	2.42	1.49	1.44
17	a	825	CLA	C1C-C2C	2.42	1.49	1.44
17	K	4003	CLA	C4C-C3C	2.42	1.49	1.45
17	2	611	CLA	C1C-C2C	2.42	1.49	1.44
17	B	821	CLA	C1C-C2C	2.42	1.49	1.44
17	9	611	CLA	C4C-C3C	2.42	1.49	1.45
17	A	818	CLA	CHD-C4C	2.42	1.48	1.41
17	4	608	CLA	C1C-C2C	2.42	1.49	1.44
17	7	603	CLA	C1C-C2C	2.42	1.49	1.44
17	A	836	CLA	CHD-C4C	2.42	1.48	1.41
17	A	812	CLA	CHD-C4C	2.42	1.48	1.41
17	1	308	CLA	C1C-C2C	2.42	1.49	1.44
17	a	856	CLA	C4C-C3C	2.42	1.49	1.45
17	G	104	CLA	C1C-C2C	2.43	1.49	1.44
17	a	825	CLA	CHD-C4C	2.43	1.48	1.41
17	1	312	CLA	C4C-C3C	2.43	1.49	1.45
17	a	839	CLA	CHD-C4C	2.43	1.48	1.41
17	a	807	CLA	CHD-C4C	2.43	1.48	1.41
17	B	822	CLA	C4C-C3C	2.43	1.49	1.45
17	a	809	CLA	C1C-C2C	2.43	1.49	1.44
17	6	310	CLA	CHD-C4C	2.43	1.48	1.41
17	A	801	CLA	C1C-C2C	2.43	1.49	1.44
17	3	303	CLA	C4C-C3C	2.43	1.49	1.45
17	3	312	CLA	C4C-C3C	2.43	1.49	1.45
17	7	613	CLA	C4C-C3C	2.43	1.49	1.45
17	a	819	CLA	CHD-C4C	2.43	1.48	1.41
17	B	815	CLA	C1C-C2C	2.43	1.49	1.44
17	A	813	CLA	C4C-C3C	2.43	1.49	1.45
17	K	4002	CLA	C4C-C3C	2.43	1.49	1.45
17	a	832	CLA	C4C-C3C	2.43	1.49	1.45
17	a	842	CLA	C1C-C2C	2.43	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	303	CLA	C1C-C2C	2.43	1.49	1.44
17	K	4002	CLA	C1C-C2C	2.43	1.49	1.44
17	B	828	CLA	C1C-C2C	2.43	1.49	1.44
17	b	832	CLA	CHD-C4C	2.43	1.48	1.41
17	A	830	CLA	CHD-C4C	2.43	1.48	1.41
17	6	314	CLA	C4C-C3C	2.43	1.49	1.45
17	a	817	CLA	CHD-C4C	2.43	1.48	1.41
17	B	823	CLA	C1C-C2C	2.43	1.49	1.44
17	a	832	CLA	C1C-C2C	2.43	1.49	1.44
17	b	803	CLA	CHD-C4C	2.43	1.48	1.41
17	a	804	CLA	C1C-C2C	2.44	1.49	1.44
17	a	816	CLA	C1C-C2C	2.44	1.49	1.44
17	9	603	CLA	CHD-C4C	2.44	1.48	1.41
17	B	833	CLA	CHD-C4C	2.44	1.48	1.41
17	3	311	CLA	C1C-C2C	2.44	1.49	1.44
17	b	820	CLA	C1C-C2C	2.44	1.49	1.44
17	a	815	CLA	C1C-C2C	2.44	1.49	1.44
17	2	604	CLA	C4C-C3C	2.44	1.49	1.45
17	b	808	CLA	CHD-C4C	2.44	1.48	1.41
17	B	813	CLA	C1C-C2C	2.44	1.49	1.44
17	1	312	CLA	CHD-C4C	2.44	1.48	1.41
17	1	314	CLA	C4C-C3C	2.44	1.49	1.45
17	3	306	CLA	CHD-C4C	2.44	1.48	1.41
17	b	825	CLA	CHD-C4C	2.44	1.48	1.41
17	j	3002	CLA	C4C-C3C	2.44	1.49	1.45
17	8	307	CLA	CHD-C4C	2.44	1.48	1.41
17	1	313	CLA	C4C-C3C	2.44	1.49	1.45
17	9	601	CLA	C4C-C3C	2.44	1.49	1.45
17	b	811	CLA	C1C-C2C	2.44	1.49	1.44
17	a	843	CLA	CHD-C4C	2.44	1.48	1.41
17	A	820	CLA	C4C-C3C	2.44	1.49	1.45
17	a	837	CLA	C4C-C3C	2.44	1.49	1.45
17	3	302	CLA	C1C-C2C	2.44	1.49	1.44
17	6	306	CLA	C4C-C3C	2.44	1.49	1.45
17	B	840	CLA	CHD-C4C	2.44	1.48	1.41
17	b	803	CLA	C1B-CHB	2.44	1.46	1.40
17	A	808	CLA	CHD-C4C	2.44	1.48	1.41
17	a	824	CLA	CHD-C4C	2.44	1.48	1.41
17	7	603	CLA	CHD-C4C	2.44	1.48	1.41
17	a	823	CLA	C1C-C2C	2.44	1.49	1.44
17	a	827	CLA	C1C-C2C	2.45	1.49	1.44
17	8	308	CLA	C1C-C2C	2.45	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	610	CLA	CHD-C4C	2.45	1.48	1.41
17	B	830	CLA	CHD-C4C	2.45	1.48	1.41
17	8	302	CLA	C4C-C3C	2.45	1.49	1.45
17	B	808	CLA	C4C-C3C	2.45	1.49	1.45
17	A	801	CLA	CHD-C4C	2.45	1.48	1.41
17	9	613	CLA	C4C-C3C	2.45	1.49	1.45
17	B	828	CLA	CHD-C4C	2.45	1.48	1.41
17	2	612	CLA	C4C-C3C	2.45	1.49	1.45
17	A	803	CLA	C1C-C2C	2.45	1.49	1.44
17	a	856	CLA	CHD-C4C	2.45	1.48	1.41
17	a	838	CLA	CHD-C4C	2.45	1.48	1.41
17	A	823	CLA	C1C-C2C	2.45	1.49	1.44
17	A	823	CLA	C4C-C3C	2.45	1.49	1.45
17	B	804	CLA	C1C-C2C	2.45	1.49	1.44
17	6	305	CLA	C4C-C3C	2.45	1.49	1.45
17	A	810	CLA	C1C-C2C	2.45	1.49	1.44
17	L	202	CLA	C4C-C3C	2.45	1.49	1.45
17	a	839	CLA	C1C-C2C	2.45	1.49	1.44
17	B	803	CLA	C1C-C2C	2.45	1.49	1.44
17	b	838	CLA	CHD-C4C	2.45	1.48	1.41
17	1	309	CLA	CHD-C4C	2.45	1.48	1.41
17	9	614	CLA	CHD-C4C	2.45	1.48	1.41
17	B	806	CLA	C1C-C2C	2.45	1.49	1.44
17	8	307	CLA	C1C-C2C	2.45	1.49	1.44
17	G	103	CLA	CHD-C4C	2.46	1.48	1.41
17	a	810	CLA	C4C-C3C	2.46	1.49	1.45
17	A	807	CLA	CHD-C4C	2.46	1.48	1.41
17	7	602	CLA	C1C-C2C	2.46	1.49	1.44
17	a	827	CLA	CHD-C4C	2.46	1.48	1.41
17	7	612	CLA	C4C-C3C	2.46	1.49	1.45
17	F	304	CLA	C1C-C2C	2.46	1.49	1.44
17	A	804	CLA	CHD-C4C	2.46	1.48	1.41
17	b	828	CLA	CHD-C4C	2.46	1.48	1.41
17	b	802	CLA	CHD-C4C	2.46	1.48	1.41
17	k	1401	CLA	C1C-C2C	2.46	1.49	1.44
17	g	101	CLA	CHD-C4C	2.46	1.48	1.41
17	A	811	CLA	C4C-C3C	2.46	1.49	1.45
17	B	813	CLA	C4C-C3C	2.46	1.49	1.45
17	b	804	CLA	C1C-C2C	2.46	1.49	1.44
17	B	811	CLA	CHD-C4C	2.46	1.48	1.41
17	b	805	CLA	C4C-C3C	2.46	1.49	1.45
17	b	831	CLA	CHD-C4C	2.46	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	835	CLA	CHD-C4C	2.46	1.48	1.41
17	4	609	CLA	C1C-C2C	2.46	1.49	1.44
17	3	311	CLA	C4C-C3C	2.46	1.49	1.45
17	a	804	CLA	CHD-C4C	2.46	1.48	1.41
17	1	304	CLA	C4C-C3C	2.46	1.49	1.45
17	4	601	CLA	CHD-C4C	2.46	1.48	1.41
17	B	806	CLA	CHD-C4C	2.46	1.48	1.41
17	a	840	CLA	CHD-C4C	2.46	1.48	1.41
17	b	838	CLA	C1C-C2C	2.46	1.49	1.44
17	B	832	CLA	CHD-C4C	2.46	1.48	1.41
17	A	821	CLA	CHD-C4C	2.46	1.48	1.41
17	2	613	CLA	C4C-C3C	2.47	1.49	1.45
17	8	303	CLA	C4C-C3C	2.47	1.49	1.45
17	a	802	CLA	CHD-C4C	2.47	1.48	1.41
17	2	611	CLA	CHD-C4C	2.47	1.48	1.41
17	6	312	CLA	CHD-C4C	2.47	1.48	1.41
17	4	612	CLA	CHD-C4C	2.47	1.48	1.41
17	A	804	CLA	C1C-C2C	2.47	1.49	1.44
17	F	301	CLA	CHD-C4C	2.47	1.48	1.41
17	a	834	CLA	C1C-C2C	2.47	1.49	1.44
17	b	826	CLA	C1C-C2C	2.47	1.49	1.44
17	B	824	CLA	CHD-C4C	2.47	1.48	1.41
17	a	836	CLA	CHD-C4C	2.47	1.48	1.41
17	l	204	CLA	CHD-C4C	2.47	1.48	1.41
17	B	804	CLA	C4C-C3C	2.47	1.49	1.45
17	3	309	CLA	C1C-C2C	2.47	1.49	1.44
17	a	814	CLA	CHD-C4C	2.47	1.48	1.41
19	1	301	LHG	O8-C23	2.47	1.45	1.33
17	B	805	CLA	CHD-C4C	2.47	1.48	1.41
17	A	817	CLA	C4C-C3C	2.47	1.49	1.45
17	A	809	CLA	CHD-C4C	2.47	1.48	1.41
17	B	808	CLA	CHD-C4C	2.47	1.48	1.41
17	B	819	CLA	C4C-C3C	2.47	1.49	1.45
17	b	834	CLA	CHD-C4C	2.47	1.48	1.41
17	A	807	CLA	C1C-C2C	2.47	1.49	1.44
17	B	817	CLA	CHD-C4C	2.47	1.48	1.41
17	b	830	CLA	C4C-C3C	2.47	1.49	1.45
17	7	612	CLA	CHD-C4C	2.47	1.48	1.41
17	1	304	CLA	CHD-C4C	2.47	1.48	1.41
17	9	612	CLA	C4C-C3C	2.47	1.49	1.45
17	A	825	CLA	CHD-C4C	2.47	1.48	1.41
17	8	310	CLA	CHD-C4C	2.48	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	314	CLA	CHD-C4C	2.48	1.48	1.41
17	G	101	CLA	CHD-C4C	2.48	1.48	1.41
17	4	611	CLA	CHD-C4C	2.48	1.48	1.41
17	B	803	CLA	C1B-CHB	2.48	1.46	1.40
17	A	806	CLA	CHD-C4C	2.48	1.48	1.41
17	l	202	CLA	CHD-C4C	2.48	1.48	1.41
17	A	825	CLA	C4C-C3C	2.48	1.49	1.45
17	A	835	CLA	C4C-C3C	2.48	1.49	1.45
17	A	812	CLA	C1C-C2C	2.48	1.49	1.44
17	8	305	CLA	CHD-C4C	2.48	1.48	1.41
17	a	833	CLA	C1C-C2C	2.48	1.49	1.44
17	7	611	CLA	CHD-C4C	2.48	1.48	1.41
17	g	102	CLA	CHD-C4C	2.48	1.48	1.41
17	A	802	CLA	C1C-C2C	2.48	1.49	1.44
17	B	807	CLA	C1C-C2C	2.48	1.49	1.44
17	A	838	CLA	CHD-C4C	2.48	1.48	1.41
17	a	841	CLA	CHD-C4C	2.48	1.48	1.41
17	3	301	CLA	C4C-C3C	2.48	1.49	1.45
17	B	816	CLA	C4C-C3C	2.48	1.49	1.45
17	4	609	CLA	CHD-C4C	2.48	1.48	1.41
17	b	816	CLA	C1B-CHB	2.48	1.46	1.40
17	a	832	CLA	CHD-C4C	2.48	1.48	1.41
17	B	837	CLA	CHD-C4C	2.48	1.48	1.41
17	B	830	CLA	C1C-C2C	2.48	1.49	1.44
17	b	841	CLA	C1C-C2C	2.48	1.49	1.44
17	9	602	CLA	CHD-C4C	2.48	1.48	1.41
17	b	822	CLA	C1C-C2C	2.48	1.49	1.44
17	g	103	CLA	C4C-C3C	2.48	1.49	1.45
17	2	608	CLA	CHD-C4C	2.48	1.48	1.41
17	b	823	CLA	CHD-C4C	2.49	1.48	1.41
17	6	305	CLA	CHD-C4C	2.49	1.48	1.41
17	3	303	CLA	CHD-C4C	2.49	1.48	1.41
17	b	812	CLA	CHD-C4C	2.49	1.48	1.41
17	2	603	CLA	CHD-C4C	2.49	1.48	1.41
17	1	306	CLA	CHD-C4C	2.49	1.48	1.41
17	a	810	CLA	CHD-C4C	2.49	1.48	1.41
17	7	608	CLA	C1B-CHB	2.49	1.46	1.40
17	b	832	CLA	C4C-C3C	2.49	1.49	1.45
17	B	813	CLA	CHD-C4C	2.49	1.48	1.41
17	6	315	CLA	C4C-C3C	2.49	1.49	1.45
17	6	313	CLA	CHD-C4C	2.49	1.48	1.41
17	4	614	CLA	CHD-C4C	2.49	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	609	CLA	C1C-C2C	2.49	1.49	1.44
17	K	4002	CLA	CHD-C4C	2.49	1.48	1.41
17	b	813	CLA	CHD-C4C	2.49	1.48	1.41
17	b	818	CLA	CHD-C4C	2.50	1.48	1.41
17	a	819	CLA	C1C-C2C	2.50	1.49	1.44
17	A	841	CLA	C1C-C2C	2.50	1.49	1.44
17	B	839	CLA	CHD-C4C	2.50	1.48	1.41
17	B	812	CLA	CHD-C4C	2.50	1.48	1.41
17	G	104	CLA	CHD-C4C	2.50	1.48	1.41
17	B	827	CLA	C1B-CHB	2.50	1.46	1.40
17	A	808	CLA	C1C-C2C	2.50	1.49	1.44
17	a	829	CLA	CHD-C4C	2.50	1.48	1.41
17	A	815	CLA	CHD-C4C	2.50	1.48	1.41
17	6	306	CLA	CHD-C4C	2.50	1.48	1.41
17	8	302	CLA	CHD-C4C	2.50	1.48	1.41
17	4	610	CLA	CHD-C4C	2.50	1.48	1.41
17	b	806	CLA	C1C-C2C	2.50	1.49	1.44
17	B	831	CLA	CHD-C4C	2.50	1.48	1.41
17	A	803	CLA	CHD-C4C	2.50	1.48	1.41
17	b	824	CLA	CHD-C4C	2.50	1.48	1.41
17	f	7002	CLA	C1C-C2C	2.50	1.49	1.44
17	3	313	CLA	C4C-C3C	2.50	1.49	1.45
17	A	840	CLA	C1C-C2C	2.50	1.49	1.44
17	L	203	CLA	CHD-C4C	2.50	1.48	1.41
17	9	601	CLA	CHD-C4C	2.50	1.48	1.41
17	b	824	CLA	C1C-C2C	2.50	1.49	1.44
17	2	609	CLA	C1C-C2C	2.50	1.49	1.44
17	A	809	CLA	C1C-C2C	2.50	1.49	1.44
17	k	1401	CLA	CHD-C4C	2.50	1.48	1.41
17	b	839	CLA	C1C-C2C	2.50	1.49	1.44
17	6	307	CLA	CHD-C4C	2.50	1.48	1.41
17	B	804	CLA	CHD-C4C	2.50	1.48	1.41
17	a	815	CLA	CHD-C4C	2.50	1.48	1.41
17	B	836	CLA	C1C-C2C	2.51	1.49	1.44
17	b	816	CLA	C4C-C3C	2.51	1.49	1.45
17	1	313	CLA	CHD-C4C	2.51	1.48	1.41
17	b	835	CLA	CHD-C4C	2.51	1.48	1.41
17	A	820	CLA	CHD-C4C	2.51	1.48	1.41
17	A	840	CLA	CHD-C4C	2.51	1.48	1.41
17	F	304	CLA	C4C-C3C	2.51	1.49	1.45
17	1	315	CLA	CHD-C4C	2.51	1.48	1.41
17	b	814	CLA	CHD-C4C	2.51	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	313	CLA	CHD-C4C	2.51	1.48	1.41
17	3	311	CLA	CHD-C4C	2.51	1.48	1.41
17	A	832	CLA	CHD-C4C	2.51	1.48	1.41
17	b	832	CLA	C1C-C2C	2.51	1.49	1.44
17	b	825	CLA	C1C-C2C	2.51	1.49	1.44
17	1	310	CLA	CHD-C4C	2.51	1.48	1.41
17	7	602	CLA	CHD-C4C	2.51	1.48	1.41
17	A	828	CLA	C1C-C2C	2.51	1.49	1.44
17	B	807	CLA	CHD-C4C	2.51	1.48	1.41
17	b	829	CLA	CHD-C4C	2.51	1.48	1.41
17	b	830	CLA	CHD-C4C	2.51	1.48	1.41
17	a	856	CLA	C1B-CHB	2.51	1.46	1.40
17	A	845	CLA	C4C-C3C	2.51	1.49	1.45
17	A	824	CLA	CHD-C4C	2.51	1.48	1.41
17	A	827	CLA	CHD-C4C	2.51	1.48	1.41
17	6	316	CLA	CHD-C4C	2.51	1.48	1.41
17	b	818	CLA	C4C-C3C	2.51	1.49	1.45
17	a	846	CLA	C4C-C3C	2.51	1.49	1.45
17	1	203	CLA	CHD-C4C	2.51	1.48	1.41
17	8	309	CLA	C4C-C3C	2.51	1.49	1.45
17	B	831	CLA	C1B-CHB	2.51	1.46	1.40
17	b	807	CLA	CHD-C4C	2.51	1.48	1.41
17	4	604	CLA	C4C-C3C	2.51	1.49	1.45
17	J	3002	CLA	C4C-C3C	2.51	1.49	1.45
17	A	822	CLA	CHD-C4C	2.51	1.48	1.41
17	b	836	CLA	C1C-C2C	2.52	1.49	1.44
17	6	304	CLA	C4C-C3C	2.52	1.49	1.45
17	a	823	CLA	CHD-C4C	2.52	1.48	1.41
17	b	806	CLA	CHD-C4C	2.52	1.48	1.41
17	b	825	CLA	C1B-CHB	2.52	1.46	1.40
17	1	203	CLA	C1C-C2C	2.52	1.49	1.44
17	4	604	CLA	CHD-C4C	2.52	1.48	1.41
17	6	311	CLA	CHD-C4C	2.52	1.48	1.41
17	B	841	CLA	CHD-C4C	2.52	1.48	1.41
17	3	309	CLA	CHD-C4C	2.52	1.48	1.41
17	A	837	CLA	CHD-C4C	2.52	1.48	1.41
17	3	304	CLA	CHD-C4C	2.52	1.48	1.41
17	1	311	CLA	CHD-C4C	2.52	1.48	1.41
17	A	834	CLA	CHD-C4C	2.52	1.48	1.41
17	7	609	CLA	C1B-CHB	2.52	1.46	1.40
17	3	314	CLA	CHD-C4C	2.52	1.48	1.41
17	B	835	CLA	CHD-C4C	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	803	CLA	CHD-C4C	2.52	1.48	1.41
17	8	301	CLA	CHD-C4C	2.52	1.48	1.41
17	a	811	CLA	CHD-C4C	2.52	1.48	1.41
17	9	602	CLA	C1C-C2C	2.52	1.49	1.44
17	k	1402	CLA	CHD-C4C	2.52	1.48	1.41
17	7	610	CLA	C4C-C3C	2.52	1.49	1.45
17	B	830	CLA	C4C-C3C	2.52	1.49	1.45
17	B	829	CLA	C4C-C3C	2.52	1.49	1.45
17	7	610	CLA	CHD-C4C	2.52	1.48	1.41
17	6	309	CLA	CHD-C4C	2.52	1.48	1.41
19	6	301	LHG	O8-C23	2.52	1.45	1.33
17	1	303	CLA	CHD-C4C	2.52	1.48	1.41
17	K	4003	CLA	CHD-C4C	2.52	1.48	1.41
17	a	822	CLA	C1B-CHB	2.52	1.46	1.40
17	3	302	CLA	CHD-C4C	2.52	1.48	1.41
17	8	304	CLA	CHD-C4C	2.52	1.48	1.41
17	a	805	CLA	CHD-C4C	2.52	1.48	1.41
17	A	845	CLA	CHD-C4C	2.52	1.48	1.41
17	j	3002	CLA	CHD-C4C	2.52	1.48	1.41
17	A	811	CLA	CHD-C4C	2.53	1.48	1.41
17	B	832	CLA	C4C-C3C	2.53	1.49	1.45
17	B	829	CLA	C4B-CHC	2.53	1.46	1.40
17	B	816	CLA	CHD-C4C	2.53	1.48	1.41
17	a	820	CLA	C4C-C3C	2.53	1.49	1.45
17	2	610	CLA	CHD-C4C	2.53	1.48	1.41
17	9	612	CLA	CHD-C4C	2.53	1.48	1.41
17	a	837	CLA	CHD-C4C	2.53	1.48	1.41
17	b	841	CLA	CHD-C4C	2.53	1.48	1.41
17	A	833	CLA	CHD-C4C	2.53	1.48	1.41
17	A	827	CLA	C1C-C2C	2.53	1.49	1.44
17	6	315	CLA	CHD-C4C	2.53	1.48	1.41
17	1	308	CLA	CHD-C4C	2.53	1.48	1.41
17	a	818	CLA	CHD-C4C	2.53	1.48	1.41
17	1	305	CLA	CHD-C4C	2.53	1.48	1.41
17	L	202	CLA	CHD-C4C	2.53	1.48	1.41
17	J	3002	CLA	CHD-C4C	2.53	1.48	1.41
17	2	610	CLA	C4C-C3C	2.53	1.49	1.45
17	2	609	CLA	CHD-C4C	2.53	1.48	1.41
17	7	608	CLA	CHD-C4C	2.53	1.48	1.41
17	b	822	CLA	CHD-C4C	2.53	1.48	1.41
17	A	842	CLA	CHD-C4C	2.54	1.48	1.41
17	A	843	CLA	CHD-C4C	2.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	310	CLA	C4C-C3C	2.54	1.49	1.45
17	A	813	CLA	CHD-C4C	2.54	1.48	1.41
17	A	803	CLA	C1B-CHB	2.54	1.46	1.40
17	3	302	CLA	C1B-CHB	2.54	1.46	1.40
17	A	802	CLA	CHD-C4C	2.54	1.48	1.41
17	7	613	CLA	CHD-C4C	2.54	1.48	1.41
17	A	816	CLA	CHD-C4C	2.54	1.48	1.41
17	A	822	CLA	C4C-C3C	2.54	1.49	1.45
17	8	301	CLA	C1C-C2C	2.54	1.49	1.44
17	A	814	CLA	CHD-C4C	2.54	1.48	1.41
17	7	609	CLA	CHD-C4C	2.54	1.48	1.41
17	b	819	CLA	C4C-C3C	2.54	1.49	1.45
17	A	833	CLA	C1C-C2C	2.54	1.49	1.44
17	A	837	CLA	C4C-C3C	2.54	1.49	1.45
17	8	312	CLA	CHD-C4C	2.54	1.48	1.41
17	b	828	CLA	C1C-C2C	2.54	1.49	1.44
17	b	817	CLA	C4C-C3C	2.54	1.49	1.45
17	3	305	CLA	CHD-C4C	2.54	1.48	1.41
17	b	823	CLA	C4C-C3C	2.54	1.49	1.45
17	B	812	CLA	C4C-C3C	2.54	1.49	1.45
17	B	819	CLA	CHD-C4C	2.54	1.48	1.41
17	8	303	CLA	CHD-C4C	2.54	1.48	1.41
17	b	805	CLA	CHD-C4C	2.54	1.48	1.41
17	3	312	CLA	CHD-C4C	2.54	1.48	1.41
17	B	835	CLA	C1B-CHB	2.54	1.46	1.40
17	B	821	CLA	CHD-C4C	2.54	1.48	1.41
17	2	612	CLA	CHD-C4C	2.54	1.48	1.41
17	4	613	CLA	CHD-C4C	2.55	1.48	1.41
17	B	816	CLA	C1B-CHB	2.55	1.46	1.40
17	a	803	CLA	CHD-C4C	2.55	1.48	1.41
17	8	311	CLA	CHD-C4C	2.55	1.48	1.41
17	b	816	CLA	CHD-C4C	2.55	1.48	1.41
17	A	835	CLA	CHD-C4C	2.55	1.48	1.41
17	A	823	CLA	CHD-C4C	2.55	1.48	1.41
17	a	803	CLA	C4B-CHC	2.55	1.46	1.40
17	b	814	CLA	C1C-C2C	2.55	1.49	1.44
17	3	310	CLA	CHD-C4C	2.55	1.48	1.41
17	F	304	CLA	CHD-C4C	2.55	1.48	1.41
17	B	831	CLA	C4C-C3C	2.55	1.49	1.45
17	8	308	CLA	C1B-CHB	2.55	1.46	1.40
17	8	309	CLA	CHD-C4C	2.55	1.48	1.41
17	B	820	CLA	CHD-C4C	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	308	CLA	CHD-C4C	2.55	1.48	1.41
17	F	301	CLA	C1C-C2C	2.55	1.49	1.44
17	b	819	CLA	CHD-C4C	2.56	1.48	1.41
17	a	840	CLA	C4C-C3C	2.56	1.49	1.45
17	a	846	CLA	CHD-C4C	2.56	1.48	1.41
17	8	307	CLA	C1B-CHB	2.56	1.46	1.40
17	B	841	CLA	C1C-C2C	2.56	1.49	1.44
17	b	827	CLA	C1B-CHB	2.56	1.46	1.40
17	a	822	CLA	CHD-C4C	2.56	1.48	1.41
17	a	814	CLA	C1B-CHB	2.56	1.46	1.40
17	b	829	CLA	C4B-CHC	2.56	1.46	1.40
17	2	609	CLA	C1B-CHB	2.56	1.46	1.40
17	1	314	CLA	CHD-C4C	2.56	1.48	1.41
17	2	613	CLA	CHD-C4C	2.56	1.48	1.41
17	3	301	CLA	CHD-C4C	2.56	1.48	1.41
17	A	827	CLA	C1B-CHB	2.56	1.46	1.40
17	b	823	CLA	C1C-C2C	2.56	1.49	1.44
17	b	814	CLA	C1B-CHB	2.56	1.47	1.40
17	g	103	CLA	CHD-C4C	2.56	1.48	1.41
17	B	825	CLA	C1C-C2C	2.56	1.49	1.44
17	a	820	CLA	CHD-C4C	2.57	1.48	1.41
17	a	812	CLA	CHD-C4C	2.57	1.48	1.41
17	4	609	CLA	C1B-CHB	2.57	1.47	1.40
17	B	832	CLA	C1C-C2C	2.57	1.49	1.44
17	b	829	CLA	C4C-C3C	2.57	1.49	1.45
17	B	810	CLA	CHD-C4C	2.57	1.48	1.41
17	3	308	CLA	C1B-CHB	2.57	1.47	1.40
17	7	604	CLA	C1B-CHB	2.57	1.47	1.40
17	2	604	CLA	CHD-C4C	2.57	1.48	1.41
17	B	802	CLA	C1C-C2C	2.57	1.49	1.44
17	8	302	CLA	C1B-CHB	2.57	1.47	1.40
17	9	609	CLA	C1B-CHB	2.57	1.47	1.40
17	f	7003	CLA	CHD-C4C	2.57	1.48	1.41
17	L	204	CLA	CHD-C4C	2.57	1.48	1.41
17	b	817	CLA	CHD-C4C	2.57	1.48	1.41
17	A	854	CLA	C1B-CHB	2.58	1.47	1.40
17	B	827	CLA	C1C-C2C	2.58	1.49	1.44
17	b	837	CLA	CHD-C4C	2.58	1.48	1.41
17	a	856	CLA	C4B-CHC	2.58	1.47	1.40
17	6	311	CLA	C1B-CHB	2.58	1.47	1.40
17	A	817	CLA	CHD-C4C	2.58	1.48	1.41
17	a	812	CLA	C1B-CHB	2.58	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	814	CLA	C1B-CHB	2.58	1.47	1.40
17	A	835	CLA	C1B-CHB	2.58	1.47	1.40
17	L	203	CLA	C1C-C2C	2.58	1.49	1.44
17	A	809	CLA	C1B-CHB	2.58	1.47	1.40
17	A	822	CLA	C1B-CHB	2.58	1.47	1.40
17	b	822	CLA	C1B-CHB	2.59	1.47	1.40
17	8	301	CLA	C1B-CHB	2.59	1.47	1.40
17	A	814	CLA	C4C-C3C	2.59	1.49	1.45
17	9	609	CLA	CHD-C4C	2.59	1.48	1.41
17	a	808	CLA	C1C-C2C	2.59	1.49	1.44
17	9	604	CLA	CHD-C4C	2.59	1.48	1.41
17	9	613	CLA	CHD-C4C	2.59	1.48	1.41
17	8	308	CLA	CHD-C4C	2.59	1.48	1.41
17	b	819	CLA	C1B-CHB	2.59	1.47	1.40
17	a	813	CLA	C4C-C3C	2.59	1.49	1.45
17	B	822	CLA	CHD-C4C	2.59	1.48	1.41
17	k	1403	CLA	CHD-C4C	2.59	1.48	1.41
17	A	831	CLA	C1B-CHB	2.59	1.47	1.40
17	a	834	CLA	CHD-C4C	2.59	1.48	1.41
17	4	602	CLA	CHD-C4C	2.60	1.48	1.41
17	A	841	CLA	C1B-CHB	2.60	1.47	1.40
17	6	304	CLA	CHD-C4C	2.60	1.48	1.41
17	a	814	CLA	C1C-C2C	2.60	1.49	1.44
17	a	826	CLA	C1C-C2C	2.60	1.49	1.44
17	8	313	CLA	CHD-C4C	2.60	1.48	1.41
17	b	821	CLA	CHD-C4C	2.60	1.48	1.41
17	B	829	CLA	CHD-C4C	2.60	1.48	1.41
17	2	608	CLA	C1B-CHB	2.60	1.47	1.40
17	b	817	CLA	C1B-CHB	2.60	1.47	1.40
17	7	604	CLA	CHD-C4C	2.60	1.48	1.41
17	3	309	CLA	C1B-CHB	2.60	1.47	1.40
17	A	801	CLA	C1B-CHB	2.60	1.47	1.40
17	3	315	CLA	CHD-C4C	2.60	1.48	1.41
17	A	831	CLA	CHD-C4C	2.60	1.49	1.41
17	a	809	CLA	C1B-CHB	2.60	1.47	1.40
17	B	834	CLA	CHD-C4C	2.60	1.49	1.41
17	B	808	CLA	C1B-CHB	2.61	1.47	1.40
17	a	829	CLA	C1B-CHB	2.61	1.47	1.40
17	B	814	CLA	C1B-CHB	2.61	1.47	1.40
17	b	808	CLA	C1B-CHB	2.61	1.47	1.40
17	L	203	CLA	C1B-CHB	2.61	1.47	1.40
17	a	807	CLA	C1B-CHB	2.61	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	k	1403	CLA	C4C-C3C	2.61	1.49	1.45
17	4	604	CLA	C1B-CHB	2.61	1.47	1.40
17	9	602	CLA	C1B-CHB	2.61	1.47	1.40
17	a	813	CLA	CHD-C4C	2.61	1.49	1.41
17	b	810	CLA	C1C-C2C	2.62	1.49	1.44
17	1	310	CLA	C1B-CHB	2.62	1.47	1.40
17	9	611	CLA	C1B-CHB	2.62	1.47	1.40
17	B	822	CLA	C1B-CHB	2.62	1.47	1.40
17	b	813	CLA	C4C-C3C	2.62	1.49	1.45
17	B	834	CLA	C4C-C3C	2.62	1.49	1.45
17	b	809	CLA	C1B-CHB	2.62	1.47	1.40
17	4	602	CLA	C1B-CHB	2.62	1.47	1.40
17	a	832	CLA	C1B-CHB	2.62	1.47	1.40
17	B	826	CLA	C1C-C2C	2.63	1.49	1.44
17	b	809	CLA	C4B-CHC	2.63	1.47	1.40
17	a	803	CLA	C1B-CHB	2.63	1.47	1.40
17	4	614	CLA	C1B-CHB	2.63	1.47	1.40
17	B	817	CLA	C1B-CHB	2.63	1.47	1.40
17	a	828	CLA	C1C-C2C	2.63	1.49	1.44
17	a	835	CLA	C1B-CHB	2.63	1.47	1.40
17	B	805	CLA	C1B-CHB	2.63	1.47	1.40
17	4	608	CLA	C1B-CHB	2.63	1.47	1.40
17	2	602	CLA	CHD-C4C	2.63	1.49	1.41
17	A	830	CLA	C1C-C2C	2.63	1.49	1.44
17	a	831	CLA	C1B-CHB	2.63	1.47	1.40
17	b	818	CLA	C1B-CHB	2.64	1.47	1.40
17	8	312	CLA	C1B-CHB	2.64	1.47	1.40
17	7	602	CLA	C1B-CHB	2.64	1.47	1.40
17	B	802	CLA	C1B-CHB	2.64	1.47	1.40
17	a	830	CLA	C1C-C2C	2.64	1.49	1.44
17	l	204	CLA	C1B-CHB	2.64	1.47	1.40
17	3	314	CLA	C1B-CHB	2.64	1.47	1.40
17	2	604	CLA	C1B-CHB	2.65	1.47	1.40
17	9	608	CLA	C1B-CHB	2.65	1.47	1.40
17	G	104	CLA	C1B-CHB	2.65	1.47	1.40
17	2	610	CLA	C1B-CHB	2.65	1.47	1.40
17	l	203	CLA	C1B-CHB	2.65	1.47	1.40
17	A	833	CLA	C1B-CHB	2.65	1.47	1.40
17	j	3002	CLA	C1B-CHB	2.65	1.47	1.40
17	a	803	CLA	C4C-C3C	2.65	1.49	1.45
17	6	313	CLA	C1B-CHB	2.65	1.47	1.40
17	a	829	CLA	C1C-C2C	2.65	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	613	CLA	C1B-CHB	2.66	1.47	1.40
17	1	309	CLA	C1B-CHB	2.66	1.47	1.40
17	b	830	CLA	C1B-CHB	2.66	1.47	1.40
17	b	827	CLA	C1C-C2C	2.66	1.49	1.44
17	A	838	CLA	C1C-C2C	2.66	1.49	1.44
17	B	807	CLA	C1B-CHB	2.66	1.47	1.40
17	1	314	CLA	C1B-CHB	2.66	1.47	1.40
17	A	824	CLA	C4C-C3C	2.66	1.49	1.45
17	B	824	CLA	C1B-CHB	2.66	1.47	1.40
17	A	831	CLA	C4B-CHC	2.66	1.47	1.40
17	2	602	CLA	C1B-CHB	2.66	1.47	1.40
17	B	830	CLA	C1B-CHB	2.66	1.47	1.40
17	a	843	CLA	C1B-CHB	2.66	1.47	1.40
17	B	826	CLA	C1B-CHB	2.66	1.47	1.40
17	A	826	CLA	C1C-C2C	2.67	1.49	1.44
17	b	802	CLA	C1B-CHB	2.67	1.47	1.40
17	8	303	CLA	C1B-CHB	2.67	1.47	1.40
17	B	812	CLA	C1B-CHB	2.67	1.47	1.40
17	7	613	CLA	C1B-CHB	2.67	1.47	1.40
17	A	820	CLA	C1B-CHB	2.67	1.47	1.40
17	1	306	CLA	C1B-CHB	2.67	1.47	1.40
17	6	315	CLA	C1B-CHB	2.67	1.47	1.40
17	1	305	CLA	C1B-CHB	2.67	1.47	1.40
17	3	304	CLA	C1B-CHB	2.68	1.47	1.40
17	a	841	CLA	C1B-CHB	2.68	1.47	1.40
17	b	805	CLA	C1B-CHB	2.68	1.47	1.40
17	3	315	CLA	CHA-C1A	2.68	1.49	1.41
17	B	841	CLA	C1B-CHB	2.68	1.47	1.40
17	9	614	CLA	C1B-CHB	2.68	1.47	1.40
17	a	811	CLA	C1B-CHB	2.68	1.47	1.40
17	a	827	CLA	C1B-CHB	2.68	1.47	1.40
17	L	204	CLA	C1B-CHB	2.68	1.47	1.40
17	B	809	CLA	C4B-CHC	2.68	1.47	1.40
17	a	838	CLA	C1B-CHB	2.68	1.47	1.40
17	B	809	CLA	C1B-CHB	2.68	1.47	1.40
17	L	202	CLA	C1B-CHB	2.68	1.47	1.40
17	4	611	CLA	C1B-CHB	2.68	1.47	1.40
17	A	823	CLA	C1B-CHB	2.68	1.47	1.40
17	4	610	CLA	C1B-CHB	2.68	1.47	1.40
17	1	312	CLA	C1B-CHB	2.69	1.47	1.40
17	A	812	CLA	C1B-CHB	2.69	1.47	1.40
17	B	804	CLA	C1B-CHB	2.69	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	834	CLA	C1B-CHB	2.69	1.47	1.40
17	6	305	CLA	C1B-CHB	2.69	1.47	1.40
17	f	7003	CLA	C1B-CHB	2.69	1.47	1.40
17	A	818	CLA	C1B-CHB	2.69	1.47	1.40
17	B	836	CLA	C1B-CHB	2.69	1.47	1.40
17	a	818	CLA	C1B-CHB	2.69	1.47	1.40
17	A	816	CLA	C1B-CHB	2.69	1.47	1.40
17	A	854	CLA	C4B-CHC	2.69	1.47	1.40
17	B	819	CLA	C1B-CHB	2.69	1.47	1.40
17	9	603	CLA	C1B-CHB	2.69	1.47	1.40
17	b	826	CLA	C1B-CHB	2.69	1.47	1.40
17	a	842	CLA	C1B-CHB	2.69	1.47	1.40
17	A	803	CLA	C4B-CHC	2.69	1.47	1.40
17	b	819	CLA	C4B-CHC	2.69	1.47	1.40
17	A	831	CLA	C4C-C3C	2.69	1.49	1.45
17	8	305	CLA	C1B-CHB	2.69	1.47	1.40
17	6	314	CLA	C1B-CHB	2.69	1.47	1.40
17	A	842	CLA	C1B-CHB	2.69	1.47	1.40
17	A	832	CLA	C1B-CHB	2.69	1.47	1.40
17	9	610	CLA	C1B-CHB	2.69	1.47	1.40
17	a	846	CLA	C1B-CHB	2.69	1.47	1.40
17	B	815	CLA	C1B-CHB	2.69	1.47	1.40
17	7	610	CLA	C1B-CHB	2.70	1.47	1.40
17	B	810	CLA	C1B-CHB	2.70	1.47	1.40
17	B	839	CLA	C1B-CHB	2.70	1.47	1.40
17	A	845	CLA	C1B-CHB	2.70	1.47	1.40
17	b	815	CLA	C1B-CHB	2.70	1.47	1.40
17	9	613	CLA	C1B-CHB	2.70	1.47	1.40
17	F	301	CLA	C1B-CHB	2.70	1.47	1.40
17	9	604	CLA	C1B-CHB	2.70	1.47	1.40
17	A	815	CLA	C1B-CHB	2.70	1.47	1.40
17	3	301	CLA	C1B-CHB	2.70	1.47	1.40
17	4	613	CLA	C1B-CHB	2.70	1.47	1.40
17	A	838	CLA	C1B-CHB	2.70	1.47	1.40
17	b	837	CLA	C1B-CHB	2.70	1.47	1.40
17	B	818	CLA	C1B-CHB	2.70	1.47	1.40
17	6	306	CLA	C1B-CHB	2.70	1.47	1.40
17	7	603	CLA	C1B-CHB	2.70	1.47	1.40
17	8	313	CLA	CHA-C1A	2.70	1.49	1.41
17	8	313	CLA	C2C-C1C	2.71	1.49	1.43
17	B	819	CLA	C4B-CHC	2.71	1.47	1.40
17	B	808	CLA	C4B-CHC	2.71	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	824	CLA	C1B-CHB	2.71	1.47	1.40
17	a	831	CLA	C4B-CHC	2.71	1.47	1.40
17	8	311	CLA	C1B-CHB	2.71	1.47	1.40
17	a	820	CLA	C1B-CHB	2.71	1.47	1.40
17	b	829	CLA	C1B-CHB	2.71	1.47	1.40
17	3	315	CLA	C2C-C1C	2.71	1.49	1.43
17	a	807	CLA	C1C-C2C	2.71	1.49	1.44
17	a	837	CLA	C1B-CHB	2.71	1.47	1.40
17	6	312	CLA	C1B-CHB	2.71	1.47	1.40
17	6	304	CLA	C1B-CHB	2.72	1.47	1.40
17	b	824	CLA	C1B-CHB	2.72	1.47	1.40
17	B	825	CLA	C1B-CHB	2.72	1.47	1.40
17	a	801	CLA	C1B-CHB	2.72	1.47	1.40
17	a	805	CLA	C1B-CHB	2.72	1.47	1.40
17	b	802	CLA	C4B-CHC	2.72	1.47	1.40
17	6	307	CLA	C1B-CHB	2.72	1.47	1.40
17	B	828	CLA	C1B-CHB	2.72	1.47	1.40
17	a	818	CLA	C4B-CHC	2.72	1.47	1.40
17	J	3002	CLA	C1B-CHB	2.72	1.47	1.40
17	A	828	CLA	C1B-CHB	2.72	1.47	1.40
17	A	813	CLA	C1B-CHB	2.72	1.47	1.40
17	A	829	CLA	C1B-CHB	2.72	1.47	1.40
17	A	826	CLA	C1B-CHB	2.72	1.47	1.40
17	B	837	CLA	C1B-CHB	2.72	1.47	1.40
17	g	103	CLA	C1B-CHB	2.72	1.47	1.40
17	b	804	CLA	C1B-CHB	2.72	1.47	1.40
17	B	813	CLA	C1B-CHB	2.72	1.47	1.40
17	1	311	CLA	C1B-CHB	2.73	1.47	1.40
17	A	808	CLA	C4B-CHC	2.73	1.47	1.40
17	A	811	CLA	C1B-CHB	2.73	1.47	1.40
17	b	820	CLA	C1B-CHB	2.73	1.47	1.40
17	k	1401	CLA	C1B-CHB	2.73	1.47	1.40
17	8	309	CLA	C1B-CHB	2.73	1.47	1.40
17	b	838	CLA	C1B-CHB	2.73	1.47	1.40
17	a	813	CLA	C1B-CHB	2.73	1.47	1.40
17	2	603	CLA	C1B-CHB	2.73	1.47	1.40
17	g	102	CLA	C1B-CHB	2.73	1.47	1.40
17	A	825	CLA	C4B-CHC	2.73	1.47	1.40
17	3	311	CLA	C1B-CHB	2.73	1.47	1.40
17	A	836	CLA	C1B-CHB	2.73	1.47	1.40
17	b	828	CLA	C1B-CHB	2.73	1.47	1.40
17	A	821	CLA	C1B-CHB	2.73	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	601	CLA	C1B-CHB	2.73	1.47	1.40
17	A	829	CLA	C4B-CHC	2.74	1.47	1.40
17	a	811	CLA	C4B-CHC	2.74	1.47	1.40
17	A	807	CLA	C1B-CHB	2.74	1.47	1.40
17	2	610	CLA	C4B-CHC	2.74	1.47	1.40
17	b	808	CLA	C4B-CHC	2.74	1.47	1.40
17	b	832	CLA	C1B-CHB	2.74	1.47	1.40
17	a	844	CLA	C1B-CHB	2.74	1.47	1.40
17	2	612	CLA	C1B-CHB	2.74	1.47	1.40
17	1	304	CLA	C1B-CHB	2.74	1.47	1.40
17	a	806	CLA	C4B-CHC	2.74	1.47	1.40
17	b	821	CLA	C1B-CHB	2.74	1.47	1.40
17	7	610	CLA	C4B-CHC	2.74	1.47	1.40
17	B	840	CLA	C1B-CHB	2.74	1.47	1.40
17	b	835	CLA	C1B-CHB	2.74	1.47	1.40
17	G	103	CLA	C1B-CHB	2.74	1.47	1.40
17	g	101	CLA	C4B-CHC	2.74	1.47	1.40
17	a	819	CLA	C1B-CHB	2.74	1.47	1.40
17	K	4002	CLA	C1B-CHB	2.74	1.47	1.40
17	b	813	CLA	C1B-CHB	2.74	1.47	1.40
17	b	812	CLA	C1B-CHB	2.74	1.47	1.40
17	1	308	CLA	C1B-CHB	2.75	1.47	1.40
17	b	804	CLA	C4B-CHC	2.75	1.47	1.40
17	A	806	CLA	C1B-CHB	2.75	1.47	1.40
17	8	304	CLA	C1B-CHB	2.75	1.47	1.40
17	A	809	CLA	C4B-CHC	2.75	1.47	1.40
17	4	612	CLA	C4B-CHC	2.75	1.47	1.40
17	2	611	CLA	C1B-CHB	2.75	1.47	1.40
17	B	838	CLA	C4B-CHC	2.75	1.47	1.40
17	k	1403	CLA	C1B-CHB	2.75	1.47	1.40
17	f	7002	CLA	C1B-CHB	2.75	1.47	1.40
17	A	843	CLA	C4B-CHC	2.75	1.47	1.40
17	8	310	CLA	C1B-CHB	2.75	1.47	1.40
17	1	313	CLA	C1B-CHB	2.75	1.47	1.40
17	B	829	CLA	C1B-CHB	2.75	1.47	1.40
17	3	303	CLA	C1B-CHB	2.76	1.47	1.40
17	a	815	CLA	C1B-CHB	2.76	1.47	1.40
17	b	807	CLA	C1B-CHB	2.76	1.47	1.40
17	B	820	CLA	C1B-CHB	2.76	1.47	1.40
17	a	828	CLA	C1B-CHB	2.76	1.47	1.40
17	A	839	CLA	C4B-CHC	2.76	1.47	1.40
17	a	820	CLA	C4B-CHC	2.76	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	310	CLA	C1B-CHB	2.76	1.47	1.40
17	4	603	CLA	C1B-CHB	2.76	1.47	1.40
17	9	612	CLA	C1B-CHB	2.76	1.47	1.40
17	b	823	CLA	C1B-CHB	2.76	1.47	1.40
17	1	303	CLA	C1B-CHB	2.76	1.47	1.40
17	a	832	CLA	C4B-CHC	2.76	1.47	1.40
17	B	805	CLA	C4B-CHC	2.76	1.47	1.40
17	7	611	CLA	C1B-CHB	2.76	1.47	1.40
17	1	309	CLA	C4B-CHC	2.76	1.47	1.40
17	A	837	CLA	C1B-CHB	2.76	1.47	1.40
17	3	312	CLA	C1B-CHB	2.76	1.47	1.40
17	A	834	CLA	C4B-CHC	2.77	1.47	1.40
17	A	821	CLA	C4B-CHC	2.77	1.47	1.40
17	A	835	CLA	C4B-CHC	2.77	1.47	1.40
17	F	304	CLA	C1B-CHB	2.77	1.47	1.40
17	B	804	CLA	C4B-CHC	2.77	1.47	1.40
17	b	805	CLA	C4B-CHC	2.77	1.47	1.40
17	B	806	CLA	C1B-CHB	2.77	1.47	1.40
17	b	810	CLA	C1B-CHB	2.77	1.47	1.40
17	B	834	CLA	C1B-CHB	2.77	1.47	1.40
17	1	315	CLA	C1B-CHB	2.77	1.47	1.40
17	3	303	CLA	C4B-CHC	2.77	1.47	1.40
17	a	810	CLA	C1B-CHB	2.77	1.47	1.40
17	B	821	CLA	C1B-CHB	2.77	1.47	1.40
17	b	840	CLA	C4B-CHC	2.77	1.47	1.40
17	b	841	CLA	C1B-CHB	2.77	1.47	1.40
17	A	817	CLA	C1B-CHB	2.77	1.47	1.40
17	K	4003	CLA	C1B-CHB	2.77	1.47	1.40
17	A	830	CLA	C1B-CHB	2.77	1.47	1.40
17	6	305	CLA	C4B-CHC	2.77	1.47	1.40
17	6	309	CLA	C1B-CHB	2.77	1.47	1.40
17	4	601	CLA	C1B-CHB	2.78	1.47	1.40
17	A	805	CLA	C1B-CHB	2.78	1.47	1.40
17	A	832	CLA	C4B-CHC	2.78	1.47	1.40
17	k	1403	CLA	C4B-CHC	2.78	1.47	1.40
17	B	811	CLA	C4B-CHC	2.78	1.47	1.40
17	b	817	CLA	C4B-CHC	2.78	1.47	1.40
17	b	831	CLA	C1B-CHB	2.78	1.47	1.40
17	A	834	CLA	C1B-CHB	2.78	1.47	1.40
17	b	836	CLA	C4B-CHC	2.78	1.47	1.40
17	7	611	CLA	C4B-CHC	2.78	1.47	1.40
17	l	202	CLA	C4B-CHC	2.78	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	310	CLA	C1B-CHB	2.78	1.47	1.40
17	4	603	CLA	C4B-CHC	2.78	1.47	1.40
17	b	821	CLA	C4B-CHC	2.78	1.47	1.40
17	A	804	CLA	C1B-CHB	2.78	1.47	1.40
17	B	833	CLA	C1B-CHB	2.78	1.47	1.40
17	a	836	CLA	C4B-CHC	2.78	1.47	1.40
17	A	824	CLA	C4B-CHC	2.78	1.47	1.40
17	9	608	CLA	C4B-CHC	2.79	1.47	1.40
17	A	819	CLA	C1B-CHB	2.79	1.47	1.40
17	a	805	CLA	C4B-CHC	2.79	1.47	1.40
17	a	838	CLA	C1C-C2C	2.79	1.49	1.44
17	a	808	CLA	C1B-CHB	2.79	1.47	1.40
17	4	610	CLA	C4B-CHC	2.79	1.47	1.40
17	3	305	CLA	C1B-CHB	2.79	1.47	1.40
17	A	822	CLA	C4B-CHC	2.79	1.47	1.40
17	a	824	CLA	C1B-CHB	2.79	1.47	1.40
17	B	815	CLA	C4B-CHC	2.79	1.47	1.40
17	6	313	CLA	C4B-CHC	2.79	1.47	1.40
17	6	310	CLA	C4B-CHC	2.79	1.47	1.40
17	b	806	CLA	C1B-CHB	2.80	1.47	1.40
17	a	833	CLA	C1B-CHB	2.80	1.47	1.40
17	b	836	CLA	C1B-CHB	2.80	1.47	1.40
17	1	304	CLA	C4B-CHC	2.80	1.47	1.40
17	3	313	CLA	C1B-CHB	2.80	1.47	1.40
17	a	836	CLA	C1B-CHB	2.80	1.47	1.40
17	8	302	CLA	C4B-CHC	2.80	1.47	1.40
17	7	604	CLA	C4B-CHC	2.80	1.47	1.40
17	A	820	CLA	C4B-CHC	2.80	1.47	1.40
17	b	815	CLA	C4B-CHC	2.80	1.47	1.40
17	b	811	CLA	C1B-CHB	2.80	1.47	1.40
17	B	822	CLA	C4B-CHC	2.80	1.47	1.40
17	a	824	CLA	C4B-CHC	2.80	1.47	1.40
17	3	306	CLA	C1B-CHB	2.80	1.47	1.40
17	l	202	CLA	C1B-CHB	2.80	1.47	1.40
17	a	817	CLA	C1B-CHB	2.80	1.47	1.40
17	A	810	CLA	C4B-CHC	2.80	1.47	1.40
17	1	314	CLA	C4B-CHC	2.80	1.47	1.40
17	A	843	CLA	C1B-CHB	2.80	1.47	1.40
17	a	823	CLA	C1B-CHB	2.80	1.47	1.40
17	a	839	CLA	C1B-CHB	2.80	1.47	1.40
17	A	817	CLA	C4B-CHC	2.80	1.47	1.40
17	A	840	CLA	C1B-CHB	2.80	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	817	CLA	C4B-CHC	2.80	1.47	1.40
17	6	316	CLA	C1B-CHB	2.80	1.47	1.40
17	a	806	CLA	C1B-CHB	2.81	1.47	1.40
17	a	840	CLA	C4B-CHC	2.81	1.47	1.40
17	F	303	CLA	C1B-CHB	2.81	1.47	1.40
17	a	801	CLA	C4B-CHC	2.81	1.47	1.40
17	b	811	CLA	C4B-CHC	2.81	1.47	1.40
17	a	825	CLA	C4B-CHC	2.81	1.47	1.40
17	9	611	CLA	C4B-CHC	2.81	1.47	1.40
17	b	831	CLA	C4B-CHC	2.81	1.47	1.40
17	A	839	CLA	C1B-CHB	2.81	1.47	1.40
17	4	601	CLA	C4B-CHC	2.81	1.47	1.40
17	b	833	CLA	C1B-CHB	2.82	1.47	1.40
17	g	101	CLA	C1B-CHB	2.82	1.47	1.40
17	8	310	CLA	C4B-CHC	2.82	1.47	1.40
17	a	825	CLA	C1B-CHB	2.82	1.47	1.40
17	a	827	CLA	C4B-CHC	2.82	1.47	1.40
17	a	837	CLA	C4B-CHC	2.82	1.47	1.40
17	b	830	CLA	C4B-CHC	2.82	1.47	1.40
17	G	101	CLA	C1B-CHB	2.82	1.47	1.40
17	g	103	CLA	C4B-CHC	2.82	1.47	1.40
17	1	312	CLA	C4B-CHC	2.82	1.47	1.40
17	8	303	CLA	C4B-CHC	2.82	1.47	1.40
17	a	826	CLA	C4B-CHC	2.82	1.47	1.40
17	a	826	CLA	C1B-CHB	2.82	1.47	1.40
17	a	821	CLA	C4B-CHC	2.82	1.47	1.40
17	l	204	CLA	C4B-CHC	2.82	1.47	1.40
17	b	839	CLA	C1B-CHB	2.82	1.47	1.40
17	B	830	CLA	C4B-CHC	2.82	1.47	1.40
17	a	816	CLA	C1B-CHB	2.82	1.47	1.40
17	B	823	CLA	C1B-CHB	2.82	1.47	1.40
17	A	808	CLA	C1B-CHB	2.82	1.47	1.40
17	a	844	CLA	C4B-CHC	2.83	1.47	1.40
17	4	604	CLA	C4B-CHC	2.83	1.47	1.40
17	A	845	CLA	C4B-CHC	2.83	1.47	1.40
17	B	825	CLA	C4B-CHC	2.83	1.47	1.40
17	A	811	CLA	C4B-CHC	2.83	1.47	1.40
17	B	802	CLA	C4B-CHC	2.83	1.47	1.40
17	b	834	CLA	C1B-CHB	2.83	1.47	1.40
17	A	814	CLA	C4B-CHC	2.83	1.47	1.40
17	b	824	CLA	C4B-CHC	2.83	1.47	1.40
17	7	612	CLA	C4B-CHC	2.83	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	818	CLA	C4B-CHC	2.83	1.47	1.40
17	1	310	CLA	C4B-CHC	2.83	1.47	1.40
17	b	823	CLA	C4B-CHC	2.83	1.47	1.40
17	k	1402	CLA	C1B-CHB	2.83	1.47	1.40
17	B	840	CLA	C4B-CHC	2.83	1.47	1.40
17	6	315	CLA	C4B-CHC	2.83	1.47	1.40
17	2	603	CLA	C4B-CHC	2.83	1.47	1.40
17	6	306	CLA	C4B-CHC	2.83	1.47	1.40
17	a	830	CLA	C1B-CHB	2.83	1.47	1.40
17	b	835	CLA	C4B-CHC	2.83	1.47	1.40
17	a	823	CLA	C4B-CHC	2.84	1.47	1.40
17	1	311	CLA	C4B-CHC	2.84	1.47	1.40
17	2	612	CLA	C4B-CHC	2.84	1.47	1.40
17	4	611	CLA	C4B-CHC	2.84	1.47	1.40
17	B	817	CLA	C4B-CHC	2.84	1.47	1.40
17	6	304	CLA	C4B-CHC	2.84	1.47	1.40
17	6	314	CLA	C4B-CHC	2.84	1.47	1.40
17	B	811	CLA	C1B-CHB	2.84	1.47	1.40
17	b	825	CLA	C4B-CHC	2.84	1.47	1.40
17	9	610	CLA	C4B-CHC	2.84	1.47	1.40
17	B	823	CLA	C4B-CHC	2.84	1.47	1.40
17	b	813	CLA	C4B-CHC	2.84	1.47	1.40
17	b	812	CLA	C4B-CHC	2.84	1.47	1.40
17	2	611	CLA	C4B-CHC	2.84	1.47	1.40
17	7	613	CLA	C4B-CHC	2.84	1.47	1.40
17	B	836	CLA	C4B-CHC	2.84	1.47	1.40
17	a	829	CLA	C4B-CHC	2.84	1.47	1.40
17	3	312	CLA	C4B-CHC	2.84	1.47	1.40
17	b	840	CLA	C1B-CHB	2.85	1.47	1.40
17	B	832	CLA	C1B-CHB	2.85	1.47	1.40
17	3	310	CLA	C4B-CHC	2.85	1.47	1.40
17	k	1402	CLA	C4B-CHC	2.85	1.47	1.40
17	3	313	CLA	C4B-CHC	2.85	1.47	1.40
17	7	612	CLA	C1B-CHB	2.85	1.47	1.40
17	A	823	CLA	C4B-CHC	2.85	1.47	1.40
17	A	813	CLA	C4B-CHC	2.85	1.47	1.40
17	F	303	CLA	C4B-CHC	2.85	1.47	1.40
17	A	812	CLA	C4B-CHC	2.85	1.47	1.40
17	a	810	CLA	C4B-CHC	2.85	1.47	1.40
17	b	807	CLA	C4B-CHC	2.85	1.47	1.40
17	9	612	CLA	C4B-CHC	2.85	1.47	1.40
17	1	313	CLA	C4B-CHC	2.85	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	836	CLA	C4B-CHC	2.85	1.47	1.40
17	b	828	CLA	C4B-CHC	2.85	1.47	1.40
17	A	825	CLA	C1B-CHB	2.85	1.47	1.40
17	1	305	CLA	C4B-CHC	2.85	1.47	1.40
17	K	4003	CLA	C4B-CHC	2.85	1.47	1.40
17	9	604	CLA	C4B-CHC	2.86	1.47	1.40
17	b	838	CLA	C4B-CHC	2.86	1.47	1.40
17	4	612	CLA	C1B-CHB	2.86	1.47	1.40
17	a	804	CLA	C1B-CHB	2.86	1.47	1.40
17	a	840	CLA	C1B-CHB	2.86	1.47	1.40
17	9	601	CLA	C4B-CHC	2.86	1.47	1.40
17	a	846	CLA	C4B-CHC	2.86	1.47	1.40
17	A	806	CLA	C4B-CHC	2.86	1.47	1.40
17	L	202	CLA	C4B-CHC	2.86	1.47	1.40
17	a	802	CLA	C4B-CHC	2.86	1.47	1.40
17	b	837	CLA	C4B-CHC	2.86	1.47	1.40
17	b	839	CLA	C4B-CHC	2.86	1.47	1.40
17	A	818	CLA	C4B-CHC	2.86	1.47	1.40
17	9	609	CLA	C4B-CHC	2.86	1.47	1.40
17	a	822	CLA	C4B-CHC	2.86	1.47	1.40
17	B	816	CLA	C4B-CHC	2.86	1.47	1.40
17	g	102	CLA	C4B-CHC	2.87	1.47	1.40
17	F	301	CLA	C4B-CHC	2.87	1.47	1.40
17	4	613	CLA	C4B-CHC	2.87	1.47	1.40
17	2	604	CLA	C4B-CHC	2.87	1.47	1.40
17	K	4002	CLA	C4B-CHC	2.87	1.47	1.40
17	3	301	CLA	C4B-CHC	2.87	1.47	1.40
17	3	305	CLA	C4B-CHC	2.87	1.47	1.40
17	6	312	CLA	C4B-CHC	2.87	1.47	1.40
17	2	608	CLA	C4B-CHC	2.87	1.47	1.40
17	3	304	CLA	C4B-CHC	2.87	1.47	1.40
17	B	821	CLA	C4B-CHC	2.87	1.47	1.40
17	9	614	CLA	C4B-CHC	2.87	1.47	1.40
17	4	608	CLA	C4B-CHC	2.87	1.47	1.40
17	a	834	CLA	C4B-CHC	2.87	1.47	1.40
17	3	315	CLA	C3C-C4C	2.87	1.49	1.43
17	a	835	CLA	C4B-CHC	2.87	1.47	1.40
17	4	602	CLA	C4B-CHC	2.87	1.47	1.40
17	A	826	CLA	C4B-CHC	2.87	1.47	1.40
17	6	316	CLA	C4B-CHC	2.88	1.47	1.40
17	8	305	CLA	C4B-CHC	2.88	1.47	1.40
17	3	302	CLA	C4B-CHC	2.88	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	3002	CLA	C4B-CHC	2.88	1.47	1.40
17	6	307	CLA	C4B-CHC	2.88	1.47	1.40
17	b	816	CLA	C4B-CHC	2.88	1.47	1.40
17	A	801	CLA	C4B-CHC	2.88	1.47	1.40
17	G	104	CLA	C4B-CHC	2.88	1.47	1.40
17	a	804	CLA	C4B-CHC	2.88	1.47	1.40
17	B	820	CLA	C4B-CHC	2.88	1.47	1.40
17	2	602	CLA	C4B-CHC	2.88	1.47	1.40
17	8	313	CLA	C3C-C4C	2.88	1.49	1.43
17	B	839	CLA	C4B-CHC	2.88	1.47	1.40
17	3	308	CLA	C4B-CHC	2.88	1.47	1.40
17	A	830	CLA	C4B-CHC	2.88	1.47	1.40
17	8	304	CLA	C4B-CHC	2.88	1.47	1.40
17	a	830	CLA	C4B-CHC	2.88	1.47	1.40
17	a	812	CLA	C4B-CHC	2.88	1.47	1.40
17	L	204	CLA	C4B-CHC	2.88	1.47	1.40
17	A	805	CLA	C4B-CHC	2.88	1.47	1.40
17	a	813	CLA	C4B-CHC	2.88	1.47	1.40
17	B	810	CLA	C4B-CHC	2.88	1.47	1.40
17	A	837	CLA	C4B-CHC	2.88	1.47	1.40
17	1	315	CLA	C4B-CHC	2.89	1.47	1.40
17	b	834	CLA	C4B-CHC	2.89	1.47	1.40
17	b	822	CLA	C4B-CHC	2.89	1.47	1.40
17	j	3002	CLA	C4B-CHC	2.89	1.47	1.40
17	B	835	CLA	C4B-CHC	2.89	1.47	1.40
17	a	839	CLA	C4B-CHC	2.89	1.47	1.40
17	B	813	CLA	C4B-CHC	2.89	1.47	1.40
17	b	833	CLA	C4B-CHC	2.89	1.47	1.40
17	2	613	CLA	C4B-CHC	2.89	1.47	1.40
17	8	312	CLA	C4B-CHC	2.89	1.47	1.40
17	B	833	CLA	C4B-CHC	2.89	1.47	1.40
17	G	101	CLA	C4B-CHC	2.89	1.47	1.40
17	f	7002	CLA	C4B-CHC	2.89	1.47	1.40
17	a	821	CLA	C1B-CHB	2.89	1.47	1.40
17	B	818	CLA	C4B-CHC	2.89	1.47	1.40
17	8	309	CLA	C4B-CHC	2.89	1.47	1.40
17	4	609	CLA	C4B-CHC	2.89	1.47	1.40
17	1	306	CLA	C4B-CHC	2.90	1.47	1.40
17	b	820	CLA	C4B-CHC	2.90	1.47	1.40
17	A	815	CLA	C4B-CHC	2.90	1.47	1.40
17	1	308	CLA	C4B-CHC	2.90	1.47	1.40
17	A	840	CLA	C4B-CHC	2.90	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	603	CLA	C4B-CHC	2.90	1.47	1.40
17	7	608	CLA	C4B-CHC	2.90	1.47	1.40
17	A	816	CLA	C4B-CHC	2.90	1.47	1.40
17	1	303	CLA	C4B-CHC	2.90	1.47	1.40
17	9	603	CLA	C4B-CHC	2.90	1.47	1.40
17	8	311	CLA	C4B-CHC	2.90	1.47	1.40
17	a	814	CLA	C4B-CHC	2.90	1.47	1.40
17	B	806	CLA	C4B-CHC	2.91	1.47	1.40
17	B	834	CLA	C4B-CHC	2.91	1.47	1.40
17	3	311	CLA	C4B-CHC	2.91	1.47	1.40
17	B	837	CLA	C4B-CHC	2.91	1.47	1.40
17	4	614	CLA	C4B-CHC	2.91	1.47	1.40
17	9	613	CLA	C4B-CHC	2.91	1.47	1.40
17	a	843	CLA	C4B-CHC	2.91	1.47	1.40
17	b	841	CLA	C4B-CHC	2.92	1.47	1.40
17	A	804	CLA	C4B-CHC	2.92	1.47	1.40
17	f	7003	CLA	C4B-CHC	2.92	1.47	1.40
17	b	806	CLA	C4B-CHC	2.92	1.47	1.40
17	B	812	CLA	C4B-CHC	2.92	1.47	1.40
17	6	309	CLA	C4B-CHC	2.92	1.47	1.40
17	B	824	CLA	C4B-CHC	2.92	1.47	1.40
17	a	809	CLA	C4B-CHC	2.92	1.47	1.40
17	3	309	CLA	C4B-CHC	2.92	1.47	1.40
17	F	304	CLA	C4B-CHC	2.92	1.47	1.40
17	L	203	CLA	C4B-CHC	2.92	1.47	1.40
17	A	842	CLA	C4B-CHC	2.92	1.47	1.40
17	B	828	CLA	C4B-CHC	2.93	1.47	1.40
17	a	842	CLA	C4B-CHC	2.93	1.47	1.40
17	G	103	CLA	C4B-CHC	2.93	1.47	1.40
17	B	838	CLA	C1B-CHB	2.93	1.47	1.40
17	a	808	CLA	C4B-CHC	2.93	1.47	1.40
17	a	816	CLA	C4B-CHC	2.93	1.47	1.40
17	8	307	CLA	C4B-CHC	2.93	1.47	1.40
17	A	827	CLA	C4B-CHC	2.93	1.47	1.40
17	b	832	CLA	C4B-CHC	2.93	1.47	1.40
17	9	602	CLA	C4B-CHC	2.93	1.47	1.40
17	b	826	CLA	C4B-CHC	2.93	1.47	1.40
17	B	831	CLA	C4B-CHC	2.94	1.47	1.40
17	3	314	CLA	C4B-CHC	2.94	1.48	1.40
17	A	828	CLA	C4B-CHC	2.95	1.48	1.40
17	B	803	CLA	C4B-CHC	2.95	1.48	1.40
17	8	308	CLA	C4B-CHC	2.95	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	609	CLA	C4B-CHC	2.95	1.48	1.40
17	a	807	CLA	C4B-CHC	2.95	1.48	1.40
17	l	203	CLA	C4B-CHC	2.95	1.48	1.40
17	A	819	CLA	C4B-CHC	2.95	1.48	1.40
17	a	815	CLA	C4B-CHC	2.95	1.48	1.40
17	B	807	CLA	C4B-CHC	2.96	1.48	1.40
17	6	311	CLA	C4B-CHC	2.96	1.48	1.40
17	k	1401	CLA	C4B-CHC	2.96	1.48	1.40
17	a	828	CLA	C4B-CHC	2.97	1.48	1.40
17	3	306	CLA	C4B-CHC	2.97	1.48	1.40
17	b	810	CLA	C4B-CHC	2.97	1.48	1.40
17	B	827	CLA	C4B-CHC	2.98	1.48	1.40
17	a	841	CLA	C4B-CHC	2.98	1.48	1.40
17	B	832	CLA	C4B-CHC	2.99	1.48	1.40
17	A	810	CLA	C1B-CHB	2.99	1.48	1.40
17	b	803	CLA	C4B-CHC	2.99	1.48	1.40
17	B	841	CLA	C4B-CHC	2.99	1.48	1.40
17	b	814	CLA	C4B-CHC	2.99	1.48	1.40
17	B	814	CLA	C4B-CHC	2.99	1.48	1.40
17	B	826	CLA	C4B-CHC	2.99	1.48	1.40
17	A	807	CLA	C4B-CHC	3.00	1.48	1.40
17	7	602	CLA	C4B-CHC	3.00	1.48	1.40
17	7	609	CLA	C4B-CHC	3.00	1.48	1.40
17	A	833	CLA	C4B-CHC	3.00	1.48	1.40
17	A	802	CLA	C4B-CHC	3.01	1.48	1.40
17	a	833	CLA	C4B-CHC	3.01	1.48	1.40
17	A	838	CLA	C4B-CHC	3.01	1.48	1.40
17	b	827	CLA	C4B-CHC	3.03	1.48	1.40
17	a	838	CLA	C4B-CHC	3.04	1.48	1.40
17	a	819	CLA	C4B-CHC	3.05	1.48	1.40
17	A	841	CLA	C4B-CHC	3.06	1.48	1.40
17	8	301	CLA	C4B-CHC	3.07	1.48	1.40
17	3	315	CLA	CHC-C1C	3.13	1.48	1.39
17	8	313	CLA	CHC-C1C	3.14	1.48	1.39
17	B	826	CLA	OBD-CAD	3.89	1.28	1.22
17	9	601	CLA	O2A-CGA	3.89	1.45	1.32
26	8	306	CHL	O2A-CGA	3.92	1.45	1.32
17	8	312	CLA	O2A-CGA	3.93	1.45	1.32
25	9	619	LMG	O7-C10	3.94	1.45	1.34
17	K	4003	CLA	O2A-CGA	3.95	1.45	1.32
26	6	308	CHL	O2A-CGA	3.96	1.45	1.32
17	4	601	CLA	O2A-CGA	3.96	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	104	CLA	O2A-CGA	3.96	1.45	1.32
19	2	618	LHG	O7-C7	3.96	1.45	1.34
25	6	302	LMG	O7-C10	3.96	1.45	1.34
17	3	314	CLA	O2A-CGA	3.96	1.45	1.32
17	3	301	CLA	O2A-CGA	3.97	1.45	1.32
17	4	603	CLA	O2A-CGA	3.97	1.45	1.32
17	k	1403	CLA	O2A-CGA	3.98	1.46	1.32
17	3	310	CLA	OBD-CAD	3.99	1.29	1.22
19	7	618	LHG	O7-C7	3.99	1.45	1.34
17	6	316	CLA	O2A-CGA	3.99	1.46	1.32
17	6	309	CLA	O2A-CGA	3.99	1.46	1.32
19	1	319	LHG	O7-C7	3.99	1.45	1.34
17	b	821	CLA	O2A-CGA	3.99	1.46	1.32
17	k	1402	CLA	O2A-CGA	3.99	1.46	1.32
17	a	803	CLA	OBD-CAD	4.00	1.28	1.22
17	9	603	CLA	O2A-CGA	4.00	1.46	1.32
19	6	301	LHG	O7-C7	4.01	1.45	1.34
24	b	849	DGD	O2G-C1B	4.01	1.45	1.34
26	3	307	CHL	O2A-CGA	4.01	1.46	1.32
19	A	846	LHG	O7-C7	4.01	1.45	1.34
25	G	102	LMG	O7-C10	4.01	1.45	1.34
17	g	103	CLA	O2A-CGA	4.01	1.46	1.32
17	B	821	CLA	O2A-CGA	4.02	1.46	1.32
19	a	847	LHG	O8-C23	4.03	1.45	1.33
17	b	802	CLA	O2A-CGA	4.03	1.45	1.33
17	a	844	CLA	O2A-CGA	4.03	1.45	1.33
17	1	315	CLA	O2A-CGA	4.03	1.46	1.32
17	b	826	CLA	OBD-CAD	4.03	1.28	1.22
26	2	607	CHL	OBD-CAD	4.04	1.28	1.21
19	6	320	LHG	O7-C7	4.04	1.46	1.34
19	a	848	LHG	O7-C7	4.05	1.46	1.34
17	a	828	CLA	OBD-CAD	4.05	1.28	1.22
17	A	843	CLA	O2A-CGA	4.05	1.45	1.33
17	a	802	CLA	O2A-CGA	4.06	1.45	1.33
24	B	850	DGD	O2G-C1B	4.06	1.46	1.34
17	A	806	CLA	O2A-CGA	4.06	1.45	1.33
17	b	832	CLA	O2A-CGA	4.07	1.45	1.33
19	a	847	LHG	O7-C7	4.07	1.46	1.34
19	1	301	LHG	O7-C7	4.07	1.46	1.34
17	b	836	CLA	OBD-CAD	4.07	1.28	1.22
25	4	619	LMG	O7-C10	4.07	1.46	1.34
25	4	620	LMG	O7-C10	4.08	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	850	DGD	O1G-C1A	4.08	1.45	1.33
17	B	810	CLA	O2A-CGA	4.08	1.45	1.33
26	7	601	CHL	O2A-CGA	4.08	1.45	1.33
17	B	805	CLA	O2A-CGA	4.09	1.45	1.33
19	A	847	LHG	O7-C7	4.09	1.46	1.34
17	b	829	CLA	O2A-CGA	4.09	1.45	1.33
26	4	607	CHL	OBD-CAD	4.09	1.28	1.21
17	a	810	CLA	O2A-CGA	4.10	1.45	1.33
26	4	605	CHL	O2A-CGA	4.11	1.45	1.33
17	a	829	CLA	O2A-CGA	4.11	1.45	1.33
17	b	805	CLA	O2A-CGA	4.12	1.45	1.33
17	a	831	CLA	O2A-CGA	4.12	1.45	1.33
17	A	838	CLA	OBD-CAD	4.13	1.28	1.22
17	B	817	CLA	O2A-CGA	4.13	1.45	1.33
17	B	806	CLA	OBD-CAD	4.13	1.28	1.22
17	2	603	CLA	OBD-CAD	4.13	1.28	1.22
19	A	846	LHG	O8-C23	4.14	1.45	1.33
17	A	831	CLA	O2A-CGA	4.14	1.45	1.33
19	3	319	LHG	O8-C23	4.15	1.45	1.33
19	a	848	LHG	O8-C23	4.15	1.45	1.33
25	9	619	LMG	O8-C28	4.16	1.45	1.33
17	A	829	CLA	O2A-CGA	4.16	1.45	1.33
17	a	828	CLA	O2A-CGA	4.16	1.45	1.33
17	b	823	CLA	C3D-C2D	4.16	1.48	1.39
26	9	605	CHL	O2A-CGA	4.16	1.45	1.33
17	A	834	CLA	O2A-CGA	4.16	1.45	1.33
17	a	806	CLA	O2A-CGA	4.16	1.45	1.33
17	a	843	CLA	C3D-C2D	4.16	1.48	1.39
17	A	801	CLA	O2A-CGA	4.16	1.45	1.33
17	b	813	CLA	O2A-CGA	4.16	1.45	1.33
17	A	804	CLA	O2A-CGA	4.16	1.45	1.33
17	a	856	CLA	CHC-C1C	4.17	1.47	1.35
17	a	809	CLA	O2A-CGA	4.17	1.45	1.33
17	9	602	CLA	O2A-CGA	4.17	1.45	1.33
25	4	619	LMG	O8-C28	4.17	1.45	1.33
24	b	849	DGD	O1G-C1A	4.17	1.45	1.33
17	a	801	CLA	O2A-CGA	4.17	1.45	1.33
26	9	606	CHL	O2A-CGA	4.17	1.45	1.33
17	b	826	CLA	O2A-CGA	4.17	1.45	1.33
17	A	811	CLA	O2A-CGA	4.18	1.45	1.33
17	A	826	CLA	O2A-CGA	4.18	1.45	1.33
17	A	803	CLA	O2A-CGA	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	814	CLA	O2A-CGA	4.18	1.45	1.33
17	3	308	CLA	O2A-CGA	4.18	1.45	1.33
17	B	813	CLA	O2A-CGA	4.18	1.45	1.33
19	7	618	LHG	O8-C23	4.18	1.45	1.33
26	2	601	CHL	O2A-CGA	4.18	1.45	1.33
17	A	830	CLA	O2A-CGA	4.18	1.45	1.33
17	a	830	CLA	O2A-CGA	4.18	1.45	1.33
17	B	829	CLA	CHC-C1C	4.18	1.47	1.35
17	b	840	CLA	O2A-CGA	4.18	1.45	1.33
17	8	302	CLA	CHC-C1C	4.19	1.47	1.35
19	1	319	LHG	O8-C23	4.19	1.45	1.33
17	b	809	CLA	O2A-CGA	4.19	1.45	1.33
17	3	302	CLA	O2A-CGA	4.19	1.45	1.33
17	1	303	CLA	O2A-CGA	4.19	1.45	1.33
17	a	803	CLA	CHC-C1C	4.19	1.47	1.35
17	B	817	CLA	OBD-CAD	4.19	1.28	1.22
17	b	834	CLA	O2A-CGA	4.20	1.45	1.33
17	A	827	CLA	O2A-CGA	4.20	1.45	1.33
17	b	841	CLA	O2A-CGA	4.20	1.45	1.33
17	a	833	CLA	O2A-CGA	4.20	1.45	1.33
17	B	819	CLA	O2A-CGA	4.20	1.45	1.33
25	4	620	LMG	O8-C28	4.20	1.45	1.33
19	6	320	LHG	O8-C23	4.20	1.45	1.33
17	a	811	CLA	O2A-CGA	4.20	1.45	1.33
17	9	604	CLA	O2A-CGA	4.20	1.45	1.33
17	a	841	CLA	O2A-CGA	4.20	1.45	1.33
17	1	313	CLA	O2A-CGA	4.21	1.45	1.33
17	3	303	CLA	CHC-C1C	4.21	1.47	1.35
17	b	808	CLA	CHC-C1C	4.21	1.47	1.35
17	B	822	CLA	O2A-CGA	4.21	1.45	1.33
17	A	810	CLA	O2A-CGA	4.21	1.45	1.33
26	6	303	CHL	O2A-CGA	4.21	1.45	1.33
17	a	827	CLA	O2A-CGA	4.21	1.45	1.33
17	B	823	CLA	O2A-CGA	4.21	1.45	1.33
17	A	812	CLA	O2A-CGA	4.21	1.45	1.33
26	7	606	CHL	O2A-CGA	4.21	1.45	1.33
17	b	818	CLA	O2A-CGA	4.21	1.45	1.33
17	b	823	CLA	O2A-CGA	4.22	1.45	1.33
17	a	804	CLA	O2A-CGA	4.22	1.45	1.33
26	2	607	CHL	O2A-CGA	4.22	1.45	1.33
17	A	833	CLA	O2A-CGA	4.22	1.45	1.33
17	B	819	CLA	CHC-C1C	4.22	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	603	CLA	OBD-CAD	4.22	1.28	1.22
17	g	102	CLA	O2A-CGA	4.22	1.45	1.33
17	a	807	CLA	O2A-CGA	4.22	1.45	1.33
26	1	302	CHL	O2A-CGA	4.22	1.45	1.33
17	1	312	CLA	O2A-CGA	4.23	1.45	1.33
17	1	309	CLA	CHC-C1C	4.23	1.47	1.35
17	b	840	CLA	CHC-C1C	4.23	1.47	1.35
17	B	802	CLA	O2A-CGA	4.23	1.45	1.33
17	b	830	CLA	O2A-CGA	4.23	1.45	1.33
17	a	842	CLA	O2A-CGA	4.23	1.45	1.33
17	F	303	CLA	CHC-C1C	4.23	1.47	1.35
17	b	803	CLA	O2A-CGA	4.23	1.45	1.33
17	b	810	CLA	O2A-CGA	4.24	1.45	1.33
25	G	102	LMG	O8-C28	4.24	1.45	1.33
17	a	836	CLA	CHC-C1C	4.24	1.47	1.35
17	a	834	CLA	O2A-CGA	4.24	1.45	1.33
17	b	806	CLA	OBD-CAD	4.24	1.28	1.22
17	A	834	CLA	CHC-C1C	4.24	1.47	1.35
17	a	856	CLA	O2A-CGA	4.24	1.45	1.33
17	B	806	CLA	O2A-CGA	4.24	1.45	1.33
17	B	838	CLA	O2A-CGA	4.24	1.45	1.33
17	B	825	CLA	O2A-CGA	4.24	1.45	1.33
17	B	831	CLA	O2A-CGA	4.24	1.45	1.33
17	a	826	CLA	O2A-CGA	4.24	1.45	1.33
17	1	304	CLA	O2A-CGA	4.24	1.45	1.33
17	6	315	CLA	O2A-CGA	4.24	1.45	1.33
17	1	308	CLA	O2A-CGA	4.24	1.45	1.33
17	2	611	CLA	O2A-CGA	4.25	1.45	1.33
26	9	607	CHL	O2A-CGA	4.25	1.45	1.33
17	3	312	CLA	CHC-C1C	4.25	1.47	1.35
17	9	608	CLA	O2A-CGA	4.25	1.45	1.33
17	1	304	CLA	CHC-C1C	4.25	1.47	1.35
26	9	607	CHL	OBD-CAD	4.25	1.28	1.21
17	9	612	CLA	O2A-CGA	4.25	1.45	1.33
17	a	822	CLA	O2A-CGA	4.25	1.45	1.33
17	7	611	CLA	CHC-C1C	4.25	1.47	1.35
26	9	605	CHL	OBD-CAD	4.25	1.28	1.21
17	B	803	CLA	O2A-CGA	4.25	1.45	1.33
17	4	603	CLA	CHC-C1C	4.25	1.47	1.35
19	A	847	LHG	O8-C23	4.25	1.45	1.33
17	A	854	CLA	CHC-C1C	4.25	1.47	1.35
26	4	606	CHL	O2A-CGA	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	829	CLA	CHC-C1C	4.25	1.47	1.35
17	4	614	CLA	O2A-CGA	4.25	1.45	1.33
17	6	305	CLA	O2A-CGA	4.25	1.45	1.33
17	A	832	CLA	O2A-CGA	4.25	1.45	1.33
17	A	809	CLA	O2A-CGA	4.26	1.45	1.33
17	b	827	CLA	O2A-CGA	4.26	1.45	1.33
17	b	832	CLA	C3D-C2D	4.26	1.49	1.39
17	b	819	CLA	CHC-C1C	4.26	1.47	1.35
26	4	607	CHL	O2A-CGA	4.26	1.45	1.33
25	6	302	LMG	O8-C28	4.26	1.45	1.33
17	9	608	CLA	CHC-C1C	4.26	1.47	1.35
17	B	818	CLA	O2A-CGA	4.26	1.45	1.33
17	g	101	CLA	CHC-C1C	4.26	1.47	1.35
17	A	814	CLA	O2A-CGA	4.26	1.45	1.33
17	6	314	CLA	O2A-CGA	4.26	1.45	1.33
17	B	809	CLA	CHC-C1C	4.26	1.47	1.35
17	a	804	CLA	C3D-C2D	4.26	1.49	1.39
17	A	836	CLA	O2A-CGA	4.27	1.45	1.33
17	A	843	CLA	CHC-C1C	4.27	1.47	1.35
19	2	618	LHG	O8-C23	4.27	1.45	1.33
17	B	827	CLA	O2A-CGA	4.27	1.45	1.33
17	a	817	CLA	CHC-C1C	4.27	1.47	1.35
17	L	202	CLA	CHC-C1C	4.27	1.47	1.35
17	b	802	CLA	CHC-C1C	4.27	1.47	1.35
17	A	828	CLA	OBD-CAD	4.27	1.28	1.22
17	A	839	CLA	OBD-CAD	4.27	1.28	1.22
17	7	610	CLA	CHC-C1C	4.27	1.47	1.35
26	7	607	CHL	O2A-CGA	4.27	1.45	1.33
17	B	841	CLA	O2A-CGA	4.27	1.45	1.33
17	8	307	CLA	O2A-CGA	4.27	1.45	1.33
17	B	826	CLA	C3D-C2D	4.27	1.49	1.39
17	a	818	CLA	CHC-C1C	4.27	1.47	1.35
17	2	608	CLA	CHC-C1C	4.27	1.47	1.35
17	A	824	CLA	CHC-C1C	4.27	1.47	1.35
17	4	612	CLA	CHC-C1C	4.27	1.47	1.35
26	2	606	CHL	O2A-CGA	4.27	1.45	1.33
17	B	820	CLA	O2A-CGA	4.27	1.45	1.33
17	a	824	CLA	CHC-C1C	4.27	1.47	1.35
17	A	829	CLA	OBD-CAD	4.27	1.28	1.22
17	B	834	CLA	O2A-CGA	4.27	1.45	1.33
17	7	608	CLA	O2A-CGA	4.27	1.45	1.33
17	7	611	CLA	O2A-CGA	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	824	CLA	O2A-CGA	4.28	1.45	1.33
17	A	802	CLA	O2A-CGA	4.28	1.45	1.33
17	1	305	CLA	O2A-CGA	4.28	1.45	1.33
17	B	830	CLA	O2A-CGA	4.28	1.45	1.33
17	a	820	CLA	CHC-C1C	4.28	1.47	1.35
17	b	831	CLA	O2A-CGA	4.28	1.45	1.33
17	1	312	CLA	CHC-C1C	4.28	1.47	1.35
17	b	805	CLA	CHC-C1C	4.28	1.47	1.35
17	3	311	CLA	O2A-CGA	4.28	1.45	1.33
17	a	832	CLA	O2A-CGA	4.28	1.45	1.33
17	a	846	CLA	O2A-CGA	4.28	1.45	1.33
17	7	603	CLA	O2A-CGA	4.28	1.45	1.33
17	7	608	CLA	CHC-C1C	4.28	1.47	1.35
26	1	307	CHL	O2A-CGA	4.28	1.45	1.33
17	9	601	CLA	CHC-C1C	4.28	1.47	1.35
17	B	838	CLA	OBD-CAD	4.28	1.28	1.22
17	7	612	CLA	CHC-C1C	4.28	1.47	1.35
17	1	314	CLA	O2A-CGA	4.28	1.45	1.33
17	B	838	CLA	CHC-C1C	4.28	1.47	1.35
17	B	814	CLA	O2A-CGA	4.28	1.45	1.33
17	a	811	CLA	CHC-C1C	4.28	1.47	1.35
17	a	805	CLA	O2A-CGA	4.28	1.45	1.33
17	A	839	CLA	CHC-C1C	4.28	1.47	1.35
17	A	825	CLA	CHC-C1C	4.28	1.47	1.35
26	4	615	CHL	OBD-CAD	4.28	1.28	1.21
17	6	310	CLA	CHC-C1C	4.28	1.47	1.35
17	4	611	CLA	O2A-CGA	4.28	1.45	1.33
17	b	817	CLA	O2A-CGA	4.28	1.45	1.33
17	a	824	CLA	O2A-CGA	4.29	1.45	1.33
17	a	829	CLA	OBD-CAD	4.29	1.28	1.22
17	a	819	CLA	O2A-CGA	4.29	1.46	1.33
17	a	843	CLA	OBD-CAD	4.29	1.28	1.22
17	l	203	CLA	O2A-CGA	4.29	1.46	1.33
17	8	310	CLA	CHC-C1C	4.29	1.47	1.35
17	A	854	CLA	O2A-CGA	4.29	1.46	1.33
17	7	612	CLA	O2A-CGA	4.29	1.46	1.33
17	B	836	CLA	OBD-CAD	4.29	1.28	1.22
17	a	825	CLA	CHC-C1C	4.29	1.47	1.35
17	b	811	CLA	O2A-CGA	4.29	1.46	1.33
17	2	610	CLA	CHC-C1C	4.29	1.47	1.35
17	7	609	CLA	O2A-CGA	4.29	1.46	1.33
17	B	840	CLA	O2A-CGA	4.29	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	807	CLA	O2A-CGA	4.29	1.46	1.33
17	A	810	CLA	CHC-C1C	4.29	1.47	1.35
26	2	601	CHL	OBD-CAD	4.29	1.28	1.21
26	1	302	CHL	OBD-CAD	4.29	1.28	1.21
17	6	313	CLA	O2A-CGA	4.29	1.46	1.33
17	F	301	CLA	O2A-CGA	4.29	1.46	1.33
17	6	305	CLA	CHC-C1C	4.29	1.47	1.35
17	A	838	CLA	O2A-CGA	4.29	1.46	1.33
17	l	202	CLA	CHC-C1C	4.29	1.47	1.35
17	4	611	CLA	CHC-C1C	4.29	1.47	1.35
17	L	204	CLA	C3D-C2D	4.29	1.49	1.39
26	7	607	CHL	OBD-CAD	4.29	1.28	1.21
17	4	608	CLA	CHC-C1C	4.29	1.47	1.35
17	B	832	CLA	C3D-C2D	4.29	1.49	1.39
17	4	601	CLA	CHC-C1C	4.29	1.47	1.35
17	L	203	CLA	O2A-CGA	4.30	1.46	1.33
17	6	304	CLA	O2A-CGA	4.30	1.46	1.33
17	F	304	CLA	O2A-CGA	4.30	1.46	1.33
17	b	819	CLA	O2A-CGA	4.30	1.46	1.33
17	9	603	CLA	CHC-C1C	4.30	1.47	1.35
17	a	824	CLA	C3D-C2D	4.30	1.49	1.39
17	A	819	CLA	O2A-CGA	4.30	1.46	1.33
17	a	828	CLA	C3D-C2D	4.30	1.49	1.39
17	f	7003	CLA	O2A-CGA	4.30	1.46	1.33
17	a	825	CLA	O2A-CGA	4.30	1.46	1.33
17	B	808	CLA	CHC-C1C	4.30	1.47	1.35
17	6	310	CLA	O2A-CGA	4.30	1.46	1.33
17	A	805	CLA	O2A-CGA	4.30	1.46	1.33
17	1	309	CLA	O2A-CGA	4.30	1.46	1.33
17	8	305	CLA	CHC-C1C	4.30	1.47	1.35
17	8	301	CLA	O2A-CGA	4.30	1.46	1.33
17	6	313	CLA	CHC-C1C	4.30	1.47	1.35
17	9	612	CLA	CHC-C1C	4.30	1.47	1.35
17	b	829	CLA	C3D-C2D	4.30	1.49	1.39
17	7	602	CLA	O2A-CGA	4.30	1.46	1.33
17	6	314	CLA	CHC-C1C	4.30	1.47	1.35
17	4	612	CLA	O2A-CGA	4.30	1.46	1.33
26	9	615	CHL	OBD-CAD	4.30	1.28	1.21
17	a	808	CLA	O2A-CGA	4.31	1.46	1.33
17	A	803	CLA	CHC-C1C	4.31	1.47	1.35
17	a	835	CLA	CHC-C1C	4.31	1.47	1.35
17	4	609	CLA	O2A-CGA	4.31	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	311	CLA	O2A-CGA	4.31	1.46	1.33
17	b	839	CLA	CHC-C1C	4.31	1.47	1.35
17	6	315	CLA	CHC-C1C	4.31	1.47	1.35
17	3	309	CLA	O2A-CGA	4.31	1.46	1.33
17	B	840	CLA	CHC-C1C	4.31	1.47	1.35
17	a	821	CLA	CHC-C1C	4.31	1.47	1.35
17	b	838	CLA	CHC-C1C	4.31	1.47	1.35
17	3	303	CLA	O2A-CGA	4.31	1.46	1.33
17	B	805	CLA	C3D-C2D	4.31	1.49	1.39
17	b	816	CLA	CHC-C1C	4.31	1.47	1.35
17	A	835	CLA	O2A-CGA	4.31	1.46	1.33
17	1	306	CLA	O2A-CGA	4.31	1.46	1.33
17	B	826	CLA	O2A-CGA	4.31	1.46	1.33
17	k	1403	CLA	CHC-C1C	4.31	1.47	1.35
17	A	817	CLA	CHC-C1C	4.31	1.47	1.35
17	b	817	CLA	OBD-CAD	4.31	1.28	1.22
17	A	803	CLA	OBD-CAD	4.31	1.28	1.22
17	1	314	CLA	CHC-C1C	4.31	1.47	1.35
17	B	811	CLA	O2A-CGA	4.32	1.46	1.33
17	2	604	CLA	O2A-CGA	4.32	1.46	1.33
26	1	307	CHL	OBD-CAD	4.32	1.28	1.21
17	B	809	CLA	O2A-CGA	4.32	1.46	1.33
17	B	833	CLA	CHC-C1C	4.32	1.47	1.35
17	9	609	CLA	O2A-CGA	4.32	1.46	1.33
26	6	303	CHL	OBD-CAD	4.32	1.28	1.21
17	A	836	CLA	CHC-C1C	4.32	1.47	1.35
17	b	833	CLA	O2A-CGA	4.32	1.46	1.33
17	1	308	CLA	C3D-C2D	4.32	1.49	1.39
17	b	837	CLA	O2A-CGA	4.32	1.46	1.33
17	6	305	CLA	OBD-CAD	4.32	1.28	1.22
17	B	840	CLA	OBD-CAD	4.32	1.28	1.22
17	A	821	CLA	CHC-C1C	4.32	1.47	1.35
17	b	811	CLA	CHC-C1C	4.32	1.47	1.35
17	6	312	CLA	CHC-C1C	4.32	1.47	1.35
17	8	310	CLA	O2A-CGA	4.32	1.46	1.33
26	7	606	CHL	OBD-CAD	4.32	1.28	1.21
17	A	813	CLA	CHC-C1C	4.32	1.47	1.35
17	a	832	CLA	C3D-C2D	4.32	1.49	1.39
17	a	836	CLA	O2A-CGA	4.32	1.46	1.33
17	1	313	CLA	CHC-C1C	4.32	1.47	1.35
26	2	606	CHL	OBD-CAD	4.32	1.28	1.21
17	6	306	CLA	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	837	CLA	CHC-C1C	4.32	1.47	1.35
17	A	820	CLA	O2A-CGA	4.32	1.46	1.33
17	b	817	CLA	CHC-C1C	4.32	1.47	1.35
17	A	816	CLA	O2A-CGA	4.33	1.46	1.33
17	9	614	CLA	O2A-CGA	4.33	1.46	1.33
17	b	831	CLA	CHC-C1C	4.33	1.47	1.35
26	6	308	CHL	OBD-CAD	4.33	1.28	1.21
17	4	604	CLA	O2A-CGA	4.33	1.46	1.33
17	A	828	CLA	O2A-CGA	4.33	1.46	1.33
17	3	313	CLA	CHC-C1C	4.33	1.48	1.35
17	A	808	CLA	O2A-CGA	4.33	1.46	1.33
17	a	823	CLA	O2A-CGA	4.33	1.46	1.33
17	a	839	CLA	CHC-C1C	4.33	1.48	1.35
17	A	845	CLA	O2A-CGA	4.33	1.46	1.33
17	7	603	CLA	OBD-CAD	4.33	1.28	1.22
17	B	838	CLA	C3D-C2D	4.33	1.49	1.39
17	8	309	CLA	O2A-CGA	4.33	1.46	1.33
17	B	833	CLA	O2A-CGA	4.33	1.46	1.33
17	A	812	CLA	C3D-C2D	4.33	1.49	1.39
17	G	103	CLA	O2A-CGA	4.33	1.46	1.33
17	b	833	CLA	CHC-C1C	4.33	1.48	1.35
17	9	611	CLA	CHC-C1C	4.33	1.48	1.35
17	f	7002	CLA	CHC-C1C	4.33	1.48	1.35
17	b	821	CLA	CHC-C1C	4.33	1.48	1.35
17	b	840	CLA	C3D-C2D	4.33	1.49	1.39
17	A	811	CLA	OBD-CAD	4.33	1.28	1.22
17	b	818	CLA	CHC-C1C	4.33	1.48	1.35
17	b	838	CLA	O2A-CGA	4.33	1.46	1.33
17	2	603	CLA	O2A-CGA	4.33	1.46	1.33
17	F	301	CLA	CHC-C1C	4.33	1.48	1.35
17	b	823	CLA	OBD-CAD	4.34	1.28	1.22
17	6	314	CLA	OBD-CAD	4.34	1.28	1.22
17	1	315	CLA	CHC-C1C	4.34	1.48	1.35
17	B	832	CLA	O2A-CGA	4.34	1.46	1.33
17	4	604	CLA	CHC-C1C	4.34	1.48	1.35
17	4	610	CLA	CHC-C1C	4.34	1.48	1.35
17	a	813	CLA	O2A-CGA	4.34	1.46	1.33
17	9	614	CLA	CHC-C1C	4.34	1.48	1.35
26	7	614	CHL	OBD-CAD	4.34	1.28	1.21
17	2	612	CLA	O2A-CGA	4.34	1.46	1.33
17	A	841	CLA	O2A-CGA	4.34	1.46	1.33
17	b	822	CLA	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	808	CLA	CHC-C1C	4.34	1.48	1.35
17	b	829	CLA	OBD-CAD	4.34	1.28	1.22
17	a	838	CLA	OBD-CAD	4.34	1.28	1.22
17	4	602	CLA	O2A-CGA	4.34	1.46	1.33
17	7	604	CLA	O2A-CGA	4.34	1.46	1.33
17	B	828	CLA	C3D-C2D	4.34	1.49	1.39
17	K	4003	CLA	CHC-C1C	4.34	1.48	1.35
17	4	608	CLA	O2A-CGA	4.34	1.46	1.33
17	7	602	CLA	C3D-C2D	4.34	1.49	1.39
17	8	309	CLA	CHC-C1C	4.34	1.48	1.35
17	A	818	CLA	O2A-CGA	4.34	1.46	1.33
17	a	828	CLA	CHC-C1C	4.34	1.48	1.35
17	b	828	CLA	O2A-CGA	4.34	1.46	1.33
17	a	806	CLA	CHC-C1C	4.34	1.48	1.35
17	A	835	CLA	CHC-C1C	4.34	1.48	1.35
17	b	812	CLA	O2A-CGA	4.34	1.46	1.33
17	B	814	CLA	C3D-C2D	4.34	1.49	1.39
26	2	605	CHL	OBD-CAD	4.34	1.28	1.21
17	B	839	CLA	CHC-C1C	4.34	1.48	1.35
17	6	306	CLA	CHC-C1C	4.34	1.48	1.35
17	2	604	CLA	CHC-C1C	4.34	1.48	1.35
26	4	605	CHL	OBD-CAD	4.35	1.29	1.21
17	a	835	CLA	O2A-CGA	4.35	1.46	1.33
17	a	801	CLA	CHC-C1C	4.35	1.48	1.35
17	a	803	CLA	O2A-CGA	4.35	1.46	1.33
17	B	804	CLA	CHC-C1C	4.35	1.48	1.35
26	2	614	CHL	OBD-CAD	4.35	1.29	1.21
17	3	306	CLA	O2A-CGA	4.35	1.46	1.33
17	2	603	CLA	C3D-C2D	4.35	1.49	1.39
17	b	820	CLA	O2A-CGA	4.35	1.46	1.33
17	6	316	CLA	CHC-C1C	4.35	1.48	1.35
17	b	805	CLA	OBD-CAD	4.35	1.28	1.22
17	A	810	CLA	C3D-C2D	4.35	1.49	1.39
17	8	308	CLA	O2A-CGA	4.35	1.46	1.33
17	a	835	CLA	C3D-C2D	4.35	1.49	1.39
17	B	815	CLA	CHC-C1C	4.35	1.48	1.35
26	3	307	CHL	OBD-CAD	4.35	1.29	1.21
17	3	301	CLA	CHC-C1C	4.35	1.48	1.35
17	B	836	CLA	CHC-C1C	4.35	1.48	1.35
17	b	815	CLA	O2A-CGA	4.35	1.46	1.33
17	8	302	CLA	O2A-CGA	4.35	1.46	1.33
17	b	812	CLA	CHC-C1C	4.35	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	818	CLA	CHC-C1C	4.35	1.48	1.35
17	4	614	CLA	CHC-C1C	4.35	1.48	1.35
17	A	824	CLA	O2A-CGA	4.35	1.46	1.33
17	3	312	CLA	O2A-CGA	4.35	1.46	1.33
17	b	803	CLA	OBD-CAD	4.36	1.28	1.22
17	B	836	CLA	O2A-CGA	4.36	1.46	1.33
17	B	816	CLA	O2A-CGA	4.36	1.46	1.33
17	a	842	CLA	CHC-C1C	4.36	1.48	1.35
17	A	819	CLA	C3D-C2D	4.36	1.49	1.39
17	7	613	CLA	C3D-C2D	4.36	1.49	1.39
26	7	605	CHL	OBD-CAD	4.36	1.29	1.21
17	2	612	CLA	CHC-C1C	4.36	1.48	1.35
17	3	310	CLA	CHC-C1C	4.36	1.48	1.35
17	7	608	CLA	OBD-CAD	4.36	1.28	1.22
17	a	840	CLA	C3D-C2D	4.36	1.49	1.39
17	9	614	CLA	C3D-C2D	4.36	1.49	1.39
17	B	823	CLA	CHC-C1C	4.36	1.48	1.35
26	7	601	CHL	OBD-CAD	4.36	1.29	1.21
26	9	606	CHL	OBD-CAD	4.36	1.29	1.21
17	j	3002	CLA	CHC-C1C	4.36	1.48	1.35
17	7	613	CLA	OBD-CAD	4.36	1.28	1.22
17	b	836	CLA	O2A-CGA	4.36	1.46	1.33
17	2	609	CLA	O2A-CGA	4.36	1.46	1.33
17	A	804	CLA	CHC-C1C	4.36	1.48	1.35
17	L	204	CLA	O2A-CGA	4.36	1.46	1.33
17	L	202	CLA	O2A-CGA	4.36	1.46	1.33
17	a	841	CLA	CHC-C1C	4.36	1.48	1.35
17	B	824	CLA	OBD-CAD	4.36	1.28	1.22
17	a	844	CLA	CHC-C1C	4.36	1.48	1.35
17	a	840	CLA	CHC-C1C	4.36	1.48	1.35
17	b	815	CLA	CHC-C1C	4.36	1.48	1.35
17	A	825	CLA	O2A-CGA	4.36	1.46	1.33
17	b	809	CLA	CHC-C1C	4.36	1.48	1.35
17	7	613	CLA	CHC-C1C	4.36	1.48	1.35
17	4	610	CLA	O2A-CGA	4.36	1.46	1.33
17	A	828	CLA	C3D-C2D	4.36	1.49	1.39
17	2	611	CLA	CHC-C1C	4.36	1.48	1.35
17	2	602	CLA	O2A-CGA	4.36	1.46	1.33
17	3	314	CLA	CHC-C1C	4.36	1.48	1.35
17	B	831	CLA	CHC-C1C	4.36	1.48	1.35
17	b	804	CLA	CHC-C1C	4.36	1.48	1.35
17	b	820	CLA	CHC-C1C	4.36	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	816	CLA	O2A-CGA	4.36	1.46	1.33
17	B	837	CLA	O2A-CGA	4.36	1.46	1.33
17	g	103	CLA	CHC-C1C	4.37	1.48	1.35
17	B	828	CLA	CHC-C1C	4.37	1.48	1.35
17	a	804	CLA	OBD-CAD	4.37	1.28	1.22
17	A	840	CLA	O2A-CGA	4.37	1.46	1.33
17	B	805	CLA	CHC-C1C	4.37	1.48	1.35
17	8	311	CLA	CHC-C1C	4.37	1.48	1.35
17	a	839	CLA	O2A-CGA	4.37	1.46	1.33
17	A	839	CLA	O2A-CGA	4.37	1.46	1.33
17	g	102	CLA	CHC-C1C	4.37	1.48	1.35
17	a	812	CLA	C3D-C2D	4.37	1.49	1.39
17	B	827	CLA	C3D-C2D	4.37	1.49	1.39
17	A	811	CLA	CHC-C1C	4.37	1.48	1.35
17	B	820	CLA	CHC-C1C	4.37	1.48	1.35
17	a	820	CLA	O2A-CGA	4.37	1.46	1.33
17	1	311	CLA	CHC-C1C	4.37	1.48	1.35
17	9	613	CLA	C3D-C2D	4.37	1.49	1.39
17	A	807	CLA	O2A-CGA	4.37	1.46	1.33
17	A	806	CLA	C3D-C2D	4.37	1.49	1.39
17	A	824	CLA	C3D-C2D	4.37	1.49	1.39
17	A	831	CLA	CHC-C1C	4.37	1.48	1.35
17	1	310	CLA	O2A-CGA	4.37	1.46	1.33
17	4	613	CLA	CHC-C1C	4.37	1.48	1.35
17	2	613	CLA	CHC-C1C	4.37	1.48	1.35
17	A	854	CLA	OBD-CAD	4.37	1.28	1.22
17	B	808	CLA	O2A-CGA	4.37	1.46	1.33
17	3	305	CLA	CHC-C1C	4.37	1.48	1.35
17	b	826	CLA	C3D-C2D	4.37	1.49	1.39
17	B	829	CLA	O2A-CGA	4.37	1.46	1.33
17	B	834	CLA	CHC-C1C	4.37	1.48	1.35
17	a	813	CLA	CHC-C1C	4.37	1.48	1.35
17	k	1402	CLA	CHC-C1C	4.37	1.48	1.35
17	7	610	CLA	OBD-CAD	4.37	1.28	1.22
17	b	806	CLA	O2A-CGA	4.37	1.46	1.33
17	b	836	CLA	CHC-C1C	4.37	1.48	1.35
17	b	808	CLA	O2A-CGA	4.37	1.46	1.33
17	b	834	CLA	CHC-C1C	4.37	1.48	1.35
17	a	822	CLA	CHC-C1C	4.37	1.48	1.35
17	a	821	CLA	C3D-C2D	4.37	1.49	1.39
17	B	813	CLA	C3D-C2D	4.37	1.49	1.39
17	A	840	CLA	CHC-C1C	4.37	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	610	CLA	OBD-CAD	4.38	1.28	1.22
17	a	834	CLA	CHC-C1C	4.38	1.48	1.35
17	9	610	CLA	CHC-C1C	4.38	1.48	1.35
17	a	832	CLA	CHC-C1C	4.38	1.48	1.35
17	B	816	CLA	CHC-C1C	4.38	1.48	1.35
17	b	810	CLA	C3D-C2D	4.38	1.49	1.39
17	8	305	CLA	O2A-CGA	4.38	1.46	1.33
17	9	611	CLA	O2A-CGA	4.38	1.46	1.33
17	b	827	CLA	C3D-C2D	4.38	1.49	1.39
17	b	835	CLA	CHC-C1C	4.38	1.48	1.35
17	A	814	CLA	CHC-C1C	4.38	1.48	1.35
17	7	604	CLA	CHC-C1C	4.38	1.48	1.35
17	3	311	CLA	CHC-C1C	4.38	1.48	1.35
17	A	837	CLA	CHC-C1C	4.38	1.48	1.35
17	A	842	CLA	O2A-CGA	4.38	1.46	1.33
17	b	825	CLA	O2A-CGA	4.38	1.46	1.33
17	B	823	CLA	C3D-C2D	4.38	1.49	1.39
17	a	829	CLA	C3D-C2D	4.38	1.49	1.39
17	A	832	CLA	CHC-C1C	4.38	1.48	1.35
17	B	817	CLA	CHC-C1C	4.38	1.48	1.35
17	4	613	CLA	C3D-C2D	4.38	1.49	1.39
17	b	814	CLA	O2A-CGA	4.38	1.46	1.33
17	b	834	CLA	C3D-C2D	4.38	1.49	1.39
17	B	812	CLA	O2A-CGA	4.38	1.46	1.33
17	1	305	CLA	CHC-C1C	4.38	1.48	1.35
17	A	845	CLA	CHC-C1C	4.38	1.48	1.35
17	6	304	CLA	C3D-C2D	4.38	1.49	1.39
17	b	839	CLA	OBD-CAD	4.38	1.28	1.22
17	6	304	CLA	CHC-C1C	4.38	1.48	1.35
17	A	805	CLA	CHC-C1C	4.38	1.48	1.35
17	b	828	CLA	CHC-C1C	4.38	1.48	1.35
17	f	7002	CLA	C3D-C2D	4.38	1.49	1.39
17	a	804	CLA	CHC-C1C	4.38	1.48	1.35
17	A	816	CLA	CHC-C1C	4.38	1.48	1.35
17	A	820	CLA	CHC-C1C	4.38	1.48	1.35
17	6	309	CLA	C3D-C2D	4.38	1.49	1.39
17	a	810	CLA	C3D-C2D	4.38	1.49	1.39
17	b	839	CLA	C3D-C2D	4.38	1.49	1.39
17	1	310	CLA	OBD-CAD	4.38	1.28	1.22
17	A	807	CLA	OBD-CAD	4.38	1.28	1.22
17	J	3002	CLA	CHC-C1C	4.38	1.48	1.35
17	2	608	CLA	O2A-CGA	4.38	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	204	CLA	CHC-C1C	4.38	1.48	1.35
17	b	808	CLA	C3D-C2D	4.39	1.49	1.39
17	3	304	CLA	CHC-C1C	4.39	1.48	1.35
17	G	101	CLA	C3D-C2D	4.39	1.49	1.39
17	F	304	CLA	OBD-CAD	4.39	1.28	1.22
17	a	810	CLA	CHC-C1C	4.39	1.48	1.35
17	A	838	CLA	C3D-C2D	4.39	1.49	1.39
17	b	835	CLA	OBD-CAD	4.39	1.28	1.22
17	b	806	CLA	C3D-C2D	4.39	1.49	1.39
17	A	822	CLA	O2A-CGA	4.39	1.46	1.33
17	4	609	CLA	C3D-C2D	4.39	1.49	1.39
17	a	838	CLA	O2A-CGA	4.39	1.46	1.33
17	b	830	CLA	CHC-C1C	4.39	1.48	1.35
26	8	306	CHL	OBD-CAD	4.39	1.29	1.21
17	A	823	CLA	O2A-CGA	4.39	1.46	1.33
17	a	840	CLA	O2A-CGA	4.39	1.46	1.33
17	B	823	CLA	OBD-CAD	4.39	1.28	1.22
17	B	811	CLA	CHC-C1C	4.39	1.48	1.35
17	1	308	CLA	CHC-C1C	4.39	1.48	1.35
17	A	822	CLA	CHC-C1C	4.39	1.48	1.35
17	6	309	CLA	CHC-C1C	4.39	1.48	1.35
17	1	310	CLA	CHC-C1C	4.39	1.48	1.35
17	G	101	CLA	CHC-C1C	4.39	1.48	1.35
17	G	103	CLA	CHC-C1C	4.39	1.48	1.35
17	A	831	CLA	OBD-CAD	4.39	1.28	1.22
17	A	812	CLA	CHC-C1C	4.39	1.48	1.35
17	A	829	CLA	CHC-C1C	4.39	1.48	1.35
17	a	843	CLA	O2A-CGA	4.39	1.46	1.33
17	8	304	CLA	CHC-C1C	4.39	1.48	1.35
17	b	824	CLA	O2A-CGA	4.40	1.46	1.33
17	B	839	CLA	C3D-C2D	4.40	1.49	1.39
17	7	612	CLA	C3D-C2D	4.40	1.49	1.39
17	8	312	CLA	CHC-C1C	4.40	1.48	1.35
17	a	839	CLA	OBD-CAD	4.40	1.28	1.22
17	b	828	CLA	OBD-CAD	4.40	1.28	1.22
17	b	820	CLA	C3D-C2D	4.40	1.49	1.39
17	B	840	CLA	C3D-C2D	4.40	1.49	1.39
17	b	814	CLA	OBD-CAD	4.40	1.28	1.22
17	k	1401	CLA	CHC-C1C	4.40	1.48	1.35
17	a	831	CLA	OBD-CAD	4.40	1.28	1.22
17	8	310	CLA	OBD-CAD	4.40	1.28	1.22
17	A	835	CLA	C3D-C2D	4.40	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	826	CLA	CHC-C1C	4.40	1.48	1.35
17	a	826	CLA	OBD-CAD	4.40	1.28	1.22
17	1	306	CLA	C3D-C2D	4.40	1.49	1.39
17	B	825	CLA	C3D-C2D	4.40	1.49	1.39
17	b	807	CLA	O2A-CGA	4.40	1.46	1.33
17	f	7003	CLA	CHC-C1C	4.40	1.48	1.35
17	9	613	CLA	CHC-C1C	4.40	1.48	1.35
17	B	822	CLA	CHC-C1C	4.40	1.48	1.35
17	b	838	CLA	C3D-C2D	4.40	1.49	1.39
17	B	804	CLA	C3D-C2D	4.40	1.49	1.39
17	a	831	CLA	CHC-C1C	4.41	1.48	1.35
17	A	842	CLA	C3D-C2D	4.41	1.49	1.39
17	3	306	CLA	CHC-C1C	4.41	1.48	1.35
17	K	4002	CLA	CHC-C1C	4.41	1.48	1.35
17	4	611	CLA	C3D-C2D	4.41	1.49	1.39
17	k	1401	CLA	C3D-C2D	4.41	1.49	1.39
17	a	805	CLA	C3D-C2D	4.41	1.49	1.39
17	A	829	CLA	C3D-C2D	4.41	1.49	1.39
17	B	810	CLA	C3D-C2D	4.41	1.49	1.39
17	B	812	CLA	CHC-C1C	4.41	1.48	1.35
17	b	810	CLA	OBD-CAD	4.41	1.28	1.22
17	2	611	CLA	C3D-C2D	4.41	1.49	1.39
17	3	306	CLA	C3D-C2D	4.41	1.49	1.39
17	b	828	CLA	C3D-C2D	4.41	1.49	1.39
17	a	823	CLA	CHC-C1C	4.41	1.48	1.35
17	4	602	CLA	C3D-C2D	4.41	1.49	1.39
17	B	808	CLA	C3D-C2D	4.41	1.49	1.39
17	a	812	CLA	CHC-C1C	4.41	1.48	1.35
17	2	603	CLA	CHC-C1C	4.41	1.48	1.35
17	A	834	CLA	C3D-C2D	4.41	1.49	1.39
17	a	827	CLA	C3D-C2D	4.41	1.49	1.39
17	B	810	CLA	CHC-C1C	4.42	1.48	1.35
17	B	830	CLA	CHC-C1C	4.42	1.48	1.35
17	a	815	CLA	C3D-C2D	4.42	1.49	1.39
17	A	817	CLA	C3D-C2D	4.42	1.49	1.39
17	9	604	CLA	CHC-C1C	4.42	1.48	1.35
17	b	814	CLA	C3D-C2D	4.42	1.49	1.39
17	A	818	CLA	CHC-C1C	4.42	1.48	1.35
17	a	830	CLA	CHC-C1C	4.42	1.48	1.35
17	a	802	CLA	CHC-C1C	4.42	1.48	1.35
17	f	7003	CLA	C3D-C2D	4.42	1.49	1.39
17	A	801	CLA	OBD-CAD	4.42	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	601	CLA	C3D-C2D	4.42	1.49	1.39
17	a	833	CLA	OBD-CAD	4.42	1.28	1.22
17	g	103	CLA	C3D-C2D	4.42	1.49	1.39
17	A	830	CLA	CHC-C1C	4.42	1.48	1.35
17	a	856	CLA	OBD-CAD	4.42	1.28	1.22
17	3	305	CLA	C3D-C2D	4.42	1.49	1.39
17	A	839	CLA	C3D-C2D	4.42	1.49	1.39
17	a	812	CLA	O2A-CGA	4.42	1.46	1.33
17	a	809	CLA	CHC-C1C	4.42	1.48	1.35
17	a	846	CLA	CHC-C1C	4.42	1.48	1.35
17	A	824	CLA	OBD-CAD	4.42	1.28	1.22
17	b	809	CLA	OBD-CAD	4.42	1.28	1.22
17	B	835	CLA	CHC-C1C	4.42	1.48	1.35
17	A	813	CLA	C3D-C2D	4.42	1.49	1.39
17	6	307	CLA	CHC-C1C	4.42	1.48	1.35
17	B	828	CLA	O2A-CGA	4.42	1.46	1.33
17	G	104	CLA	CHC-C1C	4.42	1.48	1.35
17	a	843	CLA	CHC-C1C	4.42	1.48	1.35
17	A	807	CLA	C3D-C2D	4.42	1.49	1.39
17	F	304	CLA	CHC-C1C	4.42	1.48	1.35
17	B	815	CLA	O2A-CGA	4.42	1.46	1.33
17	B	831	CLA	C3D-C2D	4.42	1.49	1.39
17	b	825	CLA	OBD-CAD	4.42	1.28	1.22
17	A	801	CLA	CHC-C1C	4.42	1.48	1.35
17	9	609	CLA	C3D-C2D	4.43	1.49	1.39
17	a	842	CLA	C3D-C2D	4.43	1.49	1.39
17	9	608	CLA	OBD-CAD	4.43	1.28	1.22
17	k	1402	CLA	OBD-CAD	4.43	1.28	1.22
17	B	802	CLA	C3D-C2D	4.43	1.49	1.39
17	8	303	CLA	CHC-C1C	4.43	1.48	1.35
17	B	810	CLA	OBD-CAD	4.43	1.28	1.22
17	A	813	CLA	O2A-CGA	4.43	1.46	1.33
17	b	813	CLA	CHC-C1C	4.43	1.48	1.35
17	4	611	CLA	OBD-CAD	4.43	1.28	1.22
17	1	303	CLA	C3D-C2D	4.43	1.49	1.39
17	b	825	CLA	C3D-C2D	4.43	1.49	1.39
17	a	836	CLA	OBD-CAD	4.43	1.28	1.22
17	1	202	CLA	O2A-CGA	4.43	1.46	1.33
17	A	815	CLA	C3D-C2D	4.43	1.49	1.39
17	7	603	CLA	CHC-C1C	4.43	1.48	1.35
17	b	816	CLA	O2A-CGA	4.43	1.46	1.33
17	4	603	CLA	C3D-C2D	4.43	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	315	CLA	OBD-CAD	4.43	1.28	1.22
17	B	821	CLA	CHC-C1C	4.43	1.48	1.35
17	8	307	CLA	CHC-C1C	4.43	1.48	1.35
17	B	830	CLA	OBD-CAD	4.44	1.28	1.22
17	A	823	CLA	C3D-C2D	4.44	1.49	1.39
17	g	101	CLA	C3D-C2D	4.44	1.49	1.39
17	4	603	CLA	OBD-CAD	4.44	1.28	1.22
17	8	312	CLA	C3D-C2D	4.44	1.49	1.39
17	a	805	CLA	CHC-C1C	4.44	1.48	1.35
17	a	816	CLA	CHC-C1C	4.44	1.48	1.35
17	B	826	CLA	CHC-C1C	4.44	1.48	1.35
17	b	807	CLA	CHC-C1C	4.44	1.48	1.35
17	b	810	CLA	CHC-C1C	4.44	1.48	1.35
17	A	815	CLA	OBD-CAD	4.44	1.28	1.22
17	B	813	CLA	OBD-CAD	4.44	1.28	1.22
17	3	308	CLA	CHC-C1C	4.44	1.48	1.35
17	8	302	CLA	OBD-CAD	4.44	1.28	1.22
17	B	839	CLA	O2A-CGA	4.44	1.46	1.33
17	A	819	CLA	CHC-C1C	4.44	1.48	1.35
17	b	822	CLA	C3D-C2D	4.44	1.49	1.39
17	l	204	CLA	CHC-C1C	4.44	1.48	1.35
17	A	842	CLA	OBD-CAD	4.44	1.28	1.22
17	a	808	CLA	C3D-C2D	4.44	1.49	1.39
17	A	818	CLA	C3D-C2D	4.44	1.49	1.39
17	B	839	CLA	OBD-CAD	4.44	1.28	1.22
26	4	606	CHL	OBD-CAD	4.44	1.29	1.21
17	1	308	CLA	OBD-CAD	4.45	1.28	1.22
17	9	601	CLA	OBD-CAD	4.45	1.28	1.22
17	b	826	CLA	CHC-C1C	4.45	1.48	1.35
17	B	803	CLA	OBD-CAD	4.45	1.28	1.22
17	4	614	CLA	C3D-C2D	4.45	1.49	1.39
17	A	842	CLA	CHC-C1C	4.45	1.48	1.35
17	A	812	CLA	OBD-CAD	4.45	1.28	1.22
17	A	840	CLA	C3D-C2D	4.45	1.49	1.39
17	7	602	CLA	OBD-CAD	4.45	1.28	1.22
17	a	807	CLA	OBD-CAD	4.45	1.28	1.22
17	a	801	CLA	C3D-C2D	4.45	1.49	1.39
17	6	312	CLA	OBD-CAD	4.45	1.28	1.22
17	a	822	CLA	OBD-CAD	4.45	1.28	1.22
17	B	834	CLA	C3D-C2D	4.45	1.49	1.39
17	b	831	CLA	C3D-C2D	4.45	1.49	1.39
17	a	844	CLA	OBD-CAD	4.45	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	814	CLA	OBD-CAD	4.45	1.28	1.22
17	2	612	CLA	C3D-C2D	4.45	1.49	1.39
17	b	813	CLA	C3D-C2D	4.45	1.49	1.39
17	a	818	CLA	O2A-CGA	4.45	1.46	1.33
17	A	801	CLA	C3D-C2D	4.45	1.49	1.39
17	1	312	CLA	C3D-C2D	4.45	1.49	1.39
17	A	807	CLA	CHC-C1C	4.45	1.48	1.35
17	B	841	CLA	CHC-C1C	4.45	1.48	1.35
17	4	601	CLA	OBD-CAD	4.46	1.28	1.22
17	1	303	CLA	OBD-CAD	4.46	1.28	1.22
17	a	816	CLA	OBD-CAD	4.46	1.28	1.22
17	b	825	CLA	CHC-C1C	4.46	1.48	1.35
17	A	809	CLA	CHC-C1C	4.46	1.48	1.35
17	b	823	CLA	CHC-C1C	4.46	1.48	1.35
17	A	843	CLA	C3D-C2D	4.46	1.49	1.39
17	b	837	CLA	CHC-C1C	4.46	1.48	1.35
17	a	807	CLA	CHC-C1C	4.46	1.48	1.35
17	1	305	CLA	C3D-C2D	4.46	1.49	1.39
17	4	602	CLA	OBD-CAD	4.46	1.28	1.22
17	4	602	CLA	CHC-C1C	4.46	1.48	1.35
17	b	839	CLA	O2A-CGA	4.46	1.46	1.33
17	B	825	CLA	CHC-C1C	4.46	1.48	1.35
17	B	802	CLA	CHC-C1C	4.46	1.48	1.35
17	B	833	CLA	OBD-CAD	4.46	1.28	1.22
17	9	613	CLA	OBD-CAD	4.46	1.28	1.22
17	a	811	CLA	C3D-C2D	4.46	1.49	1.39
17	B	816	CLA	OBD-CAD	4.46	1.28	1.22
17	B	824	CLA	CHC-C1C	4.46	1.48	1.35
17	G	101	CLA	OBD-CAD	4.46	1.28	1.22
17	B	803	CLA	C3D-C2D	4.46	1.49	1.39
17	6	307	CLA	OBD-CAD	4.46	1.28	1.22
17	1	204	CLA	O2A-CGA	4.46	1.46	1.33
17	A	827	CLA	C3D-C2D	4.46	1.49	1.39
17	3	311	CLA	C3D-C2D	4.46	1.49	1.39
17	B	832	CLA	OBD-CAD	4.46	1.28	1.22
17	1	313	CLA	C3D-C2D	4.46	1.49	1.39
17	A	826	CLA	CHC-C1C	4.46	1.48	1.35
17	2	608	CLA	OBD-CAD	4.46	1.28	1.22
17	B	829	CLA	OBD-CAD	4.46	1.28	1.22
17	1	203	CLA	C3D-C2D	4.47	1.49	1.39
17	B	837	CLA	CHC-C1C	4.47	1.48	1.35
17	b	806	CLA	CHC-C1C	4.47	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	603	CLA	C3D-C2D	4.47	1.49	1.39
17	a	824	CLA	OBD-CAD	4.47	1.28	1.22
17	9	612	CLA	C3D-C2D	4.47	1.49	1.39
17	4	612	CLA	C3D-C2D	4.47	1.49	1.39
17	A	806	CLA	CHC-C1C	4.47	1.48	1.35
17	l	202	CLA	C3D-C2D	4.47	1.49	1.39
17	a	816	CLA	C3D-C2D	4.47	1.49	1.39
17	3	314	CLA	OBD-CAD	4.47	1.28	1.22
17	a	826	CLA	C3D-C2D	4.47	1.49	1.39
17	B	817	CLA	C3D-C2D	4.47	1.49	1.39
17	b	811	CLA	OBD-CAD	4.47	1.28	1.22
17	9	602	CLA	C3D-C2D	4.47	1.49	1.39
17	B	835	CLA	C3D-C2D	4.47	1.49	1.39
17	a	806	CLA	C3D-C2D	4.47	1.49	1.39
17	A	823	CLA	CHC-C1C	4.47	1.48	1.35
17	B	822	CLA	C3D-C2D	4.47	1.49	1.39
17	B	837	CLA	OBD-CAD	4.47	1.28	1.22
17	B	824	CLA	C3D-C2D	4.47	1.49	1.39
17	F	304	CLA	C3D-C2D	4.47	1.49	1.39
17	G	104	CLA	C3D-C2D	4.47	1.49	1.39
17	A	826	CLA	C3D-C2D	4.47	1.49	1.39
17	a	835	CLA	OBD-CAD	4.47	1.28	1.22
17	4	609	CLA	CHC-C1C	4.47	1.48	1.35
17	4	609	CLA	OBD-CAD	4.47	1.28	1.22
17	9	609	CLA	CHC-C1C	4.47	1.48	1.35
17	3	314	CLA	C3D-C2D	4.47	1.49	1.39
17	L	203	CLA	OBD-CAD	4.48	1.28	1.22
17	b	822	CLA	CHC-C1C	4.48	1.48	1.35
17	A	816	CLA	C3D-C2D	4.48	1.49	1.39
17	B	813	CLA	CHC-C1C	4.48	1.48	1.35
17	b	824	CLA	C3D-C2D	4.48	1.49	1.39
17	b	804	CLA	C3D-C2D	4.48	1.49	1.39
17	9	602	CLA	OBD-CAD	4.48	1.28	1.22
17	F	303	CLA	C3D-C2D	4.48	1.49	1.39
17	3	301	CLA	C3D-C2D	4.48	1.49	1.39
17	K	4002	CLA	C3D-C2D	4.48	1.49	1.39
17	6	306	CLA	C3D-C2D	4.48	1.49	1.39
17	L	202	CLA	C3D-C2D	4.48	1.49	1.39
17	9	611	CLA	C3D-C2D	4.48	1.49	1.39
17	a	834	CLA	C3D-C2D	4.48	1.49	1.39
17	A	833	CLA	CHC-C1C	4.48	1.48	1.35
17	A	809	CLA	OBD-CAD	4.48	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	303	CLA	C3D-C2D	4.48	1.49	1.39
17	b	835	CLA	C3D-C2D	4.48	1.49	1.39
17	2	602	CLA	C3D-C2D	4.48	1.49	1.39
17	8	302	CLA	C3D-C2D	4.48	1.49	1.39
17	A	819	CLA	OBD-CAD	4.48	1.28	1.22
17	b	837	CLA	C3D-C2D	4.48	1.49	1.39
17	6	309	CLA	OBD-CAD	4.48	1.28	1.22
17	b	841	CLA	CHC-C1C	4.48	1.48	1.35
17	A	832	CLA	C3D-C2D	4.48	1.49	1.39
17	A	814	CLA	OBD-CAD	4.48	1.28	1.22
17	B	820	CLA	C3D-C2D	4.48	1.49	1.39
17	9	603	CLA	C3D-C2D	4.49	1.49	1.39
17	B	807	CLA	CHC-C1C	4.49	1.48	1.35
17	7	611	CLA	C3D-C2D	4.49	1.49	1.39
17	A	804	CLA	C3D-C2D	4.49	1.49	1.39
17	B	811	CLA	OBD-CAD	4.49	1.28	1.22
17	3	309	CLA	OBD-CAD	4.49	1.28	1.22
17	B	807	CLA	OBD-CAD	4.49	1.28	1.22
17	1	310	CLA	C3D-C2D	4.49	1.49	1.39
17	6	307	CLA	C3D-C2D	4.49	1.49	1.39
17	9	604	CLA	C3D-C2D	4.49	1.49	1.39
17	a	839	CLA	C3D-C2D	4.49	1.49	1.39
17	1	306	CLA	CHC-C1C	4.49	1.48	1.35
17	a	808	CLA	CHC-C1C	4.49	1.48	1.35
17	7	609	CLA	OBD-CAD	4.49	1.28	1.22
17	1	314	CLA	C3D-C2D	4.49	1.49	1.39
17	a	829	CLA	CHC-C1C	4.49	1.48	1.35
17	a	811	CLA	OBD-CAD	4.49	1.28	1.22
17	b	808	CLA	OBD-CAD	4.49	1.28	1.22
17	1	309	CLA	C3D-C2D	4.49	1.49	1.39
17	8	312	CLA	OBD-CAD	4.49	1.28	1.22
17	3	313	CLA	C3D-C2D	4.49	1.49	1.39
17	f	7002	CLA	OBD-CAD	4.49	1.28	1.22
17	7	604	CLA	C3D-C2D	4.49	1.49	1.39
17	2	610	CLA	C3D-C2D	4.49	1.49	1.39
17	9	601	CLA	C3D-C2D	4.49	1.49	1.39
17	b	818	CLA	OBD-CAD	4.49	1.28	1.22
17	6	311	CLA	C3D-C2D	4.49	1.49	1.39
17	A	822	CLA	C3D-C2D	4.50	1.49	1.39
17	A	841	CLA	OBD-CAD	4.50	1.28	1.22
17	B	811	CLA	C3D-C2D	4.50	1.49	1.39
17	B	806	CLA	CHC-C1C	4.50	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	832	CLA	CHC-C1C	4.50	1.48	1.35
17	A	811	CLA	C3D-C2D	4.50	1.49	1.39
17	b	841	CLA	OBD-CAD	4.50	1.28	1.22
17	1	304	CLA	OBD-CAD	4.50	1.28	1.22
17	F	303	CLA	OBD-CAD	4.50	1.28	1.22
17	g	103	CLA	OBD-CAD	4.50	1.28	1.22
17	a	830	CLA	C3D-C2D	4.50	1.49	1.39
17	L	203	CLA	C3D-C2D	4.50	1.49	1.39
17	A	845	CLA	C3D-C2D	4.50	1.49	1.39
17	B	806	CLA	C3D-C2D	4.50	1.49	1.39
17	b	824	CLA	CHC-C1C	4.50	1.48	1.35
17	B	829	CLA	C3D-C2D	4.50	1.49	1.39
17	3	312	CLA	C3D-C2D	4.50	1.49	1.39
17	A	808	CLA	OBD-CAD	4.50	1.28	1.22
17	9	610	CLA	OBD-CAD	4.50	1.28	1.22
17	1	309	CLA	OBD-CAD	4.50	1.28	1.22
17	L	204	CLA	OBD-CAD	4.50	1.28	1.22
17	A	815	CLA	CHC-C1C	4.50	1.48	1.35
17	6	311	CLA	OBD-CAD	4.50	1.28	1.22
17	B	825	CLA	OBD-CAD	4.51	1.28	1.22
17	4	612	CLA	OBD-CAD	4.51	1.28	1.22
17	B	816	CLA	C3D-C2D	4.51	1.49	1.39
17	a	831	CLA	C3D-C2D	4.51	1.49	1.39
17	a	812	CLA	OBD-CAD	4.51	1.28	1.22
17	3	305	CLA	OBD-CAD	4.51	1.28	1.22
17	3	312	CLA	OBD-CAD	4.51	1.28	1.22
17	b	803	CLA	CHC-C1C	4.51	1.48	1.35
17	b	802	CLA	C3D-C2D	4.51	1.49	1.39
17	A	841	CLA	C3D-C2D	4.51	1.49	1.39
17	A	821	CLA	OBD-CAD	4.51	1.28	1.22
17	a	814	CLA	CHC-C1C	4.51	1.48	1.35
17	8	311	CLA	C3D-C2D	4.51	1.49	1.39
17	B	805	CLA	OBD-CAD	4.51	1.28	1.22
17	A	802	CLA	OBD-CAD	4.51	1.28	1.22
17	B	837	CLA	C3D-C2D	4.51	1.49	1.39
17	B	827	CLA	CHC-C1C	4.51	1.48	1.35
17	A	828	CLA	CHC-C1C	4.51	1.48	1.35
17	b	816	CLA	OBD-CAD	4.51	1.28	1.22
17	4	610	CLA	OBD-CAD	4.51	1.28	1.22
17	3	309	CLA	C3D-C2D	4.51	1.49	1.39
17	B	836	CLA	C3D-C2D	4.51	1.49	1.39
17	A	837	CLA	C3D-C2D	4.51	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	308	CLA	C3D-C2D	4.51	1.49	1.39
17	L	203	CLA	CHC-C1C	4.51	1.48	1.35
17	b	838	CLA	OBD-CAD	4.51	1.28	1.22
17	B	821	CLA	OBD-CAD	4.51	1.28	1.22
17	B	835	CLA	OBD-CAD	4.51	1.28	1.22
17	6	316	CLA	C3D-C2D	4.51	1.49	1.39
17	8	305	CLA	C3D-C2D	4.52	1.49	1.39
17	B	833	CLA	C3D-C2D	4.52	1.49	1.39
17	l	204	CLA	C3D-C2D	4.52	1.49	1.39
17	a	833	CLA	CHC-C1C	4.52	1.48	1.35
17	b	807	CLA	OBD-CAD	4.52	1.28	1.22
17	4	608	CLA	C3D-C2D	4.52	1.49	1.39
17	6	311	CLA	CHC-C1C	4.52	1.48	1.35
17	3	304	CLA	C3D-C2D	4.52	1.49	1.39
17	1	305	CLA	OBD-CAD	4.52	1.28	1.22
17	A	834	CLA	OBD-CAD	4.52	1.28	1.22
17	6	305	CLA	C3D-C2D	4.52	1.49	1.39
17	b	817	CLA	C3D-C2D	4.52	1.49	1.39
17	1	203	CLA	OBD-CAD	4.52	1.28	1.22
17	3	304	CLA	OBD-CAD	4.52	1.28	1.22
17	2	602	CLA	CHC-C1C	4.52	1.48	1.35
17	2	602	CLA	OBD-CAD	4.52	1.28	1.22
17	F	301	CLA	OBD-CAD	4.52	1.28	1.22
17	2	613	CLA	C3D-C2D	4.52	1.49	1.39
17	A	833	CLA	C3D-C2D	4.52	1.49	1.39
17	a	822	CLA	C3D-C2D	4.52	1.49	1.39
17	2	612	CLA	OBD-CAD	4.52	1.28	1.22
17	7	608	CLA	C3D-C2D	4.52	1.49	1.39
17	a	818	CLA	C3D-C2D	4.52	1.49	1.39
17	a	817	CLA	C3D-C2D	4.52	1.49	1.39
17	A	833	CLA	OBD-CAD	4.52	1.28	1.22
17	A	816	CLA	OBD-CAD	4.52	1.28	1.22
17	9	604	CLA	OBD-CAD	4.52	1.28	1.22
17	l	204	CLA	OBD-CAD	4.52	1.28	1.22
17	G	103	CLA	C3D-C2D	4.52	1.49	1.39
17	b	827	CLA	CHC-C1C	4.52	1.48	1.35
17	k	1402	CLA	C3D-C2D	4.52	1.49	1.39
17	8	304	CLA	C3D-C2D	4.52	1.49	1.39
17	A	827	CLA	OBD-CAD	4.52	1.28	1.22
17	B	804	CLA	OBD-CAD	4.52	1.28	1.22
17	B	841	CLA	C3D-C2D	4.52	1.49	1.39
17	6	315	CLA	C3D-C2D	4.52	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	315	CLA	OBD-CAD	4.52	1.28	1.22
17	b	837	CLA	OBD-CAD	4.52	1.28	1.22
17	b	841	CLA	C3D-C2D	4.53	1.49	1.39
17	A	820	CLA	OBD-CAD	4.53	1.28	1.22
17	A	843	CLA	OBD-CAD	4.53	1.28	1.22
17	k	1403	CLA	C3D-C2D	4.53	1.49	1.39
17	a	802	CLA	OBD-CAD	4.53	1.28	1.22
17	8	301	CLA	C3D-C2D	4.53	1.49	1.39
17	b	827	CLA	OBD-CAD	4.53	1.28	1.22
17	A	817	CLA	OBD-CAD	4.53	1.28	1.22
17	b	820	CLA	OBD-CAD	4.53	1.28	1.22
17	A	841	CLA	CHC-C1C	4.53	1.48	1.35
17	g	102	CLA	C3D-C2D	4.53	1.49	1.39
17	7	602	CLA	CHC-C1C	4.53	1.48	1.35
17	A	810	CLA	OBD-CAD	4.53	1.28	1.22
17	B	831	CLA	OBD-CAD	4.53	1.28	1.22
17	A	808	CLA	C3D-C2D	4.53	1.49	1.39
17	a	846	CLA	C3D-C2D	4.53	1.49	1.39
17	a	856	CLA	O2D-CGD	4.53	1.44	1.33
17	8	303	CLA	C3D-C2D	4.53	1.49	1.39
17	4	604	CLA	C3D-C2D	4.53	1.49	1.39
17	a	814	CLA	C3D-C2D	4.53	1.49	1.39
17	b	819	CLA	OBD-CAD	4.53	1.28	1.22
17	a	825	CLA	C3D-C2D	4.53	1.49	1.39
17	j	3002	CLA	C3D-C2D	4.53	1.49	1.39
17	B	821	CLA	C3D-C2D	4.53	1.49	1.39
17	a	841	CLA	C3D-C2D	4.53	1.49	1.39
17	3	303	CLA	OBD-CAD	4.53	1.28	1.22
17	b	822	CLA	OBD-CAD	4.53	1.28	1.22
17	A	832	CLA	OBD-CAD	4.53	1.28	1.22
17	A	804	CLA	OBD-CAD	4.53	1.28	1.22
17	1	311	CLA	OBD-CAD	4.53	1.28	1.22
17	8	308	CLA	CHC-C1C	4.53	1.48	1.35
17	a	827	CLA	CHC-C1C	4.53	1.48	1.35
17	a	838	CLA	C3D-C2D	4.53	1.49	1.39
17	6	304	CLA	OBD-CAD	4.54	1.28	1.22
17	3	309	CLA	CHC-C1C	4.54	1.48	1.35
17	F	301	CLA	C3D-C2D	4.54	1.49	1.39
17	A	813	CLA	OBD-CAD	4.54	1.28	1.22
17	g	101	CLA	OBD-CAD	4.54	1.28	1.22
17	a	815	CLA	CHC-C1C	4.54	1.48	1.35
17	3	302	CLA	CHC-C1C	4.54	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	609	CLA	OBD-CAD	4.54	1.28	1.22
17	b	831	CLA	OBD-CAD	4.54	1.28	1.22
17	7	612	CLA	OBD-CAD	4.54	1.28	1.22
17	2	604	CLA	OBD-CAD	4.54	1.28	1.22
17	g	102	CLA	OBD-CAD	4.54	1.28	1.22
17	6	310	CLA	C3D-C2D	4.54	1.49	1.39
17	B	809	CLA	C3D-C2D	4.54	1.49	1.39
17	1	303	CLA	CHC-C1C	4.54	1.48	1.35
17	b	830	CLA	C3D-C2D	4.54	1.49	1.39
17	a	823	CLA	OBD-CAD	4.54	1.28	1.22
17	9	608	CLA	C3D-C2D	4.54	1.49	1.39
17	b	811	CLA	C3D-C2D	4.54	1.49	1.39
17	3	302	CLA	OBD-CAD	4.54	1.28	1.22
17	9	610	CLA	C3D-C2D	4.54	1.49	1.39
17	B	832	CLA	CHC-C1C	4.54	1.48	1.35
17	B	819	CLA	OBD-CAD	4.54	1.28	1.22
17	B	841	CLA	OBD-CAD	4.54	1.28	1.22
17	9	602	CLA	CHC-C1C	4.54	1.48	1.35
17	a	809	CLA	OBD-CAD	4.54	1.28	1.22
17	B	812	CLA	OBD-CAD	4.54	1.28	1.22
17	1	315	CLA	C3D-C2D	4.54	1.49	1.39
17	b	836	CLA	C3D-C2D	4.54	1.49	1.39
17	6	312	CLA	C3D-C2D	4.54	1.49	1.39
17	a	819	CLA	CHC-C1C	4.55	1.48	1.35
17	B	818	CLA	OBD-CAD	4.55	1.28	1.22
17	4	613	CLA	OBD-CAD	4.55	1.28	1.22
17	9	614	CLA	OBD-CAD	4.55	1.28	1.22
17	A	802	CLA	CHC-C1C	4.55	1.48	1.35
17	B	807	CLA	C3D-C2D	4.55	1.49	1.39
17	8	301	CLA	CHC-C1C	4.55	1.48	1.35
17	3	311	CLA	OBD-CAD	4.55	1.28	1.22
17	b	809	CLA	C3D-C2D	4.55	1.49	1.39
17	a	821	CLA	OBD-CAD	4.55	1.28	1.22
17	b	833	CLA	OBD-CAD	4.55	1.28	1.22
17	a	830	CLA	OBD-CAD	4.55	1.28	1.22
17	6	316	CLA	OBD-CAD	4.55	1.28	1.22
17	a	832	CLA	OBD-CAD	4.55	1.28	1.22
17	B	819	CLA	C3D-C2D	4.55	1.49	1.39
17	a	807	CLA	C3D-C2D	4.55	1.49	1.39
17	a	820	CLA	C3D-C2D	4.55	1.49	1.39
17	b	833	CLA	C3D-C2D	4.55	1.49	1.39
17	A	822	CLA	OBD-CAD	4.55	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	815	CLA	C3D-C2D	4.55	1.49	1.39
17	3	310	CLA	C3D-C2D	4.55	1.49	1.39
17	3	308	CLA	OBD-CAD	4.55	1.28	1.22
17	8	309	CLA	OBD-CAD	4.55	1.28	1.22
17	8	301	CLA	OBD-CAD	4.55	1.28	1.22
17	b	804	CLA	OBD-CAD	4.56	1.28	1.22
17	B	803	CLA	CHC-C1C	4.56	1.48	1.35
17	a	825	CLA	OBD-CAD	4.56	1.28	1.22
17	B	815	CLA	C3D-C2D	4.56	1.49	1.39
17	a	813	CLA	C3D-C2D	4.56	1.49	1.39
17	a	818	CLA	OBD-CAD	4.56	1.28	1.22
17	A	823	CLA	OBD-CAD	4.56	1.28	1.22
17	A	827	CLA	CHC-C1C	4.56	1.48	1.35
17	a	827	CLA	OBD-CAD	4.56	1.28	1.22
17	A	805	CLA	C3D-C2D	4.56	1.49	1.39
17	a	833	CLA	C3D-C2D	4.56	1.49	1.39
17	j	3002	CLA	OBD-CAD	4.56	1.28	1.22
17	9	612	CLA	OBD-CAD	4.56	1.28	1.22
17	2	604	CLA	C3D-C2D	4.56	1.49	1.39
17	8	310	CLA	C3D-C2D	4.56	1.49	1.39
17	A	845	CLA	OBD-CAD	4.56	1.28	1.22
17	B	830	CLA	C3D-C2D	4.56	1.49	1.39
17	J	3002	CLA	C3D-C2D	4.56	1.49	1.39
17	a	840	CLA	OBD-CAD	4.56	1.28	1.22
17	4	614	CLA	OBD-CAD	4.56	1.28	1.22
17	2	609	CLA	C3D-C2D	4.56	1.49	1.39
17	8	309	CLA	C3D-C2D	4.56	1.49	1.39
17	b	813	CLA	OBD-CAD	4.56	1.28	1.22
17	b	816	CLA	C3D-C2D	4.56	1.49	1.39
17	k	1401	CLA	OBD-CAD	4.57	1.28	1.22
17	a	819	CLA	C3D-C2D	4.57	1.49	1.39
17	B	814	CLA	CHC-C1C	4.57	1.48	1.35
17	2	609	CLA	CHC-C1C	4.57	1.48	1.35
17	l	203	CLA	CHC-C1C	4.57	1.48	1.35
17	b	821	CLA	C3D-C2D	4.57	1.49	1.39
17	b	803	CLA	C3D-C2D	4.57	1.49	1.39
17	a	837	CLA	C3D-C2D	4.57	1.49	1.39
17	4	610	CLA	C3D-C2D	4.57	1.49	1.39
17	1	313	CLA	OBD-CAD	4.57	1.28	1.22
17	K	4003	CLA	C3D-C2D	4.57	1.49	1.39
17	G	103	CLA	OBD-CAD	4.57	1.29	1.22
17	A	820	CLA	C3D-C2D	4.57	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	817	CLA	OBD-CAD	4.57	1.29	1.22
17	a	808	CLA	OBD-CAD	4.57	1.29	1.22
17	a	823	CLA	C3D-C2D	4.57	1.49	1.39
17	1	306	CLA	OBD-CAD	4.57	1.29	1.22
17	k	1403	CLA	OBD-CAD	4.57	1.29	1.22
17	A	818	CLA	OBD-CAD	4.57	1.29	1.22
17	3	302	CLA	C3D-C2D	4.57	1.49	1.39
17	a	809	CLA	C3D-C2D	4.57	1.49	1.39
17	7	610	CLA	C3D-C2D	4.57	1.49	1.39
17	b	830	CLA	OBD-CAD	4.58	1.29	1.22
17	8	308	CLA	OBD-CAD	4.58	1.29	1.22
17	K	4002	CLA	OBD-CAD	4.58	1.29	1.22
17	2	611	CLA	OBD-CAD	4.58	1.29	1.22
17	A	830	CLA	C3D-C2D	4.58	1.49	1.39
17	B	809	CLA	OBD-CAD	4.58	1.29	1.22
17	2	609	CLA	OBD-CAD	4.58	1.29	1.22
17	B	827	CLA	OBD-CAD	4.58	1.29	1.22
17	a	836	CLA	C3D-C2D	4.58	1.49	1.39
17	1	314	CLA	OBD-CAD	4.58	1.29	1.22
17	7	604	CLA	OBD-CAD	4.58	1.29	1.22
17	A	836	CLA	C3D-C2D	4.58	1.49	1.39
17	A	837	CLA	OBD-CAD	4.58	1.29	1.22
17	A	836	CLA	OBD-CAD	4.59	1.29	1.22
17	4	608	CLA	OBD-CAD	4.59	1.29	1.22
17	b	807	CLA	C3D-C2D	4.59	1.49	1.39
17	a	803	CLA	C3D-C2D	4.59	1.49	1.39
17	7	609	CLA	CHC-C1C	4.59	1.48	1.35
17	f	7003	CLA	OBD-CAD	4.59	1.29	1.22
17	2	608	CLA	C3D-C2D	4.59	1.49	1.39
17	b	821	CLA	OBD-CAD	4.59	1.29	1.22
17	b	814	CLA	CHC-C1C	4.59	1.48	1.35
17	7	609	CLA	C3D-C2D	4.59	1.49	1.39
17	a	806	CLA	OBD-CAD	4.59	1.29	1.22
17	6	310	CLA	OBD-CAD	4.59	1.29	1.22
17	6	314	CLA	C3D-C2D	4.60	1.49	1.39
17	8	307	CLA	OBD-CAD	4.60	1.29	1.22
17	A	826	CLA	OBD-CAD	4.60	1.29	1.22
17	L	202	CLA	OBD-CAD	4.60	1.29	1.22
17	a	846	CLA	OBD-CAD	4.60	1.29	1.22
17	A	804	CLA	O2D-CGD	4.60	1.44	1.33
17	B	828	CLA	OBD-CAD	4.60	1.29	1.22
17	a	819	CLA	OBD-CAD	4.60	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	308	CLA	C3D-C2D	4.60	1.49	1.39
17	A	838	CLA	CHC-C1C	4.60	1.48	1.35
17	a	856	CLA	C3D-C2D	4.60	1.49	1.39
17	a	805	CLA	OBD-CAD	4.60	1.29	1.22
17	b	805	CLA	C3D-C2D	4.60	1.49	1.39
17	a	814	CLA	OBD-CAD	4.60	1.29	1.22
17	B	808	CLA	OBD-CAD	4.60	1.29	1.22
17	8	303	CLA	OBD-CAD	4.60	1.29	1.22
17	A	814	CLA	C3D-C2D	4.60	1.49	1.39
17	6	313	CLA	C3D-C2D	4.60	1.49	1.39
17	4	604	CLA	OBD-CAD	4.60	1.29	1.22
17	a	810	CLA	OBD-CAD	4.60	1.29	1.22
17	B	834	CLA	OBD-CAD	4.60	1.29	1.22
17	b	819	CLA	C3D-C2D	4.61	1.49	1.39
17	B	820	CLA	OBD-CAD	4.61	1.29	1.22
17	a	841	CLA	OBD-CAD	4.61	1.29	1.22
17	8	311	CLA	OBD-CAD	4.61	1.29	1.22
17	A	802	CLA	C3D-C2D	4.61	1.49	1.39
17	G	104	CLA	OBD-CAD	4.61	1.29	1.22
17	2	613	CLA	OBD-CAD	4.61	1.29	1.22
17	a	844	CLA	C3D-C2D	4.61	1.49	1.39
17	8	304	CLA	OBD-CAD	4.61	1.29	1.22
17	8	307	CLA	C3D-C2D	4.61	1.49	1.39
17	b	824	CLA	OBD-CAD	4.61	1.29	1.22
17	B	802	CLA	OBD-CAD	4.61	1.29	1.22
17	K	4003	CLA	OBD-CAD	4.61	1.29	1.22
17	1	311	CLA	C3D-C2D	4.61	1.49	1.39
17	8	305	CLA	OBD-CAD	4.61	1.29	1.22
17	A	809	CLA	C3D-C2D	4.61	1.49	1.39
17	3	313	CLA	OBD-CAD	4.61	1.29	1.22
17	b	812	CLA	C3D-C2D	4.61	1.49	1.39
17	3	301	CLA	OBD-CAD	4.62	1.29	1.22
17	b	840	CLA	OBD-CAD	4.62	1.29	1.22
17	A	840	CLA	OBD-CAD	4.62	1.29	1.22
17	7	611	CLA	OBD-CAD	4.62	1.29	1.22
17	l	202	CLA	OBD-CAD	4.62	1.29	1.22
17	A	821	CLA	C3D-C2D	4.62	1.49	1.39
17	A	825	CLA	OBD-CAD	4.62	1.29	1.22
17	B	837	CLA	O2D-CGD	4.62	1.44	1.33
17	a	842	CLA	OBD-CAD	4.62	1.29	1.22
17	A	854	CLA	C3D-C2D	4.62	1.49	1.39
17	B	818	CLA	C3D-C2D	4.62	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	3002	CLA	OBD-CAD	4.62	1.29	1.22
17	9	611	CLA	OBD-CAD	4.63	1.29	1.22
17	b	832	CLA	OBD-CAD	4.63	1.29	1.22
17	a	838	CLA	CHC-C1C	4.63	1.48	1.35
17	6	306	CLA	OBD-CAD	4.63	1.29	1.22
17	b	834	CLA	OBD-CAD	4.64	1.29	1.22
17	A	805	CLA	O2D-CGD	4.64	1.45	1.33
17	b	812	CLA	OBD-CAD	4.64	1.29	1.22
17	1	312	CLA	OBD-CAD	4.64	1.29	1.22
17	b	802	CLA	OBD-CAD	4.64	1.29	1.22
17	B	815	CLA	OBD-CAD	4.64	1.29	1.22
17	b	809	CLA	O2D-CGD	4.65	1.45	1.33
17	A	806	CLA	OBD-CAD	4.65	1.29	1.22
17	a	834	CLA	OBD-CAD	4.65	1.29	1.22
17	3	306	CLA	OBD-CAD	4.65	1.29	1.22
17	A	854	CLA	O2D-CGD	4.65	1.45	1.33
17	b	813	CLA	O2D-CGD	4.65	1.45	1.33
17	1	304	CLA	C3D-C2D	4.65	1.50	1.39
17	A	805	CLA	OBD-CAD	4.65	1.29	1.22
17	B	812	CLA	C3D-C2D	4.65	1.50	1.39
17	b	804	CLA	O2D-CGD	4.65	1.45	1.33
17	B	814	CLA	O2D-CGD	4.66	1.45	1.33
17	a	820	CLA	OBD-CAD	4.66	1.29	1.22
17	A	803	CLA	C3D-C2D	4.66	1.50	1.39
17	a	837	CLA	OBD-CAD	4.66	1.29	1.22
17	A	825	CLA	C3D-C2D	4.66	1.50	1.39
17	b	818	CLA	C3D-C2D	4.67	1.50	1.39
17	B	825	CLA	O2D-CGD	4.67	1.45	1.33
17	b	815	CLA	OBD-CAD	4.67	1.29	1.22
17	b	837	CLA	O2D-CGD	4.68	1.45	1.33
26	7	601	CHL	O2D-CGD	4.68	1.45	1.33
17	b	808	CLA	O2D-CGD	4.69	1.45	1.33
17	A	814	CLA	O2D-CGD	4.69	1.45	1.33
17	b	829	CLA	O2D-CGD	4.70	1.45	1.33
17	A	830	CLA	OBD-CAD	4.70	1.29	1.22
17	6	313	CLA	OBD-CAD	4.70	1.29	1.22
17	A	835	CLA	OBD-CAD	4.71	1.29	1.22
26	2	601	CHL	O2D-CGD	4.71	1.45	1.33
17	a	839	CLA	O2D-CGD	4.71	1.45	1.33
17	a	828	CLA	O2D-CGD	4.73	1.45	1.33
18	a	845	PQN	C10-C5	4.74	1.48	1.40
17	b	832	CLA	O2D-CGD	4.74	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	801	CLA	O2D-CGD	4.74	1.45	1.33
17	a	813	CLA	OBD-CAD	4.74	1.29	1.22
17	b	825	CLA	O2D-CGD	4.74	1.45	1.33
17	b	815	CLA	O2D-CGD	4.74	1.45	1.33
17	A	831	CLA	C3D-C2D	4.75	1.50	1.39
17	a	801	CLA	OBD-CAD	4.75	1.29	1.22
17	9	614	CLA	O2D-CGD	4.75	1.45	1.33
17	a	838	CLA	O2D-CGD	4.76	1.45	1.33
17	b	806	CLA	O2D-CGD	4.76	1.45	1.33
26	1	302	CHL	O2D-CGD	4.76	1.45	1.33
17	B	822	CLA	OBD-CAD	4.76	1.29	1.22
17	B	826	CLA	O2D-CGD	4.76	1.45	1.33
17	b	814	CLA	O2D-CGD	4.76	1.45	1.33
17	A	828	CLA	O2D-CGD	4.76	1.45	1.33
18	B	842	PQN	C10-C5	4.77	1.48	1.40
17	b	810	CLA	O2D-CGD	4.77	1.45	1.33
17	a	804	CLA	O2D-CGD	4.78	1.45	1.33
17	A	839	CLA	O2D-CGD	4.78	1.45	1.33
17	B	832	CLA	O2D-CGD	4.78	1.45	1.33
17	a	815	CLA	OBD-CAD	4.79	1.29	1.22
17	B	829	CLA	O2D-CGD	4.79	1.45	1.33
17	a	834	CLA	O2D-CGD	4.79	1.45	1.33
17	b	841	CLA	O2D-CGD	4.79	1.45	1.33
17	G	101	CLA	O2D-CGD	4.80	1.45	1.33
17	a	802	CLA	C3D-C2D	4.80	1.50	1.39
17	a	801	CLA	O2D-CGD	4.80	1.45	1.33
17	B	838	CLA	O2D-CGD	4.81	1.45	1.33
17	4	614	CLA	O2D-CGD	4.81	1.45	1.33
17	a	831	CLA	O2D-CGD	4.81	1.45	1.33
17	A	838	CLA	O2D-CGD	4.81	1.45	1.33
17	b	824	CLA	O2D-CGD	4.82	1.45	1.33
17	2	603	CLA	O2D-CGD	4.82	1.45	1.33
17	a	829	CLA	O2D-CGD	4.82	1.45	1.33
17	a	815	CLA	O2D-CGD	4.83	1.45	1.33
17	B	812	CLA	O2D-CGD	4.83	1.45	1.33
17	2	613	CLA	O2D-CGD	4.83	1.45	1.33
17	b	812	CLA	O2D-CGD	4.83	1.45	1.33
17	A	829	CLA	O2D-CGD	4.83	1.45	1.33
17	a	807	CLA	O2D-CGD	4.83	1.45	1.33
17	B	841	CLA	O2D-CGD	4.83	1.45	1.33
26	6	303	CHL	O2D-CGD	4.83	1.45	1.33
17	a	821	CLA	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	601	CLA	O2D-CGD	4.84	1.45	1.33
17	A	821	CLA	O2D-CGD	4.84	1.45	1.33
17	B	822	CLA	O2D-CGD	4.84	1.45	1.33
17	a	805	CLA	O2D-CGD	4.84	1.45	1.33
17	B	803	CLA	O2D-CGD	4.84	1.45	1.33
17	B	824	CLA	O2D-CGD	4.84	1.45	1.33
17	B	813	CLA	O2D-CGD	4.85	1.45	1.33
18	b	842	PQN	C10-C5	4.85	1.49	1.40
17	a	814	CLA	O2D-CGD	4.85	1.45	1.33
17	B	833	CLA	O2D-CGD	4.85	1.45	1.33
17	A	834	CLA	O2D-CGD	4.86	1.45	1.33
17	B	821	CLA	O2D-CGD	4.86	1.45	1.33
17	B	815	CLA	O2D-CGD	4.86	1.45	1.33
17	F	301	CLA	O2D-CGD	4.86	1.45	1.33
17	k	1401	CLA	O2D-CGD	4.87	1.45	1.33
17	A	802	CLA	O2D-CGD	4.87	1.45	1.33
17	B	820	CLA	O2D-CGD	4.87	1.45	1.33
17	a	826	CLA	O2D-CGD	4.87	1.45	1.33
17	A	832	CLA	O2D-CGD	4.87	1.45	1.33
17	B	836	CLA	O2D-CGD	4.88	1.45	1.33
17	b	803	CLA	O2D-CGD	4.88	1.45	1.33
17	a	843	CLA	O2D-CGD	4.88	1.45	1.33
17	A	827	CLA	O2D-CGD	4.88	1.45	1.33
17	a	827	CLA	O2D-CGD	4.88	1.45	1.33
18	A	844	PQN	C10-C5	4.88	1.49	1.40
17	A	835	CLA	O2D-CGD	4.88	1.45	1.33
17	b	807	CLA	O2D-CGD	4.88	1.45	1.33
17	1	314	CLA	O2D-CGD	4.88	1.45	1.33
17	B	834	CLA	O2D-CGD	4.88	1.45	1.33
17	B	808	CLA	O2D-CGD	4.88	1.45	1.33
26	7	605	CHL	O2D-CGD	4.88	1.45	1.33
17	B	804	CLA	O2D-CGD	4.88	1.45	1.33
17	1	303	CLA	O2D-CGD	4.88	1.45	1.33
17	4	603	CLA	O2D-CGD	4.88	1.45	1.33
17	B	802	CLA	O2D-CGD	4.89	1.45	1.33
17	9	602	CLA	O2D-CGD	4.89	1.45	1.33
17	b	820	CLA	O2D-CGD	4.89	1.45	1.33
17	A	826	CLA	O2D-CGD	4.89	1.45	1.33
17	B	809	CLA	O2D-CGD	4.89	1.45	1.33
17	a	812	CLA	O2D-CGD	4.89	1.45	1.33
17	a	809	CLA	O2D-CGD	4.89	1.45	1.33
17	b	834	CLA	O2D-CGD	4.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	g	103	CLA	O2D-CGD	4.90	1.45	1.33
17	A	806	CLA	O2D-CGD	4.90	1.45	1.33
17	B	818	CLA	O2D-CGD	4.90	1.45	1.33
26	2	607	CHL	O2D-CGD	4.90	1.45	1.33
17	B	817	CLA	O2D-CGD	4.90	1.45	1.33
17	K	4002	CLA	O2D-CGD	4.90	1.45	1.33
17	B	810	CLA	O2D-CGD	4.90	1.45	1.33
17	A	831	CLA	O2D-CGD	4.90	1.45	1.33
17	b	821	CLA	O2D-CGD	4.90	1.45	1.33
26	9	607	CHL	O2D-CGD	4.90	1.45	1.33
17	a	833	CLA	O2D-CGD	4.91	1.45	1.33
17	7	602	CLA	O2D-CGD	4.91	1.45	1.33
17	8	302	CLA	O2D-CGD	4.91	1.45	1.33
17	a	810	CLA	O2D-CGD	4.91	1.45	1.33
17	6	315	CLA	O2D-CGD	4.91	1.45	1.33
17	B	806	CLA	O2D-CGD	4.92	1.45	1.33
17	B	830	CLA	O2D-CGD	4.92	1.45	1.33
17	8	303	CLA	O2D-CGD	4.92	1.45	1.33
17	1	312	CLA	O2D-CGD	4.92	1.45	1.33
17	1	306	CLA	O2D-CGD	4.92	1.45	1.33
17	A	820	CLA	O2D-CGD	4.92	1.45	1.33
17	a	818	CLA	O2D-CGD	4.92	1.45	1.33
17	A	819	CLA	O2D-CGD	4.92	1.45	1.33
17	a	844	CLA	O2D-CGD	4.92	1.45	1.33
17	9	603	CLA	O2D-CGD	4.92	1.45	1.33
26	4	605	CHL	O2D-CGD	4.92	1.45	1.33
17	7	610	CLA	O2D-CGD	4.92	1.45	1.33
17	g	101	CLA	O2D-CGD	4.92	1.45	1.33
17	9	604	CLA	O2D-CGD	4.92	1.45	1.33
17	3	304	CLA	O2D-CGD	4.92	1.45	1.33
26	2	605	CHL	O2D-CGD	4.92	1.45	1.33
17	a	817	CLA	O2D-CGD	4.92	1.45	1.33
17	4	601	CLA	O2D-CGD	4.93	1.45	1.33
17	A	810	CLA	O2D-CGD	4.93	1.45	1.33
17	A	840	CLA	O2D-CGD	4.93	1.45	1.33
17	b	836	CLA	O2D-CGD	4.93	1.45	1.33
26	4	607	CHL	O2D-CGD	4.93	1.45	1.33
17	b	816	CLA	O2D-CGD	4.93	1.45	1.33
17	A	842	CLA	O2D-CGD	4.93	1.45	1.33
17	8	312	CLA	O2D-CGD	4.93	1.45	1.33
17	1	304	CLA	O2D-CGD	4.93	1.45	1.33
17	B	827	CLA	O2D-CGD	4.93	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	g	102	CLA	O2D-CGD	4.93	1.45	1.33
17	A	816	CLA	O2D-CGD	4.93	1.45	1.33
17	b	811	CLA	O2D-CGD	4.93	1.45	1.33
26	1	307	CHL	O2D-CGD	4.93	1.45	1.33
17	6	304	CLA	O2D-CGD	4.94	1.45	1.33
17	a	840	CLA	O2D-CGD	4.94	1.45	1.33
17	3	301	CLA	O2D-CGD	4.94	1.45	1.33
17	4	604	CLA	O2D-CGD	4.94	1.45	1.33
17	b	805	CLA	O2D-CGD	4.94	1.45	1.33
17	A	845	CLA	O2D-CGD	4.94	1.45	1.33
17	b	822	CLA	O2D-CGD	4.94	1.45	1.33
17	b	833	CLA	O2D-CGD	4.94	1.45	1.33
17	a	802	CLA	O2D-CGD	4.94	1.45	1.33
17	7	609	CLA	O2D-CGD	4.94	1.45	1.33
17	a	808	CLA	O2D-CGD	4.94	1.45	1.33
17	b	826	CLA	O2D-CGD	4.94	1.45	1.33
26	7	607	CHL	O2D-CGD	4.95	1.45	1.33
17	L	202	CLA	O2D-CGD	4.95	1.45	1.33
17	A	818	CLA	O2D-CGD	4.95	1.45	1.33
17	A	833	CLA	O2D-CGD	4.95	1.45	1.33
17	a	836	CLA	O2D-CGD	4.95	1.45	1.33
17	f	7003	CLA	O2D-CGD	4.95	1.45	1.33
17	A	830	CLA	O2D-CGD	4.95	1.45	1.33
17	B	831	CLA	O2D-CGD	4.95	1.45	1.33
17	B	828	CLA	O2D-CGD	4.95	1.45	1.33
17	7	608	CLA	O2D-CGD	4.95	1.45	1.33
17	6	305	CLA	O2D-CGD	4.95	1.45	1.33
17	B	839	CLA	O2D-CGD	4.95	1.45	1.33
17	4	611	CLA	O2D-CGD	4.95	1.45	1.33
17	A	817	CLA	O2D-CGD	4.95	1.45	1.33
17	b	802	CLA	O2D-CGD	4.96	1.45	1.33
17	2	602	CLA	O2D-CGD	4.96	1.45	1.33
17	A	815	CLA	O2D-CGD	4.96	1.45	1.33
17	1	311	CLA	O2D-CGD	4.96	1.45	1.33
17	7	604	CLA	O2D-CGD	4.96	1.45	1.33
17	b	817	CLA	O2D-CGD	4.96	1.45	1.33
17	a	803	CLA	O2D-CGD	4.96	1.45	1.33
17	3	302	CLA	O2D-CGD	4.96	1.45	1.33
17	1	309	CLA	O2D-CGD	4.96	1.45	1.33
26	8	306	CHL	O2D-CGD	4.96	1.45	1.33
17	A	803	CLA	O2D-CGD	4.96	1.45	1.33
17	k	1403	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	819	CLA	O2D-CGD	4.96	1.45	1.33
17	3	305	CLA	O2D-CGD	4.96	1.45	1.33
17	b	827	CLA	O2D-CGD	4.96	1.45	1.33
17	B	805	CLA	O2D-CGD	4.96	1.45	1.33
17	B	819	CLA	O2D-CGD	4.97	1.45	1.33
17	2	610	CLA	O2D-CGD	4.97	1.45	1.33
26	7	606	CHL	O2D-CGD	4.97	1.45	1.33
17	F	303	CLA	O2D-CGD	4.97	1.45	1.33
17	4	610	CLA	O2D-CGD	4.97	1.45	1.33
17	B	835	CLA	O2D-CGD	4.97	1.45	1.33
17	b	831	CLA	O2D-CGD	4.97	1.45	1.33
17	1	315	CLA	O2D-CGD	4.97	1.45	1.33
17	6	309	CLA	O2D-CGD	4.97	1.45	1.33
17	A	809	CLA	O2D-CGD	4.97	1.45	1.33
17	A	836	CLA	O2D-CGD	4.97	1.45	1.33
17	2	604	CLA	O2D-CGD	4.97	1.45	1.33
17	9	613	CLA	O2D-CGD	4.97	1.45	1.33
17	b	818	CLA	O2D-CGD	4.98	1.45	1.33
17	B	840	CLA	O2D-CGD	4.98	1.45	1.33
17	a	813	CLA	O2D-CGD	4.98	1.45	1.33
17	b	840	CLA	O2D-CGD	4.98	1.45	1.33
17	6	313	CLA	O2D-CGD	4.98	1.45	1.33
17	a	846	CLA	O2D-CGD	4.98	1.45	1.33
17	G	103	CLA	O2D-CGD	4.98	1.45	1.33
17	a	842	CLA	O2D-CGD	4.98	1.45	1.33
17	9	608	CLA	O2D-CGD	4.98	1.45	1.33
17	l	203	CLA	O2D-CGD	4.98	1.45	1.33
17	B	811	CLA	O2D-CGD	4.98	1.45	1.33
17	9	609	CLA	O2D-CGD	4.98	1.45	1.33
26	4	606	CHL	O2D-CGD	4.99	1.45	1.33
17	b	830	CLA	O2D-CGD	4.99	1.45	1.33
17	k	1402	CLA	O2D-CGD	4.99	1.45	1.33
17	6	307	CLA	O2D-CGD	4.99	1.45	1.33
17	A	808	CLA	O2D-CGD	4.99	1.45	1.33
17	3	308	CLA	O2D-CGD	4.99	1.45	1.33
17	l	204	CLA	O2D-CGD	4.99	1.45	1.33
26	9	605	CHL	O2D-CGD	4.99	1.45	1.33
17	b	823	CLA	O2D-CGD	4.99	1.45	1.33
26	9	606	CHL	O2D-CGD	4.99	1.45	1.33
17	4	612	CLA	O2D-CGD	4.99	1.45	1.33
17	3	303	CLA	O2D-CGD	4.99	1.45	1.33
17	9	610	CLA	O2D-CGD	4.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	307	CLA	O2D-CGD	4.99	1.45	1.33
17	b	835	CLA	O2D-CGD	4.99	1.45	1.33
17	8	304	CLA	O2D-CGD	5.00	1.45	1.33
17	a	841	CLA	O2D-CGD	5.00	1.45	1.33
17	L	204	CLA	O2D-CGD	5.00	1.45	1.33
17	A	823	CLA	O2D-CGD	5.00	1.45	1.33
17	6	310	CLA	O2D-CGD	5.00	1.45	1.33
17	A	807	CLA	O2D-CGD	5.00	1.45	1.33
17	3	306	CLA	O2D-CGD	5.00	1.45	1.33
17	L	203	CLA	O2D-CGD	5.00	1.45	1.33
17	b	828	CLA	O2D-CGD	5.00	1.45	1.33
17	7	603	CLA	O2D-CGD	5.00	1.45	1.33
17	3	314	CLA	O2D-CGD	5.00	1.45	1.33
26	6	308	CHL	O2D-CGD	5.00	1.45	1.33
17	1	202	CLA	O2D-CGD	5.00	1.45	1.33
17	A	824	CLA	O2D-CGD	5.00	1.45	1.33
26	2	614	CHL	O2D-CGD	5.00	1.45	1.33
17	6	316	CLA	O2D-CGD	5.00	1.45	1.33
17	3	311	CLA	O2D-CGD	5.00	1.45	1.33
17	b	838	CLA	O2D-CGD	5.01	1.45	1.33
17	8	309	CLA	O2D-CGD	5.01	1.45	1.33
17	A	813	CLA	O2D-CGD	5.01	1.45	1.33
17	G	104	CLA	O2D-CGD	5.01	1.45	1.33
17	7	611	CLA	O2D-CGD	5.01	1.45	1.33
17	b	839	CLA	O2D-CGD	5.01	1.45	1.33
17	8	305	CLA	O2D-CGD	5.01	1.45	1.33
17	8	301	CLA	O2D-CGD	5.01	1.45	1.33
17	3	312	CLA	O2D-CGD	5.01	1.45	1.33
17	2	608	CLA	O2D-CGD	5.01	1.45	1.33
17	B	816	CLA	O2D-CGD	5.01	1.45	1.33
17	1	308	CLA	O2D-CGD	5.01	1.45	1.33
17	a	832	CLA	O2D-CGD	5.01	1.45	1.33
17	4	608	CLA	O2D-CGD	5.01	1.45	1.33
17	6	314	CLA	O2D-CGD	5.01	1.45	1.33
17	3	309	CLA	O2D-CGD	5.01	1.45	1.33
17	B	823	CLA	O2D-CGD	5.01	1.45	1.33
26	7	614	CHL	O2D-CGD	5.01	1.45	1.33
17	A	837	CLA	O2D-CGD	5.01	1.45	1.33
26	3	307	CHL	O2D-CGD	5.02	1.45	1.33
17	a	823	CLA	O2D-CGD	5.02	1.45	1.33
17	9	611	CLA	O2D-CGD	5.02	1.45	1.33
17	4	613	CLA	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	305	CLA	O2D-CGD	5.02	1.45	1.33
17	A	843	CLA	O2D-CGD	5.02	1.45	1.33
17	8	310	CLA	O2D-CGD	5.02	1.45	1.33
17	6	306	CLA	O2D-CGD	5.02	1.45	1.33
17	1	310	CLA	O2D-CGD	5.02	1.45	1.33
26	9	615	CHL	O2D-CGD	5.02	1.45	1.33
17	K	4003	CLA	O2D-CGD	5.02	1.45	1.33
26	2	606	CHL	O2D-CGD	5.02	1.45	1.33
17	A	841	CLA	O2D-CGD	5.02	1.45	1.33
17	a	824	CLA	O2D-CGD	5.03	1.45	1.33
17	B	807	CLA	O2D-CGD	5.03	1.45	1.33
26	4	615	CHL	O2D-CGD	5.03	1.45	1.33
17	A	811	CLA	O2D-CGD	5.03	1.45	1.33
17	A	812	CLA	O2D-CGD	5.03	1.45	1.33
17	F	304	CLA	O2D-CGD	5.03	1.45	1.33
17	A	822	CLA	O2D-CGD	5.03	1.46	1.33
17	8	311	CLA	O2D-CGD	5.03	1.46	1.33
17	2	611	CLA	O2D-CGD	5.03	1.46	1.33
17	6	312	CLA	O2D-CGD	5.03	1.46	1.33
17	2	609	CLA	O2D-CGD	5.04	1.46	1.33
17	f	7002	CLA	O2D-CGD	5.04	1.46	1.33
17	1	313	CLA	O2D-CGD	5.04	1.46	1.33
17	a	822	CLA	O2D-CGD	5.04	1.46	1.33
17	a	830	CLA	O2D-CGD	5.04	1.46	1.33
17	a	806	CLA	C3C-C2C	5.04	1.47	1.36
17	4	609	CLA	O2D-CGD	5.04	1.46	1.33
17	7	612	CLA	O2D-CGD	5.04	1.46	1.33
17	6	311	CLA	O2D-CGD	5.04	1.46	1.33
17	a	820	CLA	O2D-CGD	5.05	1.46	1.33
17	a	837	CLA	O2D-CGD	5.05	1.46	1.33
17	4	603	CLA	C3C-C2C	5.05	1.47	1.36
17	A	825	CLA	O2D-CGD	5.05	1.46	1.33
17	a	811	CLA	O2D-CGD	5.05	1.46	1.33
17	j	3002	CLA	O2D-CGD	5.05	1.46	1.33
17	4	602	CLA	O2D-CGD	5.05	1.46	1.33
17	a	838	CLA	C3C-C2C	5.06	1.47	1.36
17	a	844	CLA	C3C-C2C	5.06	1.47	1.36
17	2	612	CLA	O2D-CGD	5.07	1.46	1.33
17	J	3002	CLA	O2D-CGD	5.07	1.46	1.33
17	7	613	CLA	O2D-CGD	5.07	1.46	1.33
17	9	612	CLA	O2D-CGD	5.08	1.46	1.33
17	8	308	CLA	O2D-CGD	5.09	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	806	CLA	O2D-CGD	5.09	1.46	1.33
17	a	825	CLA	O2D-CGD	5.10	1.46	1.33
17	9	603	CLA	C3C-C2C	5.10	1.47	1.36
17	a	816	CLA	O2D-CGD	5.10	1.46	1.33
17	a	803	CLA	C3C-C2C	5.11	1.47	1.36
17	a	819	CLA	O2D-CGD	5.11	1.46	1.33
17	a	856	CLA	C3C-C2C	5.12	1.47	1.36
17	a	843	CLA	C3C-C2C	5.12	1.47	1.36
17	3	313	CLA	O2D-CGD	5.14	1.46	1.33
17	7	603	CLA	C3C-C2C	5.14	1.47	1.36
17	b	824	CLA	C3C-C2C	5.14	1.47	1.36
17	a	835	CLA	O2D-CGD	5.14	1.46	1.33
17	b	813	CLA	C3C-C2C	5.15	1.47	1.36
17	a	821	CLA	C3C-C2C	5.16	1.47	1.36
17	B	830	CLA	C3C-C2C	5.17	1.47	1.36
17	a	836	CLA	C3C-C2C	5.19	1.47	1.36
17	b	812	CLA	C3C-C2C	5.19	1.47	1.36
17	3	315	CLA	C3B-C4B	5.19	1.49	1.40
17	a	834	CLA	C3C-C2C	5.19	1.47	1.36
17	B	816	CLA	C3C-C2C	5.19	1.47	1.36
17	4	608	CLA	C3C-C2C	5.19	1.47	1.36
17	a	801	CLA	C3C-C2C	5.20	1.47	1.36
17	4	604	CLA	C3C-C2C	5.20	1.47	1.36
17	A	806	CLA	C3C-C2C	5.20	1.47	1.36
17	6	304	CLA	C3C-C2C	5.20	1.47	1.36
17	A	842	CLA	C3C-C2C	5.20	1.47	1.36
17	A	833	CLA	C3C-C2C	5.21	1.47	1.36
17	8	304	CLA	C3C-C2C	5.21	1.47	1.36
17	f	7002	CLA	C3C-C2C	5.21	1.47	1.36
17	g	101	CLA	C3C-C2C	5.21	1.47	1.36
17	A	813	CLA	C3C-C2C	5.22	1.47	1.36
17	B	804	CLA	C3C-C2C	5.22	1.47	1.36
17	6	310	CLA	C3C-C2C	5.22	1.47	1.36
17	b	818	CLA	C3C-C2C	5.22	1.47	1.36
17	8	313	CLA	C3B-C4B	5.23	1.49	1.40
17	A	821	CLA	C3C-C2C	5.23	1.48	1.36
17	a	829	CLA	C3C-C2C	5.23	1.48	1.36
17	B	841	CLA	C3C-C2C	5.23	1.48	1.36
17	b	821	CLA	C3C-C2C	5.23	1.48	1.36
17	b	808	CLA	C3C-C2C	5.23	1.48	1.36
17	A	802	CLA	C3C-C2C	5.24	1.48	1.36
17	A	819	CLA	C3C-C2C	5.24	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	306	CLA	C3C-C2C	5.24	1.48	1.36
17	F	301	CLA	C3C-C2C	5.24	1.48	1.36
17	a	805	CLA	C3C-C2C	5.24	1.48	1.36
17	6	312	CLA	C3C-C2C	5.24	1.48	1.36
17	B	812	CLA	C3C-C2C	5.24	1.48	1.36
17	g	103	CLA	C3C-C2C	5.24	1.48	1.36
17	A	839	CLA	C3C-C2C	5.24	1.48	1.36
17	1	315	CLA	C3C-C2C	5.25	1.48	1.36
17	b	809	CLA	C3C-C2C	5.25	1.48	1.36
17	a	807	CLA	C3C-C2C	5.25	1.48	1.36
17	b	827	CLA	C3C-C2C	5.25	1.48	1.36
17	A	805	CLA	C3C-C2C	5.25	1.48	1.36
17	A	803	CLA	C3C-C2C	5.25	1.48	1.36
17	a	837	CLA	C3C-C2C	5.25	1.48	1.36
17	B	813	CLA	C3C-C2C	5.25	1.48	1.36
17	B	825	CLA	C3C-C2C	5.25	1.48	1.36
17	7	612	CLA	C3C-C2C	5.26	1.48	1.36
17	2	609	CLA	C3C-C2C	5.26	1.48	1.36
17	a	819	CLA	C3C-C2C	5.26	1.48	1.36
17	A	843	CLA	C3C-C2C	5.26	1.48	1.36
17	A	826	CLA	C3C-C2C	5.26	1.48	1.36
17	a	817	CLA	C3C-C2C	5.26	1.48	1.36
17	6	316	CLA	C3C-C2C	5.26	1.48	1.36
17	A	854	CLA	C3C-C2C	5.27	1.48	1.36
17	A	830	CLA	C3C-C2C	5.27	1.48	1.36
17	3	309	CLA	C3C-C2C	5.27	1.48	1.36
17	b	805	CLA	C3C-C2C	5.27	1.48	1.36
17	3	312	CLA	C3C-C2C	5.27	1.48	1.36
17	B	824	CLA	C3C-C2C	5.27	1.48	1.36
17	B	817	CLA	C3C-C2C	5.27	1.48	1.36
17	b	829	CLA	C3C-C2C	5.27	1.48	1.36
17	b	836	CLA	C3C-C2C	5.27	1.48	1.36
17	4	611	CLA	C3C-C2C	5.27	1.48	1.36
17	b	806	CLA	C3C-C2C	5.27	1.48	1.36
17	f	7003	CLA	C3C-C2C	5.27	1.48	1.36
17	6	313	CLA	C3C-C2C	5.28	1.48	1.36
17	a	813	CLA	C3C-C2C	5.28	1.48	1.36
17	3	302	CLA	C3C-C2C	5.28	1.48	1.36
17	b	817	CLA	C3C-C2C	5.28	1.48	1.36
17	9	602	CLA	C3C-C2C	5.28	1.48	1.36
17	1	314	CLA	C3C-C2C	5.28	1.48	1.36
17	A	829	CLA	C3C-C2C	5.28	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	k	1402	CLA	C3C-C2C	5.28	1.48	1.36
17	b	825	CLA	C3C-C2C	5.28	1.48	1.36
17	8	302	CLA	C3C-C2C	5.28	1.48	1.36
17	B	821	CLA	C3C-C2C	5.28	1.48	1.36
17	a	831	CLA	C3C-C2C	5.28	1.48	1.36
17	8	310	CLA	C3C-C2C	5.28	1.48	1.36
17	A	808	CLA	C3C-C2C	5.28	1.48	1.36
17	7	602	CLA	C3C-C2C	5.28	1.48	1.36
17	a	841	CLA	C3C-C2C	5.28	1.48	1.36
17	9	610	CLA	C3C-C2C	5.29	1.48	1.36
17	7	613	CLA	C3C-C2C	5.29	1.48	1.36
17	1	303	CLA	C3C-C2C	5.29	1.48	1.36
17	B	839	CLA	C3C-C2C	5.29	1.48	1.36
17	A	810	CLA	C3C-C2C	5.29	1.48	1.36
17	b	804	CLA	C3C-C2C	5.29	1.48	1.36
17	a	808	CLA	C3C-C2C	5.29	1.48	1.36
17	8	312	CLA	C3C-C2C	5.29	1.48	1.36
17	3	301	CLA	C3C-C2C	5.29	1.48	1.36
17	8	303	CLA	C3C-C2C	5.29	1.48	1.36
17	G	101	CLA	C3C-C2C	5.29	1.48	1.36
17	1	313	CLA	C3C-C2C	5.29	1.48	1.36
17	a	804	CLA	C3C-C2C	5.29	1.48	1.36
17	a	839	CLA	C3C-C2C	5.29	1.48	1.36
17	1	310	CLA	C3C-C2C	5.30	1.48	1.36
17	A	837	CLA	C3C-C2C	5.30	1.48	1.36
17	G	104	CLA	C3C-C2C	5.30	1.48	1.36
17	B	818	CLA	C3C-C2C	5.30	1.48	1.36
17	7	611	CLA	C3C-C2C	5.30	1.48	1.36
17	7	609	CLA	C3C-C2C	5.30	1.48	1.36
17	A	828	CLA	C3C-C2C	5.30	1.48	1.36
17	b	815	CLA	C3C-C2C	5.30	1.48	1.36
17	4	610	CLA	C3C-C2C	5.30	1.48	1.36
17	a	823	CLA	C3C-C2C	5.30	1.48	1.36
17	B	807	CLA	C3C-C2C	5.30	1.48	1.36
17	3	314	CLA	C3C-C2C	5.30	1.48	1.36
17	k	1401	CLA	C3C-C2C	5.31	1.48	1.36
17	3	303	CLA	C3C-C2C	5.31	1.48	1.36
17	B	815	CLA	C3C-C2C	5.31	1.48	1.36
17	4	613	CLA	C3C-C2C	5.31	1.48	1.36
17	4	602	CLA	C3C-C2C	5.31	1.48	1.36
17	A	836	CLA	C3C-C2C	5.31	1.48	1.36
17	6	305	CLA	C3C-C2C	5.31	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	833	CLA	C3C-C2C	5.31	1.48	1.36
17	9	614	CLA	C3C-C2C	5.31	1.48	1.36
17	A	809	CLA	C3C-C2C	5.31	1.48	1.36
17	F	304	CLA	C3C-C2C	5.31	1.48	1.36
17	a	816	CLA	C3C-C2C	5.31	1.48	1.36
17	b	831	CLA	C3C-C2C	5.32	1.48	1.36
17	b	838	CLA	C3C-C2C	5.32	1.48	1.36
17	1	312	CLA	C3C-C2C	5.32	1.48	1.36
17	3	310	CLA	C3C-C2C	5.32	1.48	1.36
17	8	308	CLA	C3C-C2C	5.32	1.48	1.36
17	b	841	CLA	C3C-C2C	5.32	1.48	1.36
17	B	829	CLA	C3C-C2C	5.32	1.48	1.36
17	b	820	CLA	C3C-C2C	5.32	1.48	1.36
17	b	823	CLA	C3C-C2C	5.32	1.48	1.36
17	a	830	CLA	C3C-C2C	5.32	1.48	1.36
17	A	835	CLA	C3C-C2C	5.32	1.48	1.36
17	3	304	CLA	C3C-C2C	5.32	1.48	1.36
17	A	816	CLA	C3C-C2C	5.33	1.48	1.36
17	A	804	CLA	C3C-C2C	5.33	1.48	1.36
17	b	828	CLA	C3C-C2C	5.33	1.48	1.36
17	B	827	CLA	C3C-C2C	5.33	1.48	1.36
17	b	835	CLA	C3C-C2C	5.33	1.48	1.36
17	l	203	CLA	C3C-C2C	5.33	1.48	1.36
17	9	608	CLA	C3C-C2C	5.33	1.48	1.36
17	l	204	CLA	C3C-C2C	5.33	1.48	1.36
17	6	314	CLA	C3C-C2C	5.33	1.48	1.36
17	9	612	CLA	C3C-C2C	5.33	1.48	1.36
17	3	305	CLA	C3C-C2C	5.33	1.48	1.36
17	L	203	CLA	C3C-C2C	5.33	1.48	1.36
17	a	826	CLA	C3C-C2C	5.33	1.48	1.36
17	2	602	CLA	C3C-C2C	5.33	1.48	1.36
17	A	838	CLA	C3C-C2C	5.33	1.48	1.36
17	B	838	CLA	C3C-C2C	5.33	1.48	1.36
17	A	825	CLA	C3C-C2C	5.34	1.48	1.36
17	A	811	CLA	C3C-C2C	5.34	1.48	1.36
17	1	309	CLA	C3C-C2C	5.34	1.48	1.36
17	g	102	CLA	C3C-C2C	5.34	1.48	1.36
17	A	801	CLA	C3C-C2C	5.34	1.48	1.36
17	B	808	CLA	C3C-C2C	5.34	1.48	1.36
17	A	822	CLA	C3C-C2C	5.34	1.48	1.36
17	A	824	CLA	C3C-C2C	5.34	1.48	1.36
17	B	810	CLA	C3C-C2C	5.34	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	306	CLA	C3C-C2C	5.34	1.48	1.36
17	A	807	CLA	C3C-C2C	5.34	1.48	1.36
17	a	818	CLA	C3C-C2C	5.34	1.48	1.36
17	b	819	CLA	C3C-C2C	5.34	1.48	1.36
17	6	311	CLA	C3C-C2C	5.34	1.48	1.36
17	F	303	CLA	C3C-C2C	5.34	1.48	1.36
17	b	833	CLA	C3C-C2C	5.34	1.48	1.36
17	9	601	CLA	C3C-C2C	5.34	1.48	1.36
17	B	820	CLA	C3C-C2C	5.34	1.48	1.36
17	b	826	CLA	C3C-C2C	5.34	1.48	1.36
17	B	822	CLA	C3C-C2C	5.34	1.48	1.36
17	K	4002	CLA	C3C-C2C	5.34	1.48	1.36
17	B	834	CLA	C3C-C2C	5.34	1.48	1.36
17	b	807	CLA	C3C-C2C	5.34	1.48	1.36
17	6	307	CLA	C3C-C2C	5.34	1.48	1.36
17	8	301	CLA	C3C-C2C	5.34	1.48	1.36
17	B	835	CLA	C3C-C2C	5.35	1.48	1.36
17	b	816	CLA	C3C-C2C	5.35	1.48	1.36
17	1	305	CLA	C3C-C2C	5.35	1.48	1.36
17	7	610	CLA	C3C-C2C	5.35	1.48	1.36
17	L	202	CLA	C3C-C2C	5.35	1.48	1.36
17	B	828	CLA	C3C-C2C	5.35	1.48	1.36
17	A	818	CLA	C3C-C2C	5.35	1.48	1.36
17	B	814	CLA	C3C-C2C	5.35	1.48	1.36
17	b	822	CLA	C3C-C2C	5.35	1.48	1.36
17	a	842	CLA	C3C-C2C	5.35	1.48	1.36
17	6	315	CLA	C3C-C2C	5.35	1.48	1.36
17	B	819	CLA	C3C-C2C	5.35	1.48	1.36
17	B	806	CLA	C3C-C2C	5.35	1.48	1.36
17	G	103	CLA	C3C-C2C	5.35	1.48	1.36
17	8	311	CLA	C3C-C2C	5.35	1.48	1.36
17	b	830	CLA	C3C-C2C	5.35	1.48	1.36
17	A	823	CLA	C3C-C2C	5.35	1.48	1.36
17	B	831	CLA	C3C-C2C	5.35	1.48	1.36
17	b	834	CLA	C3C-C2C	5.36	1.48	1.36
17	j	3002	CLA	C3C-C2C	5.36	1.48	1.36
17	2	613	CLA	C3C-C2C	5.36	1.48	1.36
17	1	202	CLA	C3C-C2C	5.36	1.48	1.36
17	9	609	CLA	C3C-C2C	5.36	1.48	1.36
17	1	308	CLA	C3C-C2C	5.36	1.48	1.36
17	2	611	CLA	C3C-C2C	5.36	1.48	1.36
17	9	613	CLA	C3C-C2C	5.36	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	308	CLA	C3C-C2C	5.36	1.48	1.36
17	a	832	CLA	C3C-C2C	5.36	1.48	1.36
17	A	814	CLA	C3C-C2C	5.36	1.48	1.36
17	A	832	CLA	C3C-C2C	5.36	1.48	1.36
17	6	309	CLA	C3C-C2C	5.36	1.48	1.36
17	B	809	CLA	C3C-C2C	5.36	1.48	1.36
17	B	802	CLA	C3C-C2C	5.36	1.48	1.36
17	A	840	CLA	C3C-C2C	5.36	1.48	1.36
17	a	825	CLA	C3C-C2C	5.36	1.48	1.36
17	3	306	CLA	C3C-C2C	5.37	1.48	1.36
17	1	304	CLA	C3C-C2C	5.37	1.48	1.36
17	1	311	CLA	C3C-C2C	5.37	1.48	1.36
17	b	832	CLA	C3C-C2C	5.37	1.48	1.36
17	A	834	CLA	C3C-C2C	5.37	1.48	1.36
17	A	812	CLA	C3C-C2C	5.37	1.48	1.36
17	3	311	CLA	C3C-C2C	5.37	1.48	1.36
17	b	802	CLA	C3C-C2C	5.37	1.48	1.36
17	a	812	CLA	C3C-C2C	5.37	1.48	1.36
17	b	814	CLA	C3C-C2C	5.37	1.48	1.36
17	a	814	CLA	C3C-C2C	5.37	1.48	1.36
17	4	609	CLA	C3C-C2C	5.38	1.48	1.36
17	a	802	CLA	C3C-C2C	5.38	1.48	1.36
17	9	604	CLA	C3C-C2C	5.38	1.48	1.36
17	J	3002	CLA	C3C-C2C	5.38	1.48	1.36
17	A	817	CLA	C3C-C2C	5.38	1.48	1.36
17	2	612	CLA	C3C-C2C	5.38	1.48	1.36
17	b	803	CLA	C3C-C2C	5.38	1.48	1.36
17	4	614	CLA	C3C-C2C	5.38	1.48	1.36
17	K	4003	CLA	C3C-C2C	5.38	1.48	1.36
17	A	815	CLA	C3C-C2C	5.38	1.48	1.36
17	A	831	CLA	C3C-C2C	5.38	1.48	1.36
17	2	603	CLA	C3C-C2C	5.39	1.48	1.36
17	b	811	CLA	C3C-C2C	5.39	1.48	1.36
17	9	611	CLA	C3C-C2C	5.39	1.48	1.36
17	a	810	CLA	C3C-C2C	5.39	1.48	1.36
17	B	805	CLA	C3C-C2C	5.40	1.48	1.36
17	2	610	CLA	C3C-C2C	5.40	1.48	1.36
17	2	604	CLA	C3C-C2C	5.40	1.48	1.36
17	2	608	CLA	C3C-C2C	5.40	1.48	1.36
17	A	820	CLA	C3C-C2C	5.40	1.48	1.36
17	a	820	CLA	C3C-C2C	5.40	1.48	1.36
17	B	837	CLA	C3C-C2C	5.40	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	612	CLA	C3C-C2C	5.40	1.48	1.36
17	7	604	CLA	C3C-C2C	5.40	1.48	1.36
17	a	835	CLA	C3C-C2C	5.40	1.48	1.36
17	8	305	CLA	C3C-C2C	5.40	1.48	1.36
17	B	811	CLA	C3C-C2C	5.41	1.48	1.36
17	8	307	CLA	C3C-C2C	5.41	1.48	1.36
17	a	822	CLA	C3C-C2C	5.41	1.48	1.36
17	L	204	CLA	C3C-C2C	5.41	1.48	1.36
17	3	313	CLA	C3C-C2C	5.41	1.48	1.36
17	B	803	CLA	C3C-C2C	5.41	1.48	1.36
17	a	824	CLA	C3C-C2C	5.41	1.48	1.36
17	4	601	CLA	C3C-C2C	5.41	1.48	1.36
17	a	833	CLA	C3C-C2C	5.41	1.48	1.36
17	B	832	CLA	C3C-C2C	5.41	1.48	1.36
17	a	811	CLA	C3C-C2C	5.42	1.48	1.36
17	a	840	CLA	C3C-C2C	5.42	1.48	1.36
17	B	836	CLA	C3C-C2C	5.42	1.48	1.36
17	a	815	CLA	C3C-C2C	5.43	1.48	1.36
17	b	810	CLA	C3C-C2C	5.43	1.48	1.36
17	8	309	CLA	C3C-C2C	5.44	1.48	1.36
17	a	846	CLA	C3C-C2C	5.45	1.48	1.36
17	b	837	CLA	C3C-C2C	5.45	1.48	1.36
17	a	809	CLA	C3C-C2C	5.45	1.48	1.36
17	b	840	CLA	C3C-C2C	5.46	1.48	1.36
17	k	1403	CLA	C3C-C2C	5.46	1.48	1.36
17	b	809	CLA	C3B-C2B	5.46	1.47	1.40
17	7	608	CLA	C3C-C2C	5.47	1.48	1.36
17	b	839	CLA	C3C-C2C	5.47	1.48	1.36
17	B	809	CLA	C3B-C2B	5.47	1.47	1.40
17	a	828	CLA	C3C-C2C	5.49	1.48	1.36
17	B	826	CLA	C3C-C2C	5.49	1.48	1.36
17	a	827	CLA	C3C-C2C	5.49	1.48	1.36
17	B	840	CLA	C3C-C2C	5.50	1.48	1.36
17	A	845	CLA	C3C-C2C	5.51	1.48	1.36
17	A	827	CLA	C3C-C2C	5.53	1.48	1.36
17	B	823	CLA	C3C-C2C	5.53	1.48	1.36
17	b	829	CLA	C3B-C2B	5.54	1.47	1.40
17	A	831	CLA	C3B-C2B	5.57	1.47	1.40
17	A	841	CLA	C3C-C2C	5.58	1.48	1.36
17	3	315	CLA	C2B-C1B	5.67	1.49	1.40
17	8	313	CLA	C2B-C1B	5.67	1.49	1.40
17	a	831	CLA	C3B-C2B	5.71	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	843	CLA	C3B-C2B	5.72	1.47	1.40
17	b	818	CLA	C3B-C2B	5.72	1.47	1.40
17	b	802	CLA	C3B-C2B	5.73	1.47	1.40
17	B	827	CLA	C3B-C2B	5.74	1.47	1.40
17	B	802	CLA	C3B-C2B	5.77	1.48	1.40
17	A	822	CLA	C3B-C2B	5.78	1.48	1.40
17	a	844	CLA	C3B-C2B	5.78	1.48	1.40
17	b	816	CLA	C3B-C2B	5.82	1.48	1.40
17	A	826	CLA	C3B-C2B	5.83	1.48	1.40
17	A	820	CLA	C3B-C2B	5.84	1.48	1.40
17	l	204	CLA	C3B-C2B	5.84	1.48	1.40
17	3	315	CLA	C3C-C2C	5.85	1.48	1.35
17	9	604	CLA	C3B-C2B	5.86	1.48	1.40
17	a	822	CLA	C3B-C2B	5.86	1.48	1.40
17	7	602	CLA	C3B-C2B	5.86	1.48	1.40
17	A	803	CLA	C3B-C2B	5.86	1.48	1.40
17	8	313	CLA	C3C-C2C	5.87	1.48	1.35
17	a	803	CLA	C3B-C2B	5.87	1.48	1.40
17	B	816	CLA	C3B-C2B	5.88	1.48	1.40
17	A	804	CLA	C3B-C2B	5.89	1.48	1.40
17	A	838	CLA	C3B-C2B	5.89	1.48	1.40
17	b	837	CLA	C3B-C2B	5.89	1.48	1.40
17	A	801	CLA	C3B-C2B	5.90	1.48	1.40
17	a	829	CLA	C3B-C2B	5.90	1.48	1.40
17	a	836	CLA	C3B-C2B	5.90	1.48	1.40
17	A	836	CLA	C3B-C2B	5.90	1.48	1.40
17	A	833	CLA	C3B-C2B	5.91	1.48	1.40
17	A	829	CLA	C3B-C2B	5.91	1.48	1.40
17	b	827	CLA	C3B-C2B	5.91	1.48	1.40
17	B	824	CLA	C3B-C2B	5.91	1.48	1.40
17	B	832	CLA	C3B-C2B	5.91	1.48	1.40
17	B	814	CLA	C3B-C2B	5.91	1.48	1.40
17	b	832	CLA	C3B-C2B	5.91	1.48	1.40
17	8	307	CLA	C3B-C2B	5.92	1.48	1.40
17	3	302	CLA	C3B-C2B	5.92	1.48	1.40
17	B	831	CLA	C3B-C2B	5.93	1.48	1.40
17	B	805	CLA	C3B-C2B	5.93	1.48	1.40
17	a	807	CLA	C3B-C2B	5.94	1.48	1.40
17	b	819	CLA	C3B-C2B	5.95	1.48	1.40
17	l	303	CLA	C3B-C2B	5.95	1.48	1.40
17	B	829	CLA	C3B-C2B	5.96	1.48	1.40
17	A	807	CLA	C3B-C2B	5.96	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	609	CLA	C3B-C2B	5.96	1.48	1.40
17	A	828	CLA	C3B-C2B	5.97	1.48	1.40
17	a	834	CLA	C3B-C2B	5.97	1.48	1.40
17	7	608	CLA	C3B-C2B	5.97	1.48	1.40
17	4	604	CLA	C3B-C2B	5.97	1.48	1.40
17	4	609	CLA	C3B-C2B	5.97	1.48	1.40
17	7	604	CLA	C3B-C2B	5.97	1.48	1.40
17	B	837	CLA	C3B-C2B	5.97	1.48	1.40
17	7	609	CLA	C3B-C2B	5.98	1.48	1.40
17	3	308	CLA	C3B-C2B	5.98	1.48	1.40
17	a	841	CLA	C3B-C2B	5.99	1.48	1.40
17	a	809	CLA	C3B-C2B	6.00	1.48	1.40
17	8	301	CLA	C3B-C2B	6.00	1.48	1.40
17	a	826	CLA	C3B-C2B	6.00	1.48	1.40
17	L	202	CLA	C3B-C2B	6.00	1.48	1.40
17	A	810	CLA	C3B-C2B	6.00	1.48	1.40
17	8	303	CLA	C3B-C2B	6.00	1.48	1.40
17	a	828	CLA	C3B-C2B	6.00	1.48	1.40
17	b	814	CLA	C3B-C2B	6.01	1.48	1.40
17	9	602	CLA	C3B-C2B	6.01	1.48	1.40
17	2	604	CLA	C3B-C2B	6.01	1.48	1.40
17	B	819	CLA	C3B-C2B	6.02	1.48	1.40
17	a	812	CLA	C3B-C2B	6.03	1.48	1.40
17	b	805	CLA	C3B-C2B	6.03	1.48	1.40
17	A	814	CLA	C3B-C2B	6.03	1.48	1.40
17	a	835	CLA	C3B-C2B	6.03	1.48	1.40
17	B	830	CLA	C3B-C2B	6.04	1.48	1.40
17	8	308	CLA	C3B-C2B	6.04	1.48	1.40
17	B	803	CLA	C3B-C2B	6.04	1.48	1.40
17	B	813	CLA	C3B-C2B	6.05	1.48	1.40
17	a	802	CLA	C3B-C2B	6.05	1.48	1.40
17	b	813	CLA	C3B-C2B	6.05	1.48	1.40
17	l	202	CLA	C3B-C2B	6.05	1.48	1.40
17	3	304	CLA	C3B-C2B	6.05	1.48	1.40
17	2	602	CLA	C3B-C2B	6.06	1.48	1.40
17	3	309	CLA	C3B-C2B	6.06	1.48	1.40
17	b	815	CLA	C3B-C2B	6.06	1.48	1.40
17	B	818	CLA	C3B-C2B	6.06	1.48	1.40
17	B	815	CLA	C3B-C2B	6.06	1.48	1.40
17	L	203	CLA	C3B-C2B	6.06	1.48	1.40
17	l	203	CLA	C3B-C2B	6.06	1.48	1.40
17	a	827	CLA	C3B-C2B	6.07	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	828	CLA	C3B-C2B	6.07	1.48	1.40
17	b	831	CLA	C3B-C2B	6.07	1.48	1.40
17	A	840	CLA	C3B-C2B	6.07	1.48	1.40
17	b	826	CLA	C3B-C2B	6.07	1.48	1.40
17	a	840	CLA	C3B-C2B	6.08	1.48	1.40
17	b	824	CLA	C3B-C2B	6.08	1.48	1.40
17	A	834	CLA	C3B-C2B	6.08	1.48	1.40
17	4	602	CLA	C3B-C2B	6.09	1.48	1.40
17	a	839	CLA	C3B-C2B	6.09	1.48	1.40
17	b	830	CLA	C3B-C2B	6.09	1.48	1.40
17	B	833	CLA	C3B-C2B	6.09	1.48	1.40
17	a	811	CLA	C3B-C2B	6.10	1.48	1.40
17	1	306	CLA	C3B-C2B	6.10	1.48	1.40
17	A	835	CLA	C3B-C2B	6.10	1.48	1.40
17	2	609	CLA	C3B-C2B	6.10	1.48	1.40
17	A	815	CLA	C3B-C2B	6.10	1.48	1.40
17	A	827	CLA	C3B-C2B	6.10	1.48	1.40
17	a	801	CLA	C3B-C2B	6.10	1.48	1.40
17	8	302	CLA	C3B-C2B	6.11	1.48	1.40
17	b	833	CLA	C3B-C2B	6.11	1.48	1.40
17	a	838	CLA	C3B-C2B	6.11	1.48	1.40
17	B	825	CLA	C3B-C2B	6.12	1.48	1.40
17	L	204	CLA	C3B-C2B	6.12	1.48	1.40
17	F	304	CLA	C3B-C2B	6.12	1.48	1.40
17	A	802	CLA	C3B-C2B	6.12	1.48	1.40
17	b	825	CLA	C3B-C2B	6.12	1.48	1.40
17	b	828	CLA	C3B-C2B	6.12	1.48	1.40
17	b	803	CLA	C3B-C2B	6.12	1.48	1.40
17	a	808	CLA	C3B-C2B	6.13	1.48	1.40
17	B	806	CLA	C3B-C2B	6.13	1.48	1.40
17	9	614	CLA	C3B-C2B	6.13	1.48	1.40
17	6	305	CLA	C3B-C2B	6.14	1.48	1.40
17	A	816	CLA	C3B-C2B	6.14	1.48	1.40
17	a	843	CLA	C3B-C2B	6.14	1.48	1.40
17	7	603	CLA	C3B-C2B	6.14	1.48	1.40
17	6	311	CLA	C3B-C2B	6.14	1.48	1.40
17	a	846	CLA	C3B-C2B	6.14	1.48	1.40
17	9	603	CLA	C3B-C2B	6.15	1.48	1.40
17	A	809	CLA	C3B-C2B	6.15	1.48	1.40
17	a	805	CLA	C3B-C2B	6.15	1.48	1.40
17	A	811	CLA	C3B-C2B	6.15	1.48	1.40
17	a	833	CLA	C3B-C2B	6.15	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	835	CLA	C3B-C2B	6.15	1.48	1.40
17	a	816	CLA	C3B-C2B	6.15	1.48	1.40
17	6	306	CLA	C3B-C2B	6.15	1.48	1.40
17	a	814	CLA	C3B-C2B	6.15	1.48	1.40
17	a	817	CLA	C3B-C2B	6.16	1.48	1.40
17	A	823	CLA	C3B-C2B	6.16	1.48	1.40
17	a	832	CLA	C3B-C2B	6.16	1.48	1.40
17	B	812	CLA	C3B-C2B	6.16	1.48	1.40
17	a	837	CLA	C3B-C2B	6.16	1.48	1.40
17	G	103	CLA	C3B-C2B	6.16	1.48	1.40
17	a	824	CLA	C3B-C2B	6.17	1.48	1.40
17	A	839	CLA	C3B-C2B	6.17	1.48	1.40
17	A	841	CLA	C3B-C2B	6.17	1.48	1.40
17	2	608	CLA	C3B-C2B	6.17	1.48	1.40
17	a	842	CLA	C3B-C2B	6.17	1.48	1.40
17	k	1402	CLA	C3B-C2B	6.17	1.48	1.40
17	6	304	CLA	C3B-C2B	6.17	1.48	1.40
17	b	835	CLA	C3B-C2B	6.17	1.48	1.40
17	A	813	CLA	C3B-C2B	6.18	1.48	1.40
17	A	819	CLA	C3B-C2B	6.18	1.48	1.40
17	b	808	CLA	C3B-C2B	6.18	1.48	1.40
17	B	823	CLA	C3B-C2B	6.18	1.48	1.40
17	a	820	CLA	C3B-C2B	6.18	1.48	1.40
17	g	101	CLA	C3B-C2B	6.18	1.48	1.40
17	F	303	CLA	C3B-C2B	6.18	1.48	1.40
17	3	305	CLA	C3B-C2B	6.18	1.48	1.40
17	B	841	CLA	C3B-C2B	6.19	1.48	1.40
17	G	104	CLA	C3B-C2B	6.19	1.48	1.40
17	6	314	CLA	C3B-C2B	6.19	1.48	1.40
17	a	815	CLA	C3B-C2B	6.19	1.48	1.40
17	f	7002	CLA	C3B-C2B	6.19	1.48	1.40
17	4	614	CLA	C3B-C2B	6.19	1.48	1.40
17	b	822	CLA	C3B-C2B	6.19	1.48	1.40
17	4	603	CLA	C3B-C2B	6.19	1.48	1.40
17	b	840	CLA	C3B-C2B	6.20	1.48	1.40
17	b	806	CLA	C3B-C2B	6.20	1.48	1.40
17	B	817	CLA	C3B-C2B	6.20	1.48	1.40
17	4	611	CLA	C3B-C2B	6.20	1.48	1.40
17	a	819	CLA	C3B-C2B	6.20	1.48	1.40
17	9	608	CLA	C3B-C2B	6.20	1.48	1.40
17	6	307	CLA	C3B-C2B	6.21	1.48	1.40
17	2	610	CLA	C3B-C2B	6.21	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	838	CLA	C3B-C2B	6.21	1.48	1.40
17	B	808	CLA	C3B-C2B	6.21	1.48	1.40
17	4	601	CLA	C3B-C2B	6.21	1.48	1.40
17	a	825	CLA	C3B-C2B	6.22	1.48	1.40
17	A	845	CLA	C3B-C2B	6.22	1.48	1.40
17	3	303	CLA	C3B-C2B	6.22	1.48	1.40
17	B	839	CLA	C3B-C2B	6.22	1.48	1.40
17	1	310	CLA	C3B-C2B	6.22	1.48	1.40
17	B	840	CLA	C3B-C2B	6.22	1.48	1.40
17	1	305	CLA	C3B-C2B	6.23	1.48	1.40
17	A	832	CLA	C3B-C2B	6.23	1.48	1.40
17	A	842	CLA	C3B-C2B	6.23	1.48	1.40
17	a	823	CLA	C3B-C2B	6.23	1.48	1.40
17	A	812	CLA	C3B-C2B	6.23	1.48	1.40
17	2	612	CLA	C3B-C2B	6.23	1.48	1.40
17	G	101	CLA	C3B-C2B	6.23	1.48	1.40
17	1	308	CLA	C3B-C2B	6.24	1.48	1.40
17	7	611	CLA	C3B-C2B	6.24	1.48	1.40
17	b	821	CLA	C3B-C2B	6.24	1.48	1.40
17	a	856	CLA	C3B-C2B	6.24	1.48	1.40
17	b	823	CLA	C3B-C2B	6.25	1.48	1.40
17	F	301	CLA	C3B-C2B	6.25	1.48	1.40
17	b	804	CLA	C3B-C2B	6.25	1.48	1.40
17	b	841	CLA	C3B-C2B	6.26	1.48	1.40
17	A	817	CLA	C3B-C2B	6.26	1.48	1.40
17	b	810	CLA	C3B-C2B	6.26	1.48	1.40
17	b	807	CLA	C3B-C2B	6.26	1.48	1.40
17	9	611	CLA	C3B-C2B	6.26	1.48	1.40
17	B	834	CLA	C3B-C2B	6.26	1.48	1.40
17	8	304	CLA	C3B-C2B	6.26	1.48	1.40
17	9	610	CLA	C3B-C2B	6.26	1.48	1.40
17	B	804	CLA	C3B-C2B	6.26	1.48	1.40
17	b	817	CLA	C3B-C2B	6.26	1.48	1.40
17	b	820	CLA	C3B-C2B	6.27	1.48	1.40
17	6	313	CLA	C3B-C2B	6.27	1.48	1.40
17	2	613	CLA	C3B-C2B	6.27	1.48	1.40
17	2	603	CLA	C3B-C2B	6.27	1.48	1.40
18	B	842	PQN	C3-C2	6.27	1.49	1.35
17	b	834	CLA	C3B-C2B	6.27	1.48	1.40
17	1	313	CLA	C3B-C2B	6.28	1.48	1.40
17	9	613	CLA	C3B-C2B	6.28	1.48	1.40
17	B	810	CLA	C3B-C2B	6.28	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	844	PQN	C3-C2	6.28	1.49	1.35
17	2	611	CLA	C3B-C2B	6.29	1.48	1.40
17	4	610	CLA	C3B-C2B	6.29	1.48	1.40
17	9	601	CLA	C3B-C2B	6.29	1.48	1.40
17	k	1401	CLA	C3B-C2B	6.29	1.48	1.40
17	a	806	CLA	C3B-C2B	6.29	1.48	1.40
17	7	610	CLA	C3B-C2B	6.30	1.48	1.40
17	g	103	CLA	C3B-C2B	6.30	1.48	1.40
17	1	304	CLA	C3B-C2B	6.30	1.48	1.40
17	1	314	CLA	C3B-C2B	6.31	1.48	1.40
17	8	312	CLA	C3B-C2B	6.31	1.48	1.40
17	B	826	CLA	C3B-C2B	6.31	1.48	1.40
17	B	821	CLA	C3B-C2B	6.31	1.48	1.40
17	4	613	CLA	C3B-C2B	6.31	1.48	1.40
17	b	839	CLA	C3B-C2B	6.31	1.48	1.40
17	a	821	CLA	C3B-C2B	6.31	1.48	1.40
17	8	310	CLA	C3B-C2B	6.31	1.48	1.40
17	7	613	CLA	C3B-C2B	6.31	1.48	1.40
17	a	810	CLA	C3B-C2B	6.32	1.48	1.40
17	1	312	CLA	C3B-C2B	6.32	1.48	1.40
17	A	825	CLA	C3B-C2B	6.32	1.48	1.40
17	4	608	CLA	C3B-C2B	6.32	1.48	1.40
17	B	822	CLA	C3B-C2B	6.33	1.48	1.40
17	A	805	CLA	C3B-C2B	6.33	1.48	1.40
17	8	305	CLA	C3B-C2B	6.33	1.48	1.40
17	b	812	CLA	C3B-C2B	6.33	1.48	1.40
17	A	824	CLA	C3B-C2B	6.33	1.48	1.40
17	g	102	CLA	C3B-C2B	6.34	1.48	1.40
17	B	807	CLA	C3B-C2B	6.34	1.48	1.40
17	9	612	CLA	C3B-C2B	6.34	1.48	1.40
17	A	818	CLA	C3B-C2B	6.34	1.48	1.40
17	6	309	CLA	C3B-C2B	6.34	1.48	1.40
17	A	806	CLA	C3B-C2B	6.34	1.48	1.40
17	1	309	CLA	C3B-C2B	6.35	1.48	1.40
17	K	4002	CLA	C3B-C2B	6.35	1.48	1.40
17	1	311	CLA	C3B-C2B	6.35	1.48	1.40
17	B	820	CLA	C3B-C2B	6.35	1.48	1.40
17	A	821	CLA	C3B-C2B	6.36	1.48	1.40
18	b	842	PQN	C3-C2	6.36	1.49	1.35
17	K	4003	CLA	C3B-C2B	6.36	1.48	1.40
17	3	301	CLA	C3B-C2B	6.36	1.48	1.40
17	3	311	CLA	C3B-C2B	6.37	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	k	1403	CLA	C3B-C2B	6.37	1.48	1.40
17	6	315	CLA	C3B-C2B	6.37	1.48	1.40
17	6	316	CLA	C3B-C2B	6.38	1.48	1.40
17	3	314	CLA	C3B-C2B	6.38	1.48	1.40
17	3	312	CLA	C3B-C2B	6.38	1.48	1.40
17	A	837	CLA	C3B-C2B	6.38	1.48	1.40
17	6	310	CLA	C3B-C2B	6.38	1.48	1.40
17	7	612	CLA	C3B-C2B	6.39	1.48	1.40
17	J	3002	CLA	C3B-C2B	6.39	1.48	1.40
17	6	312	CLA	C3B-C2B	6.40	1.48	1.40
17	3	313	CLA	C3B-C2B	6.40	1.48	1.40
17	8	309	CLA	C3B-C2B	6.40	1.48	1.40
17	1	315	CLA	C3B-C2B	6.40	1.48	1.40
17	f	7003	CLA	C3B-C2B	6.41	1.48	1.40
17	3	310	CLA	C3B-C2B	6.41	1.48	1.40
17	a	813	CLA	C3B-C2B	6.42	1.48	1.40
17	4	612	CLA	C3B-C2B	6.42	1.48	1.40
17	8	311	CLA	C3B-C2B	6.42	1.48	1.40
18	a	845	PQN	C3-C2	6.43	1.49	1.35
17	j	3002	CLA	C3B-C2B	6.47	1.48	1.40
17	A	854	CLA	C3B-C2B	6.49	1.48	1.40
17	a	818	CLA	C3B-C2B	6.50	1.48	1.40
17	3	306	CLA	C3B-C2B	6.50	1.48	1.40
17	A	830	CLA	C3B-C2B	6.53	1.49	1.40
17	A	808	CLA	C3B-C2B	6.63	1.49	1.40
17	b	836	CLA	C3B-C2B	6.64	1.49	1.40
17	a	830	CLA	C3B-C2B	6.64	1.49	1.40
17	b	838	CLA	C3B-C2B	6.67	1.49	1.40
17	a	804	CLA	C3B-C2B	6.72	1.49	1.40
17	B	836	CLA	C3B-C2B	6.78	1.49	1.40
26	8	306	CHL	C3C-C2C	10.39	1.47	1.34
26	9	607	CHL	C3C-C2C	10.51	1.47	1.34
26	4	607	CHL	C3C-C2C	10.66	1.47	1.34
26	3	307	CHL	C3C-C2C	10.70	1.47	1.34
26	2	607	CHL	C3C-C2C	10.73	1.47	1.34
26	6	303	CHL	C3C-C2C	10.73	1.47	1.34
26	7	607	CHL	C3C-C2C	10.75	1.47	1.34
26	9	606	CHL	C3C-C2C	10.76	1.47	1.34
26	1	302	CHL	C3C-C2C	10.80	1.47	1.34
26	7	601	CHL	C3C-C2C	10.84	1.48	1.34
26	6	308	CHL	C3C-C2C	10.85	1.48	1.34
26	9	615	CHL	C3C-C2C	10.85	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	615	CHL	C3C-C2C	10.88	1.48	1.34
26	2	606	CHL	C3C-C2C	10.89	1.48	1.34
26	7	614	CHL	C3C-C2C	10.90	1.48	1.34
26	7	606	CHL	C3C-C2C	10.94	1.48	1.34
26	4	606	CHL	C3C-C2C	10.94	1.48	1.34
26	1	307	CHL	C3C-C2C	10.94	1.48	1.34
26	2	614	CHL	C3C-C2C	10.97	1.48	1.34
26	2	601	CHL	C3C-C2C	11.00	1.48	1.34
26	9	605	CHL	C3C-C2C	11.00	1.48	1.34
26	7	605	CHL	C3C-C2C	11.02	1.48	1.34
26	4	605	CHL	C3C-C2C	11.05	1.48	1.34
26	2	605	CHL	C3C-C2C	11.10	1.48	1.34

All (7028) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	307	CHL	C1C-C2C-C3C	-9.14	102.40	111.52
26	9	607	CHL	C1C-C2C-C3C	-9.04	102.51	111.52
26	8	306	CHL	C1C-C2C-C3C	-8.95	102.60	111.52
26	4	607	CHL	C1C-C2C-C3C	-8.92	102.63	111.52
26	7	614	CHL	C1C-C2C-C3C	-8.83	102.72	111.52
26	2	607	CHL	C1C-C2C-C3C	-8.83	102.72	111.52
26	6	308	CHL	C1C-C2C-C3C	-8.72	102.83	111.52
26	9	615	CHL	C1C-C2C-C3C	-8.68	102.86	111.52
26	7	607	CHL	C1C-C2C-C3C	-8.67	102.87	111.52
26	1	307	CHL	C1C-C2C-C3C	-8.66	102.89	111.52
26	2	606	CHL	C1C-C2C-C3C	-8.65	102.90	111.52
26	9	606	CHL	C1C-C2C-C3C	-8.63	102.92	111.52
26	2	614	CHL	C1C-C2C-C3C	-8.61	102.94	111.52
26	7	606	CHL	C1C-C2C-C3C	-8.60	102.95	111.52
26	4	605	CHL	C1C-C2C-C3C	-8.58	102.97	111.52
26	9	605	CHL	C1C-C2C-C3C	-8.56	102.99	111.52
26	6	303	CHL	C1C-C2C-C3C	-8.50	103.05	111.52
26	4	615	CHL	C1C-C2C-C3C	-8.48	103.06	111.52
26	2	605	CHL	C1C-C2C-C3C	-8.48	103.07	111.52
26	2	601	CHL	C1C-C2C-C3C	-8.46	103.09	111.52
26	1	302	CHL	C1C-C2C-C3C	-8.46	103.09	111.52
26	7	605	CHL	C1C-C2C-C3C	-8.26	103.28	111.52
26	4	606	CHL	C1C-C2C-C3C	-8.19	103.36	111.52
26	7	601	CHL	C1C-C2C-C3C	-8.18	103.37	111.52
17	8	313	CLA	C3D-C2D-C1D	-7.46	99.87	106.30
17	3	315	CLA	C3D-C2D-C1D	-7.36	99.96	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	313	CLA	C3B-C2B-C1B	-7.24	100.09	106.29
17	3	315	CLA	C3B-C2B-C1B	-7.20	100.13	106.29
17	3	315	CLA	C3A-C4A-CHB	-7.05	116.20	123.88
17	8	313	CLA	C3A-C4A-CHB	-6.96	116.31	123.88
28	6	318	XAT	C18-C5-C6	-6.68	111.01	122.31
28	1	317	XAT	C18-C5-C6	-6.64	111.08	122.31
28	2	616	XAT	C38-C25-C26	-6.53	111.27	122.31
28	7	616	XAT	C18-C5-C6	-6.49	111.33	122.31
20	a	849	BCR	C15-C14-C13	-6.48	118.06	127.31
28	2	616	XAT	C18-C5-C6	-6.48	111.35	122.31
28	6	318	XAT	C38-C25-C26	-6.43	111.44	122.31
26	4	605	CHL	CBA-CAA-C2A	-6.42	106.90	115.76
28	8	315	XAT	C38-C25-C26	-6.42	111.45	122.31
26	9	605	CHL	CBA-CAA-C2A	-6.38	106.95	115.76
28	7	616	XAT	C38-C25-C26	-6.38	111.51	122.31
28	9	617	XAT	C38-C25-C26	-6.36	111.55	122.31
28	9	617	XAT	C18-C5-C6	-6.35	111.56	122.31
28	8	315	XAT	C18-C5-C6	-6.34	111.58	122.31
28	3	317	XAT	C18-C5-C6	-6.31	111.63	122.31
28	1	317	XAT	C38-C25-C26	-6.30	111.66	122.31
17	B	826	CLA	CHD-C4C-C3C	-6.22	115.54	124.92
17	a	828	CLA	CHD-C4C-C3C	-6.18	115.61	124.92
20	7	617	BCR	C24-C23-C22	-6.17	116.94	126.21
28	4	617	XAT	C38-C25-C26	-6.12	111.95	122.31
17	a	838	CLA	CHD-C4C-C3C	-6.08	115.76	124.92
17	A	828	CLA	CHD-C4C-C3C	-6.07	115.77	124.92
28	4	617	XAT	C18-C5-C6	-6.07	112.05	122.31
17	a	821	CLA	CHD-C4C-C3C	-5.99	115.89	124.92
28	3	317	XAT	C38-C25-C26	-5.98	112.19	122.31
17	B	836	CLA	CHD-C4C-C3C	-5.97	115.92	124.92
20	a	849	BCR	C24-C23-C22	-5.96	117.26	126.21
20	b	845	BCR	C7-C8-C9	-5.94	117.28	126.21
17	B	811	CLA	C1B-C2B-C3B	-5.91	101.42	106.92
20	B	844	BCR	C7-C8-C9	-5.90	117.34	126.21
20	b	844	BCR	C7-C8-C9	-5.89	117.36	126.21
17	a	809	CLA	CHD-C4C-C3C	-5.88	116.06	124.92
17	b	811	CLA	C1B-C2B-C3B	-5.88	101.45	106.92
20	j	3004	BCR	C20-C21-C22	-5.84	118.97	127.31
17	b	827	CLA	CHD-C4C-C3C	-5.84	116.11	124.92
17	A	810	CLA	CHD-C4C-C3C	-5.84	116.12	124.92
17	A	841	CLA	CHD-C4C-C3C	-5.84	116.12	124.92
17	f	7002	CLA	CHD-C4C-C3C	-5.83	116.13	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	802	CLA	CHD-C4C-C3C	-5.81	116.17	124.92
17	4	603	CLA	CHD-C4C-C3C	-5.80	116.18	124.92
17	a	830	CLA	CHD-C4C-C3C	-5.80	116.18	124.92
17	A	805	CLA	CHD-C4C-C3C	-5.80	116.18	124.92
17	A	826	CLA	CHD-C4C-C3C	-5.80	116.18	124.92
17	b	840	CLA	CHD-C4C-C3C	-5.79	116.19	124.92
20	b	843	BCR	C16-C17-C18	-5.79	119.05	127.31
17	a	808	CLA	CHD-C4C-C3C	-5.79	116.20	124.92
17	b	836	CLA	CHD-C4C-C3C	-5.77	116.22	124.92
17	B	841	CLA	CHD-C4C-C3C	-5.77	116.23	124.92
17	b	828	CLA	CHD-C4C-C3C	-5.76	116.24	124.92
20	A	852	BCR	C7-C8-C9	-5.75	117.57	126.21
17	a	826	CLA	CHD-C4C-C3C	-5.74	116.27	124.92
17	B	814	CLA	CHD-C4C-C3C	-5.73	116.28	124.92
17	a	807	CLA	CHD-C4C-C3C	-5.73	116.29	124.92
17	b	806	CLA	CHD-C4C-C3C	-5.72	116.30	124.92
17	B	838	CLA	CHD-C4C-C3C	-5.72	116.30	124.92
20	j	3004	BCR	C24-C23-C22	-5.71	117.63	126.21
17	A	819	CLA	CHD-C4C-C3C	-5.71	116.31	124.92
17	b	826	CLA	CHD-C4C-C3C	-5.71	116.31	124.92
17	A	818	CLA	CHD-C4C-C3C	-5.70	116.33	124.92
17	a	856	CLA	C1C-NC-C4C	-5.70	103.78	107.06
17	a	821	CLA	C1C-NC-C4C	-5.70	103.78	107.06
20	7	617	BCR	C15-C14-C13	-5.69	119.19	127.31
17	A	830	CLA	CHD-C4C-C3C	-5.69	116.35	124.92
17	A	854	CLA	CHD-C4C-C3C	-5.68	116.35	124.92
17	B	837	CLA	CHD-C4C-C3C	-5.68	116.35	124.92
17	b	811	CLA	CHD-C4C-C3C	-5.68	116.36	124.92
17	b	804	CLA	CHD-C4C-C3C	-5.68	116.36	124.92
17	a	801	CLA	CHD-C4C-C3C	-5.68	116.36	124.92
17	3	306	CLA	CHD-C4C-C3C	-5.68	116.36	124.92
17	a	823	CLA	CHD-C4C-C3C	-5.67	116.37	124.92
17	A	829	CLA	CHD-C4C-C3C	-5.67	116.37	124.92
17	b	839	CLA	CHD-C4C-C3C	-5.67	116.38	124.92
17	B	825	CLA	CHD-C4C-C3C	-5.65	116.40	124.92
17	b	822	CLA	CHD-C4C-C3C	-5.65	116.40	124.92
17	a	816	CLA	CHD-C4C-C3C	-5.65	116.40	124.92
17	A	821	CLA	CHD-C4C-C3C	-5.64	116.41	124.92
17	B	806	CLA	CHD-C4C-C3C	-5.63	116.44	124.92
17	B	827	CLA	CHD-C4C-C3C	-5.62	116.45	124.92
17	9	602	CLA	CHD-C4C-C3C	-5.62	116.45	124.92
17	a	815	CLA	CHD-C4C-C3C	-5.61	116.47	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	805	CLA	CHD-C4C-C3C	-5.61	116.47	124.92
17	6	312	CLA	CHD-C4C-C3C	-5.61	116.47	124.92
17	b	825	CLA	CHD-C4C-C3C	-5.61	116.47	124.92
17	a	835	CLA	CHD-C4C-C3C	-5.60	116.47	124.92
17	b	814	CLA	CHD-C4C-C3C	-5.60	116.47	124.92
17	a	833	CLA	CHD-C4C-C3C	-5.60	116.48	124.92
17	a	804	CLA	CHD-C4C-C3C	-5.60	116.48	124.92
17	b	809	CLA	CHD-C4C-C3C	-5.59	116.50	124.92
17	a	843	CLA	CHD-C4C-C3C	-5.59	116.50	124.92
17	l	204	CLA	CHD-C4C-C3C	-5.58	116.51	124.92
17	B	818	CLA	CHD-C4C-C3C	-5.58	116.51	124.92
17	9	603	CLA	CHD-C4C-C3C	-5.58	116.51	124.92
17	a	806	CLA	CHD-C4C-C3C	-5.57	116.52	124.92
17	A	838	CLA	CHD-C4C-C3C	-5.57	116.52	124.92
17	A	836	CLA	C1C-NC-C4C	-5.57	103.85	107.06
17	b	820	CLA	CHD-C4C-C3C	-5.57	116.52	124.92
17	A	833	CLA	CHD-C4C-C3C	-5.57	116.52	124.92
17	B	840	CLA	CHD-C4C-C3C	-5.57	116.52	124.92
17	B	815	CLA	CHD-C4C-C3C	-5.57	116.53	124.92
17	l	203	CLA	CHD-C4C-C3C	-5.56	116.53	124.92
17	b	810	CLA	CHD-C4C-C3C	-5.56	116.54	124.92
17	B	828	CLA	CHD-C4C-C3C	-5.56	116.55	124.92
17	A	854	CLA	C1C-NC-C4C	-5.55	103.86	107.06
17	a	814	CLA	CHD-C4C-C3C	-5.55	116.55	124.92
17	6	309	CLA	CHD-C4C-C3C	-5.55	116.55	124.92
17	A	804	CLA	CHD-C4C-C3C	-5.55	116.56	124.92
20	A	851	BCR	C24-C23-C22	-5.54	117.88	126.21
17	B	824	CLA	CHD-C4C-C3C	-5.54	116.57	124.92
17	a	825	CLA	CHD-C4C-C3C	-5.54	116.58	124.92
17	b	841	CLA	CHD-C4C-C3C	-5.54	116.58	124.92
17	a	827	CLA	CHD-C4C-C3C	-5.53	116.58	124.92
17	A	821	CLA	C1C-NC-C4C	-5.53	103.88	107.06
17	a	834	CLA	CHD-C4C-C3C	-5.53	116.59	124.92
17	F	303	CLA	CHD-C4C-C3C	-5.52	116.59	124.92
17	A	840	CLA	CHD-C4C-C3C	-5.52	116.59	124.92
17	3	309	CLA	CHD-C4C-C3C	-5.52	116.59	124.92
17	A	834	CLA	CHD-C4C-C3C	-5.52	116.60	124.92
17	G	101	CLA	CHD-C4C-C3C	-5.52	116.60	124.92
17	8	312	CLA	CHD-C4C-C3C	-5.51	116.61	124.92
17	2	603	CLA	CHD-C4C-C3C	-5.51	116.61	124.92
17	a	842	CLA	CHD-C4C-C3C	-5.51	116.61	124.92
17	1	306	CLA	CHD-C4C-C3C	-5.51	116.61	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	823	CLA	CHD-C4C-C3C	-5.51	116.61	124.92
17	4	609	CLA	CHD-C4C-C3C	-5.51	116.62	124.92
17	A	836	CLA	CHD-C4C-C3C	-5.51	116.62	124.92
17	G	103	CLA	CHD-C4C-C3C	-5.51	116.62	124.92
17	A	815	CLA	CHD-C4C-C3C	-5.51	116.62	124.92
17	B	820	CLA	CHD-C4C-C3C	-5.51	116.62	124.92
17	6	310	CLA	CHD-C4C-C3C	-5.50	116.62	124.92
17	b	831	CLA	CHD-C4C-C3C	-5.50	116.62	124.92
17	a	836	CLA	CHD-C4C-C3C	-5.50	116.63	124.92
20	K	4001	BCR	C15-C14-C13	-5.50	119.46	127.31
17	b	834	CLA	CHD-C4C-C3C	-5.50	116.63	124.92
17	b	838	CLA	CHD-C4C-C3C	-5.50	116.63	124.92
17	A	803	CLA	CHD-C4C-C3C	-5.49	116.65	124.92
17	1	312	CLA	CHD-C4C-C3C	-5.49	116.65	124.92
17	A	812	CLA	CHD-C4C-C3C	-5.48	116.67	124.92
17	k	1401	CLA	CHD-C4C-C3C	-5.48	116.67	124.92
20	7	617	BCR	C11-C10-C9	-5.48	119.50	127.31
17	a	819	CLA	CHD-C4C-C3C	-5.47	116.67	124.92
17	b	824	CLA	CHD-C4C-C3C	-5.47	116.67	124.92
17	a	844	CLA	CHD-C4C-C3C	-5.47	116.67	124.92
17	4	614	CLA	CHD-C4C-C3C	-5.47	116.67	124.92
17	A	808	CLA	CHD-C4C-C3C	-5.47	116.67	124.92
17	A	827	CLA	CHD-C4C-C3C	-5.47	116.67	124.92
17	B	833	CLA	CHD-C4C-C3C	-5.47	116.68	124.92
20	j	3004	BCR	C16-C17-C18	-5.47	119.51	127.31
17	3	314	CLA	CHD-C4C-C3C	-5.47	116.68	124.92
17	A	823	CLA	CHD-C4C-C3C	-5.47	116.68	124.92
17	B	809	CLA	CHD-C4C-C3C	-5.46	116.69	124.92
17	A	801	CLA	CHD-C4C-C3C	-5.45	116.70	124.92
17	a	824	CLA	CHD-C4C-C3C	-5.45	116.70	124.92
17	a	810	CLA	CHD-C4C-C3C	-5.45	116.71	124.92
17	B	811	CLA	CHD-C4C-C3C	-5.45	116.71	124.92
17	a	840	CLA	CHD-C4C-C3C	-5.45	116.71	124.92
17	B	821	CLA	CHD-C4C-C3C	-5.44	116.71	124.92
17	K	4003	CLA	CHD-C4C-C3C	-5.44	116.71	124.92
17	8	301	CLA	CHD-C4C-C3C	-5.44	116.72	124.92
17	7	603	CLA	CHD-C4C-C3C	-5.44	116.72	124.92
17	L	204	CLA	CHD-C4C-C3C	-5.44	116.72	124.92
17	3	305	CLA	CHD-C4C-C3C	-5.44	116.72	124.92
17	a	839	CLA	CHD-C4C-C3C	-5.44	116.72	124.92
17	B	835	CLA	CHD-C4C-C3C	-5.43	116.73	124.92
17	9	610	CLA	CHD-C4C-C3C	-5.43	116.73	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	601	CLA	CHD-C4C-C3C	-5.43	116.74	124.92
17	A	816	CLA	CHD-C4C-C3C	-5.43	116.74	124.92
17	b	832	CLA	CHD-C4C-C3C	-5.43	116.74	124.92
17	B	832	CLA	CHD-C4C-C3C	-5.43	116.74	124.92
17	B	807	CLA	CHD-C4C-C3C	-5.43	116.74	124.92
17	A	802	CLA	CHD-C4C-C3C	-5.43	116.74	124.92
17	G	104	CLA	CHD-C4C-C3C	-5.42	116.74	124.92
17	8	307	CLA	CHD-C4C-C3C	-5.42	116.74	124.92
17	7	602	CLA	CHD-C4C-C3C	-5.42	116.75	124.92
17	8	311	CLA	CHD-C4C-C3C	-5.42	116.75	124.92
17	4	610	CLA	CHD-C4C-C3C	-5.42	116.75	124.92
17	a	829	CLA	CHD-C4C-C3C	-5.42	116.75	124.92
17	b	833	CLA	CHD-C4C-C3C	-5.42	116.75	124.92
17	l	202	CLA	CHD-C4C-C3C	-5.42	116.75	124.92
17	1	315	CLA	CHD-C4C-C3C	-5.42	116.75	124.92
17	L	203	CLA	CHD-C4C-C3C	-5.41	116.76	124.92
17	9	608	CLA	CHD-C4C-C3C	-5.41	116.76	124.92
17	A	807	CLA	CHD-C4C-C3C	-5.41	116.77	124.92
17	2	611	CLA	CHD-C4C-C3C	-5.41	116.77	124.92
17	b	835	CLA	CHD-C4C-C3C	-5.41	116.77	124.92
17	K	4002	CLA	CHD-C4C-C3C	-5.40	116.77	124.92
17	4	611	CLA	CHD-C4C-C3C	-5.40	116.78	124.92
17	F	301	CLA	CHD-C4C-C3C	-5.40	116.78	124.92
17	8	308	CLA	CHD-C4C-C3C	-5.40	116.78	124.92
17	a	836	CLA	C1C-NC-C4C	-5.39	103.95	107.06
17	4	602	CLA	CHD-C4C-C3C	-5.39	116.79	124.92
17	B	805	CLA	CHD-C4C-C3C	-5.39	116.79	124.92
17	A	820	CLA	CHD-C4C-C3C	-5.39	116.80	124.92
17	B	804	CLA	CHD-C4C-C3C	-5.39	116.80	124.92
17	a	837	CLA	CHD-C4C-C3C	-5.39	116.80	124.92
17	9	611	CLA	CHD-C4C-C3C	-5.39	116.80	124.92
17	6	311	CLA	CHD-C4C-C3C	-5.39	116.80	124.92
17	g	102	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
17	6	307	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
17	7	611	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
17	8	302	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
17	A	839	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
17	9	614	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
17	3	302	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
17	2	609	CLA	CHD-C4C-C3C	-5.38	116.82	124.92
17	3	311	CLA	CHD-C4C-C3C	-5.37	116.82	124.92
17	b	808	CLA	CHD-C4C-C3C	-5.37	116.82	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	305	CLA	CHD-C4C-C3C	-5.37	116.82	124.92
17	B	839	CLA	CHD-C4C-C3C	-5.37	116.82	124.92
17	3	303	CLA	CHD-C4C-C3C	-5.37	116.83	124.92
17	9	604	CLA	CHD-C4C-C3C	-5.37	116.83	124.92
17	a	832	CLA	CHD-C4C-C3C	-5.37	116.83	124.92
17	A	832	CLA	CHD-C4C-C3C	-5.36	116.83	124.92
17	b	815	CLA	CHD-C4C-C3C	-5.36	116.84	124.92
17	6	313	CLA	CHD-C4C-C3C	-5.36	116.84	124.92
17	1	308	CLA	CHD-C4C-C3C	-5.36	116.84	124.92
17	A	809	CLA	CHD-C4C-C3C	-5.36	116.84	124.92
17	b	803	CLA	CHD-C4C-C3C	-5.36	116.84	124.92
17	4	612	CLA	CHD-C4C-C3C	-5.36	116.85	124.92
17	6	306	CLA	CHD-C4C-C3C	-5.35	116.85	124.92
17	A	806	CLA	CHD-C4C-C3C	-5.35	116.86	124.92
17	B	813	CLA	CHD-C4C-C3C	-5.35	116.86	124.92
17	8	304	CLA	CHD-C4C-C3C	-5.35	116.86	124.92
17	b	821	CLA	CHD-C4C-C3C	-5.34	116.86	124.92
17	1	309	CLA	CHD-C4C-C3C	-5.34	116.87	124.92
17	b	802	CLA	CHD-C4C-C3C	-5.34	116.88	124.92
17	a	818	CLA	CHD-C4C-C3C	-5.33	116.88	124.92
17	7	608	CLA	CHD-C4C-C3C	-5.33	116.89	124.92
17	B	810	CLA	CHD-C4C-C3C	-5.33	116.89	124.92
17	1	311	CLA	CHD-C4C-C3C	-5.33	116.89	124.92
17	b	812	CLA	CHD-C4C-C3C	-5.33	116.89	124.92
17	A	825	CLA	CHD-C4C-C3C	-5.32	116.90	124.92
17	6	316	CLA	CHD-C4C-C3C	-5.32	116.90	124.92
17	6	305	CLA	CHD-C4C-C3C	-5.32	116.90	124.92
17	a	841	CLA	CHD-C4C-C3C	-5.32	116.90	124.92
17	7	609	CLA	CHD-C4C-C3C	-5.32	116.91	124.92
17	1	303	CLA	CHD-C4C-C3C	-5.32	116.91	124.92
17	2	612	CLA	CHD-C4C-C3C	-5.31	116.91	124.92
20	B	845	BCR	C24-C23-C22	-5.31	118.23	126.21
17	j	3002	CLA	CHD-C4C-C3C	-5.31	116.91	124.92
17	4	608	CLA	CHD-C4C-C3C	-5.31	116.92	124.92
17	A	842	CLA	CHD-C4C-C3C	-5.30	116.93	124.92
17	1	310	CLA	CHD-C4C-C3C	-5.30	116.93	124.92
17	a	831	CLA	CHD-C4C-C3C	-5.29	116.94	124.92
17	a	822	CLA	CHD-C4C-C3C	-5.29	116.94	124.92
17	a	817	CLA	CHD-C4C-C3C	-5.29	116.94	124.92
17	3	304	CLA	CHD-C4C-C3C	-5.29	116.95	124.92
17	4	613	CLA	CHD-C4C-C3C	-5.29	116.95	124.92
17	B	822	CLA	CHD-C4C-C3C	-5.29	116.95	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	807	CLA	CHD-C4C-C3C	-5.28	116.96	124.92
20	a	854	BCR	C7-C8-C9	-5.28	118.28	126.21
17	7	610	CLA	CHD-C4C-C3C	-5.28	116.97	124.92
17	2	602	CLA	CHD-C4C-C3C	-5.28	116.97	124.92
17	a	803	CLA	C1C-NC-C4C	-5.28	104.02	107.06
17	8	310	CLA	CHD-C4C-C3C	-5.28	116.97	124.92
17	a	846	CLA	CHD-C4C-C3C	-5.27	116.97	124.92
17	1	305	CLA	CHD-C4C-C3C	-5.27	116.97	124.92
17	A	814	CLA	CHD-C4C-C3C	-5.27	116.98	124.92
17	k	1402	CLA	CHD-C4C-C3C	-5.27	116.98	124.92
17	b	837	CLA	CHD-C4C-C3C	-5.27	116.98	124.92
17	2	613	CLA	CHD-C4C-C3C	-5.26	116.99	124.92
17	F	304	CLA	CHD-C4C-C3C	-5.26	116.99	124.92
17	9	613	CLA	CHD-C4C-C3C	-5.26	116.99	124.92
28	7	616	XAT	C6-C7-C8	-5.26	114.87	125.99
20	A	851	BCR	C20-C21-C22	-5.26	119.80	127.31
17	f	7003	CLA	CHD-C4C-C3C	-5.26	116.99	124.92
17	a	856	CLA	CHD-C4C-C3C	-5.25	117.00	124.92
17	7	613	CLA	CHD-C4C-C3C	-5.25	117.00	124.92
17	A	845	CLA	CHD-C4C-C3C	-5.25	117.00	124.92
17	9	601	CLA	CHD-C4C-C3C	-5.25	117.00	124.92
17	g	101	CLA	CHD-C4C-C3C	-5.25	117.00	124.92
17	J	3002	CLA	CHD-C4C-C3C	-5.25	117.01	124.92
17	7	612	CLA	CHD-C4C-C3C	-5.25	117.01	124.92
17	L	202	CLA	CHD-C4C-C3C	-5.24	117.02	124.92
17	3	313	CLA	CHD-C4C-C3C	-5.24	117.02	124.92
17	B	817	CLA	CHD-C4C-C3C	-5.24	117.02	124.92
28	1	317	XAT	C6-C7-C8	-5.24	114.91	125.99
17	3	310	CLA	CHD-C4C-C3C	-5.24	117.02	124.92
17	2	610	CLA	CHD-C4C-C3C	-5.24	117.02	124.92
17	6	314	CLA	CHD-C4C-C3C	-5.24	117.02	124.92
17	2	608	CLA	CHD-C4C-C3C	-5.24	117.03	124.92
17	7	604	CLA	CHD-C4C-C3C	-5.23	117.03	124.92
17	2	604	CLA	CHD-C4C-C3C	-5.23	117.03	124.92
17	9	609	CLA	CHD-C4C-C3C	-5.23	117.04	124.92
17	b	818	CLA	CHD-C4C-C3C	-5.23	117.04	124.92
17	b	816	CLA	CHD-C4C-C3C	-5.23	117.04	124.92
17	A	835	CLA	CHD-C4C-C3C	-5.23	117.04	124.92
17	B	812	CLA	CHD-C4C-C3C	-5.22	117.05	124.92
17	A	837	CLA	CHD-C4C-C3C	-5.22	117.05	124.92
17	a	812	CLA	CHD-C4C-C3C	-5.22	117.05	124.92
17	1	304	CLA	CHD-C4C-C3C	-5.22	117.05	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	819	CLA	CHD-C4C-C3C	-5.22	117.06	124.92
17	B	808	CLA	CHD-C4C-C3C	-5.21	117.06	124.92
17	A	817	CLA	CHD-C4C-C3C	-5.21	117.07	124.92
17	a	820	CLA	CHD-C4C-C3C	-5.20	117.08	124.92
17	b	823	CLA	CHD-C4C-C3C	-5.20	117.08	124.92
17	A	813	CLA	CHD-C4C-C3C	-5.20	117.08	124.92
17	9	612	CLA	CHD-C4C-C3C	-5.20	117.08	124.92
17	A	824	CLA	CHD-C4C-C3C	-5.20	117.09	124.92
17	B	831	CLA	CHD-C4C-C3C	-5.19	117.09	124.92
17	3	312	CLA	CHD-C4C-C3C	-5.19	117.09	124.92
20	7	617	BCR	C16-C17-C18	-5.18	119.91	127.31
17	6	315	CLA	CHD-C4C-C3C	-5.18	117.11	124.92
17	A	843	CLA	CHD-C4C-C3C	-5.18	117.11	124.92
17	a	802	CLA	CHD-C4C-C3C	-5.18	117.11	124.92
20	l	201	BCR	C7-C8-C9	-5.17	118.44	126.21
17	8	309	CLA	CHD-C4C-C3C	-5.17	117.12	124.92
17	8	303	CLA	CHD-C4C-C3C	-5.17	117.13	124.92
17	b	813	CLA	CHD-C4C-C3C	-5.16	117.15	124.92
17	g	103	CLA	CHD-C4C-C3C	-5.15	117.15	124.92
17	a	813	CLA	CHD-C4C-C3C	-5.15	117.16	124.92
17	a	811	CLA	CHD-C4C-C3C	-5.14	117.17	124.92
17	3	301	CLA	CHD-C4C-C3C	-5.14	117.17	124.92
17	1	313	CLA	CHD-C4C-C3C	-5.14	117.17	124.92
17	a	832	CLA	C1C-NC-C4C	-5.14	104.10	107.06
20	a	853	BCR	C24-C23-C22	-5.13	118.50	126.21
17	3	308	CLA	CHD-C4C-C3C	-5.13	117.19	124.92
20	K	4001	BCR	C16-C17-C18	-5.13	119.99	127.31
20	a	852	BCR	C16-C17-C18	-5.12	120.00	127.31
17	b	830	CLA	CHD-C4C-C3C	-5.12	117.20	124.92
28	3	317	XAT	C26-C27-C28	-5.12	115.16	125.99
20	3	318	BCR	C15-C14-C13	-5.12	120.00	127.31
17	B	816	CLA	CHD-C4C-C3C	-5.12	117.21	124.92
17	A	811	CLA	CHD-C4C-C3C	-5.11	117.22	124.92
17	4	604	CLA	CHD-C4C-C3C	-5.10	117.23	124.92
26	7	606	CHL	CBC-CAC-C3C	-5.10	105.21	112.95
17	B	830	CLA	CHD-C4C-C3C	-5.09	117.24	124.92
17	b	829	CLA	C1C-NC-C4C	-5.09	104.13	107.06
17	A	822	CLA	CHD-C4C-C3C	-5.09	117.25	124.92
17	k	1403	CLA	CHD-C4C-C3C	-5.07	117.27	124.92
17	B	834	CLA	CHD-C4C-C3C	-5.06	117.28	124.92
20	B	843	BCR	C15-C14-C13	-5.06	120.08	127.31
17	6	304	CLA	CHD-C4C-C3C	-5.06	117.29	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	817	CLA	CHD-C4C-C3C	-5.06	117.29	124.92
17	b	819	CLA	CHD-C4C-C3C	-5.05	117.31	124.92
20	I	101	BCR	C24-C23-C22	-5.05	118.63	126.21
17	A	834	CLA	C1C-NC-C4C	-5.04	104.15	107.06
17	1	314	CLA	CHD-C4C-C3C	-5.04	117.33	124.92
27	6	321	LUT	C15-C14-C13	-5.03	120.13	127.31
17	a	803	CLA	CHD-C4C-C3C	-5.03	117.34	124.92
17	B	821	CLA	C1C-NC-C4C	-5.02	104.17	107.06
17	A	803	CLA	C1C-NC-C4C	-5.01	104.17	107.06
20	j	3004	BCR	C38-C26-C25	-5.00	118.91	124.51
20	B	845	BCR	C7-C8-C9	-4.98	118.72	126.21
26	6	308	CHL	CBC-CAC-C3C	-4.96	105.42	112.95
17	b	821	CLA	C1C-NC-C4C	-4.95	104.20	107.06
17	3	314	CLA	C1C-NC-C4C	-4.95	104.21	107.06
20	a	850	BCR	C15-C14-C13	-4.95	120.24	127.31
17	b	805	CLA	CHD-C4C-C3C	-4.95	117.46	124.92
20	B	845	BCR	C16-C17-C18	-4.95	120.25	127.31
28	8	315	XAT	C26-C27-C28	-4.94	115.55	125.99
20	9	618	BCR	C15-C14-C13	-4.94	120.26	127.31
17	B	803	CLA	CHD-C4C-C3C	-4.94	117.47	124.92
17	2	610	CLA	CAA-C2A-C3A	-4.94	106.39	116.38
17	8	302	CLA	C1C-NC-C4C	-4.94	104.22	107.06
17	a	837	CLA	C1C-NC-C4C	-4.93	104.22	107.06
26	9	606	CHL	CBC-CAC-C3C	-4.93	105.47	112.95
17	3	303	CLA	C1C-NC-C4C	-4.92	104.22	107.06
17	A	810	CLA	C1C-NC-C4C	-4.92	104.23	107.06
26	2	606	CHL	CBC-CAC-C3C	-4.92	105.49	112.95
20	L	201	BCR	C7-C8-C9	-4.90	118.85	126.21
17	7	610	CLA	CAA-C2A-C3A	-4.90	106.47	116.38
28	6	318	XAT	C6-C7-C8	-4.89	115.65	125.99
17	a	801	CLA	C1C-NC-C4C	-4.88	104.25	107.06
17	a	817	CLA	C1C-NC-C4C	-4.87	104.25	107.06
20	K	4004	BCR	C16-C17-C18	-4.87	120.36	127.31
20	L	206	BCR	C20-C21-C22	-4.86	120.38	127.31
26	8	306	CHL	CBC-CAC-C3C	-4.85	105.58	112.95
17	A	831	CLA	CHD-C4C-C3C	-4.83	117.65	124.92
17	8	312	CLA	C1C-NC-C4C	-4.81	104.29	107.06
17	9	610	CLA	CAA-C2A-C3A	-4.80	106.67	116.38
17	b	829	CLA	CHD-C4C-C3C	-4.80	117.69	124.92
20	8	316	BCR	C15-C14-C13	-4.80	120.46	127.31
20	A	856	BCR	C15-C14-C13	-4.79	120.47	127.31
20	4	618	BCR	C15-C14-C13	-4.78	120.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	843	BCR	C16-C17-C18	-4.77	120.51	127.31
17	A	832	CLA	C1C-NC-C4C	-4.77	104.31	107.06
17	b	834	CLA	C1C-NC-C4C	-4.75	104.32	107.06
17	3	315	CLA	C3C-C4C-CHD	-4.75	116.90	125.03
17	A	830	CLA	C1C-NC-C4C	-4.75	104.32	107.06
17	6	312	CLA	C1C-NC-C4C	-4.74	104.33	107.06
17	B	838	CLA	C1C-NC-C4C	-4.74	104.33	107.06
17	A	826	CLA	C1C-NC-C4C	-4.74	104.33	107.06
17	a	831	CLA	C1C-NC-C4C	-4.73	104.33	107.06
17	8	313	CLA	C3C-C4C-CHD	-4.73	116.94	125.03
17	8	311	CLA	C1C-NC-C4C	-4.70	104.35	107.06
26	4	605	CHL	CBC-CAC-C3C	-4.70	105.82	112.95
17	B	829	CLA	C1C-NC-C4C	-4.70	104.35	107.06
17	a	829	CLA	C1C-NC-C4C	-4.69	104.36	107.06
20	6	319	BCR	C15-C14-C13	-4.68	120.63	127.31
17	B	818	CLA	C1C-NC-C4C	-4.67	104.37	107.06
17	A	825	CLA	C1C-NC-C4C	-4.67	104.37	107.06
26	1	307	CHL	CBC-CAC-C3C	-4.66	105.87	112.95
17	6	310	CLA	C1C-NC-C4C	-4.66	104.38	107.06
20	L	201	BCR	C15-C14-C13	-4.64	120.69	127.31
17	a	830	CLA	C1C-NC-C4C	-4.64	104.39	107.06
17	K	4003	CLA	C1C-NC-C4C	-4.64	104.39	107.06
17	3	313	CLA	C1C-NC-C4C	-4.63	104.39	107.06
17	a	818	CLA	C1C-NC-C4C	-4.63	104.39	107.06
26	9	615	CHL	CBC-CAC-C3C	-4.63	105.92	112.95
20	a	853	BCR	C28-C27-C26	-4.63	105.83	113.78
17	B	829	CLA	CHD-C4C-C3C	-4.62	117.95	124.92
17	9	608	CLA	C1C-NC-C4C	-4.62	104.40	107.06
20	a	853	BCR	C20-C21-C22	-4.62	120.72	127.31
17	4	603	CLA	C1C-NC-C4C	-4.62	104.40	107.06
17	6	312	CLA	CAA-C2A-C3A	-4.61	107.06	116.38
28	2	616	XAT	C6-C7-C8	-4.60	116.27	125.99
17	b	839	CLA	C1C-NC-C4C	-4.60	104.41	107.06
17	b	836	CLA	C1C-NC-C4C	-4.58	104.42	107.06
17	A	829	CLA	C1C-NC-C4C	-4.57	104.43	107.06
17	7	611	CLA	C1C-NC-C4C	-4.57	104.43	107.06
20	A	850	BCR	C16-C17-C18	-4.57	120.79	127.31
20	b	843	BCR	C15-C14-C13	-4.56	120.80	127.31
20	A	851	BCR	C28-C27-C26	-4.56	105.94	113.78
17	b	818	CLA	C1C-NC-C4C	-4.56	104.43	107.06
17	7	603	CLA	C1C-NC-C4C	-4.55	104.44	107.06
20	B	801	BCR	C16-C15-C14	-4.55	113.76	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	310	CLA	CAA-C2A-C3A	-4.54	107.19	116.38
20	j	3003	BCR	C28-C27-C26	-4.54	105.97	113.78
17	1	311	CLA	CAA-C2A-C3A	-4.54	107.19	116.38
17	1	312	CLA	C1C-NC-C4C	-4.54	104.44	107.06
20	a	850	BCR	C3-C4-C5	-4.54	105.97	113.78
17	a	840	CLA	C1C-NC-C4C	-4.54	104.44	107.06
20	2	617	BCR	C15-C14-C13	-4.54	120.83	127.31
17	b	809	CLA	C1C-NC-C4C	-4.54	104.44	107.06
20	B	844	BCR	C28-C27-C26	-4.54	105.98	113.78
17	A	823	CLA	C1C-NC-C4C	-4.54	104.45	107.06
26	3	307	CHL	CBC-CAC-C3C	-4.53	106.08	112.95
17	a	826	CLA	C1C-NC-C4C	-4.53	104.45	107.06
17	A	808	CLA	C1C-NC-C4C	-4.53	104.45	107.06
17	9	603	CLA	C1C-NC-C4C	-4.52	104.46	107.06
17	F	303	CLA	C1C-NC-C4C	-4.52	104.46	107.06
17	F	301	CLA	C1C-NC-C4C	-4.52	104.46	107.06
17	b	827	CLA	C1C-NC-C4C	-4.51	104.46	107.06
17	A	831	CLA	C1C-NC-C4C	-4.51	104.46	107.06
17	a	828	CLA	C1C-NC-C4C	-4.50	104.47	107.06
17	a	824	CLA	C1C-NC-C4C	-4.50	104.47	107.06
17	A	824	CLA	C1C-NC-C4C	-4.50	104.47	107.06
17	a	823	CLA	C1C-NC-C4C	-4.50	104.47	107.06
28	8	315	XAT	C35-C34-C33	-4.49	120.91	127.31
17	4	608	CLA	C1C-NC-C4C	-4.48	104.48	107.06
20	7	617	BCR	C20-C21-C22	-4.48	120.92	127.31
17	f	7002	CLA	C1C-NC-C4C	-4.48	104.48	107.06
17	B	809	CLA	C1C-NC-C4C	-4.48	104.48	107.06
17	7	610	CLA	C1C-NC-C4C	-4.47	104.48	107.06
17	9	611	CLA	C1C-NC-C4C	-4.46	104.49	107.06
17	B	836	CLA	C1C-NC-C4C	-4.46	104.49	107.06
17	b	831	CLA	C1C-NC-C4C	-4.46	104.49	107.06
28	4	617	XAT	C26-C27-C28	-4.46	116.56	125.99
20	l	206	BCR	C20-C21-C22	-4.46	120.95	127.31
26	1	302	CHL	CBC-CAC-C3C	-4.46	106.18	112.95
27	6	317	LUT	C35-C34-C33	-4.46	120.95	127.31
17	b	815	CLA	C1C-NC-C4C	-4.45	104.49	107.06
17	b	840	CLA	C1C-NC-C4C	-4.45	104.50	107.06
17	A	839	CLA	C1C-NC-C4C	-4.45	104.50	107.06
26	4	607	CHL	CBC-CAC-C3C	-4.45	106.19	112.95
27	1	320	LUT	C15-C14-C13	-4.45	120.96	127.31
28	9	617	XAT	C26-C27-C28	-4.44	116.61	125.99
17	4	611	CLA	C1C-NC-C4C	-4.44	104.50	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	845	BCR	C24-C23-C22	-4.43	119.55	126.21
17	3	306	CLA	C1C-NC-C4C	-4.43	104.50	107.06
20	B	847	BCR	C15-C14-C13	-4.43	120.99	127.31
17	B	815	CLA	C1C-NC-C4C	-4.43	104.51	107.06
20	I	101	BCR	C20-C21-C22	-4.43	120.99	127.31
17	a	842	CLA	C1C-NC-C4C	-4.42	104.51	107.06
17	B	826	CLA	C1C-NC-C4C	-4.41	104.52	107.06
17	J	3002	CLA	C1C-NC-C4C	-4.41	104.52	107.06
17	a	813	CLA	C1C-NC-C4C	-4.41	104.52	107.06
26	7	605	CHL	CBC-CAC-C3C	-4.41	106.25	112.95
17	3	305	CLA	C1C-NC-C4C	-4.41	104.52	107.06
17	B	820	CLA	C1C-NC-C4C	-4.41	104.52	107.06
17	b	824	CLA	C1C-NC-C4C	-4.41	104.52	107.06
17	g	102	CLA	C1C-NC-C4C	-4.41	104.52	107.06
26	9	605	CHL	CBC-CAC-C3C	-4.40	106.27	112.95
17	B	819	CLA	C1C-NC-C4C	-4.40	104.52	107.06
26	9	607	CHL	CBC-CAC-C3C	-4.40	106.27	112.95
17	a	846	CLA	C1C-NC-C4C	-4.40	104.53	107.06
17	a	810	CLA	C1C-NC-C4C	-4.40	104.53	107.06
26	7	614	CHL	CBC-CAC-C3C	-4.39	106.29	112.95
17	a	825	CLA	C1C-NC-C4C	-4.38	104.53	107.06
17	b	804	CLA	C1C-NC-C4C	-4.38	104.53	107.06
17	A	837	CLA	C1C-NC-C4C	-4.38	104.54	107.06
17	a	806	CLA	C1-C2-C3	-4.38	117.89	125.96
17	A	801	CLA	C1C-NC-C4C	-4.38	104.54	107.06
26	6	303	CHL	CBC-CAC-C3C	-4.38	106.31	112.95
20	1	318	BCR	C15-C14-C13	-4.37	121.07	127.31
17	b	826	CLA	C1C-NC-C4C	-4.37	104.54	107.06
17	j	3002	CLA	C1C-NC-C4C	-4.37	104.54	107.06
17	A	805	CLA	C1C-NC-C4C	-4.37	104.54	107.06
20	A	850	BCR	C3-C4-C5	-4.37	106.27	113.78
17	2	603	CLA	C1C-NC-C4C	-4.37	104.54	107.06
28	1	317	XAT	C26-C27-C28	-4.36	116.77	125.99
20	A	848	BCR	C16-C17-C18	-4.35	121.10	127.31
26	2	605	CHL	CBC-CAC-C3C	-4.35	106.35	112.95
17	B	827	CLA	C1C-NC-C4C	-4.35	104.55	107.06
26	7	601	CHL	CBC-CAC-C3C	-4.35	106.35	112.95
28	9	617	XAT	C35-C34-C33	-4.35	121.11	127.31
17	b	811	CLA	C1C-NC-C4C	-4.34	104.56	107.06
17	A	840	CLA	C1C-NC-C4C	-4.34	104.56	107.06
17	6	305	CLA	C1C-NC-C4C	-4.34	104.56	107.06
17	B	839	CLA	C1C-NC-C4C	-4.33	104.56	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	g	101	CLA	C1C-NC-C4C	-4.33	104.56	107.06
17	3	308	CLA	C1-C2-C3	-4.33	119.84	126.68
20	b	845	BCR	C28-C27-C26	-4.32	106.35	113.78
17	B	824	CLA	C1C-NC-C4C	-4.32	104.57	107.06
17	B	802	CLA	C1C-NC-C4C	-4.32	104.57	107.06
17	a	839	CLA	C1C-NC-C4C	-4.30	104.58	107.06
20	b	847	BCR	C3-C4-C5	-4.30	106.38	113.78
20	k	1404	BCR	C16-C17-C18	-4.30	121.17	127.31
17	g	101	CLA	CAA-C2A-C3A	-4.29	107.70	116.38
17	6	309	CLA	C1C-NC-C4C	-4.29	104.59	107.06
20	a	849	BCR	C20-C21-C22	-4.29	121.19	127.31
17	B	804	CLA	C1C-NC-C4C	-4.28	104.59	107.06
17	B	807	CLA	C1C-NC-C4C	-4.28	104.59	107.06
17	a	816	CLA	C1C-NC-C4C	-4.28	104.60	107.06
17	6	314	CLA	C1C-NC-C4C	-4.27	104.60	107.06
17	3	311	CLA	C1C-NC-C4C	-4.27	104.60	107.06
17	a	844	CLA	C1C-NC-C4C	-4.27	104.60	107.06
17	8	305	CLA	C1C-NC-C4C	-4.27	104.60	107.06
17	A	817	CLA	C1C-NC-C4C	-4.27	104.60	107.06
17	1	311	CLA	C1C-NC-C4C	-4.27	104.60	107.06
26	7	601	CHL	CHA-CBD-CGD	-4.26	105.12	115.00
17	B	831	CLA	C1C-NC-C4C	-4.26	104.61	107.06
17	G	101	CLA	C1C-NC-C4C	-4.25	104.61	107.06
20	g	104	BCR	C16-C17-C18	-4.25	121.24	127.31
17	f	7003	CLA	C1C-NC-C4C	-4.25	104.61	107.06
17	6	306	CLA	C1C-NC-C4C	-4.25	104.61	107.06
17	2	610	CLA	C1C-NC-C4C	-4.25	104.61	107.06
17	A	818	CLA	C1C-NC-C4C	-4.25	104.61	107.06
17	3	310	CLA	C1C-NC-C4C	-4.25	104.61	107.06
17	A	845	CLA	C1C-NC-C4C	-4.24	104.62	107.06
17	A	804	CLA	C1C-NC-C4C	-4.24	104.62	107.06
17	b	813	CLA	C1C-NC-C4C	-4.24	104.62	107.06
17	B	830	CLA	C1C-NC-C4C	-4.23	104.62	107.06
17	b	820	CLA	C1C-NC-C4C	-4.23	104.62	107.06
17	2	611	CLA	C1C-NC-C4C	-4.23	104.62	107.06
17	b	819	CLA	C1C-NC-C4C	-4.23	104.62	107.06
20	g	104	BCR	C28-C27-C26	-4.22	106.52	113.78
28	6	318	XAT	C26-C27-C28	-4.22	117.06	125.99
17	b	833	CLA	C1C-NC-C4C	-4.22	104.63	107.06
20	B	844	BCR	C3-C4-C5	-4.22	106.52	113.78
20	B	843	BCR	C20-C21-C22	-4.22	121.29	127.31
17	b	812	CLA	C1C-NC-C4C	-4.21	104.63	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	313	CLA	C1C-NC-C4C	-4.21	104.63	107.06
17	K	4002	CLA	C1C-NC-C4C	-4.21	104.63	107.06
20	I	101	BCR	C16-C17-C18	-4.21	121.30	127.31
20	b	844	BCR	C3-C4-C5	-4.21	106.54	113.78
28	8	315	XAT	C6-C7-C8	-4.21	117.10	125.99
17	4	601	CLA	C1C-NC-C4C	-4.20	104.64	107.06
20	g	104	BCR	C20-C21-C22	-4.20	121.31	127.31
17	k	1401	CLA	C1C-NC-C4C	-4.20	104.64	107.06
17	8	310	CLA	C1C-NC-C4C	-4.20	104.64	107.06
17	7	612	CLA	C1C-NC-C4C	-4.20	104.64	107.06
17	B	834	CLA	C1C-NC-C4C	-4.20	104.64	107.06
17	1	304	CLA	C1C-NC-C4C	-4.20	104.64	107.06
26	2	601	CHL	CBC-CAC-C3C	-4.20	106.58	112.95
20	A	850	BCR	C11-C10-C9	-4.20	121.32	127.31
17	A	816	CLA	C1C-NC-C4C	-4.20	104.64	107.06
17	G	103	CLA	C1C-NC-C4C	-4.20	104.64	107.06
17	b	835	CLA	C1C-NC-C4C	-4.19	104.65	107.06
17	1	308	CLA	C1C-NC-C4C	-4.19	104.65	107.06
17	B	808	CLA	C1C-NC-C4C	-4.19	104.65	107.06
17	1	315	CLA	C1C-NC-C4C	-4.18	104.65	107.06
17	B	813	CLA	C1C-NC-C4C	-4.18	104.65	107.06
28	4	617	XAT	C6-C7-C8	-4.18	117.15	125.99
26	7	601	CHL	C4A-C3A-C2A	-4.18	97.47	103.86
17	B	823	CLA	C1C-NC-C4C	-4.18	104.65	107.06
17	A	843	CLA	C1C-NC-C4C	-4.18	104.65	107.06
17	a	805	CLA	C1C-NC-C4C	-4.18	104.65	107.06
17	3	312	CLA	C1C-NC-C4C	-4.18	104.65	107.06
17	a	806	CLA	C1C-NC-C4C	-4.17	104.66	107.06
20	G	105	BCR	C20-C21-C22	-4.17	121.36	127.31
17	a	807	CLA	C1C-NC-C4C	-4.17	104.66	107.06
20	b	844	BCR	C28-C27-C26	-4.16	106.62	113.78
17	b	838	CLA	C1C-NC-C4C	-4.16	104.66	107.06
20	J	3003	BCR	C15-C14-C13	-4.16	121.38	127.31
20	G	105	BCR	C16-C17-C18	-4.16	121.38	127.31
17	9	614	CLA	C1C-NC-C4C	-4.16	104.67	107.06
17	b	810	CLA	C1C-NC-C4C	-4.15	104.67	107.06
17	A	835	CLA	C1C-NC-C4C	-4.15	104.67	107.06
17	a	804	CLA	C1C-NC-C4C	-4.15	104.67	107.06
20	b	844	BCR	C24-C23-C22	-4.15	119.98	126.21
17	A	814	CLA	C1C-NC-C4C	-4.15	104.67	107.06
17	1	309	CLA	C1C-NC-C4C	-4.14	104.67	107.06
17	4	613	CLA	C1C-NC-C4C	-4.14	104.67	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	807	CLA	C1C-NC-C4C	-4.14	104.67	107.06
17	b	805	CLA	C1C-NC-C4C	-4.14	104.67	107.06
17	L	202	CLA	C1C-NC-C4C	-4.14	104.68	107.06
17	l	202	CLA	C1C-NC-C4C	-4.13	104.68	107.06
20	A	851	BCR	C15-C14-C13	-4.13	121.41	127.31
17	1	313	CLA	C1C-NC-C4C	-4.13	104.68	107.06
17	9	601	CLA	C1C-NC-C4C	-4.13	104.68	107.06
20	j	3004	BCR	C3-C4-C5	-4.13	106.68	113.78
26	2	607	CHL	CBC-CAC-C3C	-4.13	106.68	112.95
20	A	856	BCR	C3-C4-C5	-4.13	106.68	113.78
17	A	812	CLA	C1C-NC-C4C	-4.13	104.68	107.06
17	9	610	CLA	C1C-NC-C4C	-4.12	104.68	107.06
20	b	843	BCR	C11-C10-C9	-4.11	121.44	127.31
20	l	201	BCR	C15-C14-C13	-4.11	121.44	127.31
17	a	835	CLA	C1C-NC-C4C	-4.11	104.69	107.06
17	a	834	CLA	C1C-NC-C4C	-4.11	104.69	107.06
28	1	317	XAT	C35-C34-C33	-4.11	121.45	127.31
20	G	105	BCR	C28-C27-C26	-4.10	106.73	113.78
20	L	206	BCR	C11-C10-C9	-4.10	121.46	127.31
20	b	801	BCR	C16-C17-C18	-4.10	121.47	127.31
17	4	614	CLA	C1C-NC-C4C	-4.09	104.70	107.06
17	b	816	CLA	C1C-NC-C4C	-4.09	104.70	107.06
17	9	613	CLA	C1C-NC-C4C	-4.09	104.70	107.06
17	a	808	CLA	C1C-NC-C4C	-4.09	104.70	107.06
17	4	614	CLA	C1-C2-C3	-4.09	120.22	126.68
20	B	848	BCR	C16-C17-C18	-4.09	121.48	127.31
20	b	844	BCR	C15-C14-C13	-4.09	121.48	127.31
17	6	316	CLA	C1C-NC-C4C	-4.09	104.70	107.06
17	k	1402	CLA	C1C-NC-C4C	-4.08	104.71	107.06
17	3	301	CLA	C1C-NC-C4C	-4.08	104.71	107.06
17	l	204	CLA	C1C-NC-C4C	-4.08	104.71	107.06
20	l	206	BCR	C24-C23-C22	-4.08	120.08	126.21
17	a	811	CLA	C1C-NC-C4C	-4.08	104.71	107.06
17	4	604	CLA	C1C-NC-C4C	-4.07	104.71	107.06
17	k	1403	CLA	C1C-NC-C4C	-4.07	104.71	107.06
28	3	317	XAT	C35-C34-C33	-4.07	121.50	127.31
17	A	822	CLA	C1C-NC-C4C	-4.07	104.72	107.06
17	B	811	CLA	C1C-NC-C4C	-4.06	104.72	107.06
28	9	617	XAT	C6-C7-C8	-4.06	117.40	125.99
20	A	856	BCR	C38-C26-C25	-4.06	119.96	124.51
17	F	304	CLA	C1C-NC-C4C	-4.06	104.72	107.06
17	9	612	CLA	C1C-NC-C4C	-4.06	104.72	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	851	BCR	C16-C17-C18	-4.06	121.52	127.31
20	2	617	BCR	C16-C17-C18	-4.05	121.52	127.31
17	A	819	CLA	C1C-NC-C4C	-4.05	104.72	107.06
17	4	610	CLA	C1C-NC-C4C	-4.05	104.72	107.06
17	a	814	CLA	C1C-NC-C4C	-4.04	104.73	107.06
20	A	856	BCR	C28-C27-C26	-4.04	106.83	113.78
17	8	304	CLA	C1C-NC-C4C	-4.04	104.73	107.06
17	6	307	CLA	C1C-NC-C4C	-4.04	104.73	107.06
17	b	823	CLA	C1C-NC-C4C	-4.04	104.73	107.06
20	k	1404	BCR	C15-C14-C13	-4.04	121.55	127.31
17	B	828	CLA	C1C-NC-C4C	-4.03	104.73	107.06
20	a	854	BCR	C16-C17-C18	-4.03	121.56	127.31
20	l	206	BCR	C15-C14-C13	-4.03	121.56	127.31
17	A	813	CLA	C1C-NC-C4C	-4.03	104.74	107.06
17	B	835	CLA	C1C-NC-C4C	-4.02	104.74	107.06
20	l	205	BCR	C38-C26-C25	-4.02	120.01	124.51
17	6	315	CLA	C1C-NC-C4C	-4.02	104.74	107.06
17	B	812	CLA	C1C-NC-C4C	-4.01	104.75	107.06
27	7	615	LUT	C35-C34-C33	-4.01	121.59	127.31
17	A	842	CLA	C1-C2-C3	-4.01	118.58	125.96
20	i	101	BCR	C16-C17-C18	-4.01	121.59	127.31
17	1	314	CLA	C1C-NC-C4C	-4.01	104.75	107.06
20	L	206	BCR	C16-C17-C18	-4.01	121.59	127.31
20	B	847	BCR	C24-C23-C22	-4.00	120.19	126.21
17	8	309	CLA	C1C-NC-C4C	-4.00	104.75	107.06
20	A	850	BCR	C7-C8-C9	-4.00	120.20	126.21
20	a	850	BCR	C11-C10-C9	-3.99	121.61	127.31
20	L	206	BCR	C24-C23-C22	-3.99	120.21	126.21
20	A	850	BCR	C15-C14-C13	-3.99	121.61	127.31
17	A	828	CLA	C1C-NC-C4C	-3.99	104.76	107.06
28	2	616	XAT	C26-C27-C28	-3.99	117.56	125.99
17	a	838	CLA	C1C-NC-C4C	-3.99	104.76	107.06
28	7	616	XAT	C26-C27-C28	-3.99	117.56	125.99
20	I	101	BCR	C28-C27-C26	-3.99	106.93	113.78
20	B	843	BCR	C28-C27-C26	-3.98	106.93	113.78
20	a	851	BCR	C16-C17-C18	-3.98	121.63	127.31
17	b	828	CLA	C1C-NC-C4C	-3.98	104.77	107.06
20	B	848	BCR	C33-C5-C6	-3.98	120.05	124.51
17	4	612	CLA	C1C-NC-C4C	-3.98	104.77	107.06
17	7	604	CLA	C1C-NC-C4C	-3.98	104.77	107.06
20	4	618	BCR	C28-C27-C26	-3.98	106.94	113.78
17	a	820	CLA	C1C-NC-C4C	-3.98	104.77	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	k	1404	BCR	C20-C21-C22	-3.97	121.64	127.31
20	8	316	BCR	C28-C27-C26	-3.97	106.95	113.78
17	2	612	CLA	C1C-NC-C4C	-3.97	104.77	107.06
20	g	104	BCR	C24-C23-C22	-3.97	120.25	126.21
17	2	604	CLA	C1C-NC-C4C	-3.97	104.77	107.06
17	A	809	CLA	C1C-NC-C4C	-3.97	104.77	107.06
28	3	317	XAT	C6-C7-C8	-3.97	117.60	125.99
20	b	843	BCR	C28-C27-C26	-3.96	106.97	113.78
20	6	319	BCR	C28-C27-C26	-3.96	106.97	113.78
20	A	852	BCR	C20-C21-C22	-3.96	121.66	127.31
17	b	802	CLA	C1C-NC-C4C	-3.96	104.78	107.06
17	B	833	CLA	C1C-NC-C4C	-3.96	104.78	107.06
17	b	807	CLA	C1C-NC-C4C	-3.96	104.78	107.06
20	1	318	BCR	C16-C17-C18	-3.96	121.66	127.31
17	A	815	CLA	C1C-NC-C4C	-3.95	104.78	107.06
20	1	318	BCR	C11-C10-C9	-3.95	121.67	127.31
17	A	839	CLA	C1D-CHD-C4C	-3.95	117.08	122.48
17	b	825	CLA	C1C-NC-C4C	-3.95	104.78	107.06
17	A	838	CLA	C1C-NC-C4C	-3.95	104.78	107.06
17	G	104	CLA	C1C-NC-C4C	-3.95	104.78	107.06
27	6	321	LUT	C11-C10-C9	-3.95	121.68	127.31
20	b	845	BCR	C15-C14-C13	-3.95	121.68	127.31
17	b	817	CLA	C1C-NC-C4C	-3.94	104.79	107.06
17	2	608	CLA	C1C-NC-C4C	-3.94	104.79	107.06
17	A	854	CLA	C1-C2-C3	-3.94	118.70	125.96
17	B	823	CLA	C1-C2-C3	-3.94	118.70	125.96
17	a	822	CLA	C1C-NC-C4C	-3.93	104.79	107.06
17	3	309	CLA	C1-C2-C3	-3.93	120.46	126.68
17	B	825	CLA	C1C-NC-C4C	-3.93	104.79	107.06
17	B	817	CLA	C1C-NC-C4C	-3.93	104.79	107.06
17	a	842	CLA	C1D-CHD-C4C	-3.93	117.12	122.48
17	a	821	CLA	C1D-CHD-C4C	-3.91	117.14	122.48
20	B	844	BCR	C24-C23-C22	-3.91	120.33	126.21
17	a	843	CLA	C1C-NC-C4C	-3.91	104.81	107.06
20	B	845	BCR	C3-C4-C5	-3.91	107.06	113.78
20	A	856	BCR	C16-C17-C18	-3.91	121.73	127.31
20	a	852	BCR	C15-C14-C13	-3.91	121.73	127.31
17	a	841	CLA	C1C-NC-C4C	-3.91	104.81	107.06
17	B	829	CLA	C1C-C2C-C3C	-3.91	102.59	106.92
20	k	1404	BCR	C38-C26-C25	-3.90	120.14	124.51
17	B	832	CLA	C1C-NC-C4C	-3.90	104.81	107.06
17	A	812	CLA	C1D-CHD-C4C	-3.90	117.16	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	303	CLA	C1C-NC-C4C	-3.89	104.81	107.06
17	a	812	CLA	C1C-NC-C4C	-3.89	104.82	107.06
17	B	810	CLA	C1C-NC-C4C	-3.89	104.82	107.06
20	F	305	BCR	C11-C10-C9	-3.89	121.77	127.31
17	a	824	CLA	C1-C2-C3	-3.88	118.80	125.96
17	8	313	CLA	C2C-C3C-C4C	-3.88	102.73	107.19
17	a	807	CLA	CAA-C2A-C3A	-3.88	102.17	112.81
20	A	852	BCR	C16-C17-C18	-3.88	121.77	127.31
17	b	830	CLA	C1C-NC-C4C	-3.88	104.83	107.06
20	B	846	BCR	C15-C14-C13	-3.88	121.78	127.31
17	A	821	CLA	C1C-C2C-C3C	-3.88	102.62	106.92
17	B	805	CLA	C1C-NC-C4C	-3.87	104.83	107.06
26	2	601	CHL	CHA-CBD-CGD	-3.87	106.02	115.00
17	a	821	CLA	C1C-C2C-C3C	-3.87	102.62	106.92
20	b	847	BCR	C15-C14-C13	-3.87	121.78	127.31
17	B	837	CLA	C1C-NC-C4C	-3.87	104.83	107.06
17	B	840	CLA	C1C-NC-C4C	-3.86	104.83	107.06
17	A	806	CLA	C1C-NC-C4C	-3.86	104.83	107.06
17	g	102	CLA	C1-C2-C3	-3.86	120.58	126.68
17	3	315	CLA	C2C-C3C-C4C	-3.86	102.75	107.19
17	g	101	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
20	b	847	BCR	C24-C23-C22	-3.85	120.43	126.21
17	A	833	CLA	C1C-NC-C4C	-3.85	104.84	107.06
17	A	842	CLA	C1C-NC-C4C	-3.85	104.84	107.06
20	A	856	BCR	C20-C21-C22	-3.84	121.83	127.31
17	g	103	CLA	C1C-NC-C4C	-3.84	104.85	107.06
17	3	304	CLA	C1C-NC-C4C	-3.83	104.85	107.06
17	B	822	CLA	C1C-NC-C4C	-3.83	104.85	107.06
17	7	613	CLA	C1C-NC-C4C	-3.83	104.85	107.06
20	3	318	BCR	C33-C5-C6	-3.83	120.22	124.51
17	a	844	CLA	C1-C2-C3	-3.83	118.90	125.96
17	B	841	CLA	C1C-NC-C4C	-3.83	104.85	107.06
17	9	604	CLA	C1-C2-C3	-3.83	120.63	126.68
20	6	319	BCR	C16-C17-C18	-3.83	121.85	127.31
17	L	204	CLA	C1C-NC-C4C	-3.82	104.86	107.06
20	2	617	BCR	C3-C4-C5	-3.82	107.22	113.78
17	2	613	CLA	C1C-NC-C4C	-3.81	104.86	107.06
17	B	816	CLA	C1C-NC-C4C	-3.81	104.86	107.06
17	b	829	CLA	C1C-C2C-C3C	-3.81	102.70	106.92
20	L	205	BCR	C38-C26-C25	-3.81	120.25	124.51
20	a	852	BCR	C3-C4-C5	-3.81	107.23	113.78
17	A	811	CLA	C1C-NC-C4C	-3.80	104.87	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	822	CLA	C1C-NC-C4C	-3.80	104.87	107.06
17	b	841	CLA	C1C-NC-C4C	-3.80	104.87	107.06
17	b	808	CLA	C1C-NC-C4C	-3.80	104.87	107.06
17	3	302	CLA	C1C-NC-C4C	-3.80	104.87	107.06
26	4	615	CHL	CBC-CAC-C3C	-3.80	107.18	112.95
20	A	849	BCR	C15-C14-C13	-3.80	121.89	127.31
20	B	844	BCR	C15-C14-C13	-3.80	121.89	127.31
20	9	618	BCR	C11-C10-C9	-3.80	121.89	127.31
20	a	849	BCR	C16-C17-C18	-3.80	121.89	127.31
17	b	810	CLA	C1-C2-C3	-3.79	118.97	125.96
17	4	603	CLA	C1D-CHD-C4C	-3.79	117.30	122.48
17	1	306	CLA	C1C-NC-C4C	-3.78	104.88	107.06
27	3	316	LUT	C35-C34-C33	-3.78	121.91	127.31
17	b	838	CLA	C1C-C2C-C3C	-3.78	102.72	106.92
17	A	834	CLA	C1-C2-C3	-3.78	118.99	125.96
17	b	840	CLA	C1C-C2C-C3C	-3.78	102.73	106.92
20	b	848	BCR	C33-C5-C6	-3.77	120.28	124.51
17	a	816	CLA	C1-C2-C3	-3.77	120.73	126.68
17	9	608	CLA	C1D-CHD-C4C	-3.76	117.34	122.48
17	8	313	CLA	C3C-C2C-C1C	-3.76	102.87	107.19
17	7	608	CLA	C1-C2-C3	-3.76	120.74	126.68
17	9	608	CLA	C1-C2-C3	-3.76	120.75	126.68
20	K	4004	BCR	C15-C14-C13	-3.76	121.95	127.31
17	L	203	CLA	C1C-NC-C4C	-3.75	104.90	107.06
17	A	854	CLA	C1D-CHD-C4C	-3.75	117.36	122.48
27	2	615	LUT	C35-C34-C33	-3.75	121.96	127.31
17	1	303	CLA	C1C-NC-C4C	-3.75	104.90	107.06
17	9	611	CLA	C1D-CHD-C4C	-3.75	117.36	122.48
17	G	101	CLA	C1D-CHD-C4C	-3.74	117.37	122.48
20	6	319	BCR	C33-C5-C6	-3.74	120.32	124.51
17	3	315	CLA	C3C-C2C-C1C	-3.74	102.89	107.19
17	b	832	CLA	C1C-NC-C4C	-3.74	104.90	107.06
17	A	841	CLA	C1C-NC-C4C	-3.74	104.91	107.06
17	b	836	CLA	C1D-CHD-C4C	-3.74	117.38	122.48
17	A	854	CLA	O2D-CGD-O1D	-3.74	116.31	123.82
17	a	815	CLA	C1C-NC-C4C	-3.73	104.91	107.06
17	3	308	CLA	C1C-NC-C4C	-3.73	104.91	107.06
17	1	305	CLA	C1C-NC-C4C	-3.73	104.91	107.06
17	b	809	CLA	C1C-C2C-C3C	-3.73	102.78	106.92
17	3	315	CLA	C2A-C3A-C4A	-3.73	99.49	103.78
17	a	832	CLA	C1-C2-C3	-3.72	120.80	126.68
17	4	608	CLA	C1D-CHD-C4C	-3.72	117.40	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	804	CLA	C1D-CHD-C4C	-3.72	117.40	122.48
17	l	204	CLA	C1-C2-C3	-3.72	120.80	126.68
17	a	809	CLA	C1-C2-C3	-3.71	119.11	125.96
20	J	3003	BCR	C28-C27-C26	-3.71	107.39	113.78
20	l	206	BCR	C11-C10-C9	-3.71	122.01	127.31
17	4	608	CLA	C1-C2-C3	-3.71	120.81	126.68
28	4	617	XAT	C35-C34-C33	-3.71	122.01	127.31
20	b	844	BCR	C16-C17-C18	-3.71	122.01	127.31
17	a	817	CLA	C1C-C2C-C3C	-3.71	102.80	106.92
17	A	801	CLA	CAA-C2A-C3A	-3.71	102.64	112.81
20	3	318	BCR	C16-C17-C18	-3.71	122.02	127.31
17	B	815	CLA	C1D-CHD-C4C	-3.71	117.42	122.48
17	B	806	CLA	C1C-NC-C4C	-3.71	104.92	107.06
17	8	307	CLA	C1C-NC-C4C	-3.71	104.92	107.06
17	a	833	CLA	C1C-NC-C4C	-3.70	104.92	107.06
17	F	301	CLA	C1D-CHD-C4C	-3.70	117.42	122.48
20	L	201	BCR	C33-C5-C6	-3.70	120.37	124.51
17	a	812	CLA	C1D-CHD-C4C	-3.70	117.43	122.48
17	a	804	CLA	C1-C2-C3	-3.70	119.15	125.96
17	a	828	CLA	C1D-CHD-C4C	-3.69	117.44	122.48
20	L	205	BCR	C28-C27-C26	-3.69	107.44	113.78
17	l	310	CLA	C1C-NC-C4C	-3.68	104.94	107.06
17	b	803	CLA	C1D-CHD-C4C	-3.68	117.45	122.48
20	l	318	BCR	C28-C27-C26	-3.68	107.45	113.78
17	b	814	CLA	C1D-CHD-C4C	-3.68	117.45	122.48
17	B	830	CLA	C1-C2-C3	-3.68	120.87	126.68
17	F	301	CLA	C1C-C2C-C3C	-3.68	102.84	106.92
17	7	608	CLA	C1C-NC-C4C	-3.68	104.94	107.06
17	7	611	CLA	C1D-CHD-C4C	-3.68	117.46	122.48
17	7	602	CLA	C1C-NC-C4C	-3.68	104.94	107.06
17	A	832	CLA	C1-C2-C3	-3.67	120.88	126.68
20	L	201	BCR	C38-C26-C25	-3.67	120.40	124.51
17	A	819	CLA	C1D-CHD-C4C	-3.67	117.47	122.48
17	A	803	CLA	C1C-C2C-C3C	-3.67	102.85	106.92
20	l	201	BCR	C33-C5-C6	-3.67	120.40	124.51
28	3	317	XAT	C10-C11-C12	-3.66	111.99	123.23
17	6	304	CLA	C1C-NC-C4C	-3.66	104.95	107.06
17	A	820	CLA	C1C-NC-C4C	-3.66	104.95	107.06
17	a	818	CLA	C1C-C2C-C3C	-3.66	102.86	106.92
20	l	318	BCR	C33-C5-C6	-3.66	120.41	124.51
20	a	854	BCR	C20-C21-C22	-3.66	122.09	127.31
27	1	316	LUT	C35-C34-C33	-3.66	122.09	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	304	CLA	C1C-C2C-C3C	-3.66	102.86	106.92
20	a	850	BCR	C16-C17-C18	-3.66	122.09	127.31
17	6	310	CLA	C1D-CHD-C4C	-3.66	117.49	122.48
17	8	302	CLA	C1C-C2C-C3C	-3.65	102.87	106.92
17	a	819	CLA	C1C-NC-C4C	-3.65	104.95	107.06
17	A	808	CLA	C1C-C2C-C3C	-3.65	102.87	106.92
20	4	618	BCR	C11-C10-C9	-3.65	122.10	127.31
17	b	807	CLA	C1-C2-C3	-3.65	119.24	125.96
17	2	602	CLA	C1C-NC-C4C	-3.65	104.96	107.06
20	J	3003	BCR	C20-C21-C22	-3.65	122.11	127.31
17	a	825	CLA	C1C-C2C-C3C	-3.65	102.88	106.92
17	a	830	CLA	C1C-C2C-C3C	-3.65	102.88	106.92
17	A	817	CLA	C1C-C2C-C3C	-3.65	102.88	106.92
20	A	848	BCR	C20-C21-C22	-3.65	122.11	127.31
17	8	313	CLA	C2A-C3A-C4A	-3.64	99.59	103.78
17	a	838	CLA	C1D-CHD-C4C	-3.64	117.51	122.48
17	3	303	CLA	C1C-C2C-C3C	-3.64	102.88	106.92
17	a	801	CLA	C1C-C2C-C3C	-3.64	102.88	106.92
17	B	808	CLA	C1D-CHD-C4C	-3.64	117.51	122.48
17	8	312	CLA	C1C-C2C-C3C	-3.64	102.89	106.92
17	A	836	CLA	C1C-C2C-C3C	-3.63	102.89	106.92
17	9	604	CLA	C1C-NC-C4C	-3.63	104.97	107.06
17	A	812	CLA	C1C-C2C-C3C	-3.63	102.90	106.92
17	B	810	CLA	CAA-C2A-C3A	-3.62	102.87	112.81
17	a	836	CLA	C1C-C2C-C3C	-3.62	102.90	106.92
17	B	808	CLA	C1C-C2C-C3C	-3.62	102.90	106.92
17	A	854	CLA	C1C-C2C-C3C	-3.62	102.90	106.92
20	8	316	BCR	C33-C5-C6	-3.62	120.46	124.51
17	B	819	CLA	C1C-C2C-C3C	-3.62	102.91	106.92
20	L	206	BCR	C15-C14-C13	-3.62	122.15	127.31
17	B	825	CLA	CAA-C2A-C3A	-3.62	102.90	112.81
17	3	308	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
17	A	825	CLA	C1C-C2C-C3C	-3.61	102.91	106.92
17	b	806	CLA	C1C-NC-C4C	-3.61	104.98	107.06
17	8	308	CLA	C1-C2-C3	-3.61	120.97	126.68
17	B	836	CLA	C1D-CHD-C4C	-3.61	117.55	122.48
20	3	318	BCR	C28-C27-C26	-3.60	107.58	113.78
20	K	4001	BCR	C15-C16-C17	-3.60	115.77	123.46
17	B	802	CLA	C1C-C2C-C3C	-3.60	102.93	106.92
17	1	306	CLA	C1-C2-C3	-3.60	119.33	125.96
17	b	818	CLA	C1C-C2C-C3C	-3.60	102.93	106.92
17	9	610	CLA	C1D-CHD-C4C	-3.60	117.57	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	l	203	CLA	C1C-NC-C4C	-3.60	104.99	107.06
17	7	612	CLA	C1-C2-C3	-3.60	119.33	125.96
17	6	312	CLA	C1C-C2C-C3C	-3.59	102.93	106.92
17	A	818	CLA	C1D-CHD-C4C	-3.59	117.57	122.48
17	F	303	CLA	C1C-C2C-C3C	-3.59	102.94	106.92
17	4	611	CLA	C1D-CHD-C4C	-3.59	117.58	122.48
17	4	601	CLA	C1C-C2C-C3C	-3.59	102.94	106.92
17	L	204	CLA	C1-C2-C3	-3.59	121.01	126.68
17	8	305	CLA	C1C-C2C-C3C	-3.59	102.94	106.92
20	b	844	BCR	C34-C9-C10	-3.59	117.90	122.92
17	a	835	CLA	C1D-CHD-C4C	-3.59	117.58	122.48
20	G	105	BCR	C15-C14-C13	-3.58	122.19	127.31
17	4	612	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
17	a	803	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
17	7	609	CLA	C1D-CHD-C4C	-3.58	117.59	122.48
17	f	7002	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
28	8	315	XAT	C35-C15-C14	-3.58	115.82	123.46
17	a	856	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
17	B	818	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
17	9	608	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
17	2	608	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
17	1	314	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
20	B	845	BCR	C15-C14-C13	-3.58	122.20	127.31
17	a	842	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
17	2	611	CLA	C1D-CHD-C4C	-3.57	117.60	122.48
20	k	1404	BCR	C33-C5-C6	-3.57	120.51	124.51
17	l	202	CLA	C1C-C2C-C3C	-3.57	102.96	106.92
17	A	832	CLA	C1C-C2C-C3C	-3.57	102.96	106.92
17	a	827	CLA	C1C-NC-C4C	-3.57	105.00	107.06
20	a	851	BCR	C3-C4-C5	-3.57	107.65	113.78
17	4	604	CLA	C1-C2-C3	-3.57	121.05	126.68
17	a	809	CLA	C1C-NC-C4C	-3.57	105.00	107.06
17	1	309	CLA	C1D-CHD-C4C	-3.56	117.61	122.48
17	2	610	CLA	C1C-C2C-C3C	-3.56	102.97	106.92
17	b	808	CLA	C1C-C2C-C3C	-3.56	102.97	106.92
17	a	837	CLA	C1C-C2C-C3C	-3.56	102.97	106.92
20	B	845	BCR	C37-C22-C21	-3.56	117.94	122.92
17	3	313	CLA	C1C-C2C-C3C	-3.56	102.97	106.92
17	6	305	CLA	C1C-C2C-C3C	-3.55	102.98	106.92
17	B	828	CLA	C1C-C2C-C3C	-3.55	102.98	106.92
20	K	4004	BCR	C20-C21-C22	-3.55	122.24	127.31
26	7	607	CHL	CBC-CAC-C3C	-3.55	107.56	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	848	BCR	C28-C27-C26	-3.55	107.67	113.78
17	b	819	CLA	C1C-C2C-C3C	-3.55	102.98	106.92
17	4	608	CLA	C1C-C2C-C3C	-3.55	102.98	106.92
17	f	7003	CLA	C1C-C2C-C3C	-3.55	102.98	106.92
17	1	309	CLA	C1C-C2C-C3C	-3.55	102.98	106.92
17	b	829	CLA	C1D-CHD-C4C	-3.55	117.64	122.48
17	b	804	CLA	C1C-C2C-C3C	-3.55	102.99	106.92
17	9	601	CLA	C1C-C2C-C3C	-3.54	102.99	106.92
20	b	847	BCR	C7-C8-C9	-3.54	120.89	126.21
17	8	310	CLA	C1C-C2C-C3C	-3.54	102.99	106.92
17	B	838	CLA	C1C-C2C-C3C	-3.54	102.99	106.92
17	A	833	CLA	C1C-C2C-C3C	-3.54	102.99	106.92
17	a	809	CLA	C1C-C2C-C3C	-3.54	102.99	106.92
17	B	821	CLA	C1C-C2C-C3C	-3.54	103.00	106.92
17	B	825	CLA	C1D-CHD-C4C	-3.54	117.65	122.48
17	6	312	CLA	C1D-CHD-C4C	-3.54	117.65	122.48
17	A	810	CLA	C1C-C2C-C3C	-3.54	103.00	106.92
20	a	851	BCR	C15-C14-C13	-3.54	122.26	127.31
20	a	853	BCR	C38-C26-C25	-3.53	120.55	124.51
17	G	101	CLA	C1C-C2C-C3C	-3.53	103.00	106.92
17	a	856	CLA	O2D-CGD-O1D	-3.53	116.71	123.82
20	l	201	BCR	C38-C26-C25	-3.53	120.55	124.51
17	B	814	CLA	C1D-CHD-C4C	-3.53	117.66	122.48
20	B	844	BCR	C34-C9-C10	-3.53	117.98	122.92
20	4	618	BCR	C7-C8-C9	-3.53	120.91	126.21
17	9	612	CLA	C1C-C2C-C3C	-3.53	103.01	106.92
17	a	823	CLA	C1C-C2C-C3C	-3.53	103.01	106.92
17	A	821	CLA	C1D-CHD-C4C	-3.53	117.67	122.48
17	7	610	CLA	C1C-C2C-C3C	-3.52	103.01	106.92
17	L	202	CLA	C1C-C2C-C3C	-3.52	103.01	106.92
17	b	803	CLA	C1C-NC-C4C	-3.52	105.03	107.06
17	A	830	CLA	C1-C2-C3	-3.52	119.47	125.96
17	7	613	CLA	C1C-C2C-C3C	-3.52	103.01	106.92
17	a	843	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
20	l	201	BCR	C16-C17-C18	-3.52	122.28	127.31
17	A	804	CLA	C1C-C2C-C3C	-3.52	103.01	106.92
17	a	822	CLA	C1C-C2C-C3C	-3.52	103.02	106.92
17	6	310	CLA	C1C-C2C-C3C	-3.52	103.02	106.92
17	A	834	CLA	C1C-C2C-C3C	-3.52	103.02	106.92
17	b	808	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
20	8	316	BCR	C11-C10-C9	-3.52	122.29	127.31
17	6	315	CLA	C1C-C2C-C3C	-3.52	103.02	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	826	CLA	C1D-CHD-C4C	-3.52	117.68	122.48
17	8	307	CLA	C1D-CHD-C4C	-3.52	117.68	122.48
20	6	319	BCR	C11-C10-C9	-3.52	122.29	127.31
17	J	3002	CLA	C1C-C2C-C3C	-3.52	103.02	106.92
17	b	811	CLA	C1D-CHD-C4C	-3.51	117.68	122.48
17	A	824	CLA	C1C-C2C-C3C	-3.51	103.02	106.92
17	A	843	CLA	C1C-C2C-C3C	-3.51	103.02	106.92
17	a	805	CLA	C1C-C2C-C3C	-3.51	103.02	106.92
17	a	824	CLA	C1C-C2C-C3C	-3.51	103.02	106.92
17	1	313	CLA	C1C-C2C-C3C	-3.51	103.02	106.92
17	b	837	CLA	C1C-C2C-C3C	-3.51	103.02	106.92
20	b	845	BCR	C33-C5-C6	-3.51	120.58	124.51
17	8	313	CLA	C2C-C1C-CHC	-3.51	118.36	125.47
17	a	811	CLA	C1C-C2C-C3C	-3.51	103.02	106.92
17	a	833	CLA	C1-C2-C3	-3.51	119.49	125.96
17	A	828	CLA	C1D-CHD-C4C	-3.51	117.68	122.48
20	8	316	BCR	C7-C8-C9	-3.51	120.94	126.21
17	9	602	CLA	C1C-NC-C4C	-3.51	105.03	107.06
17	1	313	CLA	C1-C2-C3	-3.51	119.49	125.96
17	A	813	CLA	C1C-C2C-C3C	-3.51	103.03	106.92
28	6	318	XAT	C35-C34-C33	-3.51	122.31	127.31
17	7	611	CLA	C1C-C2C-C3C	-3.51	103.03	106.92
17	b	834	CLA	C1C-C2C-C3C	-3.51	103.03	106.92
17	6	306	CLA	C1C-C2C-C3C	-3.51	103.03	106.92
17	A	845	CLA	C1C-C2C-C3C	-3.50	103.03	106.92
17	3	312	CLA	C1C-C2C-C3C	-3.50	103.03	106.92
17	4	602	CLA	C1C-NC-C4C	-3.50	105.04	107.06
17	A	802	CLA	C1C-NC-C4C	-3.50	105.04	107.06
20	b	846	BCR	C38-C26-C25	-3.50	120.59	124.51
17	B	838	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
17	K	4002	CLA	C1C-C2C-C3C	-3.50	103.04	106.92
17	1	312	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
17	B	804	CLA	C1C-C2C-C3C	-3.50	103.04	106.92
20	1	318	BCR	C7-C8-C9	-3.50	120.96	126.21
17	2	603	CLA	C1C-C2C-C3C	-3.50	103.04	106.92
17	4	613	CLA	C1C-C2C-C3C	-3.50	103.04	106.92
17	7	603	CLA	C1D-CHD-C4C	-3.50	117.71	122.48
17	A	838	CLA	C1-C2-C3	-3.50	119.52	125.96
20	I	101	BCR	C3-C4-C5	-3.49	107.77	113.78
17	B	839	CLA	C1-C2-C3	-3.49	119.52	125.96
17	A	836	CLA	C1D-CHD-C4C	-3.49	117.71	122.48
17	6	313	CLA	C1D-CHD-C4C	-3.49	117.71	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	303	CLA	C1D-CHD-C4C	-3.49	117.71	122.48
17	3	315	CLA	C2C-C1C-CHC	-3.49	118.41	125.47
20	9	618	BCR	C28-C27-C26	-3.49	107.78	113.78
17	A	816	CLA	C1C-C2C-C3C	-3.49	103.05	106.92
17	3	310	CLA	C1C-C2C-C3C	-3.49	103.05	106.92
17	b	820	CLA	C1-C2-C3	-3.49	121.17	126.68
20	A	851	BCR	C38-C26-C25	-3.49	120.60	124.51
17	B	836	CLA	C1C-C2C-C3C	-3.49	103.05	106.92
17	a	846	CLA	C1C-C2C-C3C	-3.49	103.05	106.92
17	b	837	CLA	C1C-NC-C4C	-3.49	105.05	107.06
17	k	1403	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
27	1	316	LUT	C18-C5-C6	-3.48	120.61	124.51
17	a	840	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	A	840	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	A	807	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	A	837	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	b	825	CLA	CAA-C2A-C3A	-3.48	103.27	112.81
27	6	321	LUT	C7-C8-C9	-3.48	120.98	126.21
17	3	311	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	b	821	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	6	313	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	B	809	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	B	837	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	b	815	CLA	C1D-CHD-C4C	-3.48	117.73	122.48
20	3	318	BCR	C38-C26-C25	-3.48	120.62	124.51
17	a	812	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	g	103	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	8	309	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
17	b	807	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
20	i	101	BCR	C28-C27-C26	-3.48	107.80	113.78
17	b	815	CLA	C1C-C2C-C3C	-3.48	103.06	106.92
20	F	305	BCR	C3-C4-C5	-3.48	107.80	113.78
17	1	315	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	6	314	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
17	1	305	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	a	856	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
17	b	811	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	9	614	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	a	833	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	4	614	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	7	603	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
20	L	205	BCR	C16-C17-C18	-3.47	122.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	841	CLA	C1-C2-C3	-3.47	119.57	125.96
17	6	311	CLA	C1-C2-C3	-3.47	119.57	125.96
17	B	840	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	9	610	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	A	830	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
17	A	811	CLA	C1C-C2C-C3C	-3.47	103.08	106.92
17	a	804	CLA	C1C-C2C-C3C	-3.47	103.08	106.92
17	3	314	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
17	g	102	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
17	B	835	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
17	2	612	CLA	C1-C2-C3	-3.46	119.58	125.96
17	9	611	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
17	B	839	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
17	1	306	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
26	7	607	CHL	C1-C2-C3	-3.46	121.21	126.68
17	b	835	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
17	B	839	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
17	a	834	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
17	b	817	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
17	9	603	CLA	C1D-CHD-C4C	-3.46	117.76	122.48
17	b	824	CLA	C1D-CHD-C4C	-3.46	117.76	122.48
27	4	616	LUT	C35-C34-C33	-3.46	122.38	127.31
17	b	820	CLA	C1C-C2C-C3C	-3.46	103.09	106.92
17	A	801	CLA	C1C-C2C-C3C	-3.45	103.09	106.92
17	6	313	CLA	C1-C2-C3	-3.45	119.59	125.96
17	3	309	CLA	C1C-NC-C4C	-3.45	105.07	107.06
17	b	836	CLA	C1-C2-C3	-3.45	119.60	125.96
20	a	853	BCR	C16-C17-C18	-3.45	122.39	127.31
17	3	306	CLA	C1D-CHD-C4C	-3.45	117.77	122.48
20	9	618	BCR	C16-C17-C18	-3.45	122.39	127.31
17	3	304	CLA	C1C-C2C-C3C	-3.45	103.09	106.92
17	8	309	CLA	C1D-CHD-C4C	-3.45	117.77	122.48
17	A	818	CLA	C1C-C2C-C3C	-3.45	103.10	106.92
17	A	839	CLA	C1C-C2C-C3C	-3.45	103.10	106.92
17	6	314	CLA	C1C-C2C-C3C	-3.45	103.10	106.92
17	a	821	CLA	CBC-CAC-C3C	-3.45	102.63	112.41
17	9	604	CLA	C1C-C2C-C3C	-3.45	103.10	106.92
17	7	604	CLA	C1C-C2C-C3C	-3.45	103.10	106.92
26	7	605	CHL	OMC-CMC-C2C	-3.45	119.89	124.29
17	4	609	CLA	C1D-CHD-C4C	-3.45	117.78	122.48
20	a	852	BCR	C33-C5-C6	-3.44	120.65	124.51
17	F	304	CLA	C1C-C2C-C3C	-3.44	103.10	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	611	CLA	C1C-C2C-C3C	-3.44	103.10	106.92
17	b	816	CLA	C1C-C2C-C3C	-3.44	103.10	106.92
17	3	301	CLA	C1C-C2C-C3C	-3.44	103.10	106.92
17	A	820	CLA	C1C-C2C-C3C	-3.44	103.10	106.92
17	K	4003	CLA	C1C-C2C-C3C	-3.44	103.10	106.92
20	A	848	BCR	C38-C26-C25	-3.44	120.66	124.51
17	8	311	CLA	C1C-C2C-C3C	-3.44	103.11	106.92
17	A	810	CLA	C1D-CHD-C4C	-3.44	117.79	122.48
17	b	828	CLA	C1C-C2C-C3C	-3.44	103.11	106.92
17	j	3002	CLA	C1C-C2C-C3C	-3.43	103.11	106.92
26	6	303	CHL	CHA-CBD-CGD	-3.43	107.03	115.00
17	9	609	CLA	C1C-NC-C4C	-3.43	105.08	107.06
17	B	811	CLA	C1C-C2C-C3C	-3.43	103.11	106.92
20	f	7004	BCR	C11-C10-C9	-3.43	122.41	127.31
17	a	811	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
17	a	844	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
17	a	839	CLA	O2D-CGD-O1D	-3.43	116.92	123.82
26	7	605	CHL	C4A-C3A-C2A	-3.43	98.61	103.86
17	4	612	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
17	4	604	CLA	C1C-C2C-C3C	-3.43	103.12	106.92
17	2	609	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
17	A	829	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
20	F	305	BCR	C15-C14-C13	-3.43	122.42	127.31
17	7	610	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
17	k	1401	CLA	C1C-C2C-C3C	-3.43	103.12	106.92
17	7	608	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
17	a	836	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
20	A	856	BCR	C33-C5-C6	-3.42	120.67	124.51
17	2	604	CLA	C1C-C2C-C3C	-3.42	103.12	106.92
20	f	7004	BCR	C3-C4-C5	-3.42	107.89	113.78
28	8	315	XAT	C10-C11-C12	-3.42	112.73	123.23
17	f	7002	CLA	C1D-CHD-C4C	-3.42	117.81	122.48
17	b	805	CLA	C1C-C2C-C3C	-3.42	103.12	106.92
17	a	835	CLA	C1C-C2C-C3C	-3.42	103.12	106.92
17	9	613	CLA	C1C-C2C-C3C	-3.42	103.12	106.92
17	B	802	CLA	C1D-CHD-C4C	-3.42	117.81	122.48
17	g	101	CLA	C1D-CHD-C4C	-3.42	117.81	122.48
17	4	611	CLA	C1C-C2C-C3C	-3.42	103.13	106.92
20	J	3003	BCR	C16-C17-C18	-3.42	122.43	127.31
17	2	613	CLA	C1C-C2C-C3C	-3.42	103.13	106.92
17	b	839	CLA	C1C-C2C-C3C	-3.42	103.13	106.92
20	j	3003	BCR	C16-C17-C18	-3.42	122.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	311	CLA	C1C-C2C-C3C	-3.42	103.13	106.92
17	6	311	CLA	C1C-NC-C4C	-3.42	105.09	107.06
18	A	844	PQN	C11-C12-C13	-3.42	121.00	126.71
17	b	822	CLA	C1C-C2C-C3C	-3.42	103.13	106.92
26	7	601	CHL	O2D-CGD-O1D	-3.41	116.95	123.82
17	1	310	CLA	C1D-CHD-C4C	-3.41	117.82	122.48
17	7	608	CLA	C1C-C2C-C3C	-3.41	103.14	106.92
17	A	841	CLA	C1C-C2C-C3C	-3.41	103.14	106.92
17	1	308	CLA	C1C-C2C-C3C	-3.41	103.14	106.92
20	K	4004	BCR	C38-C26-C25	-3.41	120.69	124.51
17	l	204	CLA	C1D-CHD-C4C	-3.41	117.83	122.48
17	B	814	CLA	C1C-NC-C4C	-3.41	105.09	107.06
20	l	205	BCR	C28-C27-C26	-3.41	107.92	113.78
17	a	820	CLA	C1C-C2C-C3C	-3.41	103.14	106.92
17	a	834	CLA	C1-C2-C3	-3.40	119.69	125.96
17	6	314	CLA	C1-C2-C3	-3.40	119.69	125.96
26	2	607	CHL	C1-C2-C3	-3.40	121.31	126.68
17	b	812	CLA	C1C-C2C-C3C	-3.40	103.15	106.92
17	b	828	CLA	C1D-CHD-C4C	-3.40	117.84	122.48
17	B	804	CLA	C1D-CHD-C4C	-3.40	117.84	122.48
17	k	1402	CLA	C1C-C2C-C3C	-3.40	103.15	106.92
27	1	320	LUT	C18-C5-C6	-3.40	120.71	124.51
17	b	825	CLA	C1D-CHD-C4C	-3.40	117.84	122.48
17	K	4003	CLA	C1D-CHD-C4C	-3.39	117.84	122.48
20	l	206	BCR	C3-C4-C5	-3.39	107.94	113.78
17	4	610	CLA	C1C-C2C-C3C	-3.39	103.16	106.92
17	B	833	CLA	C1D-CHD-C4C	-3.39	117.85	122.48
20	j	3004	BCR	C15-C14-C13	-3.39	122.47	127.31
17	a	839	CLA	C1C-C2C-C3C	-3.39	103.16	106.92
17	b	813	CLA	C1-C2-C3	-3.39	119.71	125.96
17	A	826	CLA	C1D-CHD-C4C	-3.39	117.85	122.48
17	A	805	CLA	C1C-C2C-C3C	-3.39	103.16	106.92
17	B	815	CLA	C1C-C2C-C3C	-3.39	103.16	106.92
17	B	820	CLA	C1C-C2C-C3C	-3.39	103.17	106.92
17	3	305	CLA	C1C-C2C-C3C	-3.38	103.17	106.92
17	6	316	CLA	C1C-C2C-C3C	-3.38	103.17	106.92
17	a	819	CLA	C1D-CHD-C4C	-3.38	117.86	122.48
17	b	839	CLA	C1D-CHD-C4C	-3.38	117.86	122.48
17	a	802	CLA	C1C-NC-C4C	-3.38	105.11	107.06
17	B	818	CLA	C1D-CHD-C4C	-3.38	117.86	122.48
17	b	833	CLA	C1D-CHD-C4C	-3.38	117.86	122.48
17	A	841	CLA	C1D-CHD-C4C	-3.38	117.86	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	828	CLA	C1-C2-C3	-3.38	119.73	125.96
17	a	832	CLA	C1C-C2C-C3C	-3.38	103.17	106.92
17	7	612	CLA	C1C-C2C-C3C	-3.38	103.17	106.92
17	a	805	CLA	C1D-CHD-C4C	-3.38	117.87	122.48
26	9	607	CHL	C1-C2-C3	-3.38	121.35	126.68
17	b	814	CLA	C1C-NC-C4C	-3.37	105.11	107.06
17	1	312	CLA	C1C-C2C-C3C	-3.37	103.18	106.92
17	2	612	CLA	C1C-C2C-C3C	-3.37	103.18	106.92
17	A	805	CLA	O2D-CGD-O1D	-3.37	117.04	123.82
17	4	603	CLA	C1C-C2C-C3C	-3.37	103.18	106.92
27	6	321	LUT	C18-C5-C6	-3.37	120.74	124.51
17	B	810	CLA	C1C-C2C-C3C	-3.37	103.18	106.92
17	B	812	CLA	C1C-C2C-C3C	-3.37	103.18	106.92
17	B	817	CLA	C1C-C2C-C3C	-3.37	103.19	106.92
17	B	816	CLA	C1C-C2C-C3C	-3.37	103.19	106.92
26	1	302	CHL	CHA-CBD-CGD	-3.37	107.19	115.00
17	2	612	CLA	C1D-CHD-C4C	-3.37	117.89	122.48
17	8	307	CLA	C1C-C2C-C3C	-3.36	103.19	106.92
17	2	603	CLA	C1D-CHD-C4C	-3.36	117.89	122.48
17	a	829	CLA	C1C-C2C-C3C	-3.36	103.19	106.92
20	A	849	BCR	C33-C5-C6	-3.36	120.75	124.51
17	9	609	CLA	C1D-CHD-C4C	-3.36	117.89	122.48
17	f	7003	CLA	C1D-CHD-C4C	-3.36	117.89	122.48
17	b	833	CLA	C1C-C2C-C3C	-3.36	103.19	106.92
17	B	803	CLA	C1D-CHD-C4C	-3.36	117.89	122.48
17	4	609	CLA	C1C-NC-C4C	-3.36	105.12	107.06
27	2	615	LUT	C18-C5-C6	-3.36	120.75	124.51
17	B	822	CLA	C1C-C2C-C3C	-3.36	103.19	106.92
17	b	808	CLA	O2D-CGD-O1D	-3.36	117.06	123.82
17	A	816	CLA	C1-C2-C3	-3.36	121.38	126.68
17	B	820	CLA	C1D-CHD-C4C	-3.36	117.90	122.48
17	6	311	CLA	C1D-CHD-C4C	-3.36	117.90	122.48
17	A	811	CLA	C1D-CHD-C4C	-3.36	117.90	122.48
17	G	104	CLA	C1D-CHD-C4C	-3.35	117.90	122.48
20	b	844	BCR	C20-C21-C22	-3.35	122.52	127.31
17	3	306	CLA	C1C-C2C-C3C	-3.35	103.20	106.92
26	7	601	CHL	OMC-CMC-C2C	-3.35	120.01	124.29
20	b	846	BCR	C15-C14-C13	-3.35	122.53	127.31
17	4	610	CLA	C1D-CHD-C4C	-3.35	117.90	122.48
17	6	309	CLA	C1C-C2C-C3C	-3.35	103.20	106.92
17	b	823	CLA	C1C-C2C-C3C	-3.35	103.20	106.92
17	b	831	CLA	C1C-C2C-C3C	-3.35	103.20	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	823	CLA	C1C-C2C-C3C	-3.35	103.20	106.92
17	a	826	CLA	C1C-C2C-C3C	-3.35	103.21	106.92
17	B	806	CLA	C1C-C2C-C3C	-3.35	103.21	106.92
20	b	847	BCR	C11-C10-C9	-3.35	122.53	127.31
17	8	304	CLA	C1C-C2C-C3C	-3.35	103.21	106.92
17	b	840	CLA	C1-C2-C3	-3.35	119.79	125.96
17	2	608	CLA	C1D-CHD-C4C	-3.34	117.91	122.48
17	a	807	CLA	C1C-C2C-C3C	-3.34	103.21	106.92
17	B	810	CLA	C1D-CHD-C4C	-3.34	117.91	122.48
17	A	835	CLA	C1C-C2C-C3C	-3.34	103.21	106.92
17	L	203	CLA	C1C-C2C-C3C	-3.34	103.21	106.92
17	L	204	CLA	C1C-C2C-C3C	-3.34	103.21	106.92
17	8	301	CLA	C1C-NC-C4C	-3.34	105.13	107.06
17	4	612	CLA	C1-C2-C3	-3.34	119.80	125.96
17	K	4002	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
17	a	841	CLA	C1C-C2C-C3C	-3.34	103.22	106.92
17	b	802	CLA	C1C-C2C-C3C	-3.34	103.22	106.92
17	8	303	CLA	C1C-C2C-C3C	-3.34	103.22	106.92
17	a	826	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
17	A	803	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
17	b	822	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
17	b	827	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
17	A	809	CLA	C1C-C2C-C3C	-3.34	103.22	106.92
17	b	834	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
28	1	317	XAT	C10-C11-C12	-3.34	113.00	123.23
17	a	813	CLA	C1C-C2C-C3C	-3.34	103.22	106.92
17	b	834	CLA	C1-C2-C3	-3.33	119.81	125.96
17	a	839	CLA	C1D-CHD-C4C	-3.33	117.93	122.48
17	A	814	CLA	C1D-CHD-C4C	-3.33	117.93	122.48
17	b	836	CLA	C1C-C2C-C3C	-3.33	103.23	106.92
20	a	852	BCR	C24-C23-C22	-3.33	121.21	126.21
17	l	204	CLA	C1C-C2C-C3C	-3.33	103.23	106.92
20	a	852	BCR	C28-C27-C26	-3.33	108.06	113.78
17	b	832	CLA	C1-C2-C3	-3.33	119.82	125.96
17	6	304	CLA	C1C-C2C-C3C	-3.33	103.23	106.92
17	B	823	CLA	C1C-C2C-C3C	-3.33	103.23	106.92
17	4	609	CLA	C1C-C2C-C3C	-3.33	103.23	106.92
17	a	823	CLA	C1D-CHD-C4C	-3.33	117.94	122.48
17	A	822	CLA	C1C-C2C-C3C	-3.33	103.23	106.92
17	b	824	CLA	C1C-C2C-C3C	-3.33	103.23	106.92
17	A	827	CLA	C1C-NC-C4C	-3.33	105.14	107.06
20	b	847	BCR	C38-C26-C25	-3.33	120.78	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	806	CLA	C1-C2-C3	-3.32	119.83	125.96
17	3	308	CLA	C1C-C2C-C3C	-3.32	103.23	106.92
17	a	801	CLA	CAA-C2A-C3A	-3.32	103.70	112.81
17	A	815	CLA	C1C-C2C-C3C	-3.32	103.23	106.92
20	a	853	BCR	C15-C14-C13	-3.32	122.57	127.31
20	b	845	BCR	C34-C9-C10	-3.32	118.27	122.92
26	2	605	CHL	C4A-C3A-C2A	-3.32	98.78	103.86
20	K	4001	BCR	C11-C10-C9	-3.32	122.57	127.31
17	a	809	CLA	C1D-CHD-C4C	-3.32	117.95	122.48
17	b	802	CLA	C1D-CHD-C4C	-3.32	117.95	122.48
17	b	820	CLA	C1D-CHD-C4C	-3.32	117.95	122.48
17	a	820	CLA	C1-C2-C3	-3.32	119.85	125.96
17	A	831	CLA	C1D-CHD-C4C	-3.32	117.95	122.48
17	6	307	CLA	C1C-C2C-C3C	-3.32	103.24	106.92
17	A	829	CLA	C1C-C2C-C3C	-3.31	103.24	106.92
20	L	201	BCR	C34-C9-C10	-3.31	118.28	122.92
27	9	616	LUT	C35-C34-C33	-3.31	122.58	127.31
17	F	304	CLA	C1D-CHD-C4C	-3.31	117.96	122.48
17	G	103	CLA	C1C-C2C-C3C	-3.31	103.25	106.92
17	k	1402	CLA	C1D-CHD-C4C	-3.31	117.96	122.48
17	1	304	CLA	C1D-CHD-C4C	-3.31	117.96	122.48
17	a	802	CLA	C1C-C2C-C3C	-3.31	103.25	106.92
17	a	831	CLA	C1D-CHD-C4C	-3.31	117.96	122.48
17	a	806	CLA	C1D-CHD-C4C	-3.31	117.96	122.48
17	a	810	CLA	C1C-C2C-C3C	-3.31	103.25	106.92
17	B	807	CLA	C1C-C2C-C3C	-3.31	103.25	106.92
27	1	320	LUT	C11-C10-C9	-3.31	122.59	127.31
17	2	602	CLA	C1C-C2C-C3C	-3.31	103.25	106.92
17	6	309	CLA	C1D-CHD-C4C	-3.31	117.97	122.48
20	8	316	BCR	C16-C17-C18	-3.31	122.59	127.31
17	a	842	CLA	C1-C2-C3	-3.31	119.87	125.96
20	f	7004	BCR	C15-C14-C13	-3.31	122.59	127.31
17	b	840	CLA	C1D-CHD-C4C	-3.30	117.97	122.48
17	A	831	CLA	C1C-C2C-C3C	-3.30	103.26	106.92
17	b	811	CLA	C4B-C3B-C2B	-3.30	103.85	106.92
17	3	311	CLA	C1D-CHD-C4C	-3.30	117.97	122.48
17	A	834	CLA	C1D-CHD-C4C	-3.30	117.97	122.48
17	b	816	CLA	C1D-CHD-C4C	-3.30	117.97	122.48
17	9	609	CLA	C1-C2-C3	-3.30	119.87	125.96
17	b	830	CLA	C1C-C2C-C3C	-3.30	103.26	106.92
17	A	842	CLA	C1D-CHD-C4C	-3.30	117.97	122.48
17	A	804	CLA	O2D-CGD-O1D	-3.30	117.18	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	810	CLA	C1D-CHD-C4C	-3.30	117.97	122.48
17	k	1401	CLA	C1D-CHD-C4C	-3.30	117.97	122.48
17	B	836	CLA	C1-C2-C3	-3.30	119.88	125.96
20	a	852	BCR	C11-C10-C9	-3.30	122.60	127.31
17	2	609	CLA	C1C-NC-C4C	-3.30	105.16	107.06
17	B	813	CLA	C1D-CHD-C4C	-3.30	117.98	122.48
17	1	309	CLA	C1-C2-C3	-3.30	119.88	125.96
20	b	845	BCR	C16-C17-C18	-3.30	122.61	127.31
17	8	310	CLA	C1D-CHD-C4C	-3.30	117.98	122.48
17	a	841	CLA	C1-C2-C3	-3.30	119.89	125.96
17	B	820	CLA	C1-C2-C3	-3.30	121.47	126.68
17	6	316	CLA	C1D-CHD-C4C	-3.29	117.98	122.48
17	a	803	CLA	C1D-CHD-C4C	-3.29	117.98	122.48
17	B	827	CLA	C1C-C2C-C3C	-3.29	103.27	106.92
17	8	311	CLA	C1D-CHD-C4C	-3.29	117.98	122.48
17	7	609	CLA	C1-C2-C3	-3.29	119.89	125.96
17	B	833	CLA	C1C-C2C-C3C	-3.29	103.27	106.92
17	8	308	CLA	C1C-NC-C4C	-3.29	105.16	107.06
17	7	613	CLA	C1D-CHD-C4C	-3.29	117.99	122.48
17	2	610	CLA	C1D-CHD-C4C	-3.29	117.99	122.48
17	b	827	CLA	C1C-C2C-C3C	-3.29	103.28	106.92
17	a	841	CLA	C1D-CHD-C4C	-3.29	117.99	122.48
20	A	848	BCR	C15-C14-C13	-3.28	122.62	127.31
17	a	815	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
17	b	826	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
17	1	315	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
17	8	302	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
17	A	843	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
17	b	830	CLA	C1-C2-C3	-3.28	121.50	126.68
17	4	609	CLA	C1-C2-C3	-3.28	119.92	125.96
17	b	806	CLA	C1D-CHD-C4C	-3.28	118.01	122.48
17	B	841	CLA	C1C-C2C-C3C	-3.28	103.29	106.92
17	b	839	CLA	C1-C2-C3	-3.28	119.92	125.96
20	B	846	BCR	C28-C27-C26	-3.27	108.15	113.78
17	A	838	CLA	C1C-C2C-C3C	-3.27	103.29	106.92
17	b	821	CLA	C1D-CHD-C4C	-3.27	118.01	122.48
17	a	831	CLA	C1C-C2C-C3C	-3.27	103.29	106.92
17	b	806	CLA	C1C-C2C-C3C	-3.27	103.29	106.92
17	G	104	CLA	C1C-C2C-C3C	-3.27	103.29	106.92
17	a	808	CLA	C1C-C2C-C3C	-3.27	103.30	106.92
17	3	315	CLA	C4A-NA-C1A	-3.27	104.29	107.17
26	9	615	CHL	C4A-C3A-C2A	-3.27	98.86	103.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	307	CLA	C1D-CHD-C4C	-3.26	118.02	122.48
17	9	601	CLA	C1D-CHD-C4C	-3.26	118.02	122.48
17	A	842	CLA	C1C-C2C-C3C	-3.26	103.30	106.92
17	B	829	CLA	CHC-C1C-C2C	-3.26	117.75	126.65
17	a	818	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
20	g	104	BCR	C15-C14-C13	-3.26	122.66	127.31
17	A	835	CLA	O2D-CGD-O1D	-3.26	117.26	123.82
17	B	840	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
17	B	806	CLA	C1-C2-C3	-3.26	119.95	125.96
17	B	811	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
17	7	612	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
17	3	305	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
17	9	602	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
20	b	843	BCR	C7-C8-C9	-3.26	121.32	126.21
20	A	848	BCR	C33-C5-C6	-3.26	120.86	124.51
20	a	849	BCR	C11-C10-C9	-3.26	122.66	127.31
17	a	829	CLA	C1-C2-C3	-3.26	119.96	125.96
20	K	4004	BCR	C33-C5-C6	-3.26	120.86	124.51
17	B	829	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
17	a	817	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
26	4	615	CHL	C4A-C3A-C2A	-3.25	98.88	103.86
17	1	313	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
17	A	827	CLA	C1C-C2C-C3C	-3.25	103.31	106.92
17	B	830	CLA	C1C-C2C-C3C	-3.25	103.31	106.92
17	3	303	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
17	A	817	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
17	3	312	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
17	A	840	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
20	g	104	BCR	C3-C4-C5	-3.25	108.19	113.78
20	A	850	BCR	C28-C27-C26	-3.25	108.19	113.78
17	a	844	CLA	C1C-C2C-C3C	-3.25	103.32	106.92
23	B	849	LMT	C1B-O1B-C4'	-3.25	110.08	118.00
17	a	816	CLA	C1C-C2C-C3C	-3.25	103.32	106.92
17	A	809	CLA	C1-C2-C3	-3.25	119.98	125.96
17	B	806	CLA	C1D-CHD-C4C	-3.25	118.05	122.48
17	A	833	CLA	C1-C2-C3	-3.25	119.98	125.96
17	8	305	CLA	C1D-CHD-C4C	-3.24	118.05	122.48
17	a	810	CLA	C1D-CHD-C4C	-3.24	118.05	122.48
17	a	815	CLA	C1C-C2C-C3C	-3.24	103.32	106.92
20	A	849	BCR	C16-C17-C18	-3.24	122.68	127.31
17	6	305	CLA	C1D-CHD-C4C	-3.24	118.05	122.48
17	G	103	CLA	C1D-CHD-C4C	-3.24	118.05	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	816	CLA	C1D-CHD-C4C	-3.24	118.05	122.48
20	L	206	BCR	C7-C8-C9	-3.24	121.34	126.21
27	6	321	LUT	C35-C34-C33	-3.24	122.69	127.31
20	6	319	BCR	C7-C8-C9	-3.24	121.34	126.21
20	A	848	BCR	C3-C4-C5	-3.24	108.21	113.78
17	B	828	CLA	C1D-CHD-C4C	-3.24	118.06	122.48
17	A	833	CLA	C1D-CHD-C4C	-3.24	118.06	122.48
17	8	313	CLA	C4A-NA-C1A	-3.24	104.32	107.17
17	1	310	CLA	C1C-C2C-C3C	-3.24	103.33	106.92
17	1	303	CLA	C1-C2-C3	-3.24	120.00	125.96
17	A	829	CLA	C1-C2-C3	-3.23	120.00	125.96
20	1	318	BCR	C38-C26-C25	-3.23	120.89	124.51
17	B	805	CLA	C1C-C2C-C3C	-3.23	103.33	106.92
17	2	608	CLA	C1-C2-C3	-3.23	121.57	126.68
17	B	816	CLA	C1D-CHD-C4C	-3.23	118.06	122.48
17	l	203	CLA	C1C-C2C-C3C	-3.23	103.33	106.92
20	B	801	BCR	C20-C21-C22	-3.23	122.70	127.31
17	A	801	CLA	C1D-CHD-C4C	-3.23	118.07	122.48
17	a	846	CLA	C1D-CHD-C4C	-3.23	118.07	122.48
17	A	826	CLA	C1C-C2C-C3C	-3.23	103.34	106.92
17	a	837	CLA	C1D-CHD-C4C	-3.23	118.07	122.48
17	8	308	CLA	C1D-CHD-C4C	-3.23	118.07	122.48
20	B	847	BCR	C11-C10-C9	-3.23	122.70	127.31
17	A	820	CLA	C1-C2-C3	-3.23	120.01	125.96
17	A	819	CLA	C1C-C2C-C3C	-3.23	103.34	106.92
17	6	315	CLA	C1D-CHD-C4C	-3.23	118.07	122.48
17	g	101	CLA	CBC-CAC-C3C	-3.23	103.25	112.41
17	a	828	CLA	C1C-C2C-C3C	-3.23	103.34	106.92
20	b	848	BCR	C16-C17-C18	-3.23	122.71	127.31
17	B	841	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
27	4	616	LUT	C18-C5-C6	-3.22	120.90	124.51
20	L	205	BCR	C20-C21-C22	-3.22	122.71	127.31
17	B	821	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
17	b	831	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
17	9	603	CLA	C1C-C2C-C3C	-3.22	103.35	106.92
17	A	806	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
17	2	609	CLA	C1-C2-C3	-3.22	120.02	125.96
17	g	103	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
17	B	811	CLA	C4B-C3B-C2B	-3.22	103.93	106.92
20	l	205	BCR	C20-C21-C22	-3.22	122.72	127.31
17	a	827	CLA	C1D-CHD-C4C	-3.22	118.09	122.48
17	b	812	CLA	C1D-CHD-C4C	-3.22	118.09	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	825	CLA	CHC-C1C-C2C	-3.22	117.88	126.65
17	9	609	CLA	C1C-C2C-C3C	-3.22	103.35	106.92
17	A	809	CLA	C1D-CHD-C4C	-3.22	118.09	122.48
17	a	825	CLA	C1D-CHD-C4C	-3.21	118.09	122.48
17	B	810	CLA	C1-C2-C3	-3.21	120.03	125.96
17	1	311	CLA	C1D-CHD-C4C	-3.21	118.09	122.48
17	a	829	CLA	C1D-CHD-C4C	-3.21	118.09	122.48
27	9	616	LUT	C18-C5-C6	-3.21	120.91	124.51
20	l	206	BCR	C16-C17-C18	-3.21	122.73	127.31
17	4	601	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
17	l	202	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
27	3	316	LUT	C31-C30-C29	-3.21	122.73	127.31
17	a	811	CLA	C1-C2-C3	-3.21	120.05	125.96
27	8	314	LUT	C18-C5-C6	-3.21	120.92	124.51
20	G	105	BCR	C24-C23-C22	-3.21	121.39	126.21
17	3	314	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
17	L	202	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
17	B	802	CLA	C1-C2-C3	-3.21	120.05	125.96
17	B	824	CLA	C1C-C2C-C3C	-3.21	103.36	106.92
17	L	204	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
17	A	838	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
17	a	832	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
20	B	847	BCR	C15-C16-C17	-3.20	116.62	123.46
17	B	834	CLA	C1C-C2C-C3C	-3.20	103.37	106.92
17	b	813	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
20	j	3004	BCR	C33-C5-C6	-3.20	120.92	124.51
17	3	303	CLA	C1-C2-C3	-3.20	121.62	126.68
17	b	838	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
17	2	613	CLA	O2D-CGD-O1D	-3.20	117.38	123.82
17	A	837	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
17	a	814	CLA	C1C-C2C-C3C	-3.20	103.37	106.92
17	8	304	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
17	a	807	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
17	b	829	CLA	C1-C2-C3	-3.20	120.06	125.96
17	B	803	CLA	C1C-C2C-C3C	-3.20	103.37	106.92
17	B	834	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
17	a	808	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
17	A	841	CLA	C1-C2-C3	-3.20	120.07	125.96
17	3	309	CLA	C1D-CHD-C4C	-3.20	118.12	122.48
17	a	838	CLA	C1C-C2C-C3C	-3.20	103.38	106.92
20	4	618	BCR	C16-C17-C18	-3.20	122.75	127.31
17	1	308	CLA	C1D-CHD-C4C	-3.19	118.12	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	314	LUT	C35-C34-C33	-3.19	122.75	127.31
17	b	807	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
17	B	825	CLA	C1C-C2C-C3C	-3.19	103.38	106.92
17	a	843	CLA	C1-C2-C3	-3.19	120.07	125.96
17	A	820	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
17	4	614	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
17	8	310	CLA	C1-C2-C3	-3.19	120.08	125.96
17	B	835	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
26	4	606	CHL	CBC-CAC-C3C	-3.19	108.11	112.95
17	b	810	CLA	C1C-C2C-C3C	-3.19	103.38	106.92
17	B	809	CLA	C1D-CHD-C4C	-3.19	118.13	122.48
17	B	826	CLA	C1C-C2C-C3C	-3.19	103.39	106.92
17	7	609	CLA	C1C-NC-C4C	-3.19	105.22	107.06
17	A	815	CLA	C1D-CHD-C4C	-3.19	118.13	122.48
17	B	812	CLA	C1D-CHD-C4C	-3.18	118.13	122.48
17	6	306	CLA	C1D-CHD-C4C	-3.18	118.13	122.48
17	b	819	CLA	CHC-C1C-C2C	-3.18	117.97	126.65
17	b	841	CLA	C1C-C2C-C3C	-3.18	103.39	106.92
27	7	615	LUT	C18-C5-C6	-3.18	120.95	124.51
17	A	826	CLA	C1-C2-C3	-3.18	120.09	125.96
17	b	829	CLA	CHC-C1C-C2C	-3.18	117.97	126.65
17	a	827	CLA	C1C-C2C-C3C	-3.18	103.39	106.92
17	A	824	CLA	C1-C2-C3	-3.18	120.10	125.96
20	8	316	BCR	C38-C26-C25	-3.18	120.95	124.51
17	G	103	CLA	C1-C2-C3	-3.18	121.66	126.68
20	k	1404	BCR	C24-C23-C22	-3.18	121.44	126.21
17	b	835	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
26	4	605	CHL	C4A-C3A-C2A	-3.17	99.00	103.86
17	A	843	CLA	C1-C2-C3	-3.17	120.11	125.96
17	B	805	CLA	C1D-CHD-C4C	-3.17	118.15	122.48
17	b	814	CLA	C1C-C2C-C3C	-3.17	103.40	106.92
17	8	301	CLA	C1-C2-C3	-3.17	120.11	125.96
17	A	832	CLA	C1D-CHD-C4C	-3.17	118.15	122.48
17	a	803	CLA	CHC-C1C-C2C	-3.17	118.01	126.65
17	A	828	CLA	C1-C2-C3	-3.17	120.12	125.96
17	b	826	CLA	C1C-C2C-C3C	-3.17	103.41	106.92
17	B	819	CLA	CHC-C1C-C2C	-3.17	118.01	126.65
17	b	823	CLA	C1D-CHD-C4C	-3.17	118.16	122.48
17	A	830	CLA	C1D-CHD-C4C	-3.17	118.16	122.48
17	B	824	CLA	C1D-CHD-C4C	-3.17	118.16	122.48
17	B	837	CLA	C1D-CHD-C4C	-3.17	118.16	122.48
20	K	4004	BCR	C3-C4-C5	-3.17	108.34	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	615	LUT	C15-C14-C13	-3.17	122.79	127.31
17	3	304	CLA	C1D-CHD-C4C	-3.16	118.16	122.48
17	3	302	CLA	C1-C2-C3	-3.16	120.13	125.96
17	3	315	CLA	C1D-CHD-C4C	-3.16	118.64	126.17
17	k	1403	CLA	C1D-CHD-C4C	-3.16	118.16	122.48
17	8	313	CLA	C1D-CHD-C4C	-3.16	118.64	126.17
20	9	618	BCR	C21-C20-C19	-3.16	113.54	123.23
17	B	823	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
17	a	830	CLA	C1-C2-C3	-3.16	120.14	125.96
17	1	303	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
17	L	203	CLA	C1-C2-C3	-3.16	120.14	125.96
17	a	817	CLA	CHC-C1C-C2C	-3.16	118.05	126.65
17	A	814	CLA	C1C-C2C-C3C	-3.16	103.42	106.92
17	B	837	CLA	O2D-CGD-O1D	-3.15	117.48	123.82
20	1	318	BCR	C21-C20-C19	-3.15	113.56	123.23
17	A	834	CLA	CHC-C1C-C2C	-3.15	118.05	126.65
17	A	836	CLA	CHC-C1C-C2C	-3.15	118.05	126.65
17	A	825	CLA	C1D-CHD-C4C	-3.15	118.18	122.48
17	l	203	CLA	C1D-CHD-C4C	-3.15	118.18	122.48
17	9	613	CLA	C1D-CHD-C4C	-3.15	118.18	122.48
17	A	812	CLA	C1-C2-C3	-3.15	120.15	125.96
17	a	806	CLA	C1C-C2C-C3C	-3.15	103.43	106.92
17	a	831	CLA	C1-C2-C3	-3.15	120.15	125.96
18	b	842	PQN	C11-C12-C13	-3.15	121.44	126.71
17	b	829	CLA	O2D-CGD-O1D	-3.15	117.49	123.82
17	b	837	CLA	O2D-CGD-O1D	-3.15	117.49	123.82
17	6	311	CLA	C1C-C2C-C3C	-3.15	103.43	106.92
20	3	318	BCR	C7-C8-C9	-3.15	121.48	126.21
17	A	807	CLA	C1D-CHD-C4C	-3.15	118.19	122.48
17	1	305	CLA	C1D-CHD-C4C	-3.15	118.19	122.48
17	9	612	CLA	C1D-CHD-C4C	-3.15	118.19	122.48
17	3	310	CLA	C1D-CHD-C4C	-3.15	118.19	122.48
20	F	305	BCR	C38-C26-C25	-3.14	120.99	124.51
17	a	814	CLA	C1-C2-C3	-3.14	120.17	125.96
17	8	301	CLA	C1C-C2C-C3C	-3.14	103.44	106.92
17	8	312	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
17	8	301	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
20	f	7004	BCR	C16-C17-C18	-3.14	122.83	127.31
17	A	821	CLA	CHC-C1C-C2C	-3.14	118.08	126.65
17	2	613	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
17	A	804	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
17	b	837	CLA	C1D-CHD-C4C	-3.14	118.20	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	849	DGD	C2G-O2G-C1B	-3.13	110.47	117.88
17	8	307	CLA	C1-C2-C3	-3.13	121.73	126.68
28	2	616	XAT	C10-C11-C12	-3.13	113.62	123.23
17	7	609	CLA	C1C-C2C-C3C	-3.13	103.44	106.92
17	9	614	CLA	C1D-CHD-C4C	-3.13	118.20	122.48
17	7	602	CLA	C1C-C2C-C3C	-3.13	103.45	106.92
20	F	305	BCR	C16-C17-C18	-3.13	122.84	127.31
26	2	601	CHL	C4A-C3A-C2A	-3.13	99.07	103.86
17	2	609	CLA	C1C-C2C-C3C	-3.13	103.45	106.92
17	B	831	CLA	C1C-C2C-C3C	-3.13	103.45	106.92
17	1	312	CLA	C1-C2-C3	-3.13	120.19	125.96
20	b	846	BCR	C16-C17-C18	-3.13	122.85	127.31
17	b	825	CLA	C1C-C2C-C3C	-3.13	103.45	106.92
17	A	805	CLA	C1D-CHD-C4C	-3.13	118.21	122.48
26	7	601	CHL	CBA-CAA-C2A	-3.13	111.45	115.76
17	3	302	CLA	C1C-C2C-C3C	-3.13	103.45	106.92
17	A	845	CLA	C1D-CHD-C4C	-3.12	118.21	122.48
17	B	832	CLA	C1C-C2C-C3C	-3.12	103.45	106.92
17	B	819	CLA	C1-C2-C3	-3.12	120.20	125.96
17	A	823	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
20	9	618	BCR	C38-C26-C25	-3.12	121.01	124.51
17	b	817	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
17	A	811	CLA	C1-C2-C3	-3.12	120.21	125.96
17	B	817	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
17	b	832	CLA	C1C-C2C-C3C	-3.12	103.46	106.92
17	1	305	CLA	C1-C2-C3	-3.12	120.22	125.96
17	b	805	CLA	CHC-C1C-C2C	-3.12	118.15	126.65
17	A	835	CLA	C1D-CHD-C4C	-3.12	118.23	122.48
17	J	3002	CLA	C1D-CHD-C4C	-3.12	118.23	122.48
17	a	819	CLA	C1C-C2C-C3C	-3.11	103.47	106.92
17	a	856	CLA	CHC-C1C-C2C	-3.11	118.16	126.65
17	3	309	CLA	C1C-C2C-C3C	-3.11	103.47	106.92
27	9	616	LUT	C15-C14-C13	-3.11	122.87	127.31
17	B	819	CLA	C1D-CHD-C4C	-3.11	118.23	122.48
17	1	303	CLA	C1C-C2C-C3C	-3.11	103.47	106.92
17	B	822	CLA	C1D-CHD-C4C	-3.11	118.23	122.48
17	a	830	CLA	C1D-CHD-C4C	-3.11	118.23	122.48
17	g	102	CLA	C1D-CHD-C4C	-3.11	118.23	122.48
17	8	308	CLA	C1C-C2C-C3C	-3.11	103.47	106.92
17	A	831	CLA	CHC-C1C-C2C	-3.11	118.17	126.65
17	4	602	CLA	C1C-C2C-C3C	-3.11	103.47	106.92
17	A	808	CLA	C1D-CHD-C4C	-3.11	118.24	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	816	CLA	C1D-CHD-C4C	-3.11	118.24	122.48
27	6	317	LUT	C18-C5-C6	-3.10	121.03	124.51
17	a	813	CLA	CHC-C1C-C2C	-3.10	118.18	126.65
17	3	312	CLA	C1-C2-C3	-3.10	120.24	125.96
20	a	852	BCR	C20-C21-C22	-3.10	122.88	127.31
28	2	616	XAT	C35-C34-C33	-3.10	122.88	127.31
17	4	613	CLA	C1D-CHD-C4C	-3.10	118.24	122.48
17	b	832	CLA	C1D-CHD-C4C	-3.10	118.24	122.48
20	B	843	BCR	C24-C23-C22	-3.10	121.55	126.21
17	7	602	CLA	C1D-CHD-C4C	-3.10	118.25	122.48
17	A	831	CLA	O2D-CGD-O1D	-3.10	117.58	123.82
17	b	809	CLA	C1D-CHD-C4C	-3.10	118.25	122.48
17	B	832	CLA	C1D-CHD-C4C	-3.10	118.25	122.48
17	k	1402	CLA	CHC-C1C-C2C	-3.10	118.20	126.65
17	1	314	CLA	C1D-CHD-C4C	-3.10	118.25	122.48
17	1	304	CLA	CHC-C1C-C2C	-3.10	118.20	126.65
17	4	604	CLA	C1D-CHD-C4C	-3.10	118.25	122.48
17	F	301	CLA	C1-C2-C3	-3.09	120.25	125.96
17	A	828	CLA	C1C-C2C-C3C	-3.09	103.49	106.92
17	J	3002	CLA	CHC-C1C-C2C	-3.09	118.21	126.65
17	A	821	CLA	CBC-CAC-C3C	-3.09	103.63	112.41
17	A	814	CLA	C1-C2-C3	-3.09	120.26	125.96
17	b	821	CLA	CHC-C1C-C2C	-3.09	118.22	126.65
17	A	835	CLA	CHC-C1C-C2C	-3.09	118.22	126.65
17	B	827	CLA	C1D-CHD-C4C	-3.09	118.26	122.48
17	b	811	CLA	C1-C2-C3	-3.09	120.26	125.96
17	A	806	CLA	C1C-C2C-C3C	-3.09	103.50	106.92
17	B	809	CLA	CHC-C1C-C2C	-3.09	118.23	126.65
17	a	813	CLA	C1D-CHD-C4C	-3.09	118.27	122.48
27	9	616	LUT	C10-C11-C12	-3.09	113.76	123.23
17	b	819	CLA	C1D-CHD-C4C	-3.09	118.27	122.48
20	a	852	BCR	C38-C26-C25	-3.09	121.05	124.51
17	2	608	CLA	CHC-C1C-C2C	-3.09	118.24	126.65
17	A	804	CLA	C1-C2-C3	-3.09	120.27	125.96
17	b	808	CLA	O2A-CGA-O1A	-3.08	115.89	123.55
20	2	617	BCR	C11-C10-C9	-3.08	122.91	127.31
17	9	604	CLA	C1D-CHD-C4C	-3.08	118.27	122.48
17	1	309	CLA	CHC-C1C-C2C	-3.08	118.25	126.65
17	4	604	CLA	CHC-C1C-C2C	-3.08	118.25	126.65
17	B	807	CLA	C1D-CHD-C4C	-3.08	118.27	122.48
17	B	822	CLA	C1-C2-C3	-3.08	120.28	125.96
17	A	824	CLA	C1D-CHD-C4C	-3.08	118.28	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	j	3003	BCR	C15-C14-C13	-3.08	122.92	127.31
17	A	802	CLA	C1C-C2C-C3C	-3.08	103.51	106.92
17	4	612	CLA	CHC-C1C-C2C	-3.08	118.25	126.65
26	8	306	CHL	C4A-C3A-C2A	-3.08	99.15	103.86
17	a	801	CLA	C1-C2-C3	-3.08	120.29	125.96
17	B	834	CLA	CHC-C1C-C2C	-3.08	118.26	126.65
17	9	611	CLA	CHC-C1C-C2C	-3.08	118.26	126.65
26	7	607	CHL	C4A-C3A-C2A	-3.08	99.16	103.86
17	a	821	CLA	CHC-C1C-C2C	-3.08	118.26	126.65
17	A	837	CLA	CHC-C1C-C2C	-3.07	118.26	126.65
26	1	302	CHL	O2D-CGD-O1D	-3.07	117.63	123.82
20	j	3003	BCR	C24-C23-C22	-3.07	121.59	126.21
26	1	302	CHL	CBA-CAA-C2A	-3.07	111.52	115.76
17	A	832	CLA	CHC-C1C-C2C	-3.07	118.27	126.65
17	A	817	CLA	CHC-C1C-C2C	-3.07	118.27	126.65
20	b	847	BCR	C21-C20-C19	-3.07	113.81	123.23
17	6	304	CLA	C1D-CHD-C4C	-3.07	118.29	122.48
17	a	801	CLA	C1D-CHD-C4C	-3.07	118.29	122.48
17	6	305	CLA	CHC-C1C-C2C	-3.07	118.27	126.65
17	7	604	CLA	CHC-C1C-C2C	-3.07	118.28	126.65
17	A	811	CLA	CHC-C1C-C2C	-3.07	118.28	126.65
17	a	836	CLA	CHC-C1C-C2C	-3.07	118.28	126.65
17	g	101	CLA	CMA-C3A-C2A	-3.07	110.18	116.38
17	j	3002	CLA	C1D-CHD-C4C	-3.07	118.29	122.48
17	a	820	CLA	C1D-CHD-C4C	-3.07	118.29	122.48
17	9	612	CLA	CHC-C1C-C2C	-3.07	118.29	126.65
17	b	833	CLA	C1-C2-C3	-3.07	120.31	125.96
17	a	836	CLA	C1-C2-C3	-3.07	121.84	126.68
17	K	4003	CLA	CHC-C1C-C2C	-3.07	118.29	126.65
17	A	819	CLA	C1-C2-C3	-3.06	120.31	125.96
17	3	305	CLA	CHC-C1C-C2C	-3.06	118.30	126.65
17	b	831	CLA	CHC-C1C-C2C	-3.06	118.30	126.65
17	7	604	CLA	C1D-CHD-C4C	-3.06	118.30	122.48
20	7	617	BCR	C7-C8-C9	-3.06	121.61	126.21
17	A	839	CLA	O2D-CGD-O1D	-3.06	117.66	123.82
20	8	316	BCR	C23-C24-C25	-3.06	118.68	127.25
17	7	612	CLA	CHC-C1C-C2C	-3.06	118.31	126.65
17	A	802	CLA	C1D-CHD-C4C	-3.06	118.30	122.48
17	3	313	CLA	CHC-C1C-C2C	-3.06	118.31	126.65
17	B	803	CLA	C1C-NC-C4C	-3.06	105.30	107.06
17	l	202	CLA	CHC-C1C-C2C	-3.06	118.31	126.65
17	3	312	CLA	CHC-C1C-C2C	-3.06	118.31	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	321	LUT	C23-C24-C25	-3.06	122.35	125.22
17	A	809	CLA	O2D-CGD-O1D	-3.06	117.67	123.82
17	a	828	CLA	C4C-C3C-C2C	-3.06	102.22	106.91
20	L	201	BCR	C20-C21-C22	-3.06	122.95	127.31
17	a	819	CLA	C1-C2-C3	-3.05	120.33	125.96
17	A	827	CLA	C1-C2-C3	-3.05	120.33	125.96
17	9	601	CLA	CHC-C1C-C2C	-3.05	118.32	126.65
17	B	808	CLA	CHC-C1C-C2C	-3.05	118.32	126.65
17	2	602	CLA	C1D-CHD-C4C	-3.05	118.31	122.48
20	b	846	BCR	C33-C5-C6	-3.05	121.09	124.51
17	b	841	CLA	C1D-CHD-C4C	-3.05	118.32	122.48
17	a	840	CLA	C1D-CHD-C4C	-3.05	118.32	122.48
17	1	313	CLA	CHC-C1C-C2C	-3.05	118.34	126.65
17	L	203	CLA	C1D-CHD-C4C	-3.05	118.32	122.48
17	a	820	CLA	CHC-C1C-C2C	-3.05	118.34	126.65
17	b	819	CLA	C1-C2-C3	-3.05	120.34	125.96
17	6	313	CLA	CHC-C1C-C2C	-3.05	118.34	126.65
28	9	617	XAT	C35-C15-C14	-3.05	116.96	123.46
17	6	304	CLA	C1-C2-C3	-3.04	120.35	125.96
20	6	319	BCR	C38-C26-C25	-3.04	121.10	124.51
17	b	818	CLA	CHC-C1C-C2C	-3.04	118.35	126.65
17	4	613	CLA	CHC-C1C-C2C	-3.04	118.35	126.65
17	3	310	CLA	CHC-C1C-C2C	-3.04	118.35	126.65
17	k	1403	CLA	CHC-C1C-C2C	-3.04	118.35	126.65
17	a	814	CLA	C1D-CHD-C4C	-3.04	118.33	122.48
17	b	808	CLA	CHC-C1C-C2C	-3.04	118.35	126.65
20	A	850	BCR	C20-C21-C22	-3.04	122.97	127.31
17	9	602	CLA	C1C-C2C-C3C	-3.04	103.55	106.92
20	f	7004	BCR	C38-C26-C25	-3.04	121.10	124.51
17	a	818	CLA	CHC-C1C-C2C	-3.04	118.36	126.65
17	2	604	CLA	C1D-CHD-C4C	-3.04	118.33	122.48
17	a	822	CLA	C1D-CHD-C4C	-3.04	118.33	122.48
26	7	606	CHL	C4A-C3A-C2A	-3.04	99.21	103.86
20	A	849	BCR	C24-C23-C22	-3.04	121.65	126.21
17	b	817	CLA	CHC-C1C-C2C	-3.04	118.36	126.65
17	6	304	CLA	CHC-C1C-C2C	-3.04	118.36	126.65
17	A	831	CLA	C1-C2-C3	-3.04	120.36	125.96
17	A	822	CLA	C1D-CHD-C4C	-3.04	118.33	122.48
17	A	843	CLA	CHC-C1C-C2C	-3.04	118.36	126.65
26	2	614	CHL	CBC-CAC-C3C	-3.04	108.34	112.95
17	8	310	CLA	CHC-C1C-C2C	-3.03	118.37	126.65
17	6	306	CLA	CHC-C1C-C2C	-3.03	118.38	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	837	CLA	CHC-C1C-C2C	-3.03	118.38	126.65
17	3	303	CLA	CHC-C1C-C2C	-3.03	118.38	126.65
17	7	610	CLA	CHC-C1C-C2C	-3.03	118.38	126.65
17	7	611	CLA	CHC-C1C-C2C	-3.03	118.38	126.65
17	a	824	CLA	C1D-CHD-C4C	-3.03	118.34	122.48
17	b	818	CLA	O2D-CGD-O1D	-3.03	117.72	123.82
17	A	824	CLA	CHC-C1C-C2C	-3.03	118.39	126.65
17	a	834	CLA	C1D-CHD-C4C	-3.03	118.34	122.48
20	L	201	BCR	C16-C17-C18	-3.03	122.99	127.31
17	6	312	CLA	CHC-C1C-C2C	-3.03	118.39	126.65
17	a	811	CLA	CHC-C1C-C2C	-3.03	118.40	126.65
17	9	608	CLA	CHC-C1C-C2C	-3.03	118.40	126.65
17	2	604	CLA	CHC-C1C-C2C	-3.02	118.40	126.65
17	B	824	CLA	C1-C2-C3	-3.02	120.38	125.96
17	B	831	CLA	CHC-C1C-C2C	-3.02	118.40	126.65
17	8	309	CLA	CHC-C1C-C2C	-3.02	118.40	126.65
17	8	311	CLA	CHC-C1C-C2C	-3.02	118.41	126.65
17	b	803	CLA	C1C-C2C-C3C	-3.02	103.57	106.92
17	a	840	CLA	CHC-C1C-C2C	-3.02	118.41	126.65
26	2	601	CHL	O2D-CGD-O1D	-3.02	117.74	123.82
28	2	616	XAT	C15-C14-C13	-3.02	123.00	127.31
17	A	845	CLA	CHC-C1C-C2C	-3.02	118.41	126.65
17	A	813	CLA	C1D-CHD-C4C	-3.02	118.36	122.48
17	b	809	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
17	b	835	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
17	b	834	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
17	A	822	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
17	3	302	CLA	C1D-CHD-C4C	-3.02	118.36	122.48
17	a	827	CLA	CAA-C2A-C3A	-3.02	104.54	112.81
17	4	611	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
17	L	202	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
17	2	610	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
17	a	856	CLA	CAA-C2A-C3A	-3.02	104.54	112.81
17	2	612	CLA	CHC-C1C-C2C	-3.02	118.43	126.65
20	L	201	BCR	C24-C23-C22	-3.01	121.68	126.21
17	8	305	CLA	CHC-C1C-C2C	-3.01	118.43	126.65
17	b	804	CLA	O2D-CGD-O1D	-3.01	117.76	123.82
26	4	606	CHL	C4A-C3A-C2A	-3.01	99.25	103.86
17	9	614	CLA	CHC-C1C-C2C	-3.01	118.44	126.65
17	B	831	CLA	C1D-CHD-C4C	-3.01	118.37	122.48
17	a	843	CLA	C1C-C2C-C3C	-3.01	103.58	106.92
17	B	820	CLA	CHC-C1C-C2C	-3.01	118.44	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	313	CLA	C1D-CHD-C4C	-3.01	118.37	122.48
20	1	205	BCR	C23-C24-C25	-3.01	118.82	127.25
17	7	613	CLA	CHC-C1C-C2C	-3.01	118.44	126.65
17	3	304	CLA	CHC-C1C-C2C	-3.01	118.44	126.65
17	1	314	CLA	CHC-C1C-C2C	-3.01	118.44	126.65
17	4	602	CLA	C1D-CHD-C4C	-3.01	118.37	122.48
20	B	801	BCR	C33-C5-C6	-3.01	121.14	124.51
17	B	818	CLA	CHC-C1C-C2C	-3.01	118.45	126.65
17	6	315	CLA	CHC-C1C-C2C	-3.01	118.45	126.65
17	b	818	CLA	C1D-CHD-C4C	-3.01	118.38	122.48
26	9	607	CHL	C4A-C3A-C2A	-3.01	99.26	103.86
17	B	826	CLA	C4C-C3C-C2C	-3.01	102.30	106.91
20	A	852	BCR	C20-C19-C18	-3.01	117.97	126.42
17	B	833	CLA	CHC-C1C-C2C	-3.01	118.45	126.65
26	9	606	CHL	C4A-C3A-C2A	-3.00	99.26	103.86
17	B	829	CLA	O2D-CGD-O1D	-3.00	117.78	123.82
17	b	802	CLA	CHC-C1C-C2C	-3.00	118.46	126.65
17	a	824	CLA	CHC-C1C-C2C	-3.00	118.46	126.65
17	6	310	CLA	CHC-C1C-C2C	-3.00	118.47	126.65
17	A	827	CLA	CAA-C2A-C3A	-3.00	104.59	112.81
17	b	808	CLA	CBC-CAC-C3C	-3.00	103.89	112.41
17	2	613	CLA	CHC-C1C-C2C	-3.00	118.47	126.65
17	b	824	CLA	O2D-CGD-O1D	-3.00	117.79	123.82
20	L	206	BCR	C33-C5-C6	-3.00	121.15	124.51
17	A	839	CLA	CHC-C1C-C2C	-3.00	118.47	126.65
26	2	601	CHL	OMC-CMC-C2C	-3.00	120.46	124.29
27	3	316	LUT	C15-C14-C13	-3.00	123.03	127.31
17	A	803	CLA	CHC-C1C-C2C	-3.00	118.48	126.65
17	a	808	CLA	C1-C2-C3	-3.00	120.44	125.96
26	9	605	CHL	C4A-C3A-C2A	-3.00	99.28	103.86
17	g	103	CLA	CHC-C1C-C2C	-2.99	118.48	126.65
17	f	7003	CLA	CHC-C1C-C2C	-2.99	118.48	126.65
17	9	613	CLA	CHC-C1C-C2C	-2.99	118.48	126.65
17	B	829	CLA	C1-C2-C3	-2.99	120.44	125.96
17	1	312	CLA	CHC-C1C-C2C	-2.99	118.48	126.65
17	a	802	CLA	C1D-CHD-C4C	-2.99	118.39	122.48
17	b	802	CLA	CAA-C2A-C3A	-2.99	104.60	112.81
17	F	303	CLA	CHC-C1C-C2C	-2.99	118.49	126.65
26	3	307	CHL	C4A-C3A-C2A	-2.99	99.29	103.86
17	B	805	CLA	CHC-C1C-C2C	-2.99	118.50	126.65
17	b	813	CLA	CHC-C1C-C2C	-2.99	118.50	126.65
27	4	616	LUT	C11-C10-C9	-2.99	123.05	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	827	CLA	C1D-CHD-C4C	-2.99	118.40	122.48
17	a	832	CLA	CHC-C1C-C2C	-2.99	118.50	126.65
17	B	840	CLA	C1-C2-C3	-2.99	120.45	125.96
20	8	316	BCR	C21-C20-C19	-2.99	114.07	123.23
26	6	303	CHL	O2D-CGD-O1D	-2.99	117.81	123.82
26	4	606	CHL	C1-C2-C3	-2.99	121.96	126.68
17	b	837	CLA	CHC-C1C-C2C	-2.98	118.51	126.65
26	6	308	CHL	C4A-C3A-C2A	-2.98	99.30	103.86
17	9	604	CLA	CHC-C1C-C2C	-2.98	118.51	126.65
17	a	805	CLA	CHC-C1C-C2C	-2.98	118.52	126.65
17	3	301	CLA	CHC-C1C-C2C	-2.98	118.52	126.65
17	B	811	CLA	CHC-C1C-C2C	-2.98	118.52	126.65
17	1	315	CLA	CHC-C1C-C2C	-2.98	118.52	126.65
17	A	820	CLA	CHC-C1C-C2C	-2.98	118.52	126.65
17	b	804	CLA	O1D-CGD-CBD	-2.98	119.25	124.60
27	2	615	LUT	C11-C10-C9	-2.98	123.06	127.31
17	j	3002	CLA	CHC-C1C-C2C	-2.98	118.53	126.65
17	6	307	CLA	CHC-C1C-C2C	-2.98	118.53	126.65
17	4	614	CLA	CHC-C1C-C2C	-2.98	118.53	126.65
20	B	845	BCR	C38-C26-C25	-2.97	121.18	124.51
27	6	317	LUT	C23-C24-C25	-2.97	122.43	125.22
17	1	305	CLA	CHC-C1C-C2C	-2.97	118.54	126.65
17	A	823	CLA	CHC-C1C-C2C	-2.97	118.54	126.65
28	6	318	XAT	C10-C11-C12	-2.97	114.11	123.23
17	b	807	CLA	CHC-C1C-C2C	-2.97	118.54	126.65
17	a	825	CLA	C1-C2-C3	-2.97	120.48	125.96
17	6	316	CLA	CHC-C1C-C2C	-2.97	118.55	126.65
17	B	840	CLA	CHC-C1C-C2C	-2.97	118.55	126.65
20	2	617	BCR	C33-C5-C6	-2.97	121.18	124.51
26	2	606	CHL	C4A-C3A-C2A	-2.97	99.32	103.86
20	B	847	BCR	C33-C5-C6	-2.97	121.18	124.51
17	b	805	CLA	O2D-CGD-O1D	-2.97	117.85	123.82
17	A	854	CLA	CHC-C1C-C2C	-2.97	118.55	126.65
17	9	610	CLA	CHC-C1C-C2C	-2.97	118.55	126.65
17	8	303	CLA	CHC-C1C-C2C	-2.97	118.56	126.65
17	B	821	CLA	CHC-C1C-C2C	-2.97	118.56	126.65
17	3	301	CLA	C1D-CHD-C4C	-2.97	118.43	122.48
17	3	314	CLA	CHC-C1C-C2C	-2.97	118.56	126.65
17	2	603	CLA	CHC-C1C-C2C	-2.97	118.56	126.65
27	9	616	LUT	C31-C30-C29	-2.97	123.08	127.31
17	B	812	CLA	CHC-C1C-C2C	-2.96	118.56	126.65
17	A	813	CLA	CHC-C1C-C2C	-2.96	118.57	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	849	BCR	C20-C21-C22	-2.96	123.08	127.31
17	2	611	CLA	CHC-C1C-C2C	-2.96	118.57	126.65
17	B	808	CLA	O2D-CGD-O1D	-2.96	117.86	123.82
17	B	839	CLA	CHC-C1C-C2C	-2.96	118.57	126.65
17	g	101	CLA	CHC-C1C-C2C	-2.96	118.58	126.65
17	2	610	CLA	CMA-C3A-C2A	-2.96	110.39	116.38
17	b	802	CLA	C1-C2-C3	-2.96	120.50	125.96
17	8	304	CLA	CHC-C1C-C2C	-2.96	118.58	126.65
26	2	614	CHL	C4A-C3A-C2A	-2.96	99.33	103.86
17	4	601	CLA	CHC-C1C-C2C	-2.96	118.58	126.65
17	8	302	CLA	CHC-C1C-C2C	-2.96	118.58	126.65
17	1	306	CLA	CHC-C1C-C2C	-2.96	118.58	126.65
17	3	306	CLA	CHC-C1C-C2C	-2.96	118.59	126.65
17	8	312	CLA	CHC-C1C-C2C	-2.96	118.59	126.65
17	b	812	CLA	CHC-C1C-C2C	-2.96	118.59	126.65
27	2	615	LUT	C7-C8-C9	-2.95	121.77	126.21
20	9	618	BCR	C33-C5-C6	-2.95	121.20	124.51
17	g	102	CLA	CHC-C1C-C2C	-2.95	118.59	126.65
26	4	607	CHL	C4A-C3A-C2A	-2.95	99.34	103.86
26	6	303	CHL	OMC-CMC-C2C	-2.95	120.52	124.29
28	7	616	XAT	C10-C11-C12	-2.95	114.17	123.23
17	B	817	CLA	C1-C2-C3	-2.95	120.52	125.96
26	2	607	CHL	C4A-C3A-C2A	-2.95	99.35	103.86
17	1	311	CLA	CHC-C1C-C2C	-2.95	118.60	126.65
17	A	836	CLA	C1-C2-C3	-2.95	122.02	126.68
17	A	814	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
17	6	314	CLA	CHC-C1C-C2C	-2.95	118.60	126.65
17	a	810	CLA	CHC-C1C-C2C	-2.95	118.61	126.65
17	B	817	CLA	CHC-C1C-C2C	-2.95	118.61	126.65
28	7	616	XAT	C35-C34-C33	-2.95	123.10	127.31
20	3	318	BCR	C23-C24-C25	-2.95	119.00	127.25
17	b	826	CLA	C1-C2-C3	-2.95	120.53	125.96
17	9	609	CLA	CHC-C1C-C2C	-2.95	118.62	126.65
17	A	814	CLA	CHC-C1C-C2C	-2.95	118.62	126.65
17	3	311	CLA	CHC-C1C-C2C	-2.94	118.62	126.65
17	a	801	CLA	CHC-C1C-C2C	-2.94	118.62	126.65
17	B	813	CLA	C1C-C2C-C3C	-2.94	103.66	106.92
17	A	810	CLA	CHC-C1C-C2C	-2.94	118.62	126.65
17	B	814	CLA	C1C-C2C-C3C	-2.94	103.66	106.92
17	A	854	CLA	CAA-C2A-C3A	-2.94	104.75	112.81
17	A	816	CLA	CHC-C1C-C2C	-2.94	118.63	126.65
17	a	823	CLA	CHC-C1C-C2C	-2.94	118.63	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	614	CHL	C4A-C3A-C2A	-2.94	99.36	103.86
17	A	842	CLA	CHC-C1C-C2C	-2.94	118.63	126.65
17	B	822	CLA	CHC-C1C-C2C	-2.94	118.63	126.65
26	4	607	CHL	C1-C2-C3	-2.94	122.04	126.68
20	3	318	BCR	C11-C10-C9	-2.94	123.11	127.31
20	b	844	BCR	C33-C5-C6	-2.94	121.22	124.51
17	4	610	CLA	CHC-C1C-C2C	-2.94	118.64	126.65
17	7	610	CLA	CMA-C3A-C2A	-2.94	110.44	116.38
17	a	835	CLA	CHC-C1C-C2C	-2.94	118.64	126.65
17	4	603	CLA	CHC-C1C-C2C	-2.94	118.64	126.65
20	b	843	BCR	C20-C21-C22	-2.94	123.12	127.31
17	a	825	CLA	CHC-C1C-C2C	-2.93	118.65	126.65
17	b	815	CLA	CHC-C1C-C2C	-2.93	118.65	126.65
17	a	844	CLA	CBC-CAC-C3C	-2.93	104.08	112.41
17	1	310	CLA	C1-C2-C3	-2.93	120.55	125.96
17	8	303	CLA	C1D-CHD-C4C	-2.93	118.48	122.48
17	A	801	CLA	C1-C2-C3	-2.93	120.56	125.96
17	B	835	CLA	CHC-C1C-C2C	-2.93	118.66	126.65
17	6	309	CLA	CHC-C1C-C2C	-2.93	118.66	126.65
17	a	805	CLA	C1-C2-C3	-2.93	120.56	125.96
17	a	835	CLA	O1D-CGD-CBD	-2.93	119.34	124.60
20	B	846	BCR	C33-C5-C6	-2.93	121.23	124.51
17	b	813	CLA	C1C-C2C-C3C	-2.93	103.67	106.92
17	F	304	CLA	CHC-C1C-C2C	-2.93	118.67	126.65
20	L	205	BCR	C3-C4-C5	-2.93	108.75	113.78
20	K	4001	BCR	C20-C19-C18	-2.93	118.20	126.42
17	b	805	CLA	C1D-CHD-C4C	-2.93	118.49	122.48
17	b	840	CLA	CHC-C1C-C2C	-2.93	118.67	126.65
17	a	827	CLA	C1-C2-C3	-2.92	120.57	125.96
17	l	204	CLA	CHC-C1C-C2C	-2.92	118.68	126.65
26	2	605	CHL	OMC-CMC-C2C	-2.92	120.56	124.29
17	B	813	CLA	C4C-C3C-C2C	-2.92	102.43	106.91
17	A	819	CLA	CHC-C1C-C2C	-2.92	118.68	126.65
17	B	802	CLA	CAA-C2A-C3A	-2.92	104.80	112.81
18	B	842	PQN	C11-C12-C13	-2.92	121.83	126.71
17	1	303	CLA	CHC-C1C-C2C	-2.92	118.68	126.65
20	A	848	BCR	C7-C8-C9	-2.92	121.82	126.21
17	b	816	CLA	CHC-C1C-C2C	-2.92	118.69	126.65
27	1	320	LUT	C35-C34-C33	-2.92	123.14	127.31
20	G	105	BCR	C3-C4-C5	-2.92	108.76	113.78
28	4	617	XAT	C10-C11-C12	-2.92	114.28	123.23
17	A	801	CLA	O2D-CGD-O1D	-2.92	117.95	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	846	CLA	CHC-C1C-C2C	-2.91	118.70	126.65
17	2	602	CLA	CHC-C1C-C2C	-2.91	118.70	126.65
17	4	603	CLA	CBC-CAC-C3C	-2.91	104.14	112.41
17	a	818	CLA	O2D-CGD-O1D	-2.91	117.96	123.82
27	6	317	LUT	C7-C8-C9	-2.91	121.83	126.21
17	b	830	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
17	b	811	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
17	K	4002	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
17	b	815	CLA	O2D-CGD-O1D	-2.91	117.96	123.82
17	f	7002	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
17	B	810	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
17	b	839	CLA	C4C-C3C-C2C	-2.91	102.44	106.91
17	a	839	CLA	C1-C2-C3	-2.91	120.59	125.96
17	b	833	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
17	8	307	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
17	a	826	CLA	C1-C2-C3	-2.91	120.59	125.96
17	A	806	CLA	CHC-C1C-C2C	-2.91	118.72	126.65
17	B	831	CLA	C4C-C3C-C2C	-2.91	102.45	106.91
20	G	105	BCR	C7-C8-C9	-2.91	121.84	126.21
17	b	810	CLA	C4C-C3C-C2C	-2.91	102.45	106.91
17	a	822	CLA	CHC-C1C-C2C	-2.91	118.72	126.65
17	8	302	CLA	C1-C2-C3	-2.91	122.09	126.68
17	b	839	CLA	CHC-C1C-C2C	-2.90	118.73	126.65
20	a	850	BCR	C24-C23-C22	-2.90	121.85	126.21
20	i	101	BCR	C15-C16-C17	-2.90	117.26	123.46
17	b	826	CLA	C4C-C3C-C2C	-2.90	102.45	106.91
20	g	104	BCR	C7-C8-C9	-2.90	121.85	126.21
17	B	837	CLA	CHC-C1C-C2C	-2.90	118.73	126.65
26	1	307	CHL	C4A-C3A-C2A	-2.90	99.42	103.86
17	A	818	CLA	CHC-C1C-C2C	-2.90	118.74	126.65
17	F	301	CLA	CHC-C1C-C2C	-2.90	118.74	126.65
17	7	608	CLA	CHC-C1C-C2C	-2.90	118.75	126.65
17	a	804	CLA	C1D-CHD-C4C	-2.90	118.53	122.48
17	1	306	CLA	C4C-C3C-C2C	-2.90	102.47	106.91
17	a	832	CLA	C4C-C3C-C2C	-2.90	102.47	106.91
17	a	831	CLA	CHC-C1C-C2C	-2.90	118.75	126.65
17	B	824	CLA	CHC-C1C-C2C	-2.89	118.75	126.65
17	B	815	CLA	CHC-C1C-C2C	-2.89	118.75	126.65
17	B	838	CLA	CHC-C1C-C2C	-2.89	118.75	126.65
17	B	823	CLA	C4C-C3C-C2C	-2.89	102.47	106.91
17	1	308	CLA	CHC-C1C-C2C	-2.89	118.76	126.65
17	4	608	CLA	CHC-C1C-C2C	-2.89	118.76	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	9	616	LUT	C8-C7-C6	-2.89	119.15	127.25
17	a	841	CLA	CHC-C1C-C2C	-2.89	118.76	126.65
17	b	809	CLA	CBC-CAC-C3C	-2.89	104.20	112.41
17	A	804	CLA	CHC-C1C-C2C	-2.89	118.77	126.65
17	G	101	CLA	CHC-C1C-C2C	-2.89	118.77	126.65
17	6	306	CLA	C1-C2-C3	-2.89	120.63	125.96
17	8	303	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
17	G	103	CLA	CHC-C1C-C2C	-2.89	118.77	126.65
27	7	615	LUT	C15-C14-C13	-2.89	123.19	127.31
17	b	813	CLA	C4C-C3C-C2C	-2.89	102.48	106.91
17	b	841	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
20	B	845	BCR	C11-C10-C9	-2.89	123.19	127.31
17	a	802	CLA	CHC-C1C-C2C	-2.89	118.78	126.65
17	L	204	CLA	CHC-C1C-C2C	-2.88	118.78	126.65
17	7	603	CLA	CHC-C1C-C2C	-2.88	118.78	126.65
20	K	4004	BCR	C24-C23-C22	-2.88	121.88	126.21
17	A	840	CLA	O2D-CGD-O1D	-2.88	118.02	123.82
17	9	602	CLA	C1-C2-C3	-2.88	120.65	125.96
17	B	813	CLA	CHC-C1C-C2C	-2.88	118.79	126.65
17	3	302	CLA	CHC-C1C-C2C	-2.88	118.79	126.65
17	A	812	CLA	CHC-C1C-C2C	-2.88	118.80	126.65
17	a	812	CLA	CHC-C1C-C2C	-2.88	118.80	126.65
17	k	1401	CLA	CHC-C1C-C2C	-2.88	118.80	126.65
17	1	306	CLA	C1C-C2C-C3C	-2.88	103.73	106.92
17	b	822	CLA	C1-C2-C3	-2.88	120.66	125.96
17	A	829	CLA	CHC-C1C-C2C	-2.88	118.81	126.65
20	J	3003	BCR	C24-C23-C22	-2.88	121.89	126.21
17	b	823	CLA	CHC-C1C-C2C	-2.88	118.81	126.65
28	6	318	XAT	C31-C30-C29	-2.88	123.21	127.31
20	l	201	BCR	C34-C9-C10	-2.88	118.89	122.92
20	a	850	BCR	C38-C26-C25	-2.87	121.29	124.51
17	a	846	CLA	C1-C2-C3	-2.87	120.66	125.96
17	B	813	CLA	C1-C2-C3	-2.87	120.66	125.96
17	b	838	CLA	CHC-C1C-C2C	-2.87	118.82	126.65
27	2	615	LUT	C31-C30-C29	-2.87	123.21	127.31
17	A	808	CLA	CHC-C1C-C2C	-2.87	118.82	126.65
17	b	826	CLA	CHC-C1C-C2C	-2.87	118.82	126.65
28	1	317	XAT	C35-C15-C14	-2.87	117.34	123.46
17	A	801	CLA	CHC-C1C-C2C	-2.87	118.83	126.65
28	4	617	XAT	C24-C23-C22	-2.87	104.84	110.68
17	4	602	CLA	CHC-C1C-C2C	-2.87	118.83	126.65
17	B	804	CLA	CHC-C1C-C2C	-2.87	118.83	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	815	CLA	CHC-C1C-C2C	-2.87	118.83	126.65
17	A	814	CLA	C4C-C3C-C2C	-2.87	102.51	106.91
17	B	828	CLA	C1-C2-C3	-2.87	120.68	125.96
28	4	617	XAT	C15-C14-C13	-2.86	123.22	127.31
20	6	319	BCR	C21-C20-C19	-2.86	114.45	123.23
17	B	823	CLA	CHC-C1C-C2C	-2.86	118.84	126.65
17	b	824	CLA	CHC-C1C-C2C	-2.86	118.84	126.65
17	b	820	CLA	CHC-C1C-C2C	-2.86	118.84	126.65
17	B	821	CLA	O2D-CGD-O1D	-2.86	118.06	123.82
17	b	813	CLA	O2D-CGD-O1D	-2.86	118.06	123.82
17	A	807	CLA	CHC-C1C-C2C	-2.86	118.85	126.65
17	a	801	CLA	O2D-CGD-O1D	-2.86	118.06	123.82
17	3	315	CLA	C2A-C1A-CHA	-2.86	117.76	122.63
20	B	848	BCR	C15-C14-C13	-2.86	123.23	127.31
20	B	848	BCR	C10-C11-C12	-2.86	114.46	123.23
17	B	814	CLA	C4C-C3C-C2C	-2.86	102.52	106.91
27	8	314	LUT	C23-C24-C25	-2.86	122.54	125.22
17	1	310	CLA	CHC-C1C-C2C	-2.86	118.86	126.65
20	a	854	BCR	C34-C9-C10	-2.86	118.92	122.92
17	A	805	CLA	CHC-C1C-C2C	-2.86	118.86	126.65
27	4	616	LUT	C23-C24-C25	-2.86	122.54	125.22
20	L	206	BCR	C38-C26-C25	-2.86	121.31	124.51
17	A	840	CLA	CHC-C1C-C2C	-2.85	118.86	126.65
17	B	814	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
20	K	4001	BCR	C20-C21-C22	-2.85	123.24	127.31
17	B	828	CLA	CHC-C1C-C2C	-2.85	118.86	126.65
17	a	831	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
20	a	854	BCR	C15-C14-C13	-2.85	123.24	127.31
17	b	822	CLA	CHC-C1C-C2C	-2.85	118.87	126.65
17	3	308	CLA	CHC-C1C-C2C	-2.85	118.87	126.65
17	a	831	CLA	C4C-C3C-C2C	-2.85	102.53	106.91
26	1	302	CHL	C4A-C3A-C2A	-2.85	99.50	103.86
20	a	853	BCR	C3-C4-C5	-2.85	108.88	113.78
17	b	832	CLA	C4C-C3C-C2C	-2.85	102.54	106.91
20	4	618	BCR	C33-C5-C6	-2.85	121.32	124.51
17	a	834	CLA	CHC-C1C-C2C	-2.85	118.88	126.65
17	a	802	CLA	C1-C2-C3	-2.85	120.71	125.96
17	a	812	CLA	CAA-C2A-C3A	-2.85	105.00	112.81
17	B	807	CLA	CHC-C1C-C2C	-2.85	118.89	126.65
17	A	833	CLA	CHC-C1C-C2C	-2.85	118.89	126.65
17	a	844	CLA	CHC-C1C-C2C	-2.85	118.89	126.65
17	B	816	CLA	CHC-C1C-C2C	-2.85	118.89	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	g	104	BCR	C11-C10-C9	-2.85	123.25	127.31
26	7	605	CHL	CHA-CBD-CGD	-2.85	108.40	115.00
17	B	832	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
17	a	839	CLA	CHC-C1C-C2C	-2.84	118.89	126.65
17	A	831	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
17	A	828	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
17	b	825	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
20	B	846	BCR	C11-C10-C9	-2.84	123.26	127.31
20	A	848	BCR	C11-C10-C9	-2.84	123.26	127.31
20	B	844	BCR	C33-C5-C6	-2.84	121.33	124.51
17	b	808	CLA	CAA-C2A-C3A	-2.84	105.03	112.81
17	8	313	CLA	C2A-C1A-CHA	-2.84	117.79	122.63
17	a	856	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
17	9	610	CLA	CMA-C3A-C2A	-2.84	110.64	116.38
20	b	845	BCR	C20-C21-C22	-2.84	123.26	127.31
17	B	827	CLA	C4C-C3C-C2C	-2.84	102.56	106.91
17	a	842	CLA	CHC-C1C-C2C	-2.84	118.91	126.65
17	G	104	CLA	CHC-C1C-C2C	-2.84	118.92	126.65
17	a	805	CLA	O2D-CGD-O1D	-2.83	118.12	123.82
17	b	803	CLA	C4C-C3C-C2C	-2.83	102.56	106.91
17	b	832	CLA	CHC-C1C-C2C	-2.83	118.93	126.65
17	a	826	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
20	4	618	BCR	C21-C20-C19	-2.83	114.55	123.23
17	B	805	CLA	C4C-C3C-C2C	-2.83	102.57	106.91
20	a	850	BCR	C33-C5-C6	-2.83	121.34	124.51
17	a	816	CLA	CHC-C1C-C2C	-2.83	118.94	126.65
17	A	826	CLA	C4C-C3C-C2C	-2.83	102.57	106.91
20	I	101	BCR	C8-C7-C6	-2.83	119.34	127.25
17	a	840	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
17	a	810	CLA	C1-C2-C3	-2.83	120.75	125.96
17	A	826	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
19	A	846	LHG	C5-O7-C7	-2.82	111.20	117.88
26	6	303	CHL	C4A-C3A-C2A	-2.82	99.54	103.86
20	L	205	BCR	C23-C24-C25	-2.82	119.35	127.25
20	2	617	BCR	C38-C26-C25	-2.82	121.35	124.51
17	B	808	CLA	C1-C2-C3	-2.82	120.75	125.96
17	b	814	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
26	9	605	CHL	OMC-CMC-C2C	-2.82	120.69	124.29
17	B	832	CLA	CHC-C1C-C2C	-2.82	118.95	126.65
17	a	843	CLA	CHC-C1C-C2C	-2.82	118.95	126.65
17	a	815	CLA	CHC-C1C-C2C	-2.82	118.95	126.65
17	b	841	CLA	CHC-C1C-C2C	-2.82	118.96	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	852	BCR	C34-C9-C10	-2.82	118.97	122.92
17	a	833	CLA	C1D-CHD-C4C	-2.82	118.63	122.48
17	b	828	CLA	CHC-C1C-C2C	-2.82	118.96	126.65
17	a	833	CLA	CHC-C1C-C2C	-2.82	118.97	126.65
17	B	824	CLA	C4C-C3C-C2C	-2.81	102.59	106.91
20	b	843	BCR	C24-C23-C22	-2.81	121.98	126.21
17	B	824	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
17	a	827	CLA	CHC-C1C-C2C	-2.81	118.98	126.65
17	b	804	CLA	CHC-C1C-C2C	-2.81	118.98	126.65
27	1	316	LUT	C15-C14-C13	-2.81	123.30	127.31
17	A	854	CLA	C4C-C3C-C2C	-2.81	102.60	106.91
17	B	826	CLA	C1-C2-C3	-2.81	120.78	125.96
17	7	602	CLA	CHC-C1C-C2C	-2.81	118.99	126.65
17	a	806	CLA	CHC-C1C-C2C	-2.81	118.99	126.65
17	4	609	CLA	CHC-C1C-C2C	-2.81	118.99	126.65
20	a	854	BCR	C28-C27-C26	-2.81	108.95	113.78
20	A	851	BCR	C33-C5-C6	-2.81	121.36	124.51
26	2	605	CHL	CHA-CBD-CGD	-2.81	108.49	115.00
17	3	310	CLA	CMA-C3A-C2A	-2.81	110.70	116.38
17	A	803	CLA	CAA-C2A-C3A	-2.81	105.12	112.81
17	b	823	CLA	C1-C2-C3	-2.81	120.79	125.96
17	a	804	CLA	CHC-C1C-C2C	-2.80	119.00	126.65
17	A	802	CLA	C4C-C3C-C2C	-2.80	102.61	106.91
17	A	836	CLA	C4C-C3C-C2C	-2.80	102.61	106.91
17	A	841	CLA	C4C-C3C-C2C	-2.80	102.61	106.91
20	A	852	BCR	C28-C27-C26	-2.80	108.96	113.78
17	b	833	CLA	C4C-C3C-C2C	-2.80	102.61	106.91
20	b	846	BCR	C21-C20-C19	-2.80	114.64	123.23
17	A	809	CLA	CHC-C1C-C2C	-2.80	119.01	126.65
17	1	312	CLA	C4C-C3C-C2C	-2.80	102.61	106.91
17	A	834	CLA	C4C-C3C-C2C	-2.80	102.61	106.91
17	b	836	CLA	C4C-C3C-C2C	-2.80	102.62	106.91
17	3	311	CLA	C1-C2-C3	-2.80	120.80	125.96
20	a	849	BCR	C35-C13-C14	-2.80	119.00	122.92
20	A	849	BCR	C8-C7-C6	-2.80	119.42	127.25
17	a	810	CLA	C4C-C3C-C2C	-2.80	102.62	106.91
27	1	320	LUT	C23-C24-C25	-2.80	122.60	125.22
17	A	827	CLA	CHC-C1C-C2C	-2.80	119.02	126.65
17	B	825	CLA	C4C-C3C-C2C	-2.79	102.62	106.91
26	2	607	CHL	C3B-CAB-CBB	-2.79	118.93	125.20
17	a	816	CLA	C4C-C3C-C2C	-2.79	102.62	106.91
17	A	806	CLA	C4C-C3C-C2C	-2.79	102.63	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	f	7004	BCR	C35-C13-C14	-2.79	119.01	122.92
17	6	312	CLA	CMA-C3A-C2A	-2.79	110.74	116.38
17	3	306	CLA	C4C-C3C-C2C	-2.79	102.63	106.91
17	a	824	CLA	C4C-C3C-C2C	-2.79	102.63	106.91
27	1	320	LUT	C7-C8-C9	-2.79	122.02	126.21
17	B	802	CLA	CHC-C1C-C2C	-2.79	119.05	126.65
17	1	311	CLA	CMA-C3A-C2A	-2.79	110.74	116.38
17	B	806	CLA	CHC-C1C-C2C	-2.79	119.05	126.65
17	B	830	CLA	CHC-C1C-C2C	-2.79	119.05	126.65
17	a	826	CLA	CHC-C1C-C2C	-2.79	119.05	126.65
17	b	827	CLA	CAA-C2A-C3A	-2.78	105.18	112.81
17	8	308	CLA	CHC-C1C-C2C	-2.78	119.06	126.65
27	6	317	LUT	C30-C31-C32	-2.78	114.69	123.23
17	a	806	CLA	C4C-C3C-C2C	-2.78	102.64	106.91
17	b	810	CLA	CHC-C1C-C2C	-2.78	119.06	126.65
20	K	4004	BCR	C11-C10-C9	-2.78	123.34	127.31
17	b	802	CLA	C4C-C3C-C2C	-2.78	102.64	106.91
17	B	803	CLA	C1-C2-C3	-2.78	120.83	125.96
28	3	317	XAT	C15-C14-C13	-2.78	123.34	127.31
20	4	618	BCR	C23-C24-C25	-2.78	119.47	127.25
17	a	827	CLA	C4C-C3C-C2C	-2.78	102.65	106.91
17	a	843	CLA	C4C-C3C-C2C	-2.78	102.65	106.91
17	6	311	CLA	CHC-C1C-C2C	-2.78	119.07	126.65
17	8	308	CLA	CAA-C2A-C3A	-2.78	105.20	112.81
17	a	814	CLA	C4C-C3C-C2C	-2.78	102.65	106.91
17	A	829	CLA	C4C-C3C-C2C	-2.77	102.65	106.91
17	a	809	CLA	CHC-C1C-C2C	-2.77	119.09	126.65
17	8	301	CLA	CHC-C1C-C2C	-2.77	119.09	126.65
20	1	318	BCR	C23-C24-C25	-2.77	119.49	127.25
17	a	829	CLA	CHC-C1C-C2C	-2.77	119.09	126.65
17	3	314	CLA	C4C-C3C-C2C	-2.77	102.66	106.91
17	a	807	CLA	C1-C2-C3	-2.77	120.86	125.96
17	B	802	CLA	CMA-C3A-C4A	-2.77	104.33	111.77
17	B	820	CLA	C4C-C3C-C2C	-2.77	102.66	106.91
17	B	833	CLA	C4C-C3C-C2C	-2.77	102.66	106.91
26	1	307	CHL	CHA-CBD-CGD	-2.77	108.58	115.00
17	b	807	CLA	O2D-CGD-O1D	-2.77	118.25	123.82
17	B	804	CLA	O2D-CGD-O1D	-2.77	118.25	123.82
17	b	802	CLA	CMA-C3A-C4A	-2.77	104.34	111.77
17	A	841	CLA	CHC-C1C-C2C	-2.77	119.11	126.65
17	B	815	CLA	C4C-C3C-C2C	-2.77	102.67	106.91
27	4	616	LUT	C15-C14-C13	-2.76	123.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	316	LUT	C18-C5-C6	-2.76	121.41	124.51
17	A	830	CLA	CHC-C1C-C2C	-2.76	119.11	126.65
17	A	802	CLA	CAA-C2A-C3A	-2.76	105.23	112.81
20	B	846	BCR	C21-C20-C19	-2.76	114.76	123.23
20	a	852	BCR	C7-C8-C9	-2.76	122.06	126.21
20	B	843	BCR	C7-C8-C9	-2.76	122.07	126.21
17	B	836	CLA	CHC-C1C-C2C	-2.76	119.12	126.65
17	6	309	CLA	C4C-C3C-C2C	-2.76	102.68	106.91
17	B	834	CLA	C4C-C3C-C2C	-2.76	102.68	106.91
26	1	302	CHL	OMC-CMC-C2C	-2.76	120.77	124.29
17	a	814	CLA	CHC-C1C-C2C	-2.76	119.12	126.65
17	9	603	CLA	CHC-C1C-C2C	-2.76	119.13	126.65
27	8	314	LUT	C15-C14-C13	-2.76	123.37	127.31
20	f	7004	BCR	C28-C27-C26	-2.76	109.04	113.78
17	b	803	CLA	CHC-C1C-C2C	-2.76	119.13	126.65
20	a	851	BCR	C28-C27-C26	-2.76	109.04	113.78
17	b	827	CLA	C4C-C3C-C2C	-2.76	102.68	106.91
17	K	4003	CLA	C4C-C3C-C2C	-2.76	102.68	106.91
17	A	810	CLA	C4C-C3C-C2C	-2.76	102.68	106.91
17	A	818	CLA	O1D-CGD-CBD	-2.76	119.65	124.60
17	b	836	CLA	CHC-C1C-C2C	-2.76	119.13	126.65
17	B	836	CLA	C4C-C3C-C2C	-2.76	102.68	106.91
17	A	825	CLA	C1-C2-C3	-2.75	120.88	125.96
20	7	617	BCR	C11-C12-C13	-2.75	118.68	126.42
27	6	317	LUT	C35-C15-C14	-2.75	117.59	123.46
17	a	829	CLA	C4C-C3C-C2C	-2.75	102.69	106.91
19	a	847	LHG	C5-O7-C7	-2.75	111.38	117.88
17	G	103	CLA	C4C-C3C-C2C	-2.75	102.69	106.91
17	9	602	CLA	C4C-C3C-C2C	-2.75	102.69	106.91
17	a	813	CLA	C4C-C3C-C2C	-2.75	102.69	106.91
20	B	847	BCR	C8-C7-C6	-2.75	119.56	127.25
17	A	826	CLA	CHC-C1C-C2C	-2.75	119.16	126.65
17	a	808	CLA	C4C-C3C-C2C	-2.75	102.70	106.91
17	B	807	CLA	C4C-C3C-C2C	-2.75	102.70	106.91
27	6	317	LUT	C15-C14-C13	-2.74	123.39	127.31
17	6	307	CLA	C4C-C3C-C2C	-2.74	102.70	106.91
17	9	611	CLA	C4C-C3C-C2C	-2.74	102.70	106.91
17	9	603	CLA	C4C-C3C-C2C	-2.74	102.70	106.91
17	b	815	CLA	C4C-C3C-C2C	-2.74	102.70	106.91
17	8	311	CLA	C4C-C3C-C2C	-2.74	102.70	106.91
17	B	841	CLA	O1D-CGD-CBD	-2.74	119.68	124.60
17	a	813	CLA	C1-C2-C3	-2.74	120.91	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	846	CLA	C4C-C3C-C2C	-2.74	102.70	106.91
27	4	616	LUT	C8-C7-C6	-2.74	119.58	127.25
17	a	819	CLA	C4C-C3C-C2C	-2.74	102.71	106.91
20	j	3003	BCR	C11-C10-C9	-2.74	123.40	127.31
17	B	808	CLA	O1D-CGD-CBD	-2.74	119.68	124.60
26	4	605	CHL	OMC-CMC-C2C	-2.74	120.79	124.29
17	a	801	CLA	CMA-C3A-C4A	-2.74	104.41	111.77
28	2	616	XAT	C4-C3-C2	-2.74	105.10	110.68
17	A	838	CLA	CHC-C1C-C2C	-2.74	119.18	126.65
17	9	602	CLA	CHC-C1C-C2C	-2.74	119.19	126.65
17	A	845	CLA	C4C-C3C-C2C	-2.74	102.71	106.91
17	b	831	CLA	C4C-C3C-C2C	-2.74	102.71	106.91
27	8	314	LUT	C10-C11-C12	-2.74	114.84	123.23
20	B	848	BCR	C21-C20-C19	-2.73	114.84	123.23
17	j	3002	CLA	CAA-C2A-C3A	-2.73	107.37	114.24
20	B	847	BCR	C21-C20-C19	-2.73	114.85	123.23
20	j	3004	BCR	C37-C22-C21	-2.73	119.10	122.92
17	3	305	CLA	C4C-C3C-C2C	-2.73	102.72	106.91
17	a	815	CLA	C4C-C3C-C2C	-2.73	102.72	106.91
28	7	616	XAT	C24-C23-C22	-2.73	105.12	110.68
17	a	811	CLA	C4C-C3C-C2C	-2.73	102.72	106.91
20	6	319	BCR	C23-C24-C25	-2.73	119.62	127.25
17	A	828	CLA	CHC-C1C-C2C	-2.73	119.21	126.65
17	9	608	CLA	C4C-C3C-C2C	-2.73	102.73	106.91
17	A	823	CLA	C4C-C3C-C2C	-2.73	102.73	106.91
28	3	317	XAT	C35-C15-C14	-2.73	117.64	123.46
20	8	316	BCR	C15-C16-C17	-2.73	117.64	123.46
17	A	805	CLA	C1-C2-C3	-2.72	120.94	125.96
27	3	316	LUT	C8-C7-C6	-2.72	119.63	127.25
20	b	848	BCR	C10-C11-C12	-2.72	114.88	123.23
17	9	601	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
20	2	617	BCR	C7-C8-C9	-2.72	122.12	126.21
20	4	618	BCR	C38-C26-C25	-2.72	121.46	124.51
17	3	309	CLA	CHC-C1C-C2C	-2.72	119.22	126.65
17	A	819	CLA	C4C-C3C-C2C	-2.72	102.73	106.91
17	A	835	CLA	C4C-C3C-C2C	-2.72	102.73	106.91
17	A	830	CLA	C4C-C3C-C2C	-2.72	102.73	106.91
17	b	806	CLA	CHC-C1C-C2C	-2.72	119.23	126.65
17	b	825	CLA	C1-C2-C3	-2.72	120.94	125.96
17	A	838	CLA	C4C-C3C-C2C	-2.72	102.74	106.91
17	1	311	CLA	C4C-C3C-C2C	-2.72	102.74	106.91
17	a	802	CLA	CAA-C2A-C3A	-2.72	105.35	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	827	CLA	CHC-C1C-C2C	-2.72	119.23	126.65
17	a	805	CLA	CBC-CAC-C3C	-2.72	104.70	112.41
17	a	831	CLA	O1D-CGD-CBD	-2.72	119.72	124.60
17	2	609	CLA	CHC-C1C-C2C	-2.72	119.24	126.65
17	l	204	CLA	C4C-C3C-C2C	-2.72	102.74	106.91
17	b	830	CLA	C1D-CHD-C4C	-2.71	118.77	122.48
20	J	3003	BCR	C33-C5-C6	-2.71	121.47	124.51
17	A	827	CLA	C4C-C3C-C2C	-2.71	102.75	106.91
17	A	818	CLA	C4C-C3C-C2C	-2.71	102.75	106.91
17	b	830	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
17	a	826	CLA	O1D-CGD-CBD	-2.71	119.73	124.60
17	B	838	CLA	C4C-C3C-C2C	-2.71	102.75	106.91
17	a	839	CLA	C4C-C3C-C2C	-2.71	102.75	106.91
17	B	840	CLA	C4C-C3C-C2C	-2.71	102.75	106.91
20	b	846	BCR	C7-C8-C9	-2.71	122.14	126.21
17	a	808	CLA	CHC-C1C-C2C	-2.71	119.26	126.65
20	F	305	BCR	C35-C13-C14	-2.71	119.13	122.92
17	A	804	CLA	CAA-C2A-C3A	-2.71	105.38	112.81
20	3	318	BCR	C21-C20-C19	-2.71	114.92	123.23
17	b	816	CLA	C4C-C3C-C2C	-2.71	102.75	106.91
19	7	618	LHG	C5-O7-C7	-2.71	111.47	117.88
17	b	827	CLA	C1-C2-C3	-2.71	120.97	125.96
17	2	609	CLA	CAA-C2A-C3A	-2.71	105.39	112.81
17	a	826	CLA	C4C-C3C-C2C	-2.71	102.76	106.91
26	7	601	CHL	C1-C2-C3	-2.71	120.97	125.96
17	B	809	CLA	C4C-C3C-C2C	-2.71	102.76	106.91
20	g	104	BCR	C33-C5-C6	-2.70	121.48	124.51
17	l	203	CLA	C1-C2-C3	-2.70	120.97	125.96
17	b	802	CLA	CMA-C3A-C2A	-2.70	102.80	113.77
17	4	602	CLA	C4C-C3C-C2C	-2.70	102.76	106.91
17	a	828	CLA	CHC-C1C-C2C	-2.70	119.28	126.65
17	b	834	CLA	C4C-C3C-C2C	-2.70	102.76	106.91
17	a	835	CLA	C4C-C3C-C2C	-2.70	102.76	106.91
17	2	612	CLA	C4C-C3C-C2C	-2.70	102.76	106.91
17	A	822	CLA	C4C-C3C-C2C	-2.70	102.76	106.91
17	3	309	CLA	C4C-C3C-C2C	-2.70	102.77	106.91
17	a	840	CLA	C4C-C3C-C2C	-2.70	102.77	106.91
17	a	807	CLA	C4C-C3C-C2C	-2.70	102.77	106.91
17	B	830	CLA	C4C-C3C-C2C	-2.70	102.77	106.91
17	1	308	CLA	C1-C2-C3	-2.70	120.99	125.96
17	1	310	CLA	C4C-C3C-C2C	-2.70	102.77	106.91
17	B	841	CLA	CHC-C1C-C2C	-2.70	119.30	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	848	BCR	C24-C23-C22	-2.70	122.16	126.21
17	a	830	CLA	CHC-C1C-C2C	-2.70	119.30	126.65
20	b	846	BCR	C11-C10-C9	-2.70	123.46	127.31
17	7	609	CLA	CHC-C1C-C2C	-2.70	119.30	126.65
17	l	203	CLA	CHC-C1C-C2C	-2.69	119.30	126.65
17	7	610	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	6	314	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	B	826	CLA	OBD-CAD-C3D	-2.69	123.06	128.03
28	8	315	XAT	C24-C23-C22	-2.69	105.19	110.68
17	7	612	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	B	811	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	B	841	CLA	O2D-CGD-O1D	-2.69	118.40	123.82
17	A	807	CLA	O2D-CGD-O1D	-2.69	118.40	123.82
20	G	105	BCR	C10-C11-C12	-2.69	114.97	123.23
28	7	616	XAT	C4-C3-C2	-2.69	105.20	110.68
17	j	3002	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	a	803	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	B	841	CLA	C1-C2-C3	-2.69	121.00	125.96
17	b	830	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	b	814	CLA	CHC-C1C-C2C	-2.69	119.31	126.65
17	a	808	CLA	O2D-CGD-O1D	-2.69	118.41	123.82
17	3	302	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	7	608	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	8	308	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
20	B	844	BCR	C16-C17-C18	-2.69	123.47	127.31
17	a	836	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
17	7	611	CLA	C4C-C3C-C2C	-2.69	102.79	106.91
17	L	203	CLA	CHC-C1C-C2C	-2.69	119.32	126.65
17	a	841	CLA	C4C-C3C-C2C	-2.69	102.79	106.91
27	3	316	LUT	C23-C24-C25	-2.68	122.70	125.22
17	2	604	CLA	C1-C2-C3	-2.68	121.01	125.96
17	a	806	CLA	CAA-C2A-C3A	-2.68	105.45	112.81
17	1	310	CLA	CAA-C2A-C3A	-2.68	105.45	112.81
17	g	102	CLA	C4C-C3C-C2C	-2.68	102.79	106.91
17	b	805	CLA	C4C-C3C-C2C	-2.68	102.79	106.91
17	a	837	CLA	C4C-C3C-C2C	-2.68	102.79	106.91
17	a	842	CLA	C4C-C3C-C2C	-2.68	102.79	106.91
17	B	807	CLA	C1-C2-C3	-2.68	121.02	125.96
20	L	201	BCR	C3-C4-C5	-2.68	109.17	113.78
20	a	854	BCR	C3-C4-C5	-2.68	109.17	113.78
17	B	817	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
27	1	320	LUT	C8-C7-C6	-2.68	119.75	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	301	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
17	3	311	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
17	4	611	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
17	3	309	CLA	CAA-C2A-C3A	-2.68	105.47	112.81
17	L	203	CLA	C2A-C1A-CHA	-2.68	119.17	123.92
17	A	815	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
17	A	842	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
17	A	805	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
17	A	828	CLA	O2D-CGD-O1D	-2.68	118.43	123.82
20	B	847	BCR	C28-C27-C26	-2.68	109.18	113.78
28	1	317	XAT	C4-C3-C2	-2.68	105.23	110.68
17	b	841	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
17	b	820	CLA	C4C-C3C-C2C	-2.68	102.80	106.91
17	A	810	CLA	CAA-CBA-CGA	-2.68	105.28	113.35
17	B	826	CLA	CHC-C1C-C2C	-2.68	119.35	126.65
17	a	856	CLA	C1-C2-C3	-2.68	121.03	125.96
17	G	104	CLA	C4C-C3C-C2C	-2.68	102.81	106.91
17	B	812	CLA	C4C-C3C-C2C	-2.68	102.81	106.91
17	A	802	CLA	CHC-C1C-C2C	-2.68	119.35	126.65
17	4	601	CLA	O2D-CGD-O1D	-2.67	118.44	123.82
17	k	1402	CLA	C4C-C3C-C2C	-2.67	102.81	106.91
17	l	203	CLA	C4C-C3C-C2C	-2.67	102.81	106.91
17	B	825	CLA	CHC-C1C-C2C	-2.67	119.36	126.65
26	9	605	CHL	CHA-CBD-CGD	-2.67	108.80	115.00
17	1	303	CLA	C4C-C3C-C2C	-2.67	102.81	106.91
17	b	814	CLA	C2A-C1A-CHA	-2.67	119.18	123.92
17	A	801	CLA	CMA-C3A-C4A	-2.67	104.59	111.77
17	a	809	CLA	O1D-CGD-CBD	-2.67	119.80	124.60
17	A	824	CLA	C4C-C3C-C2C	-2.67	102.81	106.91
20	2	617	BCR	C31-C1-C6	-2.67	105.98	110.31
17	B	814	CLA	C1-C2-C3	-2.67	121.04	125.96
20	b	846	BCR	C3-C4-C5	-2.67	109.19	113.78
17	A	839	CLA	C4C-C3C-C2C	-2.67	102.81	106.91
17	b	825	CLA	CHC-C1C-C2C	-2.67	119.37	126.65
17	a	819	CLA	CHC-C1C-C2C	-2.67	119.37	126.65
17	B	839	CLA	C4C-C3C-C2C	-2.67	102.82	106.91
17	a	822	CLA	C4C-C3C-C2C	-2.67	102.82	106.91
28	9	617	XAT	C4-C3-C2	-2.66	105.25	110.68
17	k	1401	CLA	C4C-C3C-C2C	-2.66	102.82	106.91
17	a	803	CLA	CAA-C2A-C3A	-2.66	105.50	112.81
17	J	3002	CLA	C4C-C3C-C2C	-2.66	102.82	106.91
17	A	833	CLA	CBC-CAC-C3C	-2.66	104.85	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	848	BCR	C21-C20-C19	-2.66	115.06	123.23
20	9	618	BCR	C23-C24-C25	-2.66	119.80	127.25
17	7	602	CLA	C4C-C3C-C2C	-2.66	102.83	106.91
20	J	3003	BCR	C38-C26-C25	-2.66	121.53	124.51
17	b	814	CLA	C4C-C3C-C2C	-2.66	102.83	106.91
26	9	606	CHL	C1-C2-C3	-2.66	122.48	126.68
17	a	838	CLA	O1D-CGD-CBD	-2.66	119.82	124.60
17	b	808	CLA	C1-C2-C3	-2.66	121.06	125.96
20	B	846	BCR	C38-C26-C25	-2.66	121.53	124.51
17	a	828	CLA	O2D-CGD-O1D	-2.66	118.47	123.82
17	1	308	CLA	C4C-C3C-C2C	-2.66	102.83	106.91
17	6	310	CLA	C4C-C3C-C2C	-2.66	102.83	106.91
17	B	803	CLA	CHC-C1C-C2C	-2.66	119.40	126.65
27	1	320	LUT	C30-C31-C32	-2.66	115.08	123.23
17	k	1403	CLA	C4C-C3C-C2C	-2.66	102.83	106.91
17	6	306	CLA	C4C-C3C-C2C	-2.66	102.83	106.91
17	L	203	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	2	611	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	b	811	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	b	823	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
20	b	845	BCR	C37-C22-C21	-2.65	119.20	122.92
17	a	825	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
28	3	317	XAT	C31-C30-C29	-2.65	123.52	127.31
17	7	602	CLA	C1-C2-C3	-2.65	121.07	125.96
28	9	617	XAT	C24-C23-C22	-2.65	105.28	110.68
17	a	830	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	8	302	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	3	308	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	A	840	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
28	6	318	XAT	C24-C23-C22	-2.65	105.28	110.68
17	g	103	CLA	O2D-CGD-O1D	-2.65	118.49	123.82
20	b	847	BCR	C15-C16-C17	-2.65	117.80	123.46
17	4	610	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	6	316	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
27	6	317	LUT	C8-C7-C6	-2.65	119.83	127.25
17	2	602	CLA	C1-C2-C3	-2.65	121.08	125.96
17	B	821	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	9	614	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	3	313	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
17	a	838	CLA	CBC-CAC-C3C	-2.65	104.89	112.41
20	a	850	BCR	C20-C21-C22	-2.65	123.53	127.31
26	7	614	CHL	CHA-CBD-CGD	-2.65	108.86	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	825	CLA	C4C-C3C-C2C	-2.65	102.85	106.91
17	a	839	CLA	C2A-C1A-CHA	-2.65	119.23	123.92
17	a	804	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
17	B	828	CLA	C4C-C3C-C2C	-2.64	102.85	106.91
26	6	308	CHL	O2D-CGD-O1D	-2.64	118.50	123.82
17	b	811	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
17	b	833	CLA	C2A-C1A-CHA	-2.64	119.23	123.92
17	6	307	CLA	CAA-C2A-C3A	-2.64	107.60	114.24
17	b	814	CLA	C1-C2-C3	-2.64	121.09	125.96
17	b	821	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
20	b	848	BCR	C28-C27-C26	-2.64	109.24	113.78
17	6	311	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
17	2	603	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
17	7	604	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
20	a	851	BCR	C20-C21-C22	-2.64	123.54	127.31
17	A	807	CLA	CAA-C2A-C3A	-2.64	105.58	112.81
20	b	801	BCR	C33-C5-C6	-2.64	121.56	124.51
17	B	814	CLA	CHC-C1C-C2C	-2.64	119.46	126.65
17	8	303	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
20	A	849	BCR	C38-C26-C25	-2.64	121.56	124.51
26	6	303	CHL	CBA-CAA-C2A	-2.64	112.12	115.76
17	b	809	CLA	O2D-CGD-O1D	-2.64	118.51	123.82
27	4	616	LUT	C7-C8-C9	-2.64	122.25	126.21
17	B	810	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
17	b	837	CLA	CBC-CAC-C3C	-2.64	104.93	112.41
19	6	320	LHG	C6-C5-C4	-2.64	105.91	111.86
17	4	609	CLA	CAA-C2A-C3A	-2.64	105.58	112.81
20	G	105	BCR	C33-C5-C6	-2.64	121.56	124.51
17	2	610	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
17	A	804	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
17	A	810	CLA	C1-C2-C3	-2.63	121.10	125.96
28	3	317	XAT	C24-C23-C22	-2.63	105.31	110.68
17	J	3002	CLA	CAA-C2A-C3A	-2.63	107.62	114.24
17	B	803	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
17	k	1403	CLA	O1D-CGD-CBD	-2.63	119.87	124.60
17	b	829	CLA	CBC-CAC-C3C	-2.63	104.93	112.41
17	a	838	CLA	C1-C2-C3	-2.63	121.11	125.96
17	a	807	CLA	CHC-C1C-C2C	-2.63	119.47	126.65
17	A	809	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
17	9	613	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
17	A	803	CLA	C1-C2-C3	-2.63	121.11	125.96
17	A	845	CLA	O2D-CGD-O1D	-2.63	118.53	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	606	CHL	O2D-CGD-O1D	-2.63	118.53	123.82
17	2	604	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
17	L	204	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
17	A	837	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
20	B	845	BCR	C34-C9-C10	-2.63	119.24	122.92
17	B	802	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
17	a	802	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
17	b	822	CLA	CBC-CAC-C3C	-2.63	104.95	112.41
17	a	812	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
17	B	806	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
17	3	312	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
17	A	816	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
17	a	843	CLA	O1D-CGD-CBD	-2.63	119.89	124.60
20	l	201	BCR	C24-C23-C22	-2.62	122.27	126.21
17	4	603	CLA	C4C-C3C-C2C	-2.62	102.88	106.91
17	L	202	CLA	C4C-C3C-C2C	-2.62	102.88	106.91
20	j	3004	BCR	C7-C8-C9	-2.62	122.27	126.21
17	8	309	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	2	613	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	4	614	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
20	b	843	BCR	C36-C18-C17	-2.62	119.25	122.92
17	9	609	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	a	818	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	2	608	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	3	303	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
20	7	617	BCR	C34-C9-C10	-2.62	119.25	122.92
17	k	1401	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
17	b	815	CLA	C1-C2-C3	-2.62	121.13	125.96
17	b	835	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	3	310	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	A	818	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
17	B	804	CLA	O1D-CGD-CBD	-2.62	119.90	124.60
17	b	820	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
26	4	606	CHL	O2D-CGD-O1D	-2.62	118.55	123.82
25	9	619	LMG	C8-O7-C10	-2.62	111.69	117.88
17	2	609	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	K	4002	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	F	304	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
17	b	828	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
20	l	205	BCR	C16-C17-C18	-2.62	123.58	127.31
17	3	305	CLA	CAA-C2A-C3A	-2.62	107.66	114.24
17	B	841	CLA	C4C-C3C-C2C	-2.62	102.90	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	312	CLA	C4C-C3C-C2C	-2.62	102.90	106.91
17	8	305	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
17	a	801	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
17	b	827	CLA	CHC-C1C-C2C	-2.61	119.52	126.65
17	F	303	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
17	b	840	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
25	6	302	LMG	C8-O7-C10	-2.61	111.71	117.88
17	8	304	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
17	k	1403	CLA	O2D-CGD-O1D	-2.61	118.57	123.82
17	9	602	CLA	O1D-CGD-CBD	-2.61	119.92	124.60
17	1	309	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
20	B	846	BCR	C16-C17-C18	-2.61	123.59	127.31
20	B	843	BCR	C27-C26-C25	-2.61	118.91	122.74
17	b	807	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
17	a	844	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
17	4	613	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
17	1	315	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
17	a	833	CLA	O2D-CGD-O1D	-2.60	118.58	123.82
17	G	101	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
20	B	843	BCR	C3-C4-C5	-2.60	109.30	113.78
17	6	315	CLA	C1-C2-C3	-2.60	121.16	125.96
17	6	313	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	a	820	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
28	2	616	XAT	C24-C23-C22	-2.60	105.38	110.68
17	B	822	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	a	823	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
26	9	606	CHL	CHA-CBD-CGD	-2.60	108.97	115.00
17	6	311	CLA	CAA-C2A-C3A	-2.60	105.68	112.81
20	a	851	BCR	C11-C10-C9	-2.60	123.60	127.31
17	4	614	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
17	a	801	CLA	O2A-CGA-O1A	-2.60	117.09	123.55
17	3	301	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	7	609	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	a	834	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
20	A	850	BCR	C24-C23-C22	-2.60	122.31	126.21
17	1	304	CLA	CBC-CAC-C3C	-2.60	105.03	112.41
17	B	835	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	a	804	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	A	807	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	B	803	CLA	CAA-C2A-C3A	-2.60	105.69	112.81
17	b	804	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	7	608	CLA	CAA-C2A-C3A	-2.60	105.69	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	609	CLA	CAA-C2A-C3A	-2.60	105.69	112.81
17	4	608	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
17	4	601	CLA	C4C-C3C-C2C	-2.60	102.93	106.91
17	6	312	CLA	C4C-C3C-C2C	-2.60	102.93	106.91
17	A	801	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
17	B	819	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
17	B	825	CLA	C1-C2-C3	-2.59	121.18	125.96
17	A	832	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
17	9	610	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
20	a	849	BCR	C8-C7-C6	-2.59	119.99	127.25
20	b	847	BCR	C20-C21-C22	-2.59	123.61	127.31
20	j	3003	BCR	C20-C21-C22	-2.59	123.61	127.31
17	B	818	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
17	b	819	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
17	a	838	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
17	b	812	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
17	a	835	CLA	CAA-C2A-C3A	-2.59	105.70	112.81
17	b	817	CLA	CAA-C2A-C3A	-2.59	105.71	112.81
17	K	4002	CLA	O2D-CGD-O1D	-2.59	118.61	123.82
17	9	601	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
17	9	609	CLA	CAA-C2A-C3A	-2.59	105.71	112.81
17	B	837	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
17	b	803	CLA	CAA-C2A-C3A	-2.59	105.71	112.81
17	3	301	CLA	O2D-CGD-O1D	-2.59	118.61	123.82
17	b	824	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
17	b	841	CLA	O1D-CGD-CBD	-2.59	119.95	124.60
17	4	612	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
17	b	806	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
17	1	313	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
17	3	304	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
20	B	846	BCR	C7-C8-C9	-2.59	122.33	126.21
17	a	817	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
17	9	612	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
17	B	808	CLA	CAA-C2A-C3A	-2.58	105.72	112.81
17	6	315	CLA	C4C-C3C-C2C	-2.58	102.94	106.91
17	A	803	CLA	C4C-C3C-C2C	-2.58	102.95	106.91
17	8	310	CLA	C4C-C3C-C2C	-2.58	102.95	106.91
17	8	307	CLA	C4C-C3C-C2C	-2.58	102.95	106.91
17	A	845	CLA	C1-C2-C3	-2.58	121.20	125.96
17	b	815	CLA	O1D-CGD-CBD	-2.58	119.97	124.60
17	9	614	CLA	O2D-CGD-O1D	-2.58	118.63	123.82
17	a	833	CLA	C4C-C3C-C2C	-2.58	102.95	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	851	BCR	C7-C8-C9	-2.58	122.33	126.21
20	B	846	BCR	C3-C4-C5	-2.58	109.35	113.78
17	b	824	CLA	C1-C2-C3	-2.58	121.21	125.96
17	9	604	CLA	C4C-C3C-C2C	-2.58	102.95	106.91
20	F	305	BCR	C28-C27-C26	-2.58	109.35	113.78
27	3	316	LUT	C7-C8-C9	-2.58	122.34	126.21
17	a	809	CLA	O2D-CGD-O1D	-2.58	118.64	123.82
17	a	809	CLA	C4C-C3C-C2C	-2.58	102.96	106.91
17	1	305	CLA	C4C-C3C-C2C	-2.57	102.96	106.91
17	B	830	CLA	O2D-CGD-O1D	-2.57	118.64	123.82
17	f	7002	CLA	C4C-C3C-C2C	-2.57	102.96	106.91
17	B	817	CLA	CAA-C2A-C3A	-2.57	105.75	112.81
20	7	617	BCR	C3-C4-C5	-2.57	109.36	113.78
17	b	806	CLA	C2A-C1A-CHA	-2.57	119.36	123.92
17	6	305	CLA	C4C-C3C-C2C	-2.57	102.97	106.91
17	B	829	CLA	C2A-C1A-CHA	-2.57	119.36	123.92
17	9	612	CLA	C1-C2-C3	-2.57	121.22	125.96
28	9	617	XAT	C31-C30-C29	-2.57	123.64	127.31
17	A	808	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
17	B	816	CLA	C4C-C3C-C2C	-2.57	102.97	106.91
17	b	817	CLA	C4C-C3C-C2C	-2.57	102.97	106.91
17	l	202	CLA	C4C-C3C-C2C	-2.57	102.97	106.91
17	l	203	CLA	C2A-C1A-CHA	-2.57	119.37	123.92
17	4	601	CLA	O1D-CGD-CBD	-2.57	119.99	124.60
17	9	602	CLA	O2D-CGD-O1D	-2.56	118.66	123.82
17	a	803	CLA	O2D-CGD-O1D	-2.56	118.66	123.82
17	a	801	CLA	CBC-CAC-C3C	-2.56	105.13	112.41
17	b	817	CLA	C1-C2-C3	-2.56	121.23	125.96
17	9	603	CLA	O1D-CGD-CBD	-2.56	120.00	124.60
17	b	833	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
17	b	832	CLA	O2A-CGA-O1A	-2.56	117.19	123.55
17	f	7003	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
17	B	808	CLA	CBC-CAC-C3C	-2.56	105.15	112.41
28	1	317	XAT	C24-C23-C22	-2.56	105.47	110.68
17	b	829	CLA	O1D-CGD-CBD	-2.56	120.01	124.60
20	I	101	BCR	C15-C14-C13	-2.56	123.66	127.31
20	A	852	BCR	C15-C14-C13	-2.56	123.66	127.31
17	F	301	CLA	C4C-C3C-C2C	-2.56	102.99	106.91
17	1	304	CLA	C4C-C3C-C2C	-2.56	102.99	106.91
17	A	813	CLA	C4C-C3C-C2C	-2.56	102.99	106.91
27	3	316	LUT	C11-C10-C9	-2.55	123.66	127.31
17	2	608	CLA	CMA-C3A-C4A	-2.55	104.91	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	318	XAT	C4-C3-C2	-2.55	105.48	110.68
17	g	103	CLA	CBC-CAC-C3C	-2.55	105.16	112.41
20	F	305	BCR	C7-C8-C9	-2.55	122.38	126.21
17	J	3002	CLA	O2D-CGD-O1D	-2.55	118.68	123.82
17	f	7003	CLA	C4C-C3C-C2C	-2.55	102.99	106.91
17	A	812	CLA	C4C-C3C-C2C	-2.55	102.99	106.91
17	a	836	CLA	CBC-CAC-C3C	-2.55	105.17	112.41
17	A	803	CLA	CBC-CAC-C3C	-2.55	105.17	112.41
27	1	316	LUT	C23-C24-C25	-2.55	122.83	125.22
17	A	811	CLA	C4C-C3C-C2C	-2.55	103.00	106.91
17	1	311	CLA	O2D-CGD-O1D	-2.55	118.69	123.82
20	J	3003	BCR	C3-C4-C5	-2.55	109.40	113.78
17	2	602	CLA	C4C-C3C-C2C	-2.55	103.00	106.91
17	7	602	CLA	O2D-CGD-O1D	-2.55	118.70	123.82
17	9	604	CLA	O2D-CGD-O1D	-2.55	118.70	123.82
17	B	804	CLA	C4C-C3C-C2C	-2.55	103.00	106.91
17	A	808	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
17	b	829	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
17	4	604	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
20	a	853	BCR	C7-C8-C9	-2.54	122.39	126.21
17	a	834	CLA	CBC-CAC-C3C	-2.54	105.20	112.41
17	B	825	CLA	O2A-CGA-O1A	-2.54	117.24	123.55
17	A	817	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
17	1	314	CLA	CBC-CAC-C3C	-2.54	105.20	112.41
17	A	843	CLA	C4C-C3C-C2C	-2.54	103.02	106.91
20	a	853	BCR	C33-C5-C6	-2.54	121.67	124.51
17	A	821	CLA	C4C-C3C-C2C	-2.54	103.02	106.91
17	4	603	CLA	O1D-CGD-CBD	-2.54	120.05	124.60
26	1	307	CHL	O2D-CGD-O1D	-2.54	118.72	123.82
20	b	843	BCR	C3-C4-C5	-2.54	109.42	113.78
17	4	609	CLA	C4C-C3C-C2C	-2.53	103.02	106.91
25	4	620	LMG	C1-O6-C5	-2.53	108.94	113.72
20	L	205	BCR	C15-C14-C13	-2.53	123.69	127.31
20	B	844	BCR	C20-C21-C22	-2.53	123.69	127.31
17	7	603	CLA	C4C-C3C-C2C	-2.53	103.02	106.91
17	A	818	CLA	C1-C2-C3	-2.53	121.29	125.96
17	b	818	CLA	C4C-C3C-C2C	-2.53	103.03	106.91
17	B	827	CLA	C1-C2-C3	-2.53	121.29	125.96
17	b	822	CLA	C4C-C3C-C2C	-2.53	103.03	106.91
17	6	312	CLA	CBC-CAC-C3C	-2.53	105.23	112.41
28	7	616	XAT	C35-C15-C14	-2.53	118.06	123.46
17	2	609	CLA	CBC-CAC-C3C	-2.53	105.23	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	820	CLA	C4C-C3C-C2C	-2.53	103.03	106.91
17	B	807	CLA	O2D-CGD-O1D	-2.53	118.73	123.82
17	A	831	CLA	O1D-CGD-CBD	-2.53	120.06	124.60
17	l	203	CLA	O2D-CGD-O1D	-2.53	118.74	123.82
17	b	812	CLA	C1-C2-C3	-2.53	121.30	125.96
17	A	828	CLA	O1D-CGD-CBD	-2.53	120.06	124.60
17	a	834	CLA	C4C-C3C-C2C	-2.53	103.03	106.91
17	A	839	CLA	C1-C2-C3	-2.53	121.30	125.96
17	B	829	CLA	CBC-CAC-C3C	-2.53	105.24	112.41
17	B	808	CLA	C4C-C3C-C2C	-2.52	103.04	106.91
17	B	805	CLA	O2D-CGD-O1D	-2.52	118.74	123.82
17	A	832	CLA	O2D-CGD-O1D	-2.52	118.74	123.82
26	6	308	CHL	CHA-CBD-CGD	-2.52	109.15	115.00
20	b	848	BCR	C8-C7-C6	-2.52	120.19	127.25
17	B	802	CLA	CBC-CAC-C3C	-2.52	105.26	112.41
17	a	821	CLA	C4C-C3C-C2C	-2.52	103.04	106.91
17	a	844	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
17	k	1402	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
17	g	103	CLA	C4C-C3C-C2C	-2.52	103.05	106.91
17	l	314	CLA	C4C-C3C-C2C	-2.52	103.05	106.91
17	B	830	CLA	C1D-CHD-C4C	-2.52	119.04	122.48
17	b	816	CLA	O2D-CGD-O1D	-2.52	118.76	123.82
20	A	850	BCR	C33-C5-C6	-2.51	121.69	124.51
26	9	615	CHL	O2D-CGD-O1D	-2.51	118.77	123.82
17	6	304	CLA	C4C-C3C-C2C	-2.51	103.06	106.91
17	b	828	CLA	C1-C2-C3	-2.51	121.33	125.96
20	l	201	BCR	C11-C10-C9	-2.51	123.73	127.31
17	A	805	CLA	CBC-CAC-C3C	-2.51	105.28	112.41
17	l	305	CLA	C2A-C1A-CHA	-2.51	119.47	123.92
20	a	851	BCR	C23-C24-C25	-2.51	120.23	127.25
17	B	804	CLA	CBC-CAC-C3C	-2.51	105.29	112.41
17	b	837	CLA	C4C-C3C-C2C	-2.51	103.06	106.91
27	8	314	LUT	C30-C31-C32	-2.51	115.54	123.23
20	l	201	BCR	C3-C4-C5	-2.51	109.47	113.78
20	K	4001	BCR	C33-C5-C6	-2.51	121.70	124.51
20	B	845	BCR	C39-C30-C25	-2.51	106.25	110.31
17	b	808	CLA	C4C-C3C-C2C	-2.51	103.07	106.91
17	4	602	CLA	C1-C2-C3	-2.50	121.34	125.96
17	b	805	CLA	C1-C2-C3	-2.50	121.34	125.96
17	l	303	CLA	O2D-CGD-O1D	-2.50	118.78	123.82
17	b	837	CLA	C1-C2-C3	-2.50	121.34	125.96
17	a	805	CLA	C4C-C3C-C2C	-2.50	103.07	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	316	BCR	C20-C21-C22	-2.50	123.74	127.31
17	f	7003	CLA	CBC-CAC-C3C	-2.50	105.31	112.41
20	A	856	BCR	C8-C7-C6	-2.50	120.25	127.25
17	L	203	CLA	CBC-CAC-C3C	-2.50	105.31	112.41
17	B	835	CLA	CAA-C2A-C3A	-2.50	105.96	112.81
17	A	802	CLA	C1-C2-C3	-2.50	121.36	125.96
17	7	613	CLA	C4C-C3C-C2C	-2.50	103.08	106.91
20	B	848	BCR	C23-C24-C25	-2.50	120.27	127.25
17	1	304	CLA	C1-C2-C3	-2.49	121.36	125.96
17	B	829	CLA	O1D-CGD-CBD	-2.49	120.12	124.60
27	3	316	LUT	C10-C11-C12	-2.49	115.58	123.23
17	7	602	CLA	C2A-C1A-CHA	-2.49	119.50	123.92
20	b	801	BCR	C8-C7-C6	-2.49	120.27	127.25
17	2	611	CLA	C1-C2-C3	-2.49	121.36	125.96
17	G	101	CLA	C2A-C1A-CHA	-2.49	119.50	123.92
17	B	816	CLA	C2A-C1A-CHA	-2.49	119.50	123.92
20	f	7004	BCR	C11-C12-C13	-2.49	119.42	126.42
17	b	809	CLA	C4C-C3C-C2C	-2.49	103.09	106.91
17	b	828	CLA	CBC-CAC-C3C	-2.49	105.34	112.41
20	l	205	BCR	C15-C14-C13	-2.49	123.76	127.31
17	a	822	CLA	C1-C2-C3	-2.49	121.38	125.96
17	9	610	CLA	CBC-CAC-C3C	-2.49	105.35	112.41
27	6	317	LUT	C11-C10-C9	-2.49	123.76	127.31
17	a	838	CLA	CHC-C1C-C2C	-2.49	119.87	126.65
17	B	818	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
17	A	840	CLA	O1D-CGD-CBD	-2.48	120.14	124.60
17	a	814	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
17	a	803	CLA	C1-C2-C3	-2.48	121.38	125.96
17	3	304	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
17	a	817	CLA	CBC-CAC-C3C	-2.48	105.37	112.41
20	j	3003	BCR	C33-C5-C6	-2.48	121.73	124.51
17	a	810	CLA	O2A-CGA-O1A	-2.48	117.39	123.55
17	B	807	CLA	C2A-C1A-CHA	-2.48	119.52	123.92
17	2	603	CLA	C1-C2-C3	-2.48	121.39	125.96
17	B	833	CLA	O2D-CGD-O1D	-2.48	118.83	123.82
17	b	838	CLA	CBC-CAC-C3C	-2.48	105.38	112.41
18	a	845	PQN	C11-C12-C13	-2.48	122.57	126.71
17	b	833	CLA	O1D-CGD-CBD	-2.48	120.16	124.60
20	k	1404	BCR	C7-C8-C9	-2.48	122.49	126.21
17	b	830	CLA	C2A-C1A-CHA	-2.48	119.53	123.92
17	B	816	CLA	O2D-CGD-O1D	-2.47	118.84	123.82
17	A	823	CLA	O1D-CGD-CBD	-2.47	120.16	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	823	CLA	CBC-CAC-C3C	-2.47	105.39	112.41
20	A	849	BCR	C28-C27-C26	-2.47	109.53	113.78
20	f	7004	BCR	C33-C5-C6	-2.47	121.74	124.51
17	b	838	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
20	B	846	BCR	C24-C23-C22	-2.47	122.50	126.21
17	B	825	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
17	a	810	CLA	CAA-CBA-CGA	-2.47	105.91	113.35
17	8	309	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
17	1	314	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
17	b	821	CLA	O1D-CGD-CBD	-2.47	120.17	124.60
19	1	301	LHG	C5-O7-C7	-2.47	112.04	117.88
17	b	808	CLA	C2A-C1A-CHA	-2.47	119.54	123.92
20	a	850	BCR	C7-C8-C9	-2.47	122.50	126.21
17	B	806	CLA	C2A-C1A-CHA	-2.47	119.54	123.92
17	a	821	CLA	O1D-CGD-CBD	-2.47	120.17	124.60
17	2	611	CLA	O2D-CGD-O1D	-2.47	118.86	123.82
17	2	608	CLA	CAA-C2A-C3A	-2.47	106.05	112.81
17	A	837	CLA	O2D-CGD-O1D	-2.47	118.86	123.82
17	a	815	CLA	O1D-CGD-CBD	-2.46	120.17	124.60
20	f	7004	BCR	C21-C20-C19	-2.46	115.67	123.23
20	B	846	BCR	C20-C21-C22	-2.46	123.80	127.31
20	K	4001	BCR	C8-C7-C6	-2.46	120.36	127.25
20	A	850	BCR	C38-C26-C25	-2.46	121.75	124.51
17	A	838	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
17	6	315	CLA	O2D-CGD-O1D	-2.46	118.87	123.82
17	A	821	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
17	7	603	CLA	CBC-CAC-C3C	-2.46	105.43	112.41
20	9	618	BCR	C7-C8-C9	-2.46	122.52	126.21
17	7	604	CLA	CAA-C2A-C3A	-2.46	106.07	112.81
17	B	811	CLA	C1-C2-C3	-2.46	121.43	125.96
20	b	801	BCR	C20-C19-C18	-2.46	119.52	126.42
17	B	829	CLA	C4C-C3C-C2C	-2.46	103.14	106.91
17	A	823	CLA	O2D-CGD-O1D	-2.45	118.88	123.82
19	6	301	LHG	C5-O7-C7	-2.45	112.08	117.88
17	A	838	CLA	CBA-CAA-C2A	-2.45	106.46	113.80
17	A	808	CLA	CBC-CAC-C3C	-2.45	105.45	112.41
17	b	830	CLA	O1D-CGD-CBD	-2.45	120.20	124.60
20	B	847	BCR	C38-C26-C25	-2.45	121.77	124.51
17	b	809	CLA	C1-C2-C3	-2.45	121.44	125.96
17	L	202	CLA	C1-C2-C3	-2.45	121.45	125.96
28	7	616	XAT	C15-C14-C13	-2.45	123.82	127.31
17	6	305	CLA	CBC-CAC-C3C	-2.45	105.46	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	f	7004	BCR	C7-C8-C9	-2.45	122.53	126.21
26	7	614	CHL	O2D-CGD-O1D	-2.45	118.90	123.82
20	B	847	BCR	C39-C30-C25	-2.45	106.34	110.31
17	7	613	CLA	CBC-CAC-C3C	-2.45	105.47	112.41
17	A	833	CLA	C4C-C3C-C2C	-2.45	103.16	106.91
17	A	835	CLA	C1-C2-C3	-2.45	121.45	125.96
17	1	305	CLA	O2D-CGD-O1D	-2.44	118.90	123.82
17	B	817	CLA	O2D-CGD-O1D	-2.44	118.90	123.82
17	A	809	CLA	C2A-C1A-CHA	-2.44	119.58	123.92
17	1	315	CLA	O2D-CGD-O1D	-2.44	118.90	123.82
17	b	838	CLA	C4C-C3C-C2C	-2.44	103.16	106.91
17	3	308	CLA	CAA-C2A-C3A	-2.44	106.11	112.81
17	b	827	CLA	O1D-CGD-CBD	-2.44	120.21	124.60
20	I	101	BCR	C27-C26-C25	-2.44	119.16	122.74
17	9	602	CLA	O2A-CGA-O1A	-2.44	117.49	123.55
17	l	203	CLA	O1D-CGD-CBD	-2.44	120.22	124.60
17	B	815	CLA	O1D-CGD-CBD	-2.44	120.22	124.60
17	a	830	CLA	O2D-CGD-O1D	-2.44	118.91	123.82
17	B	819	CLA	CBC-CAC-C3C	-2.44	105.48	112.41
17	A	806	CLA	C2A-C1A-CHA	-2.44	119.59	123.92
17	2	602	CLA	CBC-CAC-C3C	-2.44	105.49	112.41
17	l	202	CLA	O2D-CGD-O1D	-2.44	118.92	123.82
17	B	837	CLA	C2A-C1A-CHA	-2.44	119.60	123.92
17	A	807	CLA	C1-C2-C3	-2.44	121.47	125.96
17	a	808	CLA	C2A-C1A-CHA	-2.44	119.60	123.92
20	B	843	BCR	C11-C10-C9	-2.43	123.83	127.31
17	A	805	CLA	O1D-CGD-CBD	-2.43	120.23	124.60
17	7	604	CLA	C1-C2-C3	-2.43	121.47	125.96
17	1	315	CLA	CBC-CAC-C3C	-2.43	105.50	112.41
17	b	811	CLA	CBC-CAC-C3C	-2.43	105.50	112.41
17	1	314	CLA	C1-C2-C3	-2.43	121.47	125.96
17	8	312	CLA	CBC-CAC-C3C	-2.43	105.50	112.41
27	7	615	LUT	C11-C10-C9	-2.43	123.84	127.31
27	4	616	LUT	C31-C30-C29	-2.43	123.84	127.31
20	7	617	BCR	C20-C19-C18	-2.43	119.59	126.42
20	K	4004	BCR	C7-C8-C9	-2.43	122.56	126.21
17	a	856	CLA	CHA-C1A-NA	-2.43	120.53	126.18
27	7	615	LUT	C7-C8-C9	-2.43	122.56	126.21
17	4	612	CLA	CBC-CAC-C3C	-2.43	105.51	112.41
20	B	847	BCR	C20-C21-C22	-2.43	123.84	127.31
17	B	832	CLA	O2D-CGD-O1D	-2.43	118.93	123.82
20	i	101	BCR	C8-C7-C6	-2.43	120.45	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	821	CLA	O2D-CGD-O1D	-2.43	118.93	123.82
20	a	850	BCR	C28-C27-C26	-2.43	109.61	113.78
17	K	4003	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
27	1	316	LUT	C8-C7-C6	-2.43	120.46	127.25
17	b	810	CLA	C2A-C1A-CHA	-2.43	119.62	123.92
17	B	830	CLA	O1D-CGD-CBD	-2.43	120.24	124.60
17	3	311	CLA	O2D-CGD-O1D	-2.42	118.94	123.82
20	i	101	BCR	C21-C20-C19	-2.42	115.81	123.23
17	2	602	CLA	C2A-C1A-CHA	-2.42	119.63	123.92
17	6	315	CLA	O1D-CGD-CBD	-2.42	120.25	124.60
17	4	602	CLA	O1D-CGD-CBD	-2.42	120.26	124.60
20	b	846	BCR	C23-C24-C25	-2.42	120.48	127.25
17	F	301	CLA	CBC-CAC-C3C	-2.42	105.54	112.41
17	B	838	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
17	B	840	CLA	C2A-C1A-CHA	-2.42	119.63	123.92
20	K	4004	BCR	C28-C27-C26	-2.42	109.63	113.78
20	7	617	BCR	C35-C13-C14	-2.42	119.54	122.92
17	B	826	CLA	O2D-CGD-O1D	-2.41	118.96	123.82
17	l	203	CLA	CBC-CAC-C3C	-2.41	105.56	112.41
17	F	304	CLA	O2A-CGA-O1A	-2.41	117.56	123.55
17	a	837	CLA	O2D-CGD-O1D	-2.41	118.96	123.82
20	F	305	BCR	C11-C12-C13	-2.41	119.64	126.42
17	B	827	CLA	CAA-C2A-C3A	-2.41	106.20	112.81
17	9	613	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
20	B	848	BCR	C3-C4-C5	-2.41	109.64	113.78
17	4	612	CLA	C2A-C1A-CHA	-2.41	119.65	123.92
17	6	305	CLA	C1-C2-C3	-2.41	121.52	125.96
17	2	602	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
17	B	833	CLA	C1-C2-C3	-2.41	121.52	125.96
17	A	826	CLA	O1D-CGD-CBD	-2.41	120.28	124.60
17	B	837	CLA	C1-C2-C3	-2.41	121.53	125.96
17	A	807	CLA	O1D-CGD-CBD	-2.41	120.28	124.60
17	G	101	CLA	O2D-CGD-O1D	-2.40	118.98	123.82
17	B	833	CLA	C2A-C1A-CHA	-2.40	119.66	123.92
17	j	3002	CLA	O2D-CGD-O1D	-2.40	118.98	123.82
17	A	827	CLA	C2A-C1A-CHA	-2.40	119.66	123.92
26	7	606	CHL	CHA-CBD-CGD	-2.40	109.43	115.00
17	4	604	CLA	CBC-CAC-C3C	-2.40	105.59	112.41
27	7	615	LUT	C35-C15-C14	-2.40	118.34	123.46
28	9	617	XAT	C15-C14-C13	-2.40	123.89	127.31
26	9	605	CHL	C1-C2-C3	-2.40	121.54	125.96
20	k	1404	BCR	C8-C7-C6	-2.40	120.53	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	822	CLA	C2A-C1A-CHA	-2.40	119.67	123.92
17	F	304	CLA	CBC-CAC-C3C	-2.40	105.60	112.41
20	A	856	BCR	C23-C24-C25	-2.40	120.54	127.25
17	9	603	CLA	C2A-C1A-CHA	-2.40	119.67	123.92
17	A	843	CLA	CBC-CAC-C3C	-2.40	105.61	112.41
17	b	808	CLA	O1D-CGD-CBD	-2.40	120.30	124.60
17	B	808	CLA	O2A-CGA-O1A	-2.40	117.60	123.55
17	a	846	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
17	9	604	CLA	CBC-CAC-C3C	-2.40	105.61	112.41
17	8	303	CLA	C2A-C1A-CHA	-2.39	119.67	123.92
17	b	837	CLA	C2A-C1A-CHA	-2.39	119.67	123.92
17	8	312	CLA	CAA-C2A-C3A	-2.39	106.25	112.81
28	4	617	XAT	C4-C3-C2	-2.39	105.81	110.68
27	4	616	LUT	C30-C31-C32	-2.39	115.90	123.23
17	A	835	CLA	CAA-C2A-C3A	-2.39	106.26	112.81
17	b	829	CLA	C2A-C1A-CHA	-2.39	119.68	123.92
17	3	301	CLA	O1D-CGD-CBD	-2.39	120.31	124.60
17	A	819	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
26	9	605	CHL	O2D-CGD-O1D	-2.39	119.02	123.82
20	A	851	BCR	C11-C10-C9	-2.39	123.90	127.31
20	i	101	BCR	C10-C11-C12	-2.39	115.91	123.23
28	9	617	XAT	C10-C11-C12	-2.39	115.91	123.23
27	7	615	LUT	C10-C11-C12	-2.39	115.91	123.23
17	b	812	CLA	CBC-CAC-C3C	-2.38	105.64	112.41
20	g	104	BCR	C10-C11-C12	-2.38	115.92	123.23
17	A	822	CLA	C1-C2-C3	-2.38	121.56	125.96
17	a	835	CLA	O2D-CGD-O1D	-2.38	119.02	123.82
17	a	840	CLA	C1-C2-C3	-2.38	121.57	125.96
17	a	809	CLA	C2A-C1A-CHA	-2.38	119.69	123.92
17	A	816	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
17	7	604	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
20	A	848	BCR	C24-C23-C22	-2.38	122.63	126.21
20	K	4001	BCR	C28-C27-C26	-2.38	109.69	113.78
20	a	851	BCR	C33-C5-C6	-2.38	121.84	124.51
20	f	7004	BCR	C8-C7-C6	-2.38	120.58	127.25
20	2	617	BCR	C36-C18-C17	-2.38	119.59	122.92
17	A	811	CLA	CBC-CAC-C3C	-2.38	105.65	112.41
17	a	843	CLA	CBC-CAC-C3C	-2.38	105.65	112.41
17	B	822	CLA	CAA-C2A-C3A	-2.38	106.29	112.81
20	l	205	BCR	C3-C4-C5	-2.38	109.69	113.78
17	a	834	CLA	CAA-C2A-C3A	-2.38	106.29	112.81
17	a	833	CLA	CBC-CAC-C3C	-2.38	105.66	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	833	CLA	C2A-C1A-CHA	-2.38	119.70	123.92
17	6	316	CLA	O2D-CGD-O1D	-2.38	119.04	123.82
17	b	829	CLA	O2A-CGA-O1A	-2.37	117.66	123.55
17	B	814	CLA	CMA-C3A-C4A	-2.37	105.39	111.77
20	j	3003	BCR	C38-C26-C25	-2.37	121.85	124.51
17	a	810	CLA	O2D-CGD-O1D	-2.37	119.04	123.82
17	g	101	CLA	C4C-C3C-C2C	-2.37	103.27	106.91
20	B	843	BCR	C36-C18-C17	-2.37	119.60	122.92
17	1	304	CLA	C2A-C1A-CHA	-2.37	119.71	123.92
17	a	823	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
17	b	821	CLA	CBC-CAC-C3C	-2.37	105.68	112.41
20	B	846	BCR	C15-C16-C17	-2.37	118.40	123.46
20	4	618	BCR	C3-C4-C5	-2.37	109.70	113.78
17	a	818	CLA	O1D-CGD-CBD	-2.37	120.34	124.60
17	b	826	CLA	O1D-CGD-CBD	-2.37	120.34	124.60
27	3	316	LUT	C35-C15-C14	-2.37	118.40	123.46
17	b	816	CLA	C2A-C1A-CHA	-2.37	119.72	123.92
20	b	848	BCR	C15-C14-C13	-2.37	123.93	127.31
17	A	801	CLA	CBC-CAC-C3C	-2.37	105.68	112.41
17	A	820	CLA	CBC-CAC-C3C	-2.37	105.68	112.41
17	a	832	CLA	C2A-C1A-CHA	-2.37	119.72	123.92
28	1	317	XAT	C31-C30-C29	-2.37	123.93	127.31
17	1	314	CLA	O1D-CGD-CBD	-2.37	120.35	124.60
17	9	611	CLA	O2D-CGD-O1D	-2.37	119.06	123.82
20	F	305	BCR	C15-C16-C17	-2.37	118.41	123.46
20	7	617	BCR	C36-C18-C17	-2.37	119.61	122.92
17	B	813	CLA	O1D-CGD-CBD	-2.37	120.35	124.60
27	1	316	LUT	C31-C30-C29	-2.37	123.93	127.31
20	A	852	BCR	C33-C5-C6	-2.36	121.86	124.51
17	b	812	CLA	O2D-CGD-O1D	-2.36	119.06	123.82
27	4	616	LUT	C38-C25-C24	-2.36	118.59	123.68
26	9	606	CHL	OMC-CMC-C2C	-2.36	121.27	124.29
17	4	611	CLA	C1-C2-C3	-2.36	121.60	125.96
20	a	854	BCR	C20-C19-C18	-2.36	119.78	126.42
17	9	601	CLA	O1D-CGD-CBD	-2.36	120.36	124.60
20	L	206	BCR	C3-C4-C5	-2.36	109.72	113.78
17	a	812	CLA	O2D-CGD-O1D	-2.36	119.07	123.82
17	b	840	CLA	C2A-C1A-CHA	-2.36	119.73	123.92
17	A	839	CLA	CBC-CAC-C3C	-2.36	105.71	112.41
17	A	815	CLA	O2D-CGD-O1D	-2.36	119.07	123.82
17	6	310	CLA	C1-C2-C3	-2.36	121.61	125.96
17	B	816	CLA	CBC-CAC-C3C	-2.36	105.71	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	831	CLA	C2A-C1A-CHA	-2.36	119.74	123.92
17	a	811	CLA	CAA-C2A-C3A	-2.36	106.34	112.81
17	a	832	CLA	CAA-C2A-C3A	-2.36	106.34	112.81
28	6	318	XAT	C35-C15-C14	-2.36	118.43	123.46
17	b	821	CLA	O2D-CGD-O1D	-2.36	119.08	123.82
28	8	315	XAT	C30-C31-C32	-2.36	116.00	123.23
17	b	818	CLA	C1-C2-C3	-2.36	121.61	125.96
17	6	313	CLA	CBC-CAC-C3C	-2.36	105.72	112.41
17	a	806	CLA	C2A-C1A-CHA	-2.36	119.74	123.92
17	B	836	CLA	C2A-C1A-CHA	-2.36	119.74	123.92
26	4	605	CHL	O2D-CGD-O1D	-2.36	119.08	123.82
17	a	856	CLA	O2A-CGA-O1A	-2.36	117.70	123.55
17	A	820	CLA	O2D-CGD-O1D	-2.36	119.08	123.82
17	a	823	CLA	O1D-CGD-CBD	-2.35	120.37	124.60
17	6	304	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
17	A	836	CLA	CBC-CAC-C3C	-2.35	105.73	112.41
17	4	603	CLA	O2D-CGD-O1D	-2.35	119.08	123.82
17	B	822	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
17	a	811	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
17	4	613	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
27	8	314	LUT	C8-C7-C6	-2.35	120.67	127.25
17	b	805	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
17	2	604	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
17	6	304	CLA	O1D-CGD-CBD	-2.35	120.38	124.60
17	a	812	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
17	6	305	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
17	8	304	CLA	CBC-CAC-C3C	-2.35	105.74	112.41
17	B	838	CLA	O2A-CGA-O1A	-2.35	117.72	123.55
17	a	806	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
17	b	836	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
17	a	818	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
17	6	305	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
17	b	803	CLA	C1-C2-C3	-2.35	121.63	125.96
17	B	811	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
17	A	817	CLA	O2D-CGD-O1D	-2.35	119.10	123.82
17	9	602	CLA	C2A-C1A-CHA	-2.35	119.76	123.92
20	2	617	BCR	C20-C21-C22	-2.35	123.96	127.31
17	a	838	CLA	O2D-CGD-O1D	-2.35	119.10	123.82
17	B	833	CLA	O1D-CGD-CBD	-2.35	120.39	124.60
17	7	602	CLA	O1D-CGD-CBD	-2.35	120.39	124.60
20	j	3004	BCR	C20-C19-C18	-2.35	119.83	126.42
17	6	313	CLA	O2D-CGD-O1D	-2.35	119.10	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	9	616	LUT	C38-C25-C24	-2.34	118.63	123.68
19	2	618	LHG	C5-O7-C7	-2.34	112.34	117.88
17	a	806	CLA	CBC-CAC-C3C	-2.34	105.76	112.41
17	B	826	CLA	O1D-CGD-CBD	-2.34	120.39	124.60
17	b	839	CLA	C2A-C1A-CHA	-2.34	119.77	123.92
17	B	810	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
17	b	836	CLA	O1D-CGD-CBD	-2.34	120.39	124.60
17	B	835	CLA	CBC-CAC-C3C	-2.34	105.76	112.41
17	8	301	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
26	4	606	CHL	CHA-CBD-CGD	-2.34	109.57	115.00
28	4	617	XAT	C35-C15-C14	-2.34	118.47	123.46
17	4	613	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
17	a	829	CLA	O2A-CGA-O1A	-2.34	117.75	123.55
17	b	820	CLA	C2A-C1A-CHA	-2.34	119.77	123.92
17	A	854	CLA	CHA-C1A-NA	-2.34	120.75	126.18
17	1	304	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
20	A	851	BCR	C37-C22-C21	-2.34	119.65	122.92
20	L	201	BCR	C15-C16-C17	-2.34	118.47	123.46
17	6	316	CLA	CBC-CAC-C3C	-2.34	105.78	112.41
17	G	103	CLA	O2D-CGD-O1D	-2.34	119.12	123.82
20	A	856	BCR	C11-C12-C13	-2.34	119.86	126.42
17	1	303	CLA	O1D-CGD-CBD	-2.34	120.41	124.60
17	A	854	CLA	O2A-CGA-O1A	-2.33	117.75	123.55
17	1	312	CLA	O2D-CGD-O1D	-2.33	119.12	123.82
17	A	811	CLA	CAA-C2A-C3A	-2.33	106.41	112.81
17	4	611	CLA	CBC-CAC-C3C	-2.33	105.78	112.41
17	A	817	CLA	CBC-CAC-C3C	-2.33	105.78	112.41
27	2	615	LUT	C8-C7-C6	-2.33	120.72	127.25
17	a	843	CLA	C2A-C1A-CHA	-2.33	119.78	123.92
20	1	206	BCR	C7-C8-C9	-2.33	122.71	126.21
17	2	608	CLA	O2D-CGD-O1D	-2.33	119.13	123.82
26	2	614	CHL	OMC-CMC-C2C	-2.33	121.31	124.29
17	A	827	CLA	O2D-CGD-O1D	-2.33	119.13	123.82
17	3	306	CLA	O2D-CGD-O1D	-2.33	119.13	123.82
24	B	850	DGD	C2G-O2G-C1B	-2.33	112.37	117.88
17	1	303	CLA	C2A-C1A-CHA	-2.33	119.78	123.92
17	3	302	CLA	O2D-CGD-O1D	-2.33	119.13	123.82
17	A	812	CLA	CBC-CAC-C3C	-2.33	105.80	112.41
17	B	830	CLA	C2A-C1A-CHA	-2.33	119.79	123.92
17	A	837	CLA	O1D-CGD-CBD	-2.33	120.42	124.60
17	6	311	CLA	CBC-CAC-C3C	-2.33	105.80	112.41
17	a	814	CLA	O1D-CGD-CBD	-2.33	120.42	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	615	LUT	C38-C25-C24	-2.33	118.67	123.68
20	a	849	BCR	C20-C19-C18	-2.33	119.88	126.42
26	4	607	CHL	C3B-CAB-CBB	-2.33	119.97	125.20
17	6	315	CLA	CBC-CAC-C3C	-2.33	105.80	112.41
17	B	841	CLA	C2A-C1A-CHA	-2.33	119.79	123.92
17	a	807	CLA	O2A-CGA-O1A	-2.33	117.78	123.55
17	4	602	CLA	C2A-C1A-CHA	-2.33	119.80	123.92
17	b	823	CLA	C2A-C1A-CHA	-2.33	119.80	123.92
17	k	1402	CLA	CBC-CAC-C3C	-2.32	105.81	112.41
17	b	810	CLA	CAA-C2A-C3A	-2.32	106.44	112.81
17	2	603	CLA	CBC-CAC-C3C	-2.32	105.81	112.41
17	A	804	CLA	C2A-C1A-CHA	-2.32	119.80	123.92
27	7	615	LUT	C30-C31-C32	-2.32	116.11	123.23
17	9	602	CLA	CAA-C2A-C3A	-2.32	106.44	112.81
27	1	320	LUT	C15-C35-C34	-2.32	118.50	123.46
17	A	839	CLA	C2A-C1A-CHA	-2.32	119.80	123.92
20	1	206	BCR	C38-C26-C25	-2.32	121.91	124.51
17	3	305	CLA	O2D-CGD-O1D	-2.32	119.15	123.82
17	A	803	CLA	O1D-CGD-CBD	-2.32	120.43	124.60
17	B	837	CLA	CBC-CAC-C3C	-2.32	105.82	112.41
17	3	314	CLA	O2D-CGD-O1D	-2.32	119.15	123.82
17	B	815	CLA	O2D-CGD-O1D	-2.32	119.15	123.82
17	A	813	CLA	C2A-C1A-CHA	-2.32	119.81	123.92
17	a	803	CLA	CBC-CAC-C3C	-2.32	105.82	112.41
20	3	318	BCR	C15-C16-C17	-2.32	118.51	123.46
27	9	616	LUT	C7-C8-C9	-2.32	122.73	126.21
20	K	4001	BCR	C35-C13-C14	-2.32	119.67	122.92
20	j	3003	BCR	C10-C11-C12	-2.32	116.12	123.23
17	a	809	CLA	CBC-CAC-C3C	-2.32	105.83	112.41
17	3	303	CLA	CBC-CAC-C3C	-2.32	105.83	112.41
17	8	301	CLA	O1D-CGD-CBD	-2.32	120.44	124.60
25	4	619	LMG	C8-O7-C10	-2.32	112.40	117.88
27	6	321	LUT	C30-C31-C32	-2.32	116.12	123.23
17	A	811	CLA	C2A-C1A-CHA	-2.32	119.81	123.92
20	B	801	BCR	C21-C20-C19	-2.32	116.13	123.23
17	A	819	CLA	CBC-CAC-C3C	-2.32	105.84	112.41
17	A	812	CLA	C2A-C1A-CHA	-2.32	119.81	123.92
17	K	4002	CLA	O1D-CGD-CBD	-2.31	120.44	124.60
17	g	103	CLA	C2A-C1A-CHA	-2.31	119.81	123.92
17	B	833	CLA	CBC-CAC-C3C	-2.31	105.84	112.41
17	B	821	CLA	CBC-CAC-C3C	-2.31	105.84	112.41
17	4	603	CLA	C2A-C1A-CHA	-2.31	119.82	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	617	BCR	C28-C27-C26	-2.31	109.80	113.78
17	8	301	CLA	C2A-C1A-CHA	-2.31	119.82	123.92
17	a	837	CLA	CBC-CAC-C3C	-2.31	105.85	112.41
17	A	815	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
17	3	312	CLA	C2A-C1A-CHA	-2.31	119.82	123.92
27	9	616	LUT	C30-C31-C32	-2.31	116.14	123.23
17	a	807	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
17	A	820	CLA	C2A-C1A-CHA	-2.31	119.82	123.92
20	A	851	BCR	C3-C4-C5	-2.31	109.81	113.78
17	B	834	CLA	C1-C2-C3	-2.31	121.70	125.96
17	B	816	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
17	L	203	CLA	CAA-C2A-C3A	-2.31	106.48	112.81
17	B	813	CLA	O2D-CGD-O1D	-2.31	119.18	123.82
20	a	849	BCR	C33-C5-C6	-2.31	121.92	124.51
17	A	832	CLA	CBC-CAC-C3C	-2.31	105.86	112.41
17	A	833	CLA	C2A-C1A-CHA	-2.31	119.83	123.92
20	f	7004	BCR	C24-C23-C22	-2.31	122.75	126.21
17	A	805	CLA	C2A-C1A-CHA	-2.31	119.83	123.92
17	8	310	CLA	CBC-CAC-C3C	-2.31	105.86	112.41
17	a	807	CLA	O2D-CGD-O1D	-2.31	119.18	123.82
17	4	601	CLA	CBC-CAC-C3C	-2.30	105.87	112.41
17	A	818	CLA	C2A-C1A-CHA	-2.30	119.83	123.92
26	7	614	CHL	OMC-CMC-C2C	-2.30	121.35	124.29
17	a	812	CLA	C1-C2-C3	-2.30	121.71	125.96
17	l	202	CLA	C1-C2-C3	-2.30	121.71	125.96
17	B	827	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
17	A	810	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
17	b	819	CLA	CAA-C2A-C3A	-2.30	106.50	112.81
17	a	828	CLA	OBD-CAD-C3D	-2.30	123.78	128.03
17	G	104	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
17	B	828	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
17	6	312	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
17	9	603	CLA	CBC-CAC-C3C	-2.30	105.88	112.41
17	6	315	CLA	C2A-C1A-CHA	-2.30	119.84	123.92
17	b	804	CLA	CBC-CAC-C3C	-2.30	105.88	112.41
17	a	836	CLA	C2A-C1A-CHA	-2.30	119.84	123.92
17	a	856	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
17	B	812	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
17	2	604	CLA	C2A-C1A-CHA	-2.30	119.84	123.92
27	4	616	LUT	C35-C15-C14	-2.30	118.56	123.46
17	3	309	CLA	O2A-CGA-O1A	-2.30	117.85	123.55
26	4	605	CHL	CHA-CBD-CGD	-2.30	109.67	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	610	CLA	O2D-CGD-O1D	-2.30	119.20	123.82
17	A	854	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
27	2	615	LUT	C35-C15-C14	-2.30	118.56	123.46
17	A	842	CLA	CBC-CAC-C3C	-2.30	105.89	112.41
17	B	828	CLA	C2A-C1A-CHA	-2.30	119.85	123.92
17	1	311	CLA	C2A-C1A-CHA	-2.30	119.85	123.91
19	1	319	LHG	C5-O7-C7	-2.30	112.45	117.88
17	b	820	CLA	CBC-CAC-C3C	-2.30	105.89	112.41
20	F	305	BCR	C33-C5-C6	-2.29	121.94	124.51
17	9	613	CLA	CBC-CAC-C3C	-2.29	105.90	112.41
17	b	806	CLA	O2D-CGD-O1D	-2.29	119.20	123.82
17	1	314	CLA	C2A-C1A-CHA	-2.29	119.85	123.92
17	b	824	CLA	CBC-CAC-C3C	-2.29	105.90	112.41
17	a	824	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
17	B	808	CLA	C2A-C1A-CHA	-2.29	119.86	123.92
17	B	828	CLA	CBC-CAC-C3C	-2.29	105.91	112.41
17	b	841	CLA	C2A-C1A-CHA	-2.29	119.86	123.92
17	9	604	CLA	C2A-C1A-CHA	-2.29	119.86	123.92
17	4	604	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
17	8	304	CLA	CAA-C2A-C3A	-2.29	108.48	114.24
20	B	801	BCR	C10-C11-C12	-2.29	116.21	123.23
17	b	824	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
17	A	813	CLA	CBC-CAC-C3C	-2.29	105.91	112.41
20	a	853	BCR	C37-C22-C21	-2.29	119.72	122.92
17	8	303	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
17	6	316	CLA	C2A-C1A-CHA	-2.29	119.86	123.92
17	B	841	CLA	CBC-CAC-C3C	-2.29	105.92	112.41
17	6	306	CLA	CBC-CAC-C3C	-2.29	105.92	112.41
17	8	310	CLA	C2A-C1A-CHA	-2.29	119.87	123.92
17	A	822	CLA	C2A-C1A-CHA	-2.28	119.87	123.92
17	A	834	CLA	O2D-CGD-O1D	-2.28	119.22	123.82
17	1	305	CLA	CBC-CAC-C3C	-2.28	105.93	112.41
20	A	850	BCR	C23-C24-C25	-2.28	120.86	127.25
20	k	1404	BCR	C3-C4-C5	-2.28	109.85	113.78
17	l	202	CLA	CBC-CAC-C3C	-2.28	105.93	112.41
17	b	832	CLA	O2D-CGD-O1D	-2.28	119.23	123.82
27	8	314	LUT	C31-C30-C29	-2.28	124.05	127.31
17	L	204	CLA	CBC-CAC-C3C	-2.28	105.93	112.41
17	B	837	CLA	CAA-C2A-C3A	-2.28	106.55	112.81
17	3	302	CLA	O2A-CGA-O1A	-2.28	117.89	123.55
17	a	835	CLA	C1-C2-C3	-2.28	121.75	125.96
26	2	606	CHL	O2D-CGD-O1D	-2.28	119.23	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	837	CLA	O2A-CGA-O1A	-2.28	117.89	123.55
17	b	811	CLA	C2A-C1A-CHA	-2.28	119.87	123.92
17	L	202	CLA	O2D-CGD-O1D	-2.28	119.23	123.82
17	a	803	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	A	831	CLA	C2A-C1A-CHA	-2.28	119.88	123.92
17	a	835	CLA	O2A-CGA-O1A	-2.28	117.89	123.55
17	9	612	CLA	C2A-C1A-CHA	-2.28	119.88	123.92
17	A	835	CLA	O1D-CGD-CBD	-2.28	120.51	124.60
17	g	102	CLA	O2D-CGD-O1D	-2.28	119.24	123.82
17	7	612	CLA	C2A-C1A-CHA	-2.28	119.88	123.92
17	b	835	CLA	CBC-CAC-C3C	-2.28	105.95	112.41
17	B	838	CLA	CBC-CAC-C3C	-2.28	105.95	112.41
17	9	612	CLA	CBC-CAC-C3C	-2.28	105.95	112.41
20	f	7004	BCR	C20-C21-C22	-2.28	124.06	127.31
28	8	315	XAT	C4-C3-C2	-2.28	106.05	110.68
17	B	819	CLA	O2D-CGD-O1D	-2.28	119.24	123.82
26	2	607	CHL	O2D-CGD-O1D	-2.28	119.24	123.82
17	B	839	CLA	O2D-CGD-O1D	-2.27	119.24	123.82
26	2	606	CHL	CHA-CBD-CGD	-2.27	109.72	115.00
26	7	607	CHL	CBA-CAA-C2A	-2.27	112.62	115.76
20	A	849	BCR	C3-C4-C5	-2.27	109.87	113.78
19	a	848	LHG	C5-O7-C7	-2.27	112.50	117.88
26	2	614	CHL	O2D-CGD-O1D	-2.27	119.25	123.82
17	a	804	CLA	C2A-C1A-CHA	-2.27	119.89	123.92
17	A	804	CLA	CBC-CAC-C3C	-2.27	105.96	112.41
17	b	835	CLA	CAA-C2A-C3A	-2.27	106.58	112.81
17	4	609	CLA	CBC-CAC-C3C	-2.27	105.96	112.41
17	8	302	CLA	CBC-CAC-C3C	-2.27	105.96	112.41
17	B	809	CLA	CBC-CAC-C3C	-2.27	105.96	112.41
17	A	801	CLA	CMA-C3A-C2A	-2.27	104.56	113.77
17	4	612	CLA	O2D-CGD-O1D	-2.27	119.25	123.82
17	7	611	CLA	O2D-CGD-O1D	-2.27	119.25	123.82
27	6	321	LUT	C15-C35-C34	-2.27	118.62	123.46
17	b	811	CLA	O1D-CGD-CBD	-2.27	120.53	124.60
17	2	609	CLA	C2A-C1A-CHA	-2.27	119.90	123.92
17	B	817	CLA	O2A-CGA-O1A	-2.27	117.92	123.55
27	6	321	LUT	C31-C30-C29	-2.27	124.08	127.31
17	A	832	CLA	O1D-CGD-CBD	-2.27	120.53	124.60
17	2	611	CLA	CBC-CAC-C3C	-2.27	105.98	112.41
17	b	828	CLA	C2A-C1A-CHA	-2.27	119.90	123.92
17	A	825	CLA	O2D-CGD-O1D	-2.27	119.26	123.82
17	a	820	CLA	C2A-C1A-CHA	-2.27	119.90	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	823	CLA	C2A-C1A-CHA	-2.27	119.90	123.92
20	a	852	BCR	C16-C15-C14	-2.26	118.63	123.46
17	A	812	CLA	CAA-C2A-C3A	-2.26	106.60	112.81
17	8	302	CLA	C4A-NA-C1A	-2.26	103.64	106.45
17	B	821	CLA	O1D-CGD-CBD	-2.26	120.53	124.60
17	G	104	CLA	C2A-C1A-CHA	-2.26	119.90	123.92
17	L	204	CLA	O2D-CGD-O1D	-2.26	119.27	123.82
17	B	802	CLA	CMA-C3A-C2A	-2.26	104.59	113.77
17	b	819	CLA	O2D-CGD-O1D	-2.26	119.27	123.82
17	2	613	CLA	CBC-CAC-C3C	-2.26	105.99	112.41
17	F	303	CLA	CAA-C2A-C3A	-2.26	106.61	112.81
17	3	304	CLA	CBC-CAC-C3C	-2.26	105.99	112.41
17	7	611	CLA	C1-C2-C3	-2.26	121.79	125.96
17	3	310	CLA	C2A-C1A-CHA	-2.26	119.91	123.91
17	l	202	CLA	O1D-CGD-CBD	-2.26	120.54	124.60
17	9	613	CLA	O1D-CGD-CBD	-2.26	120.54	124.60
17	B	811	CLA	O2D-CGD-O1D	-2.26	119.27	123.82
17	B	827	CLA	O2A-CGA-O1A	-2.26	117.94	123.55
17	1	308	CLA	C2A-C1A-CHA	-2.26	119.91	123.92
17	7	613	CLA	C2A-C1A-CHA	-2.26	119.91	123.92
17	B	817	CLA	C2A-C1A-CHA	-2.26	119.91	123.92
17	3	302	CLA	O1D-CGD-CBD	-2.26	120.54	124.60
17	b	837	CLA	CAA-C2A-C3A	-2.26	106.62	112.81
26	7	605	CHL	O2D-CGD-O1D	-2.26	119.27	123.82
20	j	3004	BCR	C8-C7-C6	-2.26	120.93	127.25
17	K	4003	CLA	C2A-C1A-CHA	-2.26	119.91	123.92
17	8	307	CLA	O2D-CGD-O1D	-2.26	119.28	123.82
17	4	609	CLA	O2A-CGA-O1A	-2.26	117.94	123.55
17	2	609	CLA	O2D-CGD-O1D	-2.26	119.28	123.82
17	4	613	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
17	6	306	CLA	O2D-CGD-O1D	-2.26	119.28	123.82
17	6	306	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
17	g	101	CLA	C2A-C1A-CHA	-2.26	119.92	123.91
17	A	808	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
17	2	603	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
17	A	843	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
17	a	828	CLA	O1D-CGD-CBD	-2.26	120.55	124.60
17	7	608	CLA	CMA-C3A-C4A	-2.26	105.71	111.77
27	1	316	LUT	C30-C31-C32	-2.26	116.31	123.23
17	a	831	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
17	B	825	CLA	C2A-C1A-CHA	-2.26	119.92	123.92
17	8	305	CLA	O2D-CGD-O1D	-2.26	119.28	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	304	CLA	O2D-CGD-O1D	-2.26	119.28	123.82
17	k	1402	CLA	CAA-C2A-C3A	-2.25	106.63	112.81
17	A	813	CLA	C1-C2-C3	-2.25	121.80	125.96
27	1	320	LUT	C38-C25-C24	-2.25	118.83	123.68
17	b	813	CLA	C2A-C1A-CHA	-2.25	119.92	123.92
27	2	615	LUT	C38-C25-C24	-2.25	118.83	123.68
17	a	838	CLA	CAA-C2A-C3A	-2.25	106.63	112.81
17	b	807	CLA	CBC-CAC-C3C	-2.25	106.02	112.41
17	7	610	CLA	O2D-CGD-O1D	-2.25	119.29	123.82
17	B	821	CLA	C2A-C1A-CHA	-2.25	119.92	123.92
17	A	832	CLA	C2A-C1A-CHA	-2.25	119.92	123.92
17	a	832	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
27	1	316	LUT	C10-C11-C12	-2.25	116.32	123.23
19	A	847	LHG	C5-O7-C7	-2.25	112.56	117.88
17	8	307	CLA	CAA-C2A-C3A	-2.25	106.64	112.81
17	A	845	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
20	A	851	BCR	C8-C7-C6	-2.25	120.95	127.25
17	b	836	CLA	C2A-C1A-CHA	-2.25	119.93	123.92
17	7	603	CLA	C1-C2-C3	-2.25	121.81	125.96
17	b	817	CLA	O2D-CGD-O1D	-2.25	119.29	123.82
17	a	843	CLA	O2D-CGD-O1D	-2.25	119.29	123.82
17	j	3002	CLA	CBC-CAC-C3C	-2.25	106.03	112.41
17	2	610	CLA	CBC-CAC-C3C	-2.25	106.03	112.41
27	9	616	LUT	C23-C24-C25	-2.25	123.11	125.22
27	2	615	LUT	C23-C24-C25	-2.25	123.11	125.22
17	K	4003	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
17	4	602	CLA	CBC-CAC-C3C	-2.25	106.03	112.41
17	b	802	CLA	O2A-CGA-O1A	-2.25	117.97	123.55
27	8	314	LUT	C35-C15-C14	-2.25	118.67	123.46
17	a	837	CLA	C2A-C1A-CHA	-2.25	119.94	123.92
17	4	610	CLA	CBC-CAC-C3C	-2.24	106.04	112.41
17	k	1401	CLA	CBC-CAC-C3C	-2.24	106.04	112.41
17	4	614	CLA	CBC-CAC-C3C	-2.24	106.04	112.41
28	1	317	XAT	C15-C14-C13	-2.24	124.11	127.31
17	7	609	CLA	O2A-CGA-O1A	-2.24	117.98	123.55
17	b	817	CLA	CBC-CAC-C3C	-2.24	106.04	112.41
17	a	829	CLA	O2D-CGD-O1D	-2.24	119.31	123.82
17	b	841	CLA	CBC-CAC-C3C	-2.24	106.05	112.41
17	7	612	CLA	CBC-CAC-C3C	-2.24	106.05	112.41
17	1	304	CLA	O2D-CGD-O1D	-2.24	119.31	123.82
17	b	832	CLA	O1D-CGD-CBD	-2.24	120.58	124.60
17	8	313	CLA	C3A-C2A-C1A	-2.24	101.20	103.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	849	BCR	C37-C22-C21	-2.24	119.78	122.92
18	A	844	PQN	C2M-C2-C3	-2.24	119.66	124.20
17	B	829	CLA	O2A-CGA-O1A	-2.24	117.99	123.55
17	A	816	CLA	CBC-CAC-C3C	-2.24	106.05	112.41
20	k	1404	BCR	C11-C10-C9	-2.24	124.11	127.31
17	A	842	CLA	C2A-C1A-CHA	-2.24	119.95	123.92
20	K	4004	BCR	C8-C7-C6	-2.24	120.98	127.25
17	a	817	CLA	O2D-CGD-O1D	-2.24	119.31	123.82
20	b	843	BCR	C11-C12-C13	-2.24	120.13	126.42
17	l	202	CLA	C2A-C1A-CHA	-2.24	119.95	123.92
17	L	203	CLA	O2D-CGD-O1D	-2.24	119.32	123.82
27	8	314	LUT	C7-C8-C9	-2.24	122.85	126.21
20	A	849	BCR	C10-C11-C12	-2.24	116.38	123.23
20	B	846	BCR	C10-C11-C12	-2.24	116.38	123.23
17	B	813	CLA	C2A-C1A-CHA	-2.23	119.96	123.92
17	B	814	CLA	C2A-C1A-CHA	-2.23	119.96	123.92
17	7	604	CLA	CBC-CAC-C3C	-2.23	106.07	112.41
17	a	823	CLA	C2A-C1A-CHA	-2.23	119.96	123.92
20	j	3003	BCR	C3-C4-C5	-2.23	109.94	113.78
17	7	609	CLA	CBC-CAC-C3C	-2.23	106.07	112.41
17	3	304	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
17	b	810	CLA	O2D-CGD-O1D	-2.23	119.33	123.82
26	3	307	CHL	O2D-CGD-O1D	-2.23	119.33	123.82
26	4	615	CHL	O2D-CGD-O1D	-2.23	119.33	123.82
17	b	840	CLA	O2A-CGA-O1A	-2.23	118.01	123.55
17	a	832	CLA	O2D-CGD-O1D	-2.23	119.33	123.82
17	l	203	CLA	CAA-C2A-C3A	-2.23	106.69	112.81
17	a	840	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
17	b	802	CLA	C2A-C1A-CHA	-2.23	119.96	123.92
17	3	309	CLA	C2A-C1A-CHA	-2.23	119.96	123.92
17	L	202	CLA	C2A-C1A-CHA	-2.23	119.97	123.92
17	9	604	CLA	O1D-CGD-CBD	-2.23	120.60	124.60
20	a	852	BCR	C8-C7-C6	-2.23	121.01	127.25
17	1	313	CLA	C2A-C1A-CHA	-2.23	119.97	123.92
17	B	836	CLA	O2D-CGD-O1D	-2.23	119.33	123.82
17	b	822	CLA	CAA-C2A-C3A	-2.23	106.70	112.81
26	4	606	CHL	OMC-CMC-C2C	-2.23	121.45	124.29
17	B	818	CLA	CBC-CAC-C3C	-2.23	106.09	112.41
17	B	814	CLA	CAA-C2A-C3A	-2.23	106.71	112.81
17	3	301	CLA	CBC-CAC-C3C	-2.23	106.09	112.41
17	3	310	CLA	CBC-CAC-C3C	-2.23	106.09	112.41
17	3	312	CLA	CBC-CAC-C3C	-2.23	106.09	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	614	CLA	C2A-C1A-CHA	-2.23	119.97	123.92
17	3	305	CLA	O1D-CGD-CBD	-2.23	120.60	124.60
17	B	819	CLA	C2A-C1A-CHA	-2.22	119.97	123.92
17	a	822	CLA	CBC-CAC-C3C	-2.22	106.09	112.41
28	6	318	XAT	C15-C14-C13	-2.22	124.14	127.31
17	6	311	CLA	O2A-CGA-O1A	-2.22	118.03	123.55
17	7	613	CLA	O2D-CGD-O1D	-2.22	119.34	123.82
17	B	839	CLA	C2A-C1A-CHA	-2.22	119.98	123.92
20	i	101	BCR	C33-C5-C6	-2.22	122.02	124.51
17	B	832	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
17	b	825	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
27	3	316	LUT	C38-C25-C24	-2.22	118.89	123.68
17	A	824	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
17	8	309	CLA	CBC-CAC-C3C	-2.22	106.10	112.41
17	g	103	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
20	F	305	BCR	C21-C20-C19	-2.22	116.42	123.23
17	8	303	CLA	CBC-CAC-C3C	-2.22	106.10	112.41
17	b	817	CLA	C2A-C1A-CHA	-2.22	119.98	123.92
17	6	305	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
17	3	304	CLA	C2A-C1A-CHA	-2.22	119.98	123.92
17	7	613	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
17	b	840	CLA	CBC-CAC-C3C	-2.22	106.11	112.41
27	1	316	LUT	C7-C8-C9	-2.22	122.88	126.21
27	7	615	LUT	C8-C7-C6	-2.22	121.04	127.25
17	b	802	CLA	CBC-CAC-C3C	-2.22	106.11	112.41
17	K	4002	CLA	CBC-CAC-C3C	-2.22	106.11	112.41
17	A	825	CLA	C2A-C1A-CHA	-2.22	119.99	123.92
17	3	309	CLA	CBC-CAC-C3C	-2.22	106.11	112.41
26	9	615	CHL	OMC-CMC-C2C	-2.22	121.46	124.29
17	B	824	CLA	O2A-CGA-O1A	-2.22	118.05	123.55
17	b	805	CLA	O2A-CGA-O1A	-2.22	118.05	123.55
20	I	101	BCR	C11-C10-C9	-2.22	124.15	127.31
28	2	616	XAT	C30-C31-C32	-2.22	116.43	123.23
17	6	314	CLA	C2A-C1A-CHA	-2.22	119.99	123.92
17	B	837	CLA	O2A-CGA-O1A	-2.22	118.05	123.55
17	B	832	CLA	C2A-C1A-CHA	-2.21	119.99	123.92
17	A	854	CLA	CBC-CAC-C3C	-2.21	106.12	112.41
17	A	835	CLA	CBC-CAC-C3C	-2.21	106.12	112.41
27	7	615	LUT	C23-C24-C25	-2.21	123.14	125.22
17	9	602	CLA	CBC-CAC-C3C	-2.21	106.13	112.41
26	7	607	CHL	O2D-CGD-O1D	-2.21	119.37	123.82
20	7	617	BCR	C33-C5-C6	-2.21	122.03	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	825	CLA	CBC-CAC-C3C	-2.21	106.13	112.41
17	9	609	CLA	O2A-CGA-O1A	-2.21	118.06	123.55
17	2	613	CLA	C2A-C1A-CHA	-2.21	120.00	123.92
17	3	305	CLA	CBC-CAC-C3C	-2.21	106.13	112.41
17	a	819	CLA	CBC-CAC-C3C	-2.21	106.13	112.41
17	3	306	CLA	CBC-CAC-C3C	-2.21	106.13	112.41
17	1	310	CLA	O2A-CGA-O1A	-2.21	118.06	123.55
17	A	836	CLA	O2D-CGD-O1D	-2.21	119.37	123.82
20	I	101	BCR	C37-C22-C21	-2.21	119.83	122.92
17	b	819	CLA	C2A-C1A-CHA	-2.21	120.00	123.92
17	L	202	CLA	O1D-CGD-CBD	-2.21	120.63	124.60
20	a	851	BCR	C21-C20-C19	-2.21	116.45	123.23
17	4	614	CLA	C2A-C1A-CHA	-2.21	120.00	123.92
26	2	614	CHL	CHA-CBD-CGD	-2.21	109.88	115.00
17	8	308	CLA	O2A-CGA-O1A	-2.21	118.07	123.55
26	7	606	CHL	O2D-CGD-O1D	-2.21	119.38	123.82
27	2	615	LUT	C30-C31-C32	-2.21	116.46	123.23
17	4	604	CLA	CAA-C2A-C3A	-2.21	106.76	112.81
17	A	842	CLA	O2D-CGD-O1D	-2.21	119.38	123.82
20	b	843	BCR	C34-C9-C10	-2.21	119.83	122.92
17	a	813	CLA	C2A-C1A-CHA	-2.20	120.01	123.92
17	A	833	CLA	O2D-CGD-O1D	-2.20	119.38	123.82
17	a	842	CLA	CBC-CAC-C3C	-2.20	106.16	112.41
17	b	837	CLA	O1D-CGD-CBD	-2.20	120.64	124.60
17	B	809	CLA	C1-C2-C3	-2.20	121.90	125.96
20	l	206	BCR	C33-C5-C6	-2.20	122.04	124.51
17	A	810	CLA	O2A-CGA-O1A	-2.20	118.08	123.55
17	G	104	CLA	CBC-CAC-C3C	-2.20	106.16	112.41
17	7	602	CLA	CBC-CAC-C3C	-2.20	106.16	112.41
17	F	304	CLA	C1-C2-C3	-2.20	121.90	125.96
17	L	204	CLA	C2A-C1A-CHA	-2.20	120.02	123.92
17	3	313	CLA	C2A-C1A-CHA	-2.20	120.02	123.92
17	9	614	CLA	CBC-CAC-C3C	-2.20	106.16	112.41
17	4	613	CLA	CBC-CAC-C3C	-2.20	106.17	112.41
17	k	1402	CLA	C2A-C1A-CHA	-2.20	120.02	123.92
20	b	843	BCR	C27-C26-C25	-2.20	119.51	122.74
17	6	314	CLA	CBC-CAC-C3C	-2.20	106.17	112.41
20	B	801	BCR	C8-C7-C6	-2.20	121.09	127.25
20	L	205	BCR	C37-C22-C21	-2.20	119.84	122.92
27	3	316	LUT	C30-C31-C32	-2.20	116.49	123.23
17	7	608	CLA	C2A-C1A-CHA	-2.20	120.02	123.92
17	L	202	CLA	CBC-CAC-C3C	-2.20	106.17	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	618	BCR	C15-C16-C17	-2.20	118.77	123.46
17	a	856	CLA	CBC-CAC-C3C	-2.20	106.17	112.41
17	7	611	CLA	CBC-CAC-C3C	-2.20	106.17	112.41
17	a	827	CLA	O2D-CGD-O1D	-2.20	119.40	123.82
27	1	316	LUT	C38-C25-C24	-2.20	118.95	123.68
17	a	830	CLA	CBC-CAC-C3C	-2.20	106.17	112.41
17	B	810	CLA	O2A-CGA-O1A	-2.20	118.10	123.55
27	8	314	LUT	C38-C25-C24	-2.20	118.95	123.68
20	G	105	BCR	C11-C10-C9	-2.20	124.18	127.31
17	b	826	CLA	O2D-CGD-O1D	-2.20	119.40	123.82
17	B	807	CLA	CAA-C2A-C3A	-2.20	106.79	112.81
17	b	807	CLA	C2A-C1A-CHA	-2.20	120.03	123.92
17	b	824	CLA	CGD-CBD-CAD	-2.20	103.36	110.71
17	b	809	CLA	CAA-C2A-C3A	-2.19	106.79	112.81
17	g	102	CLA	CBC-CAC-C3C	-2.19	106.18	112.41
17	6	315	CLA	CAA-C2A-C3A	-2.19	106.79	112.81
20	I	101	BCR	C33-C5-C6	-2.19	122.05	124.51
17	a	835	CLA	C2A-C1A-CHA	-2.19	120.03	123.92
17	a	837	CLA	O1D-CGD-CBD	-2.19	120.66	124.60
20	B	848	BCR	C38-C26-C25	-2.19	122.05	124.51
20	a	851	BCR	C38-C26-C25	-2.19	122.05	124.51
17	6	304	CLA	CBC-CAC-C3C	-2.19	106.19	112.41
17	A	821	CLA	O2D-CGD-O1D	-2.19	119.41	123.82
17	9	603	CLA	C4A-NA-C1A	-2.19	103.73	106.45
17	G	101	CLA	CBC-CAC-C3C	-2.19	106.20	112.41
17	A	841	CLA	C2A-C1A-CHA	-2.19	120.04	123.92
20	A	856	BCR	C15-C16-C17	-2.19	118.79	123.46
17	b	830	CLA	CBC-CAC-C3C	-2.19	106.20	112.41
17	l	204	CLA	CBC-CAC-C3C	-2.19	106.20	112.41
20	F	305	BCR	C8-C7-C6	-2.19	121.13	127.25
17	2	611	CLA	C2A-C1A-CHA	-2.19	120.04	123.92
26	2	601	CHL	O1D-CGD-CBD	-2.19	120.02	124.53
17	A	809	CLA	O1D-CGD-CBD	-2.19	120.67	124.60
17	A	828	CLA	OBD-CAD-C3D	-2.19	124.00	128.03
17	4	608	CLA	CAA-C2A-C3A	-2.19	106.82	112.81
17	A	801	CLA	O2A-CGA-O1A	-2.19	118.12	123.55
20	2	617	BCR	C8-C7-C6	-2.18	121.14	127.25
17	A	829	CLA	O2D-CGD-O1D	-2.18	119.42	123.82
17	b	825	CLA	C2A-C1A-CHA	-2.18	120.05	123.92
17	3	302	CLA	C2A-C1A-CHA	-2.18	120.05	123.92
17	a	818	CLA	CBC-CAC-C3C	-2.18	106.21	112.41
17	K	4002	CLA	C2A-C1A-CHA	-2.18	120.05	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	812	CLA	C2A-C1A-CHA	-2.18	120.05	123.92
17	B	832	CLA	C6-C7-C8	-2.18	108.57	115.73
20	j	3004	BCR	C36-C18-C17	-2.18	119.87	122.92
17	a	818	CLA	C1-C2-C3	-2.18	121.94	125.96
20	b	846	BCR	C20-C21-C22	-2.18	124.20	127.31
17	1	306	CLA	O2D-CGD-O1D	-2.18	119.43	123.82
17	1	313	CLA	O2D-CGD-O1D	-2.18	119.43	123.82
17	B	818	CLA	O1D-CGD-CBD	-2.18	120.68	124.60
17	b	832	CLA	C2A-C1A-CHA	-2.18	120.05	123.92
17	A	805	CLA	O2A-CGA-O1A	-2.18	118.14	123.55
17	A	843	CLA	O2D-CGD-O1D	-2.18	119.43	123.82
20	2	617	BCR	C15-C16-C17	-2.18	118.81	123.46
20	j	3004	BCR	C11-C10-C9	-2.18	124.20	127.31
17	B	805	CLA	O1D-CGD-CBD	-2.18	120.69	124.60
17	B	807	CLA	O1D-CGD-CBD	-2.18	120.69	124.60
17	a	812	CLA	CBC-CAC-C3C	-2.18	106.23	112.41
17	a	841	CLA	CBC-CAC-C3C	-2.18	106.23	112.41
17	6	307	CLA	O2D-CGD-O1D	-2.18	119.44	123.82
17	8	302	CLA	O2D-CGD-O1D	-2.18	119.44	123.82
17	8	301	CLA	CBC-CAC-C3C	-2.18	106.23	112.41
17	b	834	CLA	O2A-CGA-O1A	-2.18	118.15	123.55
20	j	3004	BCR	C10-C11-C12	-2.18	116.56	123.23
17	4	602	CLA	O2D-CGD-O1D	-2.18	119.44	123.82
17	A	807	CLA	C2A-C1A-CHA	-2.18	120.06	123.92
17	G	103	CLA	C2A-C1A-CHA	-2.17	120.06	123.92
17	F	304	CLA	O2D-CGD-O1D	-2.17	119.44	123.82
17	a	816	CLA	CBC-CAC-C3C	-2.17	106.24	112.41
20	b	801	BCR	C20-C21-C22	-2.17	124.21	127.31
17	a	819	CLA	C2A-C1A-CHA	-2.17	120.07	123.92
17	2	612	CLA	C2A-C1A-CHA	-2.17	120.07	123.92
17	A	836	CLA	C2A-C1A-CHA	-2.17	120.07	123.92
17	A	834	CLA	CAA-C2A-C3A	-2.17	106.86	112.81
17	A	803	CLA	O2D-CGD-O1D	-2.17	119.45	123.82
17	a	842	CLA	O2A-CGA-O1A	-2.17	118.16	123.55
17	9	601	CLA	CBC-CAC-C3C	-2.17	106.25	112.41
17	8	305	CLA	C2A-C1A-CHA	-2.17	120.07	123.92
17	2	608	CLA	C2A-C1A-CHA	-2.17	120.07	123.92
26	2	601	CHL	CBA-CAA-C2A	-2.17	112.77	115.76
17	A	834	CLA	CBC-CAC-C3C	-2.17	106.26	112.41
17	3	301	CLA	C2A-C1A-CHA	-2.17	120.08	123.92
17	a	836	CLA	CAA-C2A-C3A	-2.17	106.87	112.81
17	a	809	CLA	CAA-C2A-C1A	-2.17	104.88	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	825	CLA	CAA-C2A-C1A	-2.17	104.88	111.97
17	B	825	CLA	CBC-CAC-C3C	-2.17	106.26	112.41
17	4	611	CLA	C2A-C1A-CHA	-2.17	120.08	123.92
17	9	613	CLA	C2A-C1A-CHA	-2.17	120.08	123.92
20	8	316	BCR	C10-C11-C12	-2.17	116.59	123.23
17	8	308	CLA	C2A-C1A-CHA	-2.16	120.08	123.92
17	a	817	CLA	O1D-CGD-CBD	-2.16	120.71	124.60
17	b	822	CLA	C2A-C1A-CHA	-2.16	120.08	123.92
17	1	310	CLA	C2A-C1A-CHA	-2.16	120.08	123.92
17	a	831	CLA	O2A-CGA-O1A	-2.16	118.18	123.55
17	4	602	CLA	CAA-C2A-C3A	-2.16	106.88	112.81
17	B	837	CLA	O1D-CGD-CBD	-2.16	120.72	124.60
17	a	815	CLA	C2A-C1A-CHA	-2.16	120.08	123.92
20	6	319	BCR	C15-C16-C17	-2.16	118.85	123.46
17	a	804	CLA	CAA-C2A-C3A	-2.16	106.88	112.81
17	3	311	CLA	C2A-C1A-CHA	-2.16	120.09	123.92
17	2	604	CLA	CBC-CAC-C3C	-2.16	106.28	112.41
17	B	810	CLA	CBC-CAC-C3C	-2.16	106.28	112.41
17	a	802	CLA	O2A-CGA-O1A	-2.16	118.19	123.55
20	A	852	BCR	C10-C11-C12	-2.16	116.61	123.23
17	a	829	CLA	C11-C10-C8	-2.16	108.65	115.73
17	A	816	CLA	C2A-C1A-CHA	-2.16	120.09	123.92
17	b	827	CLA	O2D-CGD-O1D	-2.16	119.48	123.82
17	9	614	CLA	O1D-CGD-CBD	-2.16	120.73	124.60
17	a	840	CLA	CBC-CAC-C3C	-2.16	106.29	112.41
17	3	303	CLA	C4A-NA-C1A	-2.16	103.78	106.45
17	b	833	CLA	CBC-CAC-C3C	-2.16	106.29	112.41
17	B	822	CLA	CBC-CAC-C3C	-2.16	106.29	112.41
17	6	310	CLA	CBC-CAC-C3C	-2.16	106.29	112.41
17	4	611	CLA	O2D-CGD-O1D	-2.16	119.48	123.82
20	A	849	BCR	C23-C24-C25	-2.16	121.22	127.25
17	B	810	CLA	C2A-C1A-CHA	-2.16	120.10	123.92
28	1	317	XAT	C8-C9-C10	-2.16	115.63	118.94
20	l	205	BCR	C8-C7-C6	-2.16	121.22	127.25
17	b	806	CLA	CBC-CAC-C3C	-2.16	106.29	112.41
17	a	802	CLA	CBC-CAC-C3C	-2.16	106.29	112.41
17	b	820	CLA	CAA-C2A-C3A	-2.15	106.90	112.81
17	A	835	CLA	C2A-C1A-CHA	-2.15	120.10	123.92
20	L	206	BCR	C28-C27-C26	-2.15	110.08	113.78
27	6	317	LUT	C10-C11-C12	-2.15	116.62	123.23
17	B	819	CLA	CAA-C2A-C3A	-2.15	106.91	112.81
17	a	808	CLA	CBC-CAC-C3C	-2.15	106.30	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	606	CHL	OMC-CMC-C2C	-2.15	121.54	124.29
26	3	307	CHL	OMC-CMC-C2C	-2.15	121.54	124.29
17	4	601	CLA	C2A-C1A-CHA	-2.15	120.10	123.92
17	4	609	CLA	C2A-C1A-CHA	-2.15	120.10	123.92
17	A	840	CLA	C2A-C1A-CHA	-2.15	120.10	123.92
26	7	601	CHL	O1D-CGD-CBD	-2.15	120.09	124.53
17	1	315	CLA	C2A-C1A-CHA	-2.15	120.10	123.92
17	3	315	CLA	C3A-C2A-C1A	-2.15	101.31	103.78
17	9	611	CLA	O1D-CGD-CBD	-2.15	120.74	124.60
20	j	3004	BCR	C16-C15-C14	-2.15	118.87	123.46
27	1	316	LUT	C35-C15-C14	-2.15	118.87	123.46
17	B	807	CLA	CBC-CAC-C3C	-2.15	106.31	112.41
26	1	307	CHL	CBA-CAA-C2A	-2.15	112.80	115.76
17	a	844	CLA	C2A-C1A-CHA	-2.15	120.11	123.92
17	B	820	CLA	C2A-C1A-CHA	-2.15	120.11	123.92
17	8	308	CLA	CBC-CAC-C3C	-2.15	106.31	112.41
17	g	102	CLA	C2A-C1A-CHA	-2.15	120.11	123.92
20	a	850	BCR	C11-C12-C13	-2.15	120.39	126.42
17	1	308	CLA	CBC-CAC-C3C	-2.15	106.32	112.41
17	6	309	CLA	C2A-C1A-CHA	-2.15	120.11	123.92
17	9	601	CLA	C2A-C1A-CHA	-2.15	120.11	123.92
20	b	845	BCR	C27-C26-C25	-2.15	119.59	122.74
17	a	825	CLA	C2A-C1A-CHA	-2.14	120.12	123.92
17	k	1401	CLA	C2A-C1A-CHA	-2.14	120.12	123.92
17	B	809	CLA	O2D-CGD-O1D	-2.14	119.50	123.82
20	2	617	BCR	C10-C11-C12	-2.14	116.65	123.23
17	A	814	CLA	O1D-CGD-CBD	-2.14	120.75	124.60
17	8	311	CLA	CBC-CAC-C3C	-2.14	106.33	112.41
20	J	3003	BCR	C23-C24-C25	-2.14	121.25	127.25
17	B	815	CLA	CBC-CAC-C3C	-2.14	106.33	112.41
17	6	307	CLA	CBC-CAC-C3C	-2.14	106.33	112.41
17	3	306	CLA	C2A-C1A-CHA	-2.14	120.12	123.92
17	8	305	CLA	CBC-CAC-C3C	-2.14	106.33	112.41
17	6	307	CLA	C2A-C1A-CHA	-2.14	120.12	123.92
17	a	856	CLA	O1D-CGD-CBD	-2.14	120.75	124.60
17	2	609	CLA	O2A-CGA-O1A	-2.14	118.23	123.55
17	a	830	CLA	C2A-C1A-CHA	-2.14	120.12	123.92
17	8	304	CLA	C2A-C1A-CHA	-2.14	120.12	123.92
17	A	840	CLA	C1-C2-C3	-2.14	122.02	125.96
20	B	845	BCR	C4-C5-C6	-2.14	119.60	122.74
20	9	618	BCR	C3-C4-C5	-2.14	110.10	113.78
17	b	818	CLA	CBC-CAC-C3C	-2.14	106.34	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	307	CHL	OMC-CMC-C2C	-2.14	121.56	124.29
17	A	830	CLA	CBC-CAC-C3C	-2.14	106.34	112.41
17	g	101	CLA	O2D-CGD-O1D	-2.14	119.52	123.82
17	9	609	CLA	C2A-C1A-CHA	-2.14	120.13	123.92
17	a	834	CLA	C2A-C1A-CHA	-2.14	120.13	123.92
17	4	610	CLA	C1-C2-C3	-2.14	122.02	125.96
20	a	850	BCR	C8-C7-C6	-2.14	121.27	127.25
17	k	1401	CLA	O1D-CGD-CBD	-2.14	120.77	124.60
17	7	604	CLA	C2A-C1A-CHA	-2.14	120.13	123.92
17	B	802	CLA	O2A-CGA-O1A	-2.14	118.25	123.55
25	G	102	LMG	C8-O7-C10	-2.13	112.83	117.88
17	8	310	CLA	O2D-CGD-O1D	-2.13	119.53	123.82
17	8	311	CLA	O2D-CGD-O1D	-2.13	119.53	123.82
17	A	810	CLA	CBC-CAC-C3C	-2.13	106.36	112.41
17	B	817	CLA	CBC-CAC-C3C	-2.13	106.36	112.41
17	f	7002	CLA	CAA-C2A-C3A	-2.13	106.96	112.81
17	a	822	CLA	CAA-C2A-C3A	-2.13	106.96	112.81
17	1	310	CLA	CBC-CAC-C3C	-2.13	106.36	112.41
17	1	303	CLA	CBC-CAC-C3C	-2.13	106.36	112.41
17	a	826	CLA	C2A-C1A-CHA	-2.13	120.14	123.92
17	b	819	CLA	CBC-CAC-C3C	-2.13	106.36	112.41
17	b	834	CLA	C2A-C1A-CHA	-2.13	120.14	123.92
17	J	3002	CLA	CBC-CAC-C3C	-2.13	106.37	112.41
20	9	618	BCR	C15-C16-C17	-2.13	118.92	123.46
17	A	837	CLA	C2A-C1A-CHA	-2.13	120.14	123.92
28	3	317	XAT	C4-C3-C2	-2.13	106.35	110.68
17	A	824	CLA	CBC-CAC-C3C	-2.13	106.37	112.41
17	4	604	CLA	O2D-CGD-O1D	-2.13	119.54	123.82
17	B	831	CLA	C2A-C1A-CHA	-2.13	120.15	123.92
17	A	832	CLA	CAA-C2A-C3A	-2.13	106.98	112.81
17	9	603	CLA	O2D-CGD-O1D	-2.13	119.54	123.82
17	3	302	CLA	CAA-C2A-C3A	-2.13	106.98	112.81
17	a	839	CLA	CBC-CAC-C3C	-2.13	106.38	112.41
20	B	845	BCR	C36-C18-C17	-2.13	119.95	122.92
17	1	313	CLA	CBC-CAC-C3C	-2.12	106.38	112.41
17	A	818	CLA	CBC-CAC-C3C	-2.12	106.38	112.41
17	3	303	CLA	C2A-C1A-CHA	-2.12	120.15	123.92
17	L	204	CLA	O1D-CGD-CBD	-2.12	120.78	124.60
17	A	830	CLA	C2A-C1A-CHA	-2.12	120.15	123.92
17	7	612	CLA	O2D-CGD-O1D	-2.12	119.55	123.82
17	b	816	CLA	C1-C2-C3	-2.12	122.04	125.96
17	b	826	CLA	OBD-CAD-C3D	-2.12	124.11	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	820	CLA	O1D-CGD-CBD	-2.12	120.79	124.60
17	9	610	CLA	O2D-CGD-O1D	-2.12	119.55	123.82
20	G	105	BCR	C16-C15-C14	-2.12	118.93	123.46
17	2	604	CLA	CAA-C2A-C3A	-2.12	106.99	112.81
17	a	813	CLA	O2D-CGD-O1D	-2.12	119.55	123.82
17	b	834	CLA	O2D-CGD-O1D	-2.12	119.55	123.82
27	6	317	LUT	C38-C25-C24	-2.12	119.11	123.68
17	3	314	CLA	CBC-CAC-C3C	-2.12	106.39	112.41
17	9	604	CLA	CAA-C2A-C3A	-2.12	107.00	112.81
28	4	617	XAT	O4-C5-C6	-2.12	57.16	58.94
17	b	834	CLA	O1D-CGD-CBD	-2.12	120.80	124.60
17	B	824	CLA	O1D-CGD-CBD	-2.12	120.80	124.60
17	1	305	CLA	O2A-CGA-O1A	-2.12	118.29	123.55
17	2	608	CLA	CBC-CAC-C3C	-2.12	106.40	112.41
17	A	812	CLA	O2D-CGD-O1D	-2.12	119.56	123.82
17	F	301	CLA	O2A-CGA-O1A	-2.12	118.29	123.55
17	A	845	CLA	C2A-C1A-CHA	-2.12	120.16	123.92
17	3	302	CLA	CBC-CAC-C3C	-2.12	106.40	112.41
20	J	3003	BCR	C10-C11-C12	-2.12	116.74	123.23
17	6	312	CLA	O1D-CGD-CBD	-2.12	120.80	124.60
17	8	309	CLA	O1D-CGD-CBD	-2.12	120.80	124.60
17	b	814	CLA	CBC-CAC-C3C	-2.12	106.40	112.41
20	A	848	BCR	C23-C24-C25	-2.12	121.33	127.25
17	8	301	CLA	CAA-C2A-C3A	-2.12	107.01	112.81
20	A	851	BCR	C20-C19-C18	-2.12	120.47	126.42
20	L	206	BCR	C11-C12-C13	-2.11	120.47	126.42
20	B	846	BCR	C8-C7-C6	-2.11	121.33	127.25
17	9	601	CLA	CAA-C2A-C3A	-2.11	107.02	112.81
17	b	812	CLA	C2A-C1A-CHA	-2.11	120.17	123.92
20	2	617	BCR	C24-C23-C22	-2.11	123.04	126.21
17	f	7003	CLA	O2A-CGA-O1A	-2.11	118.31	123.55
17	A	840	CLA	CBC-CAC-C3C	-2.11	106.42	112.41
17	B	827	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
17	6	316	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
26	4	605	CHL	C3B-CAB-CBB	-2.11	120.46	125.20
20	L	201	BCR	C21-C20-C19	-2.11	116.76	123.23
17	A	824	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
17	B	807	CLA	O2A-CGA-O1A	-2.11	118.31	123.55
17	7	603	CLA	C2A-C1A-CHA	-2.11	120.18	123.92
17	A	811	CLA	O2D-CGD-O1D	-2.11	119.58	123.82
17	4	608	CLA	O2D-CGD-O1D	-2.11	119.58	123.82
17	a	838	CLA	C4A-NA-C1A	-2.11	103.83	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	810	CLA	CBC-CAC-C3C	-2.11	106.43	112.41
28	7	616	XAT	C30-C31-C32	-2.11	116.77	123.23
17	1	311	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
17	A	829	CLA	CAA-C2A-C3A	-2.11	107.03	112.81
17	b	835	CLA	O2D-CGD-O1D	-2.11	119.58	123.82
20	b	844	BCR	C37-C22-C21	-2.11	119.97	122.92
17	b	831	CLA	CBC-CAC-C3C	-2.11	106.43	112.41
17	b	825	CLA	O2A-CGA-O1A	-2.11	118.32	123.55
20	J	3003	BCR	C8-C7-C6	-2.11	121.36	127.25
17	K	4003	CLA	CBC-CAC-C3C	-2.11	106.43	112.41
17	l	204	CLA	C2A-C1A-CHA	-2.11	120.19	123.92
17	6	306	CLA	O1D-CGD-CBD	-2.10	120.82	124.60
17	a	836	CLA	O2D-CGD-O1D	-2.10	119.58	123.82
17	G	104	CLA	O1D-CGD-CBD	-2.10	120.82	124.60
17	7	609	CLA	O2D-CGD-O1D	-2.10	119.59	123.82
17	a	811	CLA	O1D-CGD-CBD	-2.10	120.83	124.60
17	3	308	CLA	O2D-CGD-O1D	-2.10	119.59	123.82
17	b	828	CLA	O2D-CGD-O1D	-2.10	119.59	123.82
17	1	306	CLA	O1D-CGD-CBD	-2.10	120.83	124.60
17	3	311	CLA	CBC-CAC-C3C	-2.10	106.44	112.41
17	a	843	CLA	CAA-C2A-C3A	-2.10	107.05	112.81
20	L	201	BCR	C11-C10-C9	-2.10	124.31	127.31
26	8	306	CHL	OMC-CMC-C2C	-2.10	121.61	124.29
17	7	610	CLA	C2A-C1A-CHA	-2.10	120.19	123.91
17	1	306	CLA	O2A-CGA-O1A	-2.10	118.34	123.55
17	4	603	CLA	C4A-NA-C1A	-2.10	103.85	106.45
17	f	7002	CLA	O2D-CGD-O1D	-2.10	119.59	123.82
17	A	806	CLA	CAA-C2A-C3A	-2.10	107.06	112.81
17	A	821	CLA	C2A-C1A-CHA	-2.10	120.20	123.92
26	4	615	CHL	OMC-CMC-C2C	-2.10	121.61	124.29
17	a	846	CLA	C2A-C1A-CHA	-2.10	120.20	123.92
20	L	206	BCR	C37-C22-C21	-2.10	119.98	122.92
28	1	317	XAT	C30-C31-C32	-2.10	116.80	123.23
17	4	604	CLA	C2A-C1A-CHA	-2.10	120.20	123.92
26	2	607	CHL	CBA-CAA-C2A	-2.10	112.87	115.76
17	b	817	CLA	O2A-CGA-O1A	-2.10	118.35	123.55
17	6	314	CLA	O2D-CGD-O1D	-2.10	119.60	123.82
17	b	814	CLA	O1D-CGD-CBD	-2.10	120.84	124.60
26	7	606	CHL	OMC-CMC-C2C	-2.09	121.61	124.29
17	A	822	CLA	C11-C10-C8	-2.09	108.86	115.73
20	1	318	BCR	C8-C7-C6	-2.09	121.39	127.25
17	j	3002	CLA	C2A-C1A-CHA	-2.09	120.20	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	g	104	BCR	C8-C7-C6	-2.09	121.39	127.25
17	f	7003	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
17	7	611	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
17	B	805	CLA	O2A-CGA-O1A	-2.09	118.35	123.55
20	G	105	BCR	C27-C26-C25	-2.09	119.67	122.74
17	b	835	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
17	g	102	CLA	O2A-CGA-O1A	-2.09	118.35	123.55
17	2	610	CLA	O1D-CGD-CBD	-2.09	120.84	124.60
17	B	806	CLA	O2D-CGD-O1D	-2.09	119.61	123.82
17	1	312	CLA	O1D-CGD-CBD	-2.09	120.84	124.60
27	4	616	LUT	C10-C11-C12	-2.09	116.81	123.23
20	l	206	BCR	C8-C7-C6	-2.09	121.40	127.25
17	A	854	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
20	g	104	BCR	C38-C26-C25	-2.09	122.17	124.51
20	b	846	BCR	C31-C1-C6	-2.09	106.92	110.31
17	A	817	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
28	7	616	XAT	O4-C5-C6	-2.09	57.18	58.94
17	7	611	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
17	A	808	CLA	C1-C2-C3	-2.09	122.11	125.96
17	3	314	CLA	C2A-C1A-CHA	-2.09	120.22	123.92
17	a	817	CLA	C2A-C1A-CHA	-2.09	120.22	123.92
20	a	853	BCR	C8-C7-C6	-2.09	121.40	127.25
17	B	823	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
17	a	804	CLA	CBC-CAC-C3C	-2.09	106.48	112.41
17	B	840	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
19	6	320	LHG	C5-O7-C7	-2.09	112.94	117.88
25	4	620	LMG	O1-C7-C8	-2.09	106.02	110.99
17	b	823	CLA	CBC-CAC-C3C	-2.09	106.48	112.41
17	7	603	CLA	O2D-CGD-O1D	-2.09	119.62	123.82
26	9	615	CHL	CHA-CBD-CGD	-2.09	110.16	115.00
17	a	804	CLA	CAA-CBA-CGA	-2.09	107.06	113.35
17	f	7003	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
17	A	839	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
17	A	837	CLA	CBC-CAC-C3C	-2.09	106.49	112.41
17	3	305	CLA	C2A-C1A-CHA	-2.09	120.22	123.92
17	b	830	CLA	CAA-C2A-C3A	-2.09	107.09	112.81
17	l	204	CLA	O2D-CGD-O1D	-2.09	119.62	123.82
17	a	838	CLA	C2A-C1A-CHA	-2.09	120.22	123.92
17	8	312	CLA	C2A-C1A-CHA	-2.09	120.22	123.92
17	B	812	CLA	O1D-CGD-CBD	-2.09	120.86	124.60
17	F	303	CLA	O2D-CGD-O1D	-2.08	119.62	123.82
20	k	1404	BCR	C23-C24-C25	-2.08	121.42	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	828	CLA	O2A-CGA-O1A	-2.08	118.37	123.55
17	b	831	CLA	O2D-CGD-O1D	-2.08	119.62	123.82
17	8	301	CLA	O2A-CGA-O1A	-2.08	118.38	123.55
17	B	831	CLA	O2D-CGD-O1D	-2.08	119.63	123.82
17	1	315	CLA	O1D-CGD-CBD	-2.08	120.86	124.60
17	A	823	CLA	C2A-C1A-CHA	-2.08	120.23	123.92
17	3	312	CLA	O1D-CGD-CBD	-2.08	120.86	124.60
20	J	3003	BCR	C11-C10-C9	-2.08	124.34	127.31
20	A	852	BCR	C23-C24-C25	-2.08	121.43	127.25
17	1	306	CLA	CBC-CAC-C3C	-2.08	106.50	112.41
17	B	811	CLA	CBC-CAC-C3C	-2.08	106.50	112.41
17	a	824	CLA	C2A-C1A-CHA	-2.08	120.23	123.92
17	a	827	CLA	C2A-C1A-CHA	-2.08	120.23	123.92
17	b	816	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
17	f	7002	CLA	CBC-CAC-C3C	-2.08	106.51	112.41
17	L	203	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
17	3	313	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
17	J	3002	CLA	C2A-C1A-CHA	-2.08	120.23	123.92
17	1	305	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
17	8	309	CLA	C1-C2-C3	-2.08	122.13	125.96
20	6	319	BCR	C8-C7-C6	-2.08	121.44	127.25
26	4	606	CHL	C3B-CAB-CBB	-2.08	120.54	125.20
17	4	610	CLA	C2A-C1A-CHA	-2.08	120.24	123.92
20	1	318	BCR	C15-C16-C17	-2.08	119.03	123.46
17	8	312	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
20	9	618	BCR	C8-C7-C6	-2.07	121.44	127.25
17	9	608	CLA	CAA-C2A-C3A	-2.07	107.12	112.81
17	B	838	CLA	C2A-C1A-CHA	-2.07	120.24	123.92
17	3	311	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
17	B	814	CLA	CBC-CAC-C3C	-2.07	106.52	112.41
17	B	834	CLA	O2D-CGD-O1D	-2.07	119.65	123.82
17	2	602	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
17	A	819	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
17	1	308	CLA	O2D-CGD-O1D	-2.07	119.65	123.82
17	k	1403	CLA	C2A-C1A-CHA	-2.07	120.24	123.92
17	2	610	CLA	C2A-C1A-CHA	-2.07	120.24	123.91
17	B	834	CLA	C2A-C1A-CHA	-2.07	120.24	123.92
17	B	806	CLA	CAA-C2A-C3A	-2.07	107.13	112.81
17	4	610	CLA	O2D-CGD-O1D	-2.07	119.65	123.82
17	2	612	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
28	2	616	XAT	C35-C15-C14	-2.07	119.04	123.46
17	7	608	CLA	O2D-CGD-O1D	-2.07	119.65	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	313	CLA	C2A-C1A-CHA	-2.07	120.25	123.92
17	4	610	CLA	CAA-C2A-C3A	-2.07	107.14	112.81
17	4	602	CLA	O2A-CGA-O1A	-2.07	118.41	123.55
17	B	835	CLA	C2A-C1A-CHA	-2.07	120.25	123.92
17	9	609	CLA	CBC-CAC-C3C	-2.07	106.54	112.41
28	2	616	XAT	O4-C5-C6	-2.07	57.20	58.94
17	8	304	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
17	7	609	CLA	C2A-C1A-CHA	-2.07	120.25	123.92
17	8	302	CLA	C2A-C1A-CHA	-2.07	120.25	123.92
17	F	303	CLA	CBC-CAC-C3C	-2.07	106.54	112.41
17	A	807	CLA	CBC-CAC-C3C	-2.07	106.54	112.41
20	I	101	BCR	C10-C11-C12	-2.07	116.89	123.23
17	A	833	CLA	O1D-CGD-CBD	-2.07	120.89	124.60
20	b	847	BCR	C33-C5-C6	-2.07	122.19	124.51
17	A	854	CLA	C4-C3-C2	-2.07	118.18	123.69
17	A	815	CLA	C2A-C1A-CHA	-2.07	120.26	123.92
17	B	813	CLA	O2A-CGA-O1A	-2.07	118.42	123.55
20	a	852	BCR	C23-C24-C25	-2.06	121.47	127.25
17	A	822	CLA	O2D-CGD-O1D	-2.06	119.67	123.82
17	a	802	CLA	C2A-C1A-CHA	-2.06	120.26	123.92
26	4	607	CHL	O2A-CGA-O1A	-2.06	118.43	123.55
17	8	311	CLA	C2A-C1A-CHA	-2.06	120.26	123.92
17	b	834	CLA	CBC-CAC-C3C	-2.06	106.56	112.41
17	a	824	CLA	O2D-CGD-O1D	-2.06	119.67	123.82
17	g	102	CLA	O1D-CGD-CBD	-2.06	120.90	124.60
17	A	801	CLA	C2A-C1A-CHA	-2.06	120.26	123.92
17	4	608	CLA	CBC-CAC-C3C	-2.06	106.56	112.41
17	A	803	CLA	O2A-CGA-O1A	-2.06	118.43	123.55
17	B	840	CLA	O2A-CGA-O1A	-2.06	118.43	123.55
17	3	309	CLA	O2D-CGD-O1D	-2.06	119.67	123.82
20	a	854	BCR	C24-C23-C22	-2.06	123.12	126.21
17	A	806	CLA	O2D-CGD-O1D	-2.06	119.68	123.82
17	a	831	CLA	CBC-CAC-C3C	-2.06	106.57	112.41
20	l	201	BCR	C21-C20-C19	-2.06	116.92	123.23
17	1	306	CLA	CAA-C2A-C3A	-2.06	107.17	112.81
20	B	848	BCR	C7-C8-C9	-2.06	123.12	126.21
17	6	312	CLA	C2A-C1A-CHA	-2.06	120.27	123.91
17	3	306	CLA	O1D-CGD-CBD	-2.06	120.91	124.60
17	6	311	CLA	C2A-C1A-CHA	-2.06	120.27	123.92
17	B	803	CLA	O2A-CGA-O1A	-2.06	118.45	123.55
17	3	314	CLA	O1D-CGD-CBD	-2.06	120.91	124.60
17	A	824	CLA	C2A-C1A-CHA	-2.05	120.28	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	309	CLA	CBC-CAC-C3C	-2.05	106.58	112.41
17	9	608	CLA	O2D-CGD-O1D	-2.05	119.69	123.82
27	6	321	LUT	C38-C25-C24	-2.05	119.26	123.68
17	b	815	CLA	C2A-C1A-CHA	-2.05	120.28	123.92
20	A	849	BCR	C15-C16-C17	-2.05	119.08	123.46
17	a	811	CLA	O2D-CGD-O1D	-2.05	119.69	123.82
17	B	816	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
17	9	612	CLA	O1D-CGD-CBD	-2.05	120.92	124.60
20	1	318	BCR	C39-C30-C25	-2.05	106.98	110.31
17	1	312	CLA	C2A-C1A-CHA	-2.05	120.28	123.92
26	2	606	CHL	O1D-CGD-CBD	-2.05	120.30	124.53
17	9	608	CLA	CBC-CAC-C3C	-2.05	106.59	112.41
20	K	4004	BCR	C23-C24-C25	-2.05	121.51	127.25
17	A	815	CLA	CBC-CAC-C3C	-2.05	106.59	112.41
17	A	838	CLA	C2A-C1A-CHA	-2.05	120.28	123.92
17	4	614	CLA	CAA-C2A-C3A	-2.05	107.19	112.81
17	9	611	CLA	CBC-CAC-C3C	-2.05	106.60	112.41
20	b	847	BCR	C4-C5-C6	-2.05	119.73	122.74
17	a	816	CLA	C2A-C1A-CHA	-2.05	120.29	123.92
17	B	839	CLA	CBC-CAC-C3C	-2.05	106.60	112.41
17	B	823	CLA	O2A-CGA-O1A	-2.05	118.47	123.55
17	1	303	CLA	O2A-CGA-O1A	-2.05	118.47	123.55
17	3	313	CLA	CBC-CAC-C3C	-2.05	106.60	112.41
17	a	841	CLA	C2A-C1A-CHA	-2.05	120.29	123.92
17	a	819	CLA	O2D-CGD-O1D	-2.05	119.70	123.82
17	4	614	CLA	O1D-CGD-CBD	-2.05	120.93	124.60
17	b	832	CLA	CAA-C2A-C3A	-2.05	107.20	112.81
17	7	604	CLA	O1D-CGD-CBD	-2.04	120.93	124.60
17	b	824	CLA	O2A-CGA-O1A	-2.04	118.48	123.55
17	B	831	CLA	CAA-C2A-C3A	-2.04	107.21	112.81
26	6	308	CHL	OMC-CMC-C2C	-2.04	121.68	124.29
17	2	602	CLA	CAA-C2A-C3A	-2.04	107.21	112.81
17	2	602	CLA	O2A-CGA-O1A	-2.04	118.48	123.55
17	F	304	CLA	C2A-C1A-CHA	-2.04	120.30	123.92
17	l	204	CLA	O1D-CGD-CBD	-2.04	120.94	124.60
28	8	315	XAT	C8-C9-C10	-2.04	115.81	118.94
17	a	825	CLA	O2A-CGA-O1A	-2.04	118.48	123.55
17	B	804	CLA	C2A-C1A-CHA	-2.04	120.30	123.92
17	b	839	CLA	O1D-CGD-CBD	-2.04	120.94	124.60
20	j	3003	BCR	C27-C26-C25	-2.04	119.75	122.74
17	B	827	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
20	a	850	BCR	C39-C30-C25	-2.04	107.00	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	306	CHL	O2D-CGD-O1D	-2.04	119.72	123.82
20	1	201	BCR	C39-C30-C25	-2.04	107.00	110.31
17	1	309	CLA	CBC-CAC-C3C	-2.04	106.63	112.41
17	9	610	CLA	O1D-CGD-CBD	-2.04	120.94	124.60
17	a	841	CLA	O2D-CGD-O1D	-2.04	119.72	123.82
20	F	305	BCR	C20-C21-C22	-2.03	124.41	127.31
20	6	319	BCR	C10-C11-C12	-2.03	116.99	123.23
17	a	805	CLA	C2A-C1A-CHA	-2.03	120.31	123.92
17	7	608	CLA	CBC-CAC-C3C	-2.03	106.64	112.41
17	A	829	CLA	C6-C7-C8	-2.03	109.06	115.73
26	7	606	CHL	O1D-CGD-CBD	-2.03	120.33	124.53
17	3	313	CLA	O2D-CGD-O1D	-2.03	119.73	123.82
20	1	318	BCR	C10-C11-C12	-2.03	117.00	123.23
17	b	838	CLA	C2A-C1A-CHA	-2.03	120.31	123.92
17	A	822	CLA	CAA-C2A-C3A	-2.03	107.24	112.81
17	a	842	CLA	CAA-C2A-C3A	-2.03	107.24	112.81
26	9	605	CHL	O1D-CGD-CBD	-2.03	120.34	124.53
17	G	103	CLA	CBC-CAC-C3C	-2.03	106.64	112.41
17	8	304	CLA	O1D-CGD-CBD	-2.03	120.95	124.60
17	B	820	CLA	CBC-CAC-C3C	-2.03	106.65	112.41
20	i	101	BCR	C27-C26-C25	-2.03	119.76	122.74
26	4	605	CHL	C1-C2-C3	-2.03	122.22	125.96
17	B	803	CLA	CBC-CAC-C3C	-2.03	106.65	112.41
17	B	823	CLA	O2D-CGD-O1D	-2.03	119.74	123.82
17	A	836	CLA	CAA-C2A-C3A	-2.03	107.26	112.81
20	B	847	BCR	C16-C17-C18	-2.03	124.42	127.31
17	B	836	CLA	O1D-CGD-CBD	-2.03	120.96	124.60
17	A	829	CLA	CBC-CAC-C3C	-2.03	106.66	112.41
17	a	801	CLA	CGD-CBD-CAD	-2.02	103.93	110.71
17	A	830	CLA	O2D-CGD-O1D	-2.02	119.75	123.82
20	l	201	BCR	C20-C21-C22	-2.02	124.42	127.31
19	2	618	LHG	C6-C5-C4	-2.02	107.29	111.86
17	a	811	CLA	CBC-CAC-C3C	-2.02	106.67	112.41
17	A	820	CLA	C4A-NA-C1A	-2.02	103.94	106.45
17	B	826	CLA	O2A-CGA-O1A	-2.02	118.53	123.55
17	A	819	CLA	O2A-CGA-O1A	-2.02	118.53	123.55
17	a	815	CLA	CBC-CAC-C3C	-2.02	106.67	112.41
17	3	308	CLA	C2A-C1A-CHA	-2.02	120.33	123.92
17	B	802	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
17	8	312	CLA	O2D-CGD-O1D	-2.02	119.75	123.82
17	A	803	CLA	CHA-C1A-NA	-2.02	121.48	126.18
17	B	805	CLA	C2A-C1A-CHA	-2.02	120.33	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	f	7002	CLA	C2A-C1A-CHA	-2.02	120.33	123.92
17	K	4003	CLA	CAA-C2A-C3A	-2.02	107.27	112.81
17	B	818	CLA	C1-C2-C3	-2.02	122.23	125.96
17	a	807	CLA	C2A-C1A-CHA	-2.02	120.34	123.92
17	7	603	CLA	CAA-C2A-C3A	-2.02	107.27	112.81
17	9	611	CLA	O2A-CGA-O1A	-2.02	118.54	123.55
17	b	812	CLA	O1D-CGD-CBD	-2.02	120.98	124.60
17	b	826	CLA	C2A-C1A-CHA	-2.02	120.34	123.92
17	3	312	CLA	O2D-CGD-O1D	-2.02	119.76	123.82
17	b	838	CLA	O2A-CGA-O1A	-2.02	118.55	123.55
17	2	611	CLA	O2A-CGA-O1A	-2.02	118.55	123.55
17	7	611	CLA	O2A-CGA-O1A	-2.02	118.55	123.55
17	7	610	CLA	O1D-CGD-CBD	-2.01	120.98	124.60
20	j	3003	BCR	C8-C7-C6	-2.01	121.61	127.25
17	6	311	CLA	O1D-CGD-CBD	-2.01	120.98	124.60
17	a	828	CLA	C2A-C1A-CHA	-2.01	120.35	123.92
17	3	311	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
20	A	851	BCR	C7-C8-C9	-2.01	123.19	126.21
28	8	315	XAT	C15-C14-C13	-2.01	124.44	127.31
20	a	853	BCR	C11-C10-C9	-2.01	124.44	127.31
17	8	307	CLA	CBC-CAC-C3C	-2.01	106.70	112.41
17	8	305	CLA	O1D-CGD-CBD	-2.01	120.99	124.60
17	A	813	CLA	CAA-C2A-C3A	-2.01	107.30	112.81
17	A	842	CLA	O1D-CGD-CBD	-2.01	120.99	124.60
17	b	815	CLA	CBC-CAC-C3C	-2.01	106.70	112.41
17	b	831	CLA	CAA-C2A-C3A	-2.01	107.30	112.81
20	a	852	BCR	C36-C18-C17	-2.01	120.11	122.92
20	F	305	BCR	C23-C24-C25	-2.01	121.63	127.25
17	a	820	CLA	O2D-CGD-O1D	-2.01	119.78	123.82
17	B	822	CLA	O2D-CGD-O1D	-2.01	119.78	123.82
24	B	850	DGD	O1G-C1A-O1A	-2.01	118.56	123.55
20	3	318	BCR	C20-C21-C22	-2.01	124.44	127.31
20	B	848	BCR	C8-C7-C6	-2.01	121.63	127.25
17	b	838	CLA	O1D-CGD-CBD	-2.01	121.00	124.60
17	9	614	CLA	CAA-C2A-C3A	-2.01	107.31	112.81
17	k	1403	CLA	CBC-CAC-C3C	-2.01	106.71	112.41
17	a	813	CLA	O1D-CGD-CBD	-2.01	121.00	124.60
20	b	845	BCR	C10-C11-C12	-2.01	117.08	123.23
26	4	607	CHL	O2D-CGD-O1D	-2.01	119.78	123.82
20	B	843	BCR	C33-C5-C6	-2.01	122.26	124.51
17	8	311	CLA	CAA-C2A-C3A	-2.01	107.31	112.81
20	j	3003	BCR	C23-C24-C25	-2.01	121.64	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	804	CLA	O1D-CGD-CBD	-2.01	121.00	124.60
20	a	851	BCR	C31-C1-C6	-2.00	107.06	110.31
18	a	845	PQN	C2M-C2-C3	-2.00	120.14	124.20
17	a	806	CLA	O1D-CGD-CBD	-2.00	121.00	124.60
20	a	851	BCR	C10-C11-C12	-2.00	117.09	123.23
17	B	809	CLA	CAA-C2A-C3A	-2.00	107.32	112.81
17	A	843	CLA	O1D-CGD-CBD	-2.00	121.00	124.60
17	B	815	CLA	C2A-C1A-CHA	-2.00	120.37	123.92
17	B	840	CLA	O2D-CGD-O1D	-2.00	119.79	123.82
17	b	841	CLA	O2A-CGA-O1A	-2.00	118.58	123.55
17	a	820	CLA	CBC-CAC-C3C	-2.00	106.73	112.41
17	4	612	CLA	O2A-CGA-O1A	-2.00	118.58	123.55
17	B	807	CLA	CHB-C4A-NA	2.00	127.28	124.51
17	A	834	CLA	CHB-C4A-NA	2.00	127.28	124.51
25	4	620	LMG	O8-C28-C29	2.00	117.72	111.90
17	A	830	CLA	CED-O2D-CGD	2.00	120.66	115.97
17	9	611	CLA	CHB-C4A-NA	2.00	127.28	124.51
17	9	611	CLA	CMC-C2C-C1C	2.00	128.06	125.02
17	1	306	CLA	CMC-C2C-C1C	2.00	128.06	125.02
17	a	846	CLA	CMC-C2C-C1C	2.00	128.06	125.02
20	a	849	BCR	C29-C30-C25	2.01	113.61	110.48
17	6	313	CLA	C1-O2A-CGA	2.01	121.58	116.77
17	a	806	CLA	C4-C3-C5	2.01	118.77	115.29
20	j	3003	BCR	C29-C30-C25	2.01	113.61	110.48
17	b	811	CLA	CMB-C2B-C3B	2.01	128.77	124.92
26	8	306	CHL	CED-O2D-CGD	2.01	120.68	115.97
17	3	309	CLA	C5-C3-C4	2.01	119.29	114.60
26	8	306	CHL	CHB-C1B-C2B	2.01	122.55	116.99
17	f	7002	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	b	804	CLA	CMB-C2B-C3B	2.01	128.62	124.89
27	1	320	LUT	C39-C29-C28	2.01	121.30	118.10
17	a	834	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	B	823	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	B	810	CLA	CHB-C4A-NA	2.01	127.29	124.51
20	A	848	BCR	C33-C5-C4	2.01	117.27	113.45
17	a	836	CLA	C5-C3-C4	2.01	119.29	114.60
20	a	854	BCR	C37-C22-C23	2.01	121.30	118.10
17	F	303	CLA	CMB-C2B-C3B	2.01	128.62	124.89
17	9	602	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	b	817	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	8	311	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	2	604	CLA	CHB-C4A-NA	2.01	127.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	802	CLA	CED-O2D-CGD	2.01	120.69	115.97
20	L	201	BCR	C33-C5-C4	2.01	117.27	113.45
17	A	828	CLA	CHB-C4A-NA	2.01	127.30	124.51
26	9	607	CHL	CHC-C4B-C3B	2.01	123.00	118.23
17	8	311	CLA	CED-O2D-CGD	2.02	120.69	115.97
26	8	306	CHL	O2A-CGA-CBA	2.02	120.64	112.33
20	a	853	BCR	C2-C1-C6	2.02	113.63	110.48
17	B	819	CLA	CED-O2D-CGD	2.02	120.70	115.97
17	A	829	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	l	202	CLA	CMB-C2B-C3B	2.02	128.63	124.89
17	a	811	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	A	823	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	B	802	CLA	C4-C3-C5	2.02	118.79	115.29
17	A	825	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	A	806	CLA	CED-O2D-CGD	2.02	120.70	115.97
20	a	854	BCR	C29-C30-C25	2.02	113.63	110.48
17	a	811	CLA	CMC-C2C-C1C	2.02	128.08	125.02
20	F	305	BCR	C2-C1-C6	2.02	113.64	110.48
17	2	609	CLA	CED-O2D-CGD	2.02	120.70	115.97
17	a	811	CLA	CMB-C2B-C3B	2.02	128.64	124.89
17	9	609	CLA	CED-O2D-CGD	2.02	120.71	115.97
20	A	850	BCR	C38-C26-C27	2.02	117.29	113.45
17	6	310	CLA	CED-O2D-CGD	2.02	120.71	115.97
26	2	607	CHL	CHC-C4B-C3B	2.02	123.02	118.23
17	A	804	CLA	CHB-C4A-NA	2.02	127.31	124.51
20	A	852	BCR	C37-C22-C23	2.02	121.32	118.10
17	b	818	CLA	C1-O2A-CGA	2.02	121.63	116.77
17	a	843	CLA	C4-C3-C5	2.02	118.80	115.29
20	I	101	BCR	C33-C5-C4	2.03	117.30	113.45
17	b	840	CLA	CHB-C4A-NA	2.03	127.31	124.51
20	b	846	BCR	C36-C18-C19	2.03	121.33	118.10
17	B	825	CLA	CHB-C4A-NA	2.03	127.32	124.51
17	A	805	CLA	CMB-C2B-C3B	2.03	128.66	124.89
20	i	101	BCR	C2-C1-C6	2.03	113.65	110.48
17	B	829	CLA	C4-C3-C5	2.03	118.81	115.29
17	b	806	CLA	CMB-C2B-C3B	2.03	128.67	124.89
17	G	101	CLA	CMB-C2B-C3B	2.03	128.67	124.89
26	4	605	CHL	CHD-C1D-C2D	2.03	122.62	116.99
17	A	837	CLA	CHB-C4A-NA	2.03	127.33	124.51
17	7	610	CLA	CMC-C2C-C1C	2.03	128.11	125.02
17	a	808	CLA	CMB-C2B-C3B	2.04	128.67	124.89
17	k	1403	CLA	CMC-C2C-C1C	2.04	128.11	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	f	7004	BCR	C12-C13-C14	2.04	122.06	118.94
17	7	612	CLA	CMB-C2B-C3B	2.04	128.67	124.89
17	a	835	CLA	CMC-C2C-C1C	2.04	128.11	125.02
20	f	7004	BCR	C2-C1-C6	2.04	113.66	110.48
26	2	601	CHL	C1-O2A-CGA	2.04	121.66	116.77
17	l	204	CLA	CMB-C2B-C3B	2.04	128.68	124.89
17	b	831	CLA	CMC-C2C-C1C	2.04	128.11	125.02
26	4	615	CHL	CHD-C1D-C2D	2.04	122.64	116.99
17	A	828	CLA	CAC-C3C-C4C	2.04	127.71	124.83
17	b	805	CLA	CMB-C2B-C3B	2.04	128.68	124.89
26	9	605	CHL	CHD-C1D-C2D	2.04	122.64	116.99
17	k	1403	CLA	CHB-C4A-NA	2.04	127.33	124.51
26	7	614	CHL	CHB-C1B-C2B	2.04	122.64	116.99
17	K	4003	CLA	CMC-C2C-C1C	2.04	128.12	125.02
17	A	806	CLA	CHB-C4A-NA	2.04	127.33	124.51
17	b	815	CLA	CHB-C4A-NA	2.04	127.33	124.51
20	B	801	BCR	C2-C1-C6	2.04	113.67	110.48
26	9	615	CHL	CHC-C4B-C3B	2.04	123.07	118.23
17	B	815	CLA	CHB-C4A-NA	2.04	127.34	124.51
17	a	828	CLA	CMB-C2B-C3B	2.04	128.69	124.89
26	7	607	CHL	CHC-C4B-C3B	2.04	123.07	118.23
17	l	204	CLA	CHB-C4A-NA	2.05	127.34	124.51
17	b	809	CLA	CMB-C2B-C3B	2.05	128.69	124.89
17	4	604	CLA	CMB-C2B-C3B	2.05	128.69	124.89
17	a	835	CLA	CHB-C4A-NA	2.05	127.34	124.51
17	B	819	CLA	C1-O2A-CGA	2.05	121.69	116.77
20	a	850	BCR	C2-C1-C6	2.05	113.68	110.48
17	A	835	CLA	CMC-C2C-C1C	2.05	128.13	125.02
17	B	831	CLA	CMC-C2C-C1C	2.05	128.13	125.02
17	a	822	CLA	CED-O2D-CGD	2.05	120.78	115.97
17	a	812	CLA	CHB-C4A-NA	2.05	127.35	124.51
17	b	832	CLA	CHB-C4A-NA	2.05	127.35	124.51
17	b	835	CLA	CHB-C4A-NA	2.05	127.35	124.51
17	9	604	CLA	CHB-C4A-NA	2.05	127.35	124.51
17	b	806	CLA	C4-C3-C5	2.05	118.85	115.29
20	k	1404	BCR	C38-C26-C27	2.05	117.35	113.45
17	a	813	CLA	CMC-C2C-C1C	2.05	128.13	125.02
28	4	617	XAT	C18-C5-C4	2.06	116.63	114.28
17	a	821	CLA	CHB-C4A-NA	2.06	127.36	124.51
20	B	845	BCR	C8-C9-C10	2.06	122.10	118.94
17	B	812	CLA	C4-C3-C5	2.06	118.86	115.29
20	A	850	BCR	C2-C1-C6	2.06	113.69	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	802	CLA	CAC-C3C-C4C	2.06	127.73	124.83
17	B	815	CLA	CMB-C2B-C3B	2.06	128.71	124.89
17	A	834	CLA	CMC-C2C-C1C	2.06	128.14	125.02
17	a	837	CLA	CED-O2D-CGD	2.06	120.80	115.97
17	1	313	CLA	C4-C3-C5	2.06	118.86	115.29
17	a	821	CLA	CMB-C2B-C3B	2.06	128.72	124.89
17	a	805	CLA	CHB-C4A-NA	2.06	127.36	124.51
20	i	101	BCR	C37-C22-C23	2.06	121.38	118.10
17	a	802	CLA	CMC-C2C-C1C	2.06	128.15	125.02
17	4	610	CLA	CHB-C4A-NA	2.06	127.36	124.51
17	B	834	CLA	CHB-C4A-NA	2.06	127.36	124.51
20	B	801	BCR	C36-C18-C19	2.06	121.39	118.10
17	1	306	CLA	CHB-C4A-NA	2.06	127.36	124.51
17	1	310	CLA	CED-O2D-CGD	2.06	120.81	115.97
20	4	618	BCR	C37-C22-C23	2.06	121.39	118.10
26	9	615	CHL	CHD-C1D-C2D	2.06	122.71	116.99
17	1	305	CLA	CHB-C4A-NA	2.07	127.37	124.51
26	7	614	CHL	CHD-C1D-C2D	2.07	122.71	116.99
26	6	308	CHL	CHB-C1B-C2B	2.07	122.72	116.99
17	A	831	CLA	CHB-C4A-NA	2.07	127.37	124.51
17	2	608	CLA	CMC-C2C-C1C	2.07	128.16	125.02
17	b	803	CLA	C4-C3-C5	2.07	118.88	115.29
17	7	608	CLA	CMC-C2C-C1C	2.07	128.16	125.02
17	B	837	CLA	CMB-C2B-C3B	2.07	128.74	124.89
17	A	821	CLA	CHB-C4A-NA	2.07	127.38	124.51
26	1	307	CHL	CHD-C1D-C2D	2.07	122.73	116.99
17	b	837	CLA	CMB-C2B-C3B	2.07	128.74	124.89
17	1	313	CLA	CHB-C4A-NA	2.07	127.38	124.51
17	4	608	CLA	CHB-C4A-NA	2.07	127.38	124.51
26	2	605	CHL	CHD-C1D-C2D	2.07	122.73	116.99
17	f	7002	CLA	CMB-C2B-C3B	2.08	128.74	124.89
17	B	835	CLA	CED-O2D-CGD	2.08	120.84	115.97
17	1	314	CLA	CHB-C4A-NA	2.08	127.38	124.51
20	g	104	BCR	C33-C5-C4	2.08	117.39	113.45
27	4	616	LUT	C1-C2-C3	2.08	117.89	113.40
17	a	820	CLA	C4-C3-C5	2.08	118.89	115.29
20	f	7004	BCR	C37-C22-C23	2.08	121.41	118.10
20	B	848	BCR	C33-C5-C4	2.08	117.40	113.45
26	3	307	CHL	CHC-C4B-C3B	2.08	123.16	118.23
17	A	836	CLA	C5-C3-C4	2.08	119.45	114.60
17	B	820	CLA	CHB-C4A-NA	2.08	127.39	124.51
26	7	601	CHL	CHD-C1D-C2D	2.08	122.75	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	818	CLA	CHB-C4A-NA	2.08	127.39	124.51
17	B	805	CLA	CMB-C2B-C3B	2.08	128.75	124.89
17	b	805	CLA	CHB-C4A-NA	2.08	127.39	124.51
20	l	201	BCR	C33-C5-C4	2.08	117.41	113.45
17	7	604	CLA	CMC-C2C-C1C	2.08	128.18	125.02
28	3	317	XAT	C18-C5-C4	2.08	116.67	114.28
17	B	804	CLA	CHB-C4A-NA	2.08	127.39	124.51
17	2	604	CLA	CMC-C2C-C1C	2.09	128.18	125.02
20	A	856	BCR	C34-C9-C8	2.09	121.42	118.10
17	A	817	CLA	CMB-C2B-C3B	2.09	128.77	124.89
17	b	807	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	B	828	CLA	CMB-C2B-C3B	2.09	128.77	124.89
17	l	203	CLA	CHB-C4A-NA	2.09	127.40	124.51
26	7	607	CHL	CHB-C1B-C2B	2.09	122.78	116.99
17	b	830	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	6	306	CLA	CHB-C4A-NA	2.09	127.41	124.51
17	a	816	CLA	CMB-C2B-C3B	2.09	128.78	124.89
20	b	846	BCR	C2-C1-C6	2.09	113.75	110.48
17	B	808	CLA	CHB-C4A-NA	2.09	127.41	124.51
17	B	803	CLA	CED-O2D-CGD	2.10	120.88	115.97
17	a	816	CLA	CED-O2D-CGD	2.10	120.88	115.97
17	7	604	CLA	CHB-C4A-NA	2.10	127.41	124.51
17	a	824	CLA	CMB-C2B-C3B	2.10	128.78	124.89
17	A	805	CLA	CHB-C4A-NA	2.10	127.41	124.51
17	6	311	CLA	CHB-C4A-NA	2.10	127.41	124.51
17	B	838	CLA	CMB-C2B-C3B	2.10	128.79	124.89
17	B	811	CLA	CMC-C2C-C1C	2.10	128.21	125.02
17	4	604	CLA	C5-C3-C4	2.10	119.50	114.60
17	A	841	CLA	CHB-C4A-NA	2.10	127.42	124.51
20	A	848	BCR	C29-C30-C25	2.10	113.77	110.48
17	F	304	CLA	CHB-C4A-NA	2.10	127.42	124.51
20	3	318	BCR	C37-C22-C23	2.10	121.45	118.10
17	b	822	CLA	CAC-C3C-C4C	2.11	127.80	124.83
17	4	609	CLA	CHB-C4A-NA	2.11	127.42	124.51
20	B	848	BCR	C35-C13-C12	2.11	121.46	118.10
17	A	809	CLA	CHB-C4A-NA	2.11	127.43	124.51
20	G	105	BCR	C33-C5-C4	2.11	117.45	113.45
26	8	306	CHL	CHD-C1D-C2D	2.11	122.83	116.99
17	A	831	CLA	CMB-C2B-C3B	2.11	128.81	124.89
17	A	835	CLA	CHB-C4A-NA	2.11	127.43	124.51
26	6	303	CHL	CHD-C1D-C2D	2.11	122.84	116.99
17	A	814	CLA	CMB-C2B-C3B	2.11	128.81	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	f	7003	CLA	C1-O2A-CGA	2.11	121.84	116.77
17	A	811	CLA	CMC-C2C-C1C	2.11	128.22	125.02
17	B	840	CLA	CAC-C3C-C4C	2.12	127.81	124.83
17	a	827	CLA	CMC-C2C-C1C	2.12	128.23	125.02
17	b	802	CLA	CMC-C2C-C1C	2.12	128.23	125.02
17	B	834	CLA	CMC-C2C-C1C	2.12	128.23	125.02
17	l	204	CLA	C1-O2A-CGA	2.12	121.85	116.77
17	A	815	CLA	CMB-C2B-C3B	2.12	128.82	124.89
17	8	309	CLA	CMC-C2C-C1C	2.12	128.23	125.02
17	b	813	CLA	CMB-C2B-C3B	2.12	128.82	124.89
17	4	602	CLA	CHB-C4A-NA	2.12	127.44	124.51
17	1	313	CLA	CMB-C2B-C3B	2.12	128.83	124.89
20	8	316	BCR	C37-C22-C23	2.12	121.48	118.10
17	a	807	CLA	CHB-C4A-NA	2.12	127.45	124.51
17	L	203	CLA	CHB-C4A-NA	2.12	127.45	124.51
28	4	617	XAT	C19-C9-C8	2.12	121.48	118.10
17	A	811	CLA	CMB-C2B-C3B	2.13	128.84	124.89
17	3	304	CLA	CMC-C2C-C1C	2.13	128.25	125.02
17	1	304	CLA	CMB-C2B-C3B	2.13	128.84	124.89
17	A	836	CLA	CHB-C4A-NA	2.13	127.45	124.51
17	B	840	CLA	CMB-C2B-C3B	2.13	128.84	124.89
28	2	616	XAT	C18-C5-C4	2.13	116.72	114.28
20	K	4004	BCR	C33-C5-C4	2.13	117.49	113.45
17	A	840	CLA	C1-O2A-CGA	2.13	121.88	116.77
17	k	1402	CLA	CMB-C2B-C3B	2.13	128.84	124.89
17	B	809	CLA	CMC-C2C-C1C	2.13	128.25	125.02
17	4	604	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	9	618	BCR	C38-C26-C27	2.13	117.50	113.45
17	3	313	CLA	CED-O2D-CGD	2.13	120.97	115.97
17	a	802	CLA	C4-C3-C5	2.13	118.99	115.29
17	4	603	CLA	CMB-C2B-C3B	2.13	128.85	124.89
20	A	849	BCR	C34-C9-C8	2.14	121.50	118.10
17	a	841	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	8	307	CLA	CAC-C3C-C4C	2.14	127.84	124.83
26	8	306	CHL	CHC-C4B-C3B	2.14	123.29	118.23
17	6	311	CLA	CED-O2D-CGD	2.14	120.98	115.97
17	3	304	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	7	609	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	b	804	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	A	822	CLA	CMC-C2C-C1C	2.14	128.26	125.02
17	A	819	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	b	815	CLA	CMB-C2B-C3B	2.14	128.87	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	849	DGD	O6D-C5D-C6D	2.14	110.91	106.64
26	9	607	CHL	CHD-C1D-C2D	2.14	122.92	116.99
17	3	304	CLA	CMB-C2B-C3B	2.14	128.87	124.89
17	1	309	CLA	CED-O2D-CGD	2.14	121.00	115.97
20	a	849	BCR	C2-C1-C6	2.15	113.83	110.48
17	b	818	CLA	CMB-C2B-C3B	2.15	128.87	124.89
17	B	824	CLA	CHB-C4A-NA	2.15	127.48	124.51
17	a	836	CLA	C1-O2A-CGA	2.15	121.93	116.77
17	3	309	CLA	CHB-C4A-NA	2.15	127.48	124.51
17	A	820	CLA	C4-C3-C5	2.15	119.02	115.29
17	L	202	CLA	CMB-C2B-C3B	2.15	128.88	124.89
17	6	314	CLA	CMB-C2B-C3B	2.15	128.88	124.89
17	4	613	CLA	CHB-C4A-NA	2.15	127.49	124.51
17	a	821	CLA	CAC-C3C-C4C	2.15	127.86	124.83
17	b	828	CLA	CAC-C3C-C4C	2.15	127.86	124.83
17	9	601	CLA	O2A-CGA-CBA	2.15	121.20	112.33
20	B	846	BCR	C36-C18-C19	2.15	121.53	118.10
26	9	605	CHL	O2A-CGA-CBA	2.15	118.16	111.90
17	a	856	CLA	CMC-C2C-C1C	2.15	128.28	125.02
28	8	315	XAT	C20-C13-C12	2.15	121.53	118.10
17	a	829	CLA	CMB-C2B-C3B	2.15	128.89	124.89
17	9	613	CLA	CHB-C4A-NA	2.16	127.49	124.51
17	A	842	CLA	C4-C3-C5	2.16	119.03	115.29
17	8	302	CLA	C5-C3-C4	2.16	119.63	114.60
17	b	809	CLA	CAC-C3C-C4C	2.16	127.87	124.83
20	2	617	BCR	C36-C18-C19	2.16	121.54	118.10
17	9	601	CLA	CMC-C2C-C1C	2.16	128.29	125.02
26	7	614	CHL	CHC-C4B-C3B	2.16	123.34	118.23
17	9	604	CLA	C5-C3-C4	2.16	119.64	114.60
17	b	803	CLA	CMC-C2C-C1C	2.16	128.29	125.02
20	B	847	BCR	C38-C26-C27	2.16	117.55	113.45
20	B	847	BCR	C36-C18-C19	2.16	121.54	118.10
17	B	823	CLA	CED-O2D-CGD	2.16	121.03	115.97
17	A	828	CLA	C4-C3-C5	2.16	119.04	115.29
26	6	308	CHL	CHD-C1D-C2D	2.16	122.97	116.99
17	1	310	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	2	609	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	L	202	CLA	CMC-C2C-C1C	2.16	128.30	125.02
17	B	835	CLA	CMC-C2C-C1C	2.16	128.30	125.02
17	A	832	CLA	C5-C3-C4	2.16	119.65	114.60
17	B	820	CLA	CMC-C2C-C1C	2.16	128.30	125.02
17	B	823	CLA	CMB-C2B-C3B	2.16	128.91	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	806	CLA	CMB-C2B-C3B	2.16	128.91	124.89
17	B	834	CLA	CMB-C2B-C3B	2.17	128.91	124.89
17	B	811	CLA	CMB-C2B-C3B	2.17	129.08	124.92
17	8	305	CLA	CMC-C2C-C1C	2.17	128.31	125.02
17	8	310	CLA	CMB-C2B-C3B	2.17	128.92	124.89
20	B	844	BCR	C2-C1-C6	2.17	113.87	110.48
17	B	819	CLA	CHB-C4A-NA	2.17	127.51	124.51
17	a	835	CLA	CAC-C3C-C4C	2.17	127.89	124.83
28	3	317	XAT	C20-C13-C12	2.17	121.56	118.10
17	3	303	CLA	C5-C3-C4	2.17	119.67	114.60
26	9	606	CHL	C5-C3-C4	2.17	119.67	114.60
17	B	816	CLA	CHB-C4A-NA	2.17	127.52	124.51
17	k	1403	CLA	CMB-C2B-C3B	2.17	128.92	124.89
17	B	835	CLA	CHB-C4A-NA	2.17	127.52	124.51
17	f	7002	CLA	CAC-C3C-C4C	2.17	127.90	124.83
17	B	813	CLA	CMB-C2B-C3B	2.17	128.93	124.89
17	7	602	CLA	CMB-C2B-C3B	2.17	128.93	124.89
17	a	841	CLA	CMB-C2B-C3B	2.18	128.93	124.89
17	a	822	CLA	CMC-C2C-C1C	2.18	128.32	125.02
17	8	311	CLA	CMC-C2C-C1C	2.18	128.32	125.02
17	6	305	CLA	CMB-C2B-C3B	2.18	128.93	124.89
17	8	308	CLA	CED-O2D-CGD	2.18	121.07	115.97
17	1	309	CLA	CHB-C4A-NA	2.18	127.52	124.51
17	1	309	CLA	CMC-C2C-C1C	2.18	128.32	125.02
17	7	609	CLA	C4-C3-C5	2.18	119.07	115.29
17	A	812	CLA	CHB-C4A-NA	2.18	127.53	124.51
17	l	204	CLA	CMC-C2C-C1C	2.18	128.33	125.02
17	A	825	CLA	CMC-C2C-C1C	2.18	128.33	125.02
17	4	612	CLA	CMC-C2C-C1C	2.18	128.33	125.02
28	1	317	XAT	C38-C25-C24	2.18	116.78	114.28
17	B	808	CLA	C4-C3-C5	2.18	119.08	115.29
17	9	609	CLA	CHB-C4A-NA	2.18	127.53	124.51
17	b	805	CLA	CMC-C2C-C1C	2.18	128.33	125.02
17	2	612	CLA	C4-C3-C5	2.18	119.08	115.29
17	b	830	CLA	CMB-C2B-C3B	2.18	128.94	124.89
28	2	616	XAT	C38-C25-C24	2.19	116.78	114.28
17	9	608	CLA	C5-C3-C4	2.19	119.70	114.60
17	b	835	CLA	CMB-C2B-C3B	2.19	128.95	124.89
17	B	829	CLA	CMB-C2B-C3B	2.19	128.95	124.89
17	a	838	CLA	C4-C3-C5	2.19	118.44	115.85
20	4	618	BCR	C36-C18-C19	2.19	121.58	118.10
26	9	605	CHL	CHC-C4B-C3B	2.19	123.42	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	305	BCR	C37-C22-C23	2.19	121.59	118.10
17	b	808	CLA	C4-C3-C5	2.19	119.09	115.29
17	b	837	CLA	CHB-C4A-NA	2.19	127.54	124.51
20	G	105	BCR	C38-C26-C27	2.19	117.61	113.45
17	A	836	CLA	CMC-C2C-C1C	2.19	128.34	125.02
17	a	828	CLA	CMC-C2C-C1C	2.19	128.34	125.02
17	7	608	CLA	C5-C3-C4	2.19	119.72	114.60
20	A	852	BCR	C19-C18-C17	2.19	122.31	118.94
17	A	816	CLA	CMB-C2B-C3B	2.19	128.96	124.89
17	2	610	CLA	CMC-C2C-C1C	2.19	128.35	125.02
17	B	829	CLA	CMC-C2C-C1C	2.19	128.35	125.02
17	B	823	CLA	CMC-C2C-C1C	2.19	128.35	125.02
17	2	612	CLA	CMC-C2C-C1C	2.19	128.35	125.02
17	J	3002	CLA	CMC-C2C-C1C	2.19	128.35	125.02
17	B	837	CLA	CHB-C4A-NA	2.19	127.55	124.51
26	6	303	CHL	CHC-C4B-C3B	2.20	123.43	118.23
17	B	817	CLA	CMC-C2C-C1C	2.20	128.35	125.02
17	a	805	CLA	CMB-C2B-C3B	2.20	128.97	124.89
20	B	846	BCR	C37-C22-C23	2.20	121.60	118.10
17	3	312	CLA	CMB-C2B-C3B	2.20	128.97	124.89
17	B	831	CLA	CHB-C4A-NA	2.20	127.55	124.51
17	b	830	CLA	C5-C3-C4	2.20	119.73	114.60
27	6	317	LUT	C39-C29-C28	2.20	121.60	118.10
20	A	848	BCR	C38-C26-C27	2.20	117.62	113.45
17	F	304	CLA	CMB-C2B-C3B	2.20	128.97	124.89
17	G	103	CLA	C5-C3-C4	2.20	119.73	114.60
17	2	604	CLA	CMB-C2B-C3B	2.20	128.97	124.89
17	9	608	CLA	CMC-C2C-C1C	2.20	128.36	125.02
26	1	307	CHL	CHC-C4B-C3B	2.20	123.44	118.23
26	2	606	CHL	CHC-C4B-C3B	2.20	123.44	118.23
17	B	820	CLA	CMB-C2B-C3B	2.20	128.98	124.89
17	3	313	CLA	CMB-C2B-C3B	2.20	128.98	124.89
17	a	832	CLA	C5-C3-C4	2.20	119.74	114.60
28	6	318	XAT	C20-C13-C12	2.20	121.61	118.10
17	A	816	CLA	C5-C3-C4	2.20	119.74	114.60
17	8	303	CLA	CHB-C4A-NA	2.20	127.56	124.51
17	8	307	CLA	CHB-C4A-NA	2.21	127.56	124.51
20	a	852	BCR	C29-C30-C25	2.21	113.93	110.48
17	8	308	CLA	CHB-C4A-NA	2.21	127.56	124.51
17	4	609	CLA	CED-O2D-CGD	2.21	121.14	115.97
17	6	315	CLA	CMC-C2C-C1C	2.21	128.37	125.02
17	1	304	CLA	CMC-C2C-C1C	2.21	128.37	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	303	CLA	CMB-C2B-C3B	2.21	128.99	124.89
17	b	816	CLA	CHB-C4A-NA	2.21	127.57	124.51
20	b	844	BCR	C2-C1-C6	2.21	113.93	110.48
17	a	832	CLA	CMC-C2C-C1C	2.21	128.37	125.02
17	8	307	CLA	CMC-C2C-C1C	2.21	128.37	125.02
17	b	816	CLA	CMB-C2B-C3B	2.21	129.00	124.89
17	3	308	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	9	608	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	B	830	CLA	C5-C3-C4	2.21	119.77	114.60
17	b	810	CLA	CMB-C2B-C3B	2.21	129.00	124.89
17	2	608	CLA	CMB-C2B-C3B	2.21	129.00	124.89
17	a	818	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	b	814	CLA	CMB-C2B-C3B	2.22	129.00	124.89
20	b	848	BCR	C34-C9-C8	2.22	121.63	118.10
17	9	609	CLA	CMC-C2C-C1C	2.22	128.38	125.02
17	a	843	CLA	CMB-C2B-C3B	2.22	129.01	124.89
27	3	316	LUT	C18-C5-C4	2.22	118.38	114.33
17	3	308	CLA	C5-C3-C4	2.22	119.78	114.60
17	A	827	CLA	CMC-C2C-C1C	2.22	128.38	125.02
17	4	611	CLA	CMC-C2C-C1C	2.22	128.39	125.02
26	4	606	CHL	CHD-C1D-C2D	2.22	123.14	116.99
17	2	612	CLA	CMB-C2B-C3B	2.22	129.01	124.89
17	a	837	CLA	CMB-C2B-C3B	2.22	129.02	124.89
17	7	602	CLA	C4-C3-C5	2.22	119.15	115.29
17	B	802	CLA	CHB-C4A-NA	2.22	127.59	124.51
17	a	840	CLA	CMB-C2B-C3B	2.22	129.02	124.89
17	A	810	CLA	CAC-C3C-C4C	2.22	127.97	124.83
17	a	810	CLA	CMC-C2C-C1C	2.23	128.40	125.02
17	a	830	CLA	CAC-C3C-C4C	2.23	127.97	124.83
17	b	816	CLA	C1-O2A-CGA	2.23	122.11	116.77
17	3	305	CLA	CMC-C2C-C1C	2.23	128.40	125.02
28	8	315	XAT	C39-C29-C28	2.23	121.65	118.10
17	A	824	CLA	CMC-C2C-C1C	2.23	128.40	125.02
20	9	618	BCR	C36-C18-C19	2.23	121.65	118.10
17	A	818	CLA	CMB-C2B-C3B	2.23	129.03	124.89
26	9	606	CHL	CHC-C4B-C3B	2.23	123.51	118.23
17	3	313	CLA	CMC-C2C-C1C	2.23	128.40	125.02
20	1	206	BCR	C2-C1-C6	2.23	113.97	110.48
17	g	102	CLA	C5-C3-C4	2.23	119.81	114.60
17	2	608	CLA	C5-C3-C4	2.23	119.81	114.60
17	B	820	CLA	C5-C3-C4	2.23	119.81	114.60
26	4	606	CHL	CHC-C4B-C3B	2.23	123.52	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	803	CLA	CMB-C2B-C3B	2.23	129.04	124.89
17	b	802	CLA	CHB-C4A-NA	2.23	127.60	124.51
17	k	1401	CLA	CMB-C2B-C3B	2.23	129.04	124.89
17	B	817	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	4	615	CHL	CHC-C4B-C3B	2.23	123.52	118.23
17	a	831	CLA	CMB-C2B-C3B	2.23	129.04	124.89
17	b	820	CLA	C5-C3-C4	2.24	119.82	114.60
17	G	104	CLA	CMB-C2B-C3B	2.24	129.04	124.89
17	A	814	CLA	C1-O2A-CGA	2.24	122.14	116.77
17	B	832	CLA	C1-O2A-CGA	2.24	122.14	116.77
17	A	813	CLA	C1-O2A-CGA	2.24	122.14	116.77
17	B	824	CLA	CMB-C2B-C3B	2.24	129.04	124.89
17	a	825	CLA	CED-O2D-CGD	2.24	121.21	115.97
17	1	306	CLA	CMB-C2B-C3B	2.24	129.04	124.89
17	A	812	CLA	CMB-C2B-C3B	2.24	129.04	124.89
17	a	841	CLA	C4-C3-C5	2.24	119.17	115.29
20	9	618	BCR	C29-C30-C25	2.24	113.98	110.48
17	A	813	CLA	CMB-C2B-C3B	2.24	129.04	124.89
17	b	837	CLA	CAC-C3C-C4C	2.24	127.99	124.83
17	4	614	CLA	C5-C3-C4	2.24	119.83	114.60
17	b	838	CLA	CAC-C3C-C4C	2.24	127.99	124.83
17	9	614	CLA	CMB-C2B-C3B	2.24	129.05	124.89
17	L	204	CLA	CMC-C2C-C1C	2.24	128.42	125.02
20	g	104	BCR	C29-C30-C25	2.24	113.98	110.48
17	B	827	CLA	CMB-C2B-C3B	2.24	129.05	124.89
17	a	807	CLA	C4-C3-C5	2.24	119.18	115.29
17	A	835	CLA	CMB-C2B-C3B	2.24	129.05	124.89
17	6	310	CLA	CMB-C2B-C3B	2.24	129.05	124.89
17	4	614	CLA	CMC-C2C-C1C	2.24	128.42	125.02
17	b	820	CLA	CMB-C2B-C3B	2.24	129.05	124.89
17	9	603	CLA	CMB-C2B-C3B	2.24	129.05	124.89
17	9	604	CLA	CMC-C2C-C1C	2.24	128.42	125.02
17	a	806	CLA	CHB-C4A-NA	2.24	127.61	124.51
20	a	852	BCR	C38-C26-C27	2.24	117.71	113.45
17	7	611	CLA	CMB-C2B-C3B	2.24	129.06	124.89
17	b	827	CLA	CMB-C2B-C3B	2.25	129.06	124.89
17	a	838	CLA	CMB-C2B-C3B	2.25	129.06	124.89
17	a	832	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	1	308	CLA	CMB-C2B-C3B	2.25	129.06	124.89
17	b	803	CLA	CED-O2D-CGD	2.25	121.24	115.97
17	a	807	CLA	CMB-C2B-C3B	2.25	129.06	124.89
17	4	608	CLA	C5-C3-C4	2.25	119.86	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	613	CLA	CMB-C2B-C3B	2.25	129.07	124.89
17	a	818	CLA	CMC-C2C-C1C	2.25	128.44	125.02
17	3	306	CLA	CMC-C2C-C1C	2.25	128.44	125.02
17	A	812	CLA	CAC-C3C-C4C	2.25	128.01	124.83
20	6	319	BCR	C37-C22-C23	2.25	121.69	118.10
17	a	825	CLA	CMB-C2B-C3B	2.25	129.07	124.89
20	b	845	BCR	C38-C26-C27	2.25	117.73	113.45
17	B	838	CLA	CMC-C2C-C1C	2.26	128.44	125.02
17	a	809	CLA	C4-C3-C5	2.26	119.20	115.29
17	b	837	CLA	CMC-C2C-C1C	2.26	128.44	125.02
20	b	845	BCR	C29-C30-C25	2.26	114.01	110.48
17	A	814	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	4	612	CLA	CMB-C2B-C3B	2.26	129.09	124.89
17	L	203	CLA	C4-C3-C5	2.26	119.21	115.29
17	J	3002	CLA	CHB-C4A-NA	2.26	127.64	124.51
18	a	845	PQN	C2M-C2-C1	2.26	120.02	116.23
17	A	837	CLA	CMB-C2B-C3B	2.26	129.09	124.89
17	1	311	CLA	CMC-C2C-C1C	2.26	128.45	125.02
20	1	201	BCR	C8-C9-C10	2.26	122.42	118.94
17	B	841	CLA	CMB-C2B-C3B	2.26	129.09	124.89
17	b	826	CLA	CMB-C2B-C3B	2.26	129.09	124.89
28	7	616	XAT	C38-C25-C24	2.26	116.87	114.28
17	A	837	CLA	CMC-C2C-C1C	2.26	128.45	125.02
26	7	606	CHL	CHC-C4B-C3B	2.26	123.59	118.23
17	A	854	CLA	CAC-C3C-C4C	2.27	128.03	124.83
17	3	305	CLA	CMB-C2B-C3B	2.27	129.10	124.89
17	B	838	CLA	CAC-C3C-C4C	2.27	128.03	124.83
20	b	847	BCR	C36-C18-C19	2.27	121.71	118.10
17	b	807	CLA	CMB-C2B-C3B	2.27	129.10	124.89
17	4	613	CLA	CMC-C2C-C1C	2.27	128.46	125.02
17	6	306	CLA	CMB-C2B-C3B	2.27	129.11	124.89
20	b	847	BCR	C29-C30-C25	2.27	114.03	110.48
20	B	848	BCR	C37-C22-C23	2.27	121.72	118.10
17	B	819	CLA	CMC-C2C-C1C	2.27	128.47	125.02
17	8	307	CLA	C5-C3-C4	2.27	119.90	114.60
20	4	618	BCR	C38-C26-C27	2.27	117.77	113.45
17	9	601	CLA	CMB-C2B-C3B	2.27	129.11	124.89
17	b	834	CLA	CMC-C2C-C1C	2.27	128.47	125.02
17	j	3002	CLA	CMC-C2C-C1C	2.28	128.47	125.02
17	a	818	CLA	C4-C3-C5	2.28	119.24	115.29
17	B	832	CLA	C4-C3-C5	2.28	119.24	115.29
17	3	308	CLA	CMC-C2C-C1C	2.28	128.47	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	103	CLA	CMB-C2B-C3B	2.28	129.12	124.89
17	4	601	CLA	CMB-C2B-C3B	2.28	129.12	124.89
17	9	612	CLA	CMC-C2C-C1C	2.28	128.47	125.02
17	3	310	CLA	CMC-C2C-C1C	2.28	128.48	125.02
17	a	820	CLA	CMC-C2C-C1C	2.28	128.48	125.02
17	6	305	CLA	C4-C3-C5	2.28	119.25	115.29
17	a	833	CLA	CAC-C3C-C4C	2.28	128.05	124.83
20	A	852	BCR	C29-C30-C25	2.28	114.05	110.48
17	B	823	CLA	C4-C3-C5	2.28	119.25	115.29
17	A	814	CLA	CMC-C2C-C1C	2.28	128.48	125.02
17	b	825	CLA	CHB-C4A-NA	2.28	127.67	124.51
17	b	814	CLA	CAC-C3C-C4C	2.28	128.05	124.83
17	8	303	CLA	CMC-C2C-C1C	2.28	128.49	125.02
17	9	613	CLA	CMC-C2C-C1C	2.28	128.49	125.02
20	b	847	BCR	C2-C1-C6	2.29	114.05	110.48
17	a	817	CLA	CMC-C2C-C1C	2.29	128.49	125.02
17	l	202	CLA	CMC-C2C-C1C	2.29	128.49	125.02
17	b	839	CLA	CMB-C2B-C3B	2.29	129.13	124.89
17	B	831	CLA	CMB-C2B-C3B	2.29	129.13	124.89
17	4	604	CLA	CMC-C2C-C1C	2.29	128.49	125.02
17	9	609	CLA	CMB-C2B-C3B	2.29	129.13	124.89
17	B	806	CLA	CAC-C3C-C4C	2.29	128.06	124.83
20	j	3004	BCR	C38-C26-C27	2.29	117.79	113.45
17	A	805	CLA	C4-C3-C5	2.29	119.26	115.29
17	a	815	CLA	CMB-C2B-C3B	2.29	129.14	124.89
17	a	804	CLA	CAC-C3C-C4C	2.29	128.06	124.83
17	7	611	CLA	CMC-C2C-C1C	2.29	128.49	125.02
20	a	851	BCR	C33-C5-C4	2.29	117.80	113.45
17	6	312	CLA	CMB-C2B-C3B	2.29	129.14	124.89
17	3	306	CLA	CAC-C3C-C4C	2.29	128.06	124.83
17	A	818	CLA	CAC-C3C-C4C	2.29	128.06	124.83
17	B	835	CLA	CAC-C3C-C4C	2.29	128.06	124.83
17	3	312	CLA	CMC-C2C-C1C	2.29	128.50	125.02
17	9	611	CLA	CMB-C2B-C3B	2.29	129.15	124.89
17	b	807	CLA	CMC-C2C-C1C	2.29	128.50	125.02
17	a	801	CLA	CAC-C3C-C4C	2.29	128.06	124.83
17	a	812	CLA	CMB-C2B-C3B	2.29	129.15	124.89
17	a	841	CLA	CMC-C2C-C1C	2.29	128.50	125.02
26	4	606	CHL	C5-C3-C4	2.30	119.96	114.60
26	7	607	CHL	C5-C3-C4	2.30	119.96	114.60
17	l	203	CLA	CAC-C3C-C4C	2.30	128.07	124.83
17	3	303	CLA	CMB-C2B-C3B	2.30	129.15	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	810	CLA	CMB-C2B-C3B	2.30	129.15	124.89
17	3	312	CLA	C4-C3-C5	2.30	119.27	115.29
17	7	604	CLA	CMB-C2B-C3B	2.30	129.16	124.89
17	2	610	CLA	CMB-C2B-C3B	2.30	129.16	124.89
17	1	313	CLA	CMC-C2C-C1C	2.30	128.50	125.02
17	G	103	CLA	CMC-C2C-C1C	2.30	128.50	125.02
17	A	803	CLA	CAC-C3C-C4C	2.30	128.07	124.83
17	b	824	CLA	CMB-C2B-C3B	2.30	129.16	124.89
17	b	810	CLA	CMC-C2C-C1C	2.30	128.51	125.02
17	A	816	CLA	CMC-C2C-C1C	2.30	128.51	125.02
17	L	204	CLA	C5-C3-C4	2.30	119.97	114.60
17	6	316	CLA	CMB-C2B-C3B	2.30	129.16	124.89
17	A	805	CLA	CAC-C3C-C4C	2.30	128.07	124.83
17	b	810	CLA	C4-C3-C5	2.30	119.28	115.29
17	6	309	CLA	CMB-C2B-C3B	2.30	129.16	124.89
28	1	317	XAT	C20-C13-C12	2.30	121.77	118.10
17	b	804	CLA	CAC-C3C-C4C	2.30	128.08	124.83
17	2	602	CLA	CMC-C2C-C1C	2.30	128.51	125.02
17	b	835	CLA	CMC-C2C-C1C	2.30	128.51	125.02
26	1	302	CHL	C1-O2A-CGA	2.31	122.30	116.77
17	b	833	CLA	CMC-C2C-C1C	2.31	128.52	125.02
26	2	605	CHL	CHC-C4B-C3B	2.31	123.69	118.23
28	3	317	XAT	C19-C9-C8	2.31	121.77	118.10
17	2	603	CLA	CMB-C2B-C3B	2.31	129.17	124.89
17	K	4003	CLA	CMB-C2B-C3B	2.31	129.17	124.89
17	8	304	CLA	CMB-C2B-C3B	2.31	129.17	124.89
17	a	835	CLA	CMB-C2B-C3B	2.31	129.18	124.89
17	b	808	CLA	CMB-C2B-C3B	2.31	129.18	124.89
17	A	842	CLA	CMC-C2C-C1C	2.31	128.52	125.02
17	6	306	CLA	CMC-C2C-C1C	2.31	128.52	125.02
17	A	845	CLA	CMB-C2B-C3B	2.31	129.18	124.89
17	a	846	CLA	CMB-C2B-C3B	2.31	129.18	124.89
17	8	304	CLA	CMC-C2C-C1C	2.31	128.52	125.02
17	K	4002	CLA	CMB-C2B-C3B	2.31	129.18	124.89
17	a	802	CLA	CAC-C3C-C4C	2.31	128.09	124.83
17	B	808	CLA	CMB-C2B-C3B	2.31	129.18	124.89
26	2	614	CHL	CHC-C4B-C3B	2.31	123.70	118.23
17	a	816	CLA	C5-C3-C4	2.31	119.99	114.60
17	L	203	CLA	CAC-C3C-C4C	2.31	128.09	124.83
26	4	607	CHL	C5-C3-C4	2.31	119.99	114.60
17	B	832	CLA	CMC-C2C-C1C	2.31	128.53	125.02
26	2	607	CHL	C5-C3-C4	2.31	120.00	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	814	CLA	CMB-C2B-C3B	2.31	129.18	124.89
17	6	313	CLA	CMB-C2B-C3B	2.31	129.18	124.89
17	1	312	CLA	CMB-C2B-C3B	2.31	129.18	124.89
17	2	611	CLA	CMC-C2C-C1C	2.31	128.53	125.02
20	I	101	BCR	C34-C9-C8	2.31	121.78	118.10
17	B	814	CLA	CMB-C2B-C3B	2.31	129.19	124.89
17	3	306	CLA	CMB-C2B-C3B	2.32	129.19	124.89
17	4	613	CLA	CMB-C2B-C3B	2.32	129.19	124.89
17	6	313	CLA	CMC-C2C-C1C	2.32	128.53	125.02
17	A	820	CLA	CMC-C2C-C1C	2.32	128.53	125.02
17	b	825	CLA	CMB-C2B-C3B	2.32	129.19	124.89
17	A	813	CLA	C4-C3-C5	2.32	119.31	115.29
17	6	307	CLA	CMC-C2C-C1C	2.32	128.53	125.02
17	A	841	CLA	CED-O2D-CGD	2.32	121.40	115.97
17	k	1401	CLA	CMC-C2C-C1C	2.32	128.53	125.02
17	1	310	CLA	C4-C3-C5	2.32	119.31	115.29
17	6	314	CLA	C4-C3-C5	2.32	119.31	115.29
17	a	842	CLA	C4-C3-C5	2.32	119.31	115.29
26	1	302	CHL	O2A-CGA-CBA	2.32	118.65	111.90
17	9	614	CLA	CMC-C2C-C1C	2.32	128.54	125.02
17	a	823	CLA	CMB-C2B-C3B	2.32	129.20	124.89
17	b	821	CLA	CMC-C2C-C1C	2.32	128.54	125.02
17	l	204	CLA	C5-C3-C4	2.32	120.02	114.60
17	B	806	CLA	CMB-C2B-C3B	2.32	129.20	124.89
17	B	822	CLA	CMC-C2C-C1C	2.32	128.54	125.02
17	a	823	CLA	CAC-C3C-C4C	2.32	128.10	124.83
17	A	829	CLA	CMC-C2C-C1C	2.32	128.54	125.02
17	b	827	CLA	C4-C3-C5	2.32	119.32	115.29
17	9	602	CLA	CMB-C2B-C3B	2.32	129.20	124.89
17	A	838	CLA	CMB-C2B-C3B	2.32	129.21	124.89
17	j	3002	CLA	CHB-C4A-NA	2.32	127.73	124.51
20	A	850	BCR	C29-C30-C25	2.33	114.11	110.48
17	1	312	CLA	CMC-C2C-C1C	2.33	128.55	125.02
17	b	828	CLA	CMB-C2B-C3B	2.33	129.21	124.89
26	2	606	CHL	C1D-CHD-C4C	2.33	117.33	112.37
17	l	203	CLA	CMB-C2B-C3B	2.33	129.21	124.89
17	a	805	CLA	C4-C3-C5	2.33	119.33	115.29
17	a	803	CLA	CMB-C2B-C3B	2.33	129.22	124.89
26	6	308	CHL	CHC-C4B-C3B	2.33	123.75	118.23
17	b	840	CLA	CMC-C2C-C1C	2.33	128.56	125.02
17	3	311	CLA	CMC-C2C-C1C	2.33	128.56	125.02
17	a	804	CLA	C4-C3-C5	2.33	119.33	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	841	CLA	CMB-C2B-C3B	2.33	129.22	124.89
17	1	308	CLA	CMC-C2C-C1C	2.33	128.56	125.02
17	4	609	CLA	CAC-C3C-C4C	2.33	128.12	124.83
20	1	201	BCR	C29-C30-C25	2.33	114.13	110.48
17	b	839	CLA	CMC-C2C-C1C	2.33	128.56	125.02
17	b	826	CLA	CMC-C2C-C1C	2.34	128.56	125.02
17	4	611	CLA	CMB-C2B-C3B	2.34	129.23	124.89
17	a	805	CLA	CAC-C3C-C4C	2.34	128.12	124.83
17	b	811	CLA	CAC-C3C-C4C	2.34	128.13	124.83
17	a	803	CLA	CMC-C2C-C1C	2.34	128.57	125.02
17	1	314	CLA	CMC-C2C-C1C	2.34	128.57	125.02
17	7	613	CLA	CMC-C2C-C1C	2.34	128.57	125.02
17	2	609	CLA	C4-C3-C5	2.34	119.35	115.29
17	a	815	CLA	CAC-C3C-C4C	2.34	128.13	124.83
17	B	808	CLA	CMC-C2C-C1C	2.34	128.57	125.02
17	1	315	CLA	CMB-C2B-C3B	2.34	129.23	124.89
17	6	307	CLA	CMB-C2B-C3B	2.34	129.23	124.89
17	B	814	CLA	CHB-C4A-NA	2.34	127.75	124.51
17	1	305	CLA	CMB-C2B-C3B	2.34	129.24	124.89
17	B	806	CLA	C4-C3-C5	2.34	119.35	115.29
17	8	310	CLA	CMC-C2C-C1C	2.34	128.57	125.02
17	A	823	CLA	CMC-C2C-C1C	2.34	128.57	125.02
26	2	601	CHL	O2A-CGA-CBA	2.34	118.72	111.90
17	a	825	CLA	CAC-C3C-C4C	2.34	128.13	124.83
17	A	832	CLA	CMC-C2C-C1C	2.34	128.57	125.02
17	4	612	CLA	C4-C3-C5	2.34	119.36	115.29
17	1	305	CLA	CMC-C2C-C1C	2.34	128.57	125.02
17	8	308	CLA	CMB-C2B-C3B	2.34	129.24	124.89
26	9	607	CHL	C5-C3-C4	2.35	120.07	114.60
17	B	805	CLA	CHB-C4A-NA	2.35	127.75	124.51
17	a	824	CLA	CAC-C3C-C4C	2.35	128.14	124.83
17	b	829	CLA	CMC-C2C-C1C	2.35	128.58	125.02
17	6	314	CLA	CMC-C2C-C1C	2.35	128.58	125.02
17	a	846	CLA	CAC-C3C-C4C	2.35	128.14	124.83
17	2	613	CLA	CMC-C2C-C1C	2.35	128.58	125.02
20	1	318	BCR	C37-C22-C23	2.35	121.84	118.10
17	8	310	CLA	C4-C3-C5	2.35	119.36	115.29
17	7	612	CLA	CMC-C2C-C1C	2.35	128.58	125.02
17	a	842	CLA	CMB-C2B-C3B	2.35	129.25	124.89
20	A	856	BCR	C29-C30-C25	2.35	114.15	110.48
20	4	618	BCR	C29-C30-C25	2.35	114.15	110.48
20	b	848	BCR	C29-C30-C25	2.35	114.15	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	825	CLA	C4-C3-C5	2.35	119.36	115.29
17	b	811	CLA	CMC-C2C-C1C	2.35	128.58	125.02
17	B	826	CLA	CMB-C2B-C3B	2.35	129.25	124.89
20	g	104	BCR	C2-C1-C6	2.35	114.15	110.48
17	A	839	CLA	CMC-C2C-C1C	2.35	128.59	125.02
17	F	304	CLA	C4-C3-C5	2.35	119.37	115.29
17	B	836	CLA	C4-C3-C5	2.35	119.37	115.29
17	A	824	CLA	CMB-C2B-C3B	2.35	129.26	124.89
20	3	318	BCR	C29-C30-C25	2.35	114.16	110.48
17	k	1401	CLA	CAC-C3C-C4C	2.35	128.15	124.83
17	a	825	CLA	CMC-C2C-C1C	2.35	128.59	125.02
17	a	822	CLA	CMB-C2B-C3B	2.35	129.26	124.89
17	a	832	CLA	CMB-C2B-C3B	2.35	129.26	124.89
17	B	804	CLA	CMB-C2B-C3B	2.36	129.26	124.89
17	8	312	CLA	CMB-C2B-C3B	2.36	129.26	124.89
17	2	603	CLA	CMC-C2C-C1C	2.36	128.59	125.02
17	1	309	CLA	CMB-C2B-C3B	2.36	129.26	124.89
17	L	203	CLA	CMB-C2B-C3B	2.36	129.26	124.89
27	9	616	LUT	C18-C5-C4	2.36	118.63	114.33
17	B	814	CLA	CAC-C3C-C4C	2.36	128.15	124.83
17	B	810	CLA	CMB-C2B-C3B	2.36	129.27	124.89
17	a	822	CLA	C4-C3-C5	2.36	119.38	115.29
17	L	204	CLA	CMB-C2B-C3B	2.36	129.27	124.89
17	B	803	CLA	C4-C3-C5	2.36	119.38	115.29
17	7	613	CLA	CMB-C2B-C3B	2.36	129.27	124.89
17	g	102	CLA	CMC-C2C-C1C	2.36	128.60	125.02
17	a	827	CLA	CAC-C3C-C4C	2.36	128.16	124.83
17	1	306	CLA	C4-C3-C5	2.36	119.39	115.29
17	b	820	CLA	CMC-C2C-C1C	2.36	128.60	125.02
26	1	307	CHL	C1D-CHD-C4C	2.36	117.41	112.37
17	a	802	CLA	C1-O2A-CGA	2.36	122.44	116.77
17	a	814	CLA	CHB-C4A-NA	2.36	127.78	124.51
17	g	103	CLA	CMB-C2B-C3B	2.36	129.28	124.89
17	4	610	CLA	CMB-C2B-C3B	2.36	129.28	124.89
17	9	610	CLA	CMB-C2B-C3B	2.37	129.28	124.89
17	1	314	CLA	CMB-C2B-C3B	2.37	129.28	124.89
17	B	827	CLA	C4-C3-C5	2.37	119.39	115.29
17	B	833	CLA	CAC-C3C-C4C	2.37	128.17	124.83
17	a	842	CLA	CAC-C3C-C4C	2.37	128.17	124.83
17	4	602	CLA	C4-C3-C5	2.37	119.40	115.29
20	B	845	BCR	C33-C5-C4	2.37	117.94	113.45
17	A	821	CLA	CMB-C2B-C3B	2.37	129.29	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	614	CLA	CMB-C2B-C3B	2.37	129.29	124.89
17	6	309	CLA	CMC-C2C-C1C	2.37	128.61	125.02
17	B	837	CLA	CMC-C2C-C1C	2.37	128.61	125.02
17	8	305	CLA	CMB-C2B-C3B	2.37	129.29	124.89
17	A	833	CLA	CAC-C3C-C4C	2.37	128.17	124.83
17	a	840	CLA	CMC-C2C-C1C	2.37	128.61	125.02
17	b	808	CLA	CMC-C2C-C1C	2.37	128.61	125.02
17	B	821	CLA	CMB-C2B-C3B	2.37	129.29	124.89
17	B	811	CLA	CAC-C3C-C4C	2.37	128.18	124.83
28	6	318	XAT	C19-C9-C8	2.37	121.88	118.10
17	9	612	CLA	CMB-C2B-C3B	2.37	129.30	124.89
17	a	813	CLA	C4-C3-C5	2.37	119.41	115.29
17	b	817	CLA	CMC-C2C-C1C	2.37	128.62	125.02
17	7	603	CLA	CMB-C2B-C3B	2.37	129.30	124.89
17	3	310	CLA	CMB-C2B-C3B	2.38	129.30	124.89
17	a	836	CLA	CMC-C2C-C1C	2.38	128.62	125.02
26	7	606	CHL	C1D-CHD-C4C	2.38	117.44	112.37
28	7	616	XAT	C19-C9-C8	2.38	121.89	118.10
17	b	806	CLA	CAC-C3C-C4C	2.38	128.18	124.83
17	A	833	CLA	CMB-C2B-C3B	2.38	129.30	124.89
27	1	316	LUT	C18-C5-C4	2.38	118.67	114.33
20	B	845	BCR	C2-C1-C6	2.38	114.20	110.48
17	b	840	CLA	C4-C3-C5	2.38	119.42	115.29
17	A	806	CLA	CMC-C2C-C1C	2.38	128.63	125.02
26	4	605	CHL	C1-O2A-CGA	2.38	122.48	116.77
17	A	854	CLA	CMC-C2C-C1C	2.38	128.63	125.02
17	6	312	CLA	CMC-C2C-C1C	2.38	128.63	125.02
17	7	608	CLA	CAC-C3C-C4C	2.38	128.19	124.83
17	A	801	CLA	C4-C3-C5	2.38	119.42	115.29
17	7	612	CLA	C4-C3-C5	2.38	119.42	115.29
23	B	849	LMT	C1B-C2B-C3B	2.38	114.40	109.98
17	A	809	CLA	CMB-C2B-C3B	2.38	129.31	124.89
17	a	812	CLA	CMC-C2C-C1C	2.38	128.63	125.02
17	K	4002	CLA	CMC-C2C-C1C	2.38	128.63	125.02
20	8	316	BCR	C29-C30-C25	2.38	114.20	110.48
26	1	302	CHL	CHC-C4B-C3B	2.38	123.88	118.23
17	a	838	CLA	CAC-C3C-C4C	2.38	128.19	124.83
17	J	3002	CLA	CMB-C2B-C3B	2.38	129.32	124.89
17	6	305	CLA	CMC-C2C-C1C	2.38	128.64	125.02
17	A	810	CLA	CMC-C2C-C1C	2.38	128.64	125.02
20	L	205	BCR	C38-C26-C27	2.38	117.98	113.45
17	7	608	CLA	CHB-C4A-NA	2.39	127.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	318	XAT	C38-C25-C24	2.39	117.01	114.28
17	B	815	CLA	C4-C3-C5	2.39	119.43	115.29
17	4	601	CLA	CMC-C2C-C1C	2.39	128.64	125.02
17	B	809	CLA	CAC-C3C-C4C	2.39	128.20	124.83
17	B	828	CLA	CAC-C3C-C4C	2.39	128.20	124.83
17	3	303	CLA	CMC-C2C-C1C	2.39	128.64	125.02
17	a	839	CLA	CMC-C2C-C1C	2.39	128.64	125.02
17	A	818	CLA	CMC-C2C-C1C	2.39	128.64	125.02
17	B	825	CLA	CMB-C2B-C3B	2.39	129.33	124.89
17	2	608	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	4	607	CHL	C1D-CHD-C4C	2.39	117.47	112.37
17	A	827	CLA	CAC-C3C-C4C	2.39	128.20	124.83
17	B	812	CLA	CMB-C2B-C3B	2.39	129.33	124.89
17	9	604	CLA	CAC-C3C-C4C	2.39	128.21	124.83
17	b	832	CLA	CMC-C2C-C1C	2.39	128.65	125.02
27	1	320	LUT	C18-C5-C4	2.39	118.70	114.33
17	6	311	CLA	C4-C3-C5	2.39	119.44	115.29
17	A	813	CLA	CMC-C2C-C1C	2.39	128.65	125.02
17	F	304	CLA	CMC-C2C-C1C	2.39	128.65	125.02
17	F	301	CLA	C4-C3-C5	2.40	119.44	115.29
17	6	315	CLA	CMB-C2B-C3B	2.40	129.34	124.89
17	2	611	CLA	CMB-C2B-C3B	2.40	129.34	124.89
18	A	844	PQN	C2M-C2-C1	2.40	120.25	116.23
17	8	305	CLA	CAC-C3C-C4C	2.40	128.21	124.83
17	L	204	CLA	CAC-C3C-C4C	2.40	128.21	124.83
17	3	309	CLA	CMB-C2B-C3B	2.40	129.34	124.89
26	9	606	CHL	C1D-CHD-C4C	2.40	117.49	112.37
17	9	613	CLA	CMB-C2B-C3B	2.40	129.34	124.89
17	b	829	CLA	C4-C3-C5	2.40	119.45	115.29
17	A	820	CLA	CMB-C2B-C3B	2.40	129.35	124.89
17	9	608	CLA	CAC-C3C-C4C	2.40	128.22	124.83
17	b	825	CLA	CMC-C2C-C1C	2.40	128.66	125.02
20	g	104	BCR	C38-C26-C27	2.40	118.01	113.45
17	g	102	CLA	CMB-C2B-C3B	2.40	129.35	124.89
17	b	809	CLA	CMC-C2C-C1C	2.41	128.67	125.02
17	7	608	CLA	CMB-C2B-C3B	2.41	129.35	124.89
17	2	602	CLA	CMB-C2B-C3B	2.41	129.35	124.89
17	6	312	CLA	CAC-C3C-C4C	2.41	128.22	124.83
17	B	826	CLA	CMC-C2C-C1C	2.41	128.67	125.02
17	1	309	CLA	C4-C3-C5	2.41	119.46	115.29
17	8	302	CLA	CMC-C2C-C1C	2.41	128.67	125.02
17	a	839	CLA	CAC-C3C-C4C	2.41	128.23	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	814	CLA	C4-C3-C5	2.41	119.47	115.29
17	8	302	CLA	CMB-C2B-C3B	2.41	129.36	124.89
17	8	307	CLA	CMB-C2B-C3B	2.41	129.36	124.89
17	B	803	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	K	4001	BCR	C29-C30-C25	2.41	114.25	110.48
17	4	602	CLA	CMC-C2C-C1C	2.41	128.68	125.02
17	A	819	CLA	CMC-C2C-C1C	2.41	128.68	125.02
20	9	618	BCR	C37-C22-C23	2.41	121.94	118.10
17	1	303	CLA	CMC-C2C-C1C	2.41	128.68	125.02
17	3	311	CLA	CMB-C2B-C3B	2.41	129.37	124.89
20	b	801	BCR	C35-C13-C12	2.41	121.94	118.10
17	B	830	CLA	CMB-C2B-C3B	2.41	129.37	124.89
17	4	608	CLA	CMB-C2B-C3B	2.41	129.37	124.89
27	4	616	LUT	C18-C5-C4	2.41	118.74	114.33
17	b	820	CLA	CAC-C3C-C4C	2.41	128.24	124.83
17	b	821	CLA	CMB-C2B-C3B	2.41	129.37	124.89
17	4	609	CLA	CMB-C2B-C3B	2.41	129.37	124.89
17	1	311	CLA	CMB-C2B-C3B	2.41	129.37	124.89
17	A	828	CLA	CMC-C2C-C1C	2.41	128.68	125.02
17	B	819	CLA	CMB-C2B-C3B	2.42	129.38	124.89
17	A	806	CLA	C1-O2A-CGA	2.42	122.57	116.77
17	b	816	CLA	CMC-C2C-C1C	2.42	128.69	125.02
17	8	301	CLA	CMB-C2B-C3B	2.42	129.38	124.89
17	9	610	CLA	CMC-C2C-C1C	2.42	128.69	125.02
26	7	605	CHL	CHC-C4B-C3B	2.42	123.96	118.23
17	8	309	CLA	CMB-C2B-C3B	2.42	129.38	124.89
17	a	822	CLA	CAC-C3C-C4C	2.42	128.24	124.83
20	a	854	BCR	C8-C9-C10	2.42	122.65	118.94
17	A	815	CLA	CMC-C2C-C1C	2.42	128.69	125.02
20	A	856	BCR	C2-C1-C6	2.42	114.26	110.48
17	A	827	CLA	CMB-C2B-C3B	2.42	129.38	124.89
17	a	809	CLA	CMC-C2C-C1C	2.42	128.69	125.02
20	G	105	BCR	C29-C30-C25	2.42	114.26	110.48
17	4	601	CLA	CAC-C3C-C4C	2.42	128.25	124.83
17	b	803	CLA	O2D-CGD-CBD	2.42	115.63	111.30
17	6	310	CLA	CMC-C2C-C1C	2.42	128.69	125.02
17	A	815	CLA	CAC-C3C-C4C	2.42	128.25	124.83
17	A	829	CLA	CAC-C3C-C4C	2.42	128.25	124.83
20	L	205	BCR	C29-C30-C25	2.42	114.27	110.48
17	a	819	CLA	CMB-C2B-C3B	2.42	129.39	124.89
17	b	811	CLA	C4-C3-C5	2.42	119.49	115.29
20	B	846	BCR	C38-C26-C27	2.42	118.05	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	819	CLA	C4-C3-C5	2.42	119.50	115.29
17	A	823	CLA	CMB-C2B-C3B	2.42	129.39	124.89
17	b	823	CLA	CMB-C2B-C3B	2.42	129.39	124.89
26	7	607	CHL	C1D-CHD-C4C	2.43	117.54	112.37
17	b	814	CLA	CMC-C2C-C1C	2.43	128.70	125.02
17	A	801	CLA	CAC-C3C-C4C	2.43	128.25	124.83
20	A	852	BCR	C8-C9-C10	2.43	122.67	118.94
26	1	302	CHL	C1D-CHD-C4C	2.43	117.55	112.37
17	G	101	CLA	CAC-C3C-C4C	2.43	128.25	124.83
20	L	201	BCR	C8-C9-C10	2.43	122.67	118.94
17	B	839	CLA	CMC-C2C-C1C	2.43	128.70	125.02
17	3	301	CLA	CMC-C2C-C1C	2.43	128.70	125.02
17	a	822	CLA	O2A-CGA-CBA	2.43	118.97	111.90
17	7	610	CLA	CMB-C2B-C3B	2.43	129.40	124.89
17	A	822	CLA	CMB-C2B-C3B	2.43	129.40	124.89
17	B	818	CLA	CMB-C2B-C3B	2.43	129.40	124.89
20	6	319	BCR	C29-C30-C25	2.43	114.28	110.48
17	a	814	CLA	O2A-CGA-CBA	2.43	118.97	111.90
17	8	311	CLA	CMB-C2B-C3B	2.43	129.41	124.89
17	1	310	CLA	CMB-C2B-C3B	2.43	129.41	124.89
17	6	304	CLA	CMC-C2C-C1C	2.43	128.71	125.02
20	b	847	BCR	C33-C5-C4	2.43	118.07	113.45
17	1	305	CLA	C4-C3-C5	2.43	119.51	115.29
26	6	308	CHL	C1D-CHD-C4C	2.43	117.56	112.37
17	1	311	CLA	CAC-C3C-C4C	2.44	128.27	124.83
17	A	801	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	b	815	CLA	CMC-C2C-C1C	2.44	128.72	125.02
17	B	814	CLA	CMC-C2C-C1C	2.44	128.72	125.02
17	b	809	CLA	C4-C3-C5	2.44	119.52	115.29
17	a	807	CLA	CAC-C3C-C4C	2.44	128.27	124.83
17	B	806	CLA	CMC-C2C-C1C	2.44	128.72	125.02
17	B	813	CLA	CMC-C2C-C1C	2.44	128.72	125.02
17	f	7003	CLA	CMB-C2B-C3B	2.44	129.42	124.89
17	1	303	CLA	C4-C3-C5	2.44	119.52	115.29
17	G	104	CLA	CMC-C2C-C1C	2.44	128.72	125.02
17	B	812	CLA	CMC-C2C-C1C	2.44	128.72	125.02
17	A	821	CLA	CAC-C3C-C4C	2.44	128.27	124.83
17	3	314	CLA	CMC-C2C-C1C	2.44	128.72	125.02
20	a	852	BCR	C33-C5-C4	2.44	118.09	113.45
17	4	609	CLA	C4-C3-C5	2.44	119.53	115.29
17	b	803	CLA	CHB-C4A-NA	2.44	127.89	124.51
28	6	318	XAT	C18-C5-C4	2.44	117.08	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	l	202	CLA	O2A-CGA-CBA	2.44	119.01	111.90
17	A	812	CLA	CMC-C2C-C1C	2.45	128.73	125.02
17	2	608	CLA	CAC-C3C-C4C	2.45	128.28	124.83
17	a	843	CLA	CMC-C2C-C1C	2.45	128.73	125.02
26	7	601	CHL	C1D-CHD-C4C	2.45	117.59	112.37
17	6	304	CLA	C4-C3-C5	2.45	119.54	115.29
17	b	813	CLA	CMC-C2C-C1C	2.45	128.73	125.02
17	F	301	CLA	CMB-C2B-C3B	2.45	129.44	124.89
17	b	802	CLA	CAC-C3C-C4C	2.45	128.29	124.83
17	a	815	CLA	CMC-C2C-C1C	2.45	128.74	125.02
17	a	801	CLA	C4-C3-C5	2.45	119.54	115.29
17	6	311	CLA	CMB-C2B-C3B	2.45	129.44	124.89
17	6	316	CLA	CMC-C2C-C1C	2.45	128.74	125.02
17	B	803	CLA	CMC-C2C-C1C	2.45	128.74	125.02
17	9	609	CLA	C4-C3-C5	2.45	119.55	115.29
17	b	830	CLA	CMC-C2C-C1C	2.45	128.74	125.02
17	A	845	CLA	CAC-C3C-C4C	2.45	128.29	124.83
17	b	812	CLA	CMB-C2B-C3B	2.45	129.45	124.89
17	a	828	CLA	C4-C3-C5	2.46	119.55	115.29
17	b	839	CLA	CAC-C3C-C4C	2.46	128.29	124.83
17	3	308	CLA	CMB-C2B-C3B	2.46	129.45	124.89
17	a	803	CLA	C4-C3-C5	2.46	119.55	115.29
28	8	315	XAT	C18-C5-C4	2.46	117.09	114.28
17	A	804	CLA	C4-C3-C5	2.46	119.55	115.29
17	F	304	CLA	C1-O2A-CGA	2.46	122.67	116.77
26	2	601	CHL	CHC-C4B-C3B	2.46	124.06	118.23
17	A	807	CLA	CAC-C3C-C4C	2.46	128.30	124.83
26	3	307	CHL	C1D-CHD-C4C	2.46	117.62	112.37
17	l	204	CLA	CAC-C3C-C4C	2.46	128.30	124.83
17	F	303	CLA	CMC-C2C-C1C	2.46	128.75	125.02
17	B	805	CLA	CAC-C3C-C4C	2.46	128.30	124.83
28	1	317	XAT	C18-C5-C4	2.46	117.10	114.28
17	3	314	CLA	CMB-C2B-C3B	2.46	129.47	124.89
17	6	304	CLA	CMB-C2B-C3B	2.46	129.47	124.89
17	B	815	CLA	CMC-C2C-C1C	2.46	128.76	125.02
17	4	609	CLA	CMC-C2C-C1C	2.47	128.76	125.02
17	a	833	CLA	CMB-C2B-C3B	2.47	129.47	124.89
27	6	317	LUT	C18-C5-C4	2.47	118.84	114.33
17	2	602	CLA	C4-C3-C5	2.47	119.57	115.29
17	A	827	CLA	O2A-CGA-CBA	2.47	119.09	111.90
17	a	830	CLA	C4-C3-C5	2.47	119.58	115.29
17	b	822	CLA	CMC-C2C-C1C	2.47	128.77	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	818	CLA	CAC-C3C-C4C	2.47	128.32	124.83
26	7	605	CHL	C1D-CHD-C4C	2.47	117.64	112.37
17	B	828	CLA	CMC-C2C-C1C	2.47	128.77	125.02
17	9	602	CLA	C4-C3-C5	2.47	119.58	115.29
20	J	3003	BCR	C38-C26-C27	2.47	118.15	113.45
17	a	856	CLA	C4-C3-C5	2.47	119.58	115.29
17	b	808	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	G	101	CLA	CMC-C2C-C1C	2.48	128.78	125.02
17	l	202	CLA	CAC-C3C-C4C	2.48	128.32	124.83
17	g	101	CLA	CAC-C3C-C4C	2.48	128.32	124.83
28	2	616	XAT	C19-C9-C8	2.48	122.05	118.10
17	A	801	CLA	CMC-C2C-C1C	2.48	128.78	125.02
17	a	816	CLA	CMC-C2C-C1C	2.48	128.78	125.02
17	B	837	CLA	C4-C3-C5	2.48	119.59	115.29
20	1	318	BCR	C29-C30-C25	2.48	114.35	110.48
17	A	804	CLA	CAC-C3C-C4C	2.48	128.33	124.83
26	2	607	CHL	C1D-CHD-C4C	2.48	117.66	112.37
17	B	803	CLA	C3B-C4B-NB	2.48	112.42	109.21
17	a	812	CLA	CAC-C3C-C4C	2.48	128.33	124.83
17	B	836	CLA	CMC-C2C-C1C	2.48	128.78	125.02
17	A	806	CLA	CMB-C2B-C3B	2.48	129.50	124.89
17	A	829	CLA	C4-C3-C5	2.48	119.60	115.29
17	b	827	CLA	CAC-C3C-C4C	2.48	128.33	124.83
26	4	606	CHL	C1D-CHD-C4C	2.48	117.67	112.37
17	A	816	CLA	CAC-C3C-C4C	2.49	128.34	124.83
17	a	825	CLA	C4-C3-C5	2.49	119.60	115.29
17	a	831	CLA	CMC-C2C-C1C	2.49	128.79	125.02
17	a	836	CLA	CAC-C3C-C4C	2.49	128.34	124.83
17	B	823	CLA	CAC-C3C-C4C	2.49	128.34	124.83
17	b	814	CLA	C4-C3-C5	2.49	119.61	115.29
17	3	301	CLA	CMB-C2B-C3B	2.49	129.51	124.89
17	a	805	CLA	CMC-C2C-C1C	2.49	128.80	125.02
20	B	843	BCR	C29-C30-C25	2.49	114.37	110.48
17	L	203	CLA	CMC-C2C-C1C	2.49	128.80	125.02
17	8	312	CLA	CAC-C3C-C4C	2.49	128.34	124.83
17	4	602	CLA	CMB-C2B-C3B	2.49	129.52	124.89
17	A	819	CLA	C4-C3-C5	2.49	119.61	115.29
17	3	302	CLA	CMB-C2B-C3B	2.49	129.52	124.89
17	A	820	CLA	CAC-C3C-C4C	2.49	128.35	124.83
17	A	842	CLA	CMB-C2B-C3B	2.49	129.52	124.89
17	B	814	CLA	C4-C3-C5	2.50	119.62	115.29
17	8	301	CLA	C4-C3-C5	2.50	119.62	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	205	BCR	C2-C1-C6	2.50	114.38	110.48
17	1	315	CLA	CMC-C2C-C1C	2.50	128.81	125.02
26	9	615	CHL	C1D-CHD-C4C	2.50	117.70	112.37
17	b	808	CLA	CAC-C3C-C4C	2.50	128.35	124.83
17	9	610	CLA	CAC-C3C-C4C	2.50	128.35	124.83
17	A	832	CLA	CMB-C2B-C3B	2.50	129.53	124.89
17	A	841	CLA	CMB-C2B-C3B	2.50	129.53	124.89
26	6	303	CHL	O2A-CGA-CBA	2.50	119.18	111.90
17	f	7003	CLA	CMC-C2C-C1C	2.50	128.81	125.02
17	a	802	CLA	CGD-CBD-CAD	2.50	119.10	110.71
17	A	821	CLA	CMC-C2C-C1C	2.50	128.82	125.02
17	B	807	CLA	CMB-C2B-C3B	2.50	129.54	124.89
17	B	810	CLA	CMC-C2C-C1C	2.50	128.82	125.02
17	3	302	CLA	CMC-C2C-C1C	2.51	128.82	125.02
20	j	3004	BCR	C2-C1-C6	2.51	114.40	110.48
17	F	303	CLA	CAC-C3C-C4C	2.51	128.37	124.83
17	B	816	CLA	CMB-C2B-C3B	2.51	129.55	124.89
26	8	306	CHL	C1D-CHD-C4C	2.51	117.72	112.37
17	a	823	CLA	CMC-C2C-C1C	2.51	128.82	125.02
17	A	809	CLA	C4-C3-C5	2.51	119.64	115.29
20	3	318	BCR	C38-C26-C27	2.51	118.21	113.45
17	a	834	CLA	CAC-C3C-C4C	2.51	128.37	124.83
17	L	202	CLA	CAC-C3C-C4C	2.51	128.37	124.83
17	a	801	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	B	820	CLA	CAC-C3C-C4C	2.51	128.37	124.83
17	B	807	CLA	CMC-C2C-C1C	2.51	128.83	125.02
17	B	824	CLA	O2A-CGA-CBA	2.51	119.21	111.90
17	j	3002	CLA	CMB-C2B-C3B	2.51	129.56	124.89
17	A	825	CLA	C4-C3-C5	2.51	119.65	115.29
20	G	105	BCR	C2-C1-C6	2.51	114.41	110.48
17	A	819	CLA	CMB-C2B-C3B	2.51	129.56	124.89
17	6	315	CLA	C4-C3-C5	2.51	119.65	115.29
17	A	817	CLA	CAC-C3C-C4C	2.51	128.38	124.83
26	7	614	CHL	C1D-CHD-C4C	2.52	117.73	112.37
17	2	609	CLA	CMB-C2B-C3B	2.52	129.56	124.89
17	b	811	CLA	CAB-C3B-C2B	2.52	129.75	124.92
17	b	819	CLA	C4-C3-C5	2.52	119.66	115.29
17	4	614	CLA	CAC-C3C-C4C	2.52	128.38	124.83
17	b	837	CLA	C4-C3-C5	2.52	119.66	115.29
17	a	802	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	a	829	CLA	C4-C3-C5	2.52	119.66	115.29
17	A	807	CLA	CMC-C2C-C1C	2.52	128.84	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	803	CLA	C3B-C4B-NB	2.52	112.47	109.21
17	B	811	CLA	CAB-C3B-C2B	2.52	129.76	124.92
17	a	831	CLA	C4-C3-C5	2.52	119.66	115.29
17	B	813	CLA	C4-C3-C5	2.52	119.66	115.29
26	4	605	CHL	C1D-CHD-C4C	2.52	117.75	112.37
17	a	826	CLA	CAC-C3C-C4C	2.52	128.39	124.83
17	a	837	CLA	CMC-C2C-C1C	2.52	128.85	125.02
17	9	608	CLA	CMB-C2B-C3B	2.52	129.57	124.89
17	b	832	CLA	C4-C3-C5	2.53	119.67	115.29
17	a	846	CLA	C4-C3-C5	2.53	119.67	115.29
17	A	843	CLA	C4-C3-C5	2.53	119.67	115.29
17	a	842	CLA	CMC-C2C-C1C	2.53	128.85	125.02
17	b	822	CLA	CMB-C2B-C3B	2.53	129.59	124.89
17	B	818	CLA	CMC-C2C-C1C	2.53	128.85	125.02
17	A	834	CLA	CAC-C3C-C4C	2.53	128.40	124.83
26	4	615	CHL	C1D-CHD-C4C	2.53	117.77	112.37
17	A	840	CLA	CMC-C2C-C1C	2.53	128.86	125.02
17	B	839	CLA	CMB-C2B-C3B	2.53	129.59	124.89
17	7	604	CLA	C4-C3-C5	2.53	119.68	115.29
26	2	601	CHL	C1D-CHD-C4C	2.53	117.77	112.37
17	4	608	CLA	O2A-CGA-CBA	2.53	119.27	111.90
17	b	835	CLA	CAC-C3C-C4C	2.53	128.41	124.83
17	4	610	CLA	C4-C3-C5	2.54	119.69	115.29
17	A	803	CLA	CMC-C2C-C1C	2.54	128.87	125.02
17	g	101	CLA	CMC-C2C-C1C	2.54	128.87	125.02
17	6	311	CLA	CMC-C2C-C1C	2.54	128.87	125.02
17	4	612	CLA	CAC-C3C-C4C	2.54	128.41	124.83
17	b	826	CLA	CAC-C3C-C4C	2.54	128.41	124.83
17	K	4003	CLA	CAC-C3C-C4C	2.54	128.41	124.83
26	6	303	CHL	C1D-CHD-C4C	2.54	117.79	112.37
17	B	824	CLA	CMC-C2C-C1C	2.54	128.88	125.02
17	L	202	CLA	C4-C3-C5	2.55	119.70	115.29
17	b	841	CLA	C4-C3-C5	2.55	119.71	115.29
17	A	840	CLA	CAC-C3C-C4C	2.55	128.42	124.83
17	b	811	CLA	O2A-CGA-CBA	2.55	119.31	111.90
17	b	828	CLA	CMC-C2C-C1C	2.55	128.89	125.02
17	B	827	CLA	CMC-C2C-C1C	2.55	128.89	125.02
17	9	611	CLA	CAC-C3C-C4C	2.55	128.43	124.83
26	2	614	CHL	C1D-CHD-C4C	2.55	117.81	112.37
17	1	309	CLA	CAC-C3C-C4C	2.55	128.43	124.83
17	a	816	CLA	CAC-C3C-C4C	2.56	128.43	124.83
17	3	309	CLA	CMC-C2C-C1C	2.56	128.90	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	808	CLA	CAC-C3C-C4C	2.56	128.44	124.83
17	b	803	CLA	CAC-C3C-C4C	2.56	128.44	124.83
28	8	315	XAT	C19-C9-C8	2.56	122.17	118.10
17	A	802	CLA	CMC-C2C-C1C	2.56	128.90	125.02
17	B	803	CLA	CMB-C2B-C3B	2.56	129.64	124.89
28	9	617	XAT	C38-C25-C24	2.56	117.21	114.28
17	b	822	CLA	C4-C3-C5	2.56	119.73	115.29
17	A	812	CLA	C4-C3-C5	2.56	119.73	115.29
20	a	850	BCR	C33-C5-C4	2.56	118.31	113.45
17	b	831	CLA	CAC-C3C-C4C	2.56	128.44	124.83
17	b	803	CLA	CMB-C2B-C3B	2.56	129.64	124.89
17	7	610	CLA	CAC-C3C-C4C	2.56	128.44	124.83
17	B	841	CLA	CAC-C3C-C4C	2.56	128.44	124.83
17	A	818	CLA	C4-C3-C5	2.56	119.73	115.29
17	1	310	CLA	CMC-C2C-C1C	2.56	128.91	125.02
17	l	203	CLA	CMC-C2C-C1C	2.57	128.91	125.02
17	b	813	CLA	C4-C3-C5	2.57	119.74	115.29
17	8	309	CLA	C4-C3-C5	2.57	119.74	115.29
26	7	601	CHL	O2A-CGA-CBA	2.57	119.37	111.90
26	6	303	CHL	C4-C3-C5	2.57	119.75	115.29
17	B	825	CLA	C4-C3-C5	2.57	119.75	115.29
17	3	304	CLA	CAC-C3C-C4C	2.57	128.45	124.83
17	2	604	CLA	C4-C3-C5	2.57	119.75	115.29
20	B	845	BCR	C23-C22-C21	2.57	122.89	118.94
17	A	845	CLA	C4-C3-C5	2.57	119.75	115.29
17	B	816	CLA	CMC-C2C-C1C	2.57	128.92	125.02
26	2	605	CHL	C1D-CHD-C4C	2.57	117.86	112.37
20	6	319	BCR	C38-C26-C27	2.57	118.33	113.45
17	A	839	CLA	C4-C3-C5	2.57	119.75	115.29
17	a	813	CLA	CMB-C2B-C3B	2.57	129.67	124.89
20	8	316	BCR	C38-C26-C27	2.58	118.34	113.45
17	a	812	CLA	C4-C3-C5	2.58	119.76	115.29
17	a	839	CLA	C4-C3-C5	2.58	119.76	115.29
17	A	854	CLA	C4-C3-C5	2.58	119.76	115.29
17	8	308	CLA	CMC-C2C-C1C	2.58	128.93	125.02
17	a	818	CLA	CAC-C3C-C4C	2.58	128.47	124.83
17	b	838	CLA	CMC-C2C-C1C	2.58	128.93	125.02
17	A	843	CLA	CMC-C2C-C1C	2.58	128.93	125.02
17	F	304	CLA	CAC-C3C-C4C	2.58	128.47	124.83
17	B	811	CLA	O2A-CGA-CBA	2.58	119.41	111.90
17	A	804	CLA	CMC-C2C-C1C	2.58	128.93	125.02
17	a	801	CLA	CMC-C2C-C1C	2.58	128.93	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	308	CLA	CAC-C3C-C4C	2.58	128.47	124.83
20	1	318	BCR	C38-C26-C27	2.58	118.35	113.45
17	a	811	CLA	C4-C3-C5	2.58	119.77	115.29
20	A	850	BCR	C33-C5-C4	2.58	118.35	113.45
17	b	825	CLA	CAC-C3C-C4C	2.58	128.47	124.83
17	4	611	CLA	CAC-C3C-C4C	2.58	128.47	124.83
17	A	808	CLA	CAC-C3C-C4C	2.58	128.47	124.83
17	A	830	CLA	C4-C3-C5	2.58	119.77	115.29
17	A	805	CLA	CMC-C2C-C1C	2.59	128.94	125.02
18	b	842	PQN	C14-C13-C15	2.59	119.78	115.29
17	a	835	CLA	C4-C3-C5	2.59	119.78	115.29
20	j	3004	BCR	C33-C5-C4	2.59	118.36	113.45
17	A	808	CLA	O2A-CGA-CBA	2.59	119.43	111.90
17	B	821	CLA	CMC-C2C-C1C	2.59	128.95	125.02
17	a	810	CLA	CAC-C3C-C4C	2.59	128.48	124.83
17	B	815	CLA	CAC-C3C-C4C	2.59	128.49	124.83
17	A	804	CLA	O2A-CGA-CBA	2.59	119.45	111.90
17	2	611	CLA	CAC-C3C-C4C	2.60	128.49	124.83
17	4	610	CLA	CMC-C2C-C1C	2.60	128.96	125.02
17	6	311	CLA	CAC-C3C-C4C	2.60	128.49	124.83
17	K	4002	CLA	CAC-C3C-C4C	2.60	128.49	124.83
17	8	312	CLA	CMC-C2C-C1C	2.60	128.96	125.02
17	A	820	CLA	O2A-CGA-CBA	2.60	119.46	111.90
26	9	607	CHL	C1D-CHD-C4C	2.60	117.91	112.37
17	l	203	CLA	O2A-CGA-CBA	2.60	119.46	111.90
17	B	835	CLA	CMB-C2B-C3B	2.60	129.72	124.89
17	B	819	CLA	C4-C3-C5	2.60	119.80	115.29
17	B	827	CLA	CAC-C3C-C4C	2.60	128.50	124.83
28	4	617	XAT	C38-C25-C24	2.60	117.26	114.28
17	A	833	CLA	O2A-CGA-CBA	2.60	119.47	111.90
17	3	311	CLA	CAC-C3C-C4C	2.60	128.50	124.83
17	a	833	CLA	CMC-C2C-C1C	2.60	128.97	125.02
17	8	301	CLA	CMC-C2C-C1C	2.60	128.97	125.02
28	1	317	XAT	C19-C9-C8	2.60	122.25	118.10
17	a	830	CLA	CMB-C2B-C3B	2.60	129.72	124.89
17	a	808	CLA	CAC-C3C-C4C	2.60	128.50	124.83
26	7	601	CHL	CHC-C4B-C3B	2.60	124.40	118.23
17	B	815	CLA	O2A-CGA-CBA	2.61	119.48	111.90
17	a	827	CLA	CMB-C2B-C3B	2.61	129.73	124.89
17	1	304	CLA	O2A-CGA-CBA	2.61	119.48	111.90
17	A	843	CLA	O2A-CGA-CBA	2.61	119.49	111.90
17	b	812	CLA	C4-C3-C5	2.61	119.81	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	j	3003	BCR	C38-C26-C27	2.61	118.40	113.45
17	6	310	CLA	CAC-C3C-C4C	2.61	128.51	124.83
17	a	836	CLA	O2A-CGA-CBA	2.61	119.49	111.90
17	a	827	CLA	C4-C3-C5	2.61	119.81	115.29
20	B	844	BCR	C29-C30-C25	2.61	114.56	110.48
17	a	808	CLA	O2A-CGA-CBA	2.61	119.50	111.90
17	G	103	CLA	CAC-C3C-C4C	2.61	128.51	124.83
17	B	822	CLA	CMB-C2B-C3B	2.61	129.74	124.89
17	A	802	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	9	602	CLA	CMC-C2C-C1C	2.61	128.98	125.02
17	8	309	CLA	CAC-C3C-C4C	2.61	128.51	124.83
17	3	309	CLA	CAC-C3C-C4C	2.61	128.52	124.83
17	b	807	CLA	CAC-C3C-C4C	2.61	128.52	124.83
17	3	302	CLA	C4-C3-C5	2.62	119.83	115.29
17	f	7003	CLA	CAC-C3C-C4C	2.62	128.52	124.83
17	a	824	CLA	O2A-CGA-CBA	2.62	119.52	111.90
17	L	202	CLA	O2A-CGA-CBA	2.62	119.52	111.90
17	a	819	CLA	C3B-C4B-NB	2.62	112.60	109.21
17	b	819	CLA	CMB-C2B-C3B	2.62	129.75	124.89
17	b	823	CLA	CMC-C2C-C1C	2.62	129.00	125.02
17	6	313	CLA	CAC-C3C-C4C	2.62	128.53	124.83
17	a	821	CLA	CMC-C2C-C1C	2.62	129.00	125.02
24	B	850	DGD	O6D-C5D-C6D	2.62	111.88	106.64
17	2	603	CLA	CAC-C3C-C4C	2.62	128.53	124.83
20	B	843	BCR	C2-C1-C6	2.62	114.58	110.48
17	9	611	CLA	C4-C3-C5	2.62	119.84	115.29
17	a	840	CLA	C4-C3-C5	2.62	119.84	115.29
17	9	601	CLA	CAC-C3C-C4C	2.63	128.53	124.83
17	B	819	CLA	O2A-CGA-CBA	2.63	119.54	111.90
17	B	809	CLA	C4-C3-C5	2.63	119.84	115.29
17	1	312	CLA	CAC-C3C-C4C	2.63	128.53	124.83
17	a	826	CLA	CMC-C2C-C1C	2.63	129.01	125.02
17	B	822	CLA	C4-C3-C5	2.63	119.85	115.29
17	B	822	CLA	CAC-C3C-C4C	2.63	128.54	124.83
17	7	608	CLA	O2A-CGA-CBA	2.63	119.56	111.90
17	A	819	CLA	CAC-C3C-C4C	2.63	128.54	124.83
26	9	605	CHL	C1D-CHD-C4C	2.63	117.98	112.37
20	b	843	BCR	C2-C1-C6	2.63	114.60	110.48
17	2	602	CLA	CAC-C3C-C4C	2.63	128.54	124.83
17	A	802	CLA	C3B-C4B-NB	2.63	112.62	109.21
17	a	810	CLA	C4-C3-C5	2.64	119.86	115.29
20	b	844	BCR	C33-C5-C4	2.64	118.45	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	832	CLA	CAC-C3C-C4C	2.64	128.55	124.83
23	B	849	LMT	O5B-C1B-C2B	2.64	115.38	110.30
17	b	815	CLA	C4-C3-C5	2.64	119.86	115.29
17	A	814	CLA	C4-C3-C5	2.64	119.87	115.29
17	A	809	CLA	CMC-C2C-C1C	2.64	129.02	125.02
17	b	824	CLA	O2A-CGA-CBA	2.64	119.58	111.90
17	7	602	CLA	CMC-C2C-C1C	2.64	129.03	125.02
17	a	804	CLA	CMC-C2C-C1C	2.64	129.03	125.02
17	a	833	CLA	O2A-CGA-CBA	2.64	119.59	111.90
17	6	309	CLA	CAC-C3C-C4C	2.64	128.56	124.83
17	A	830	CLA	CAC-C3C-C4C	2.64	128.56	124.83
17	b	836	CLA	C4-C3-C5	2.64	119.87	115.29
17	b	834	CLA	CAC-C3C-C4C	2.64	128.56	124.83
17	A	822	CLA	O2A-CGA-CBA	2.64	119.59	111.90
17	a	811	CLA	CAC-C3C-C4C	2.64	128.56	124.83
17	A	802	CLA	CAC-C3C-C4C	2.64	128.56	124.83
17	f	7003	CLA	C4-C3-C5	2.64	119.88	115.29
17	3	306	CLA	O2A-CGA-CBA	2.65	119.60	111.90
17	A	802	CLA	C4-C3-C5	2.65	119.88	115.29
19	a	847	LHG	O8-C23-C24	2.65	119.60	111.90
17	A	836	CLA	CAC-C3C-C4C	2.65	128.56	124.83
17	A	838	CLA	CAC-C3C-C4C	2.65	128.57	124.83
17	A	826	CLA	CMC-C2C-C1C	2.65	129.04	125.02
17	A	833	CLA	C4-C3-C5	2.65	119.89	115.29
17	A	841	CLA	C3B-C4B-NB	2.65	112.64	109.21
17	a	816	CLA	O2A-CGA-CBA	2.65	119.62	111.90
17	L	203	CLA	O2A-CGA-CBA	2.65	119.62	111.90
28	7	616	XAT	C18-C5-C4	2.66	117.32	114.28
17	A	802	CLA	O2A-CGA-CBA	2.66	119.63	111.90
17	b	806	CLA	O2A-CGA-CBA	2.66	119.64	111.90
17	B	807	CLA	C4-C3-C5	2.66	119.90	115.29
17	f	7002	CLA	CMC-C2C-C1C	2.66	129.06	125.02
17	B	826	CLA	C4-C3-C5	2.66	119.91	115.29
17	4	608	CLA	CMC-C2C-C1C	2.66	129.06	125.02
20	J	3003	BCR	C29-C30-C25	2.66	114.64	110.48
17	b	815	CLA	O2A-CGA-CBA	2.66	119.65	111.90
17	B	831	CLA	O2A-CGA-CBA	2.67	119.66	111.90
17	A	803	CLA	C4-C3-C5	2.67	119.92	115.29
17	9	614	CLA	O2A-CGA-CBA	2.67	119.66	111.90
17	a	856	CLA	CAC-C3C-C4C	2.67	128.59	124.83
17	9	612	CLA	C4-C3-C5	2.67	119.92	115.29
17	7	611	CLA	C4-C3-C5	2.67	119.92	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	851	BCR	C29-C30-C25	2.67	114.65	110.48
17	7	611	CLA	CAC-C3C-C4C	2.67	128.59	124.83
17	g	103	CLA	CMC-C2C-C1C	2.67	129.07	125.02
17	a	823	CLA	O2A-CGA-CBA	2.67	119.68	111.90
17	a	814	CLA	CMC-C2C-C1C	2.67	129.08	125.02
17	1	314	CLA	C4-C3-C5	2.68	119.93	115.29
17	8	311	CLA	CAC-C3C-C4C	2.68	128.61	124.83
17	b	831	CLA	O2A-CGA-CBA	2.68	119.69	111.90
26	4	606	CHL	O2A-CGA-CBA	2.68	119.69	111.90
19	A	846	LHG	O8-C23-C24	2.68	119.69	111.90
20	B	845	BCR	C29-C30-C25	2.68	114.67	110.48
17	A	822	CLA	C4-C3-C5	2.68	119.94	115.29
17	8	304	CLA	CAC-C3C-C4C	2.68	128.61	124.83
17	B	826	CLA	C3B-C4B-NB	2.68	112.68	109.21
17	1	305	CLA	CAC-C3C-C4C	2.68	128.61	124.83
17	G	104	CLA	CAC-C3C-C4C	2.68	128.61	124.83
17	A	813	CLA	CAC-C3C-C4C	2.68	128.61	124.83
17	A	803	CLA	O2A-CGA-CBA	2.68	119.71	111.90
17	7	609	CLA	CMB-C2B-C3B	2.68	129.87	124.89
17	2	611	CLA	C4-C3-C5	2.69	119.95	115.29
17	4	602	CLA	CAC-C3C-C4C	2.69	128.62	124.83
17	B	834	CLA	C4-C3-C5	2.69	119.95	115.29
17	F	301	CLA	CAC-C3C-C4C	2.69	128.62	124.83
17	A	839	CLA	CAC-C3C-C4C	2.69	128.62	124.83
17	A	829	CLA	O2A-CGA-CBA	2.69	119.73	111.90
17	9	614	CLA	CAC-C3C-C4C	2.69	128.63	124.83
17	7	603	CLA	CMC-C2C-C1C	2.69	129.10	125.02
17	A	823	CLA	CAC-C3C-C4C	2.69	128.63	124.83
17	b	812	CLA	CMC-C2C-C1C	2.69	129.10	125.02
17	a	841	CLA	CAC-C3C-C4C	2.69	128.63	124.83
17	4	608	CLA	CAC-C3C-C4C	2.69	128.63	124.83
17	A	836	CLA	O2A-CGA-CBA	2.70	119.74	111.90
17	B	810	CLA	CAC-C3C-C4C	2.70	128.63	124.83
17	A	838	CLA	CMC-C2C-C1C	2.70	129.11	125.02
17	B	810	CLA	C4-C3-C5	2.70	119.97	115.29
17	3	311	CLA	C4-C3-C5	2.70	119.97	115.29
17	b	818	CLA	CMC-C2C-C1C	2.70	129.11	125.02
20	1	205	BCR	C38-C26-C27	2.70	118.57	113.45
17	2	604	CLA	CAC-C3C-C4C	2.70	128.64	124.83
17	a	840	CLA	CAC-C3C-C4C	2.70	128.64	124.83
17	A	806	CLA	C4-C3-C5	2.70	119.97	115.29
17	1	308	CLA	CAC-C3C-C4C	2.70	128.64	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	827	CLA	O2A-CGA-CBA	2.70	119.76	111.90
17	B	840	CLA	C4-C3-C5	2.70	119.97	115.29
25	9	619	LMG	O8-C28-C29	2.70	119.76	111.90
17	4	610	CLA	CAC-C3C-C4C	2.70	128.64	124.83
17	3	305	CLA	CAC-C3C-C4C	2.70	128.64	124.83
17	b	823	CLA	O2A-CGA-CBA	2.70	119.77	111.90
26	4	605	CHL	C4-C3-C5	2.70	119.98	115.29
17	A	811	CLA	C4-C3-C5	2.71	119.98	115.29
17	A	811	CLA	CAC-C3C-C4C	2.71	128.65	124.83
17	6	306	CLA	CAC-C3C-C4C	2.71	128.65	124.83
17	1	304	CLA	C4-C3-C5	2.71	119.98	115.29
17	2	609	CLA	CAC-C3C-C4C	2.71	128.65	124.83
17	b	828	CLA	C4-C3-C5	2.71	119.99	115.29
17	a	820	CLA	O2A-CGA-CBA	2.71	119.78	111.90
17	a	814	CLA	CAC-C3C-C4C	2.71	128.66	124.83
17	7	604	CLA	CAC-C3C-C4C	2.71	128.66	124.83
17	A	830	CLA	CMB-C2B-C3B	2.71	129.93	124.89
17	F	301	CLA	CMC-C2C-C1C	2.72	129.14	125.02
20	B	844	BCR	C33-C5-C4	2.72	118.61	113.45
17	b	823	CLA	C4-C3-C5	2.72	120.00	115.29
17	A	840	CLA	C4-C3-C5	2.72	120.00	115.29
17	B	825	CLA	CMC-C2C-C1C	2.72	129.14	125.02
17	a	834	CLA	CMC-C2C-C1C	2.72	129.14	125.02
17	3	313	CLA	CAC-C3C-C4C	2.72	128.66	124.83
17	A	809	CLA	CAC-C3C-C4C	2.72	128.66	124.83
20	2	617	BCR	C33-C5-C4	2.72	118.61	113.45
17	6	307	CLA	CAC-C3C-C4C	2.72	128.67	124.83
17	A	826	CLA	O2A-CGA-CBA	2.72	119.82	111.90
17	b	827	CLA	O2A-CGA-CBA	2.72	119.82	111.90
17	b	817	CLA	CMB-C2B-C3B	2.72	129.94	124.89
17	a	838	CLA	C3B-C4B-NB	2.72	112.73	109.21
17	b	841	CLA	CMC-C2C-C1C	2.72	129.15	125.02
17	a	839	CLA	O2A-CGA-CBA	2.72	119.82	111.90
17	A	826	CLA	CAC-C3C-C4C	2.72	128.67	124.83
17	B	814	CLA	O2A-CGA-CBA	2.73	119.83	111.90
17	B	825	CLA	CAC-C3C-C4C	2.73	128.67	124.83
17	B	824	CLA	C3B-C4B-NB	2.73	112.74	109.21
20	l	205	BCR	C29-C30-C25	2.73	114.74	110.48
17	a	835	CLA	O2A-CGA-CBA	2.73	119.84	111.90
17	a	819	CLA	CMC-C2C-C1C	2.73	129.16	125.02
17	B	804	CLA	CAC-C3C-C4C	2.73	128.68	124.83
17	B	811	CLA	C4-C3-C5	2.73	120.02	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	824	CLA	CAC-C3C-C4C	2.73	128.69	124.83
17	a	843	CLA	CAC-C3C-C4C	2.73	128.69	124.83
17	4	611	CLA	C4-C3-C5	2.73	120.03	115.29
17	B	803	CLA	CAC-C3C-C4C	2.73	128.69	124.83
17	6	315	CLA	CAC-C3C-C4C	2.74	128.69	124.83
17	3	314	CLA	CAC-C3C-C4C	2.74	128.69	124.83
17	7	613	CLA	CAC-C3C-C4C	2.74	128.69	124.83
17	a	803	CLA	O2A-CGA-CBA	2.74	119.87	111.90
17	4	603	CLA	CMC-C2C-C1C	2.74	129.17	125.02
20	b	844	BCR	C29-C30-C25	2.74	114.76	110.48
17	B	809	CLA	O2A-CGA-CBA	2.74	119.87	111.90
17	k	1402	CLA	CAC-C3C-C4C	2.74	128.69	124.83
17	a	826	CLA	C4-C3-C5	2.74	120.04	115.29
17	8	301	CLA	C3B-C4B-NB	2.74	112.75	109.21
17	2	609	CLA	CMC-C2C-C1C	2.74	129.18	125.02
17	9	608	CLA	O2A-CGA-CBA	2.74	119.88	111.90
17	1	315	CLA	CAC-C3C-C4C	2.74	128.70	124.83
17	b	810	CLA	CAC-C3C-C4C	2.74	128.70	124.83
17	l	202	CLA	C4-C3-C5	2.74	120.05	115.29
17	J	3002	CLA	CAC-C3C-C4C	2.74	128.70	124.83
17	9	613	CLA	CAC-C3C-C4C	2.74	128.70	124.83
17	9	612	CLA	CAC-C3C-C4C	2.74	128.70	124.83
17	1	313	CLA	CAC-C3C-C4C	2.75	128.70	124.83
17	2	610	CLA	CAC-C3C-C4C	2.75	128.70	124.83
17	6	305	CLA	O2A-CGA-CBA	2.75	119.89	111.90
17	l	204	CLA	O2A-CGA-CBA	2.75	119.89	111.90
17	4	613	CLA	CAC-C3C-C4C	2.75	128.71	124.83
17	8	301	CLA	CAC-C3C-C4C	2.75	128.71	124.83
20	A	856	BCR	C33-C5-C4	2.75	118.67	113.45
17	l	203	CLA	C4-C3-C5	2.75	120.06	115.29
17	B	807	CLA	CAC-C3C-C4C	2.75	128.71	124.83
17	b	834	CLA	C4-C3-C5	2.75	120.07	115.29
17	b	806	CLA	CMC-C2C-C1C	2.75	129.20	125.02
19	1	319	LHG	O8-C23-C24	2.75	119.91	111.90
17	B	839	CLA	CAC-C3C-C4C	2.75	128.72	124.83
17	B	802	CLA	CMC-C2C-C1C	2.76	129.20	125.02
17	7	609	CLA	CMC-C2C-C1C	2.76	129.20	125.02
17	A	830	CLA	CMC-C2C-C1C	2.76	129.20	125.02
17	6	314	CLA	O2A-CGA-CBA	2.76	119.94	111.90
17	A	835	CLA	C4-C3-C5	2.76	120.08	115.29
17	b	815	CLA	CAC-C3C-C4C	2.76	128.73	124.83
17	B	818	CLA	C4-C3-C5	2.76	120.08	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	8	315	XAT	C38-C25-C24	2.76	117.45	114.28
19	7	618	LHG	O8-C23-C24	2.77	119.95	111.90
17	4	603	CLA	CAC-C3C-C4C	2.77	128.73	124.83
17	a	826	CLA	O2A-CGA-CBA	2.77	119.95	111.90
17	A	842	CLA	CAC-C3C-C4C	2.77	128.73	124.83
17	a	840	CLA	C1-O2A-CGA	2.77	123.42	116.77
17	B	819	CLA	CAC-C3C-C4C	2.77	128.74	124.83
17	b	833	CLA	CAC-C3C-C4C	2.77	128.74	124.83
17	B	817	CLA	CAC-C3C-C4C	2.77	128.74	124.83
17	A	827	CLA	C4-C3-C5	2.77	120.10	115.29
17	8	310	CLA	CAC-C3C-C4C	2.77	128.74	124.83
17	3	303	CLA	CAC-C3C-C4C	2.77	128.74	124.83
17	9	602	CLA	CAC-C3C-C4C	2.77	128.74	124.83
17	g	102	CLA	CAC-C3C-C4C	2.77	128.74	124.83
17	B	830	CLA	CMC-C2C-C1C	2.78	129.23	125.02
17	f	7003	CLA	O2A-CGA-CBA	2.78	119.98	111.90
17	b	827	CLA	C3B-C4B-NB	2.78	112.80	109.21
17	4	610	CLA	O2A-CGA-CBA	2.78	119.98	111.90
17	b	820	CLA	O2A-CGA-CBA	2.78	119.98	111.90
17	2	613	CLA	CAC-C3C-C4C	2.78	128.75	124.83
17	b	818	CLA	C4-C3-C5	2.78	120.11	115.29
17	A	839	CLA	O2A-CGA-CBA	2.78	119.99	111.90
17	a	814	CLA	C3B-C4B-NB	2.78	112.81	109.21
17	1	310	CLA	CAC-C3C-C4C	2.78	128.75	124.83
17	8	305	CLA	O2A-CGA-CBA	2.78	120.00	111.90
17	b	826	CLA	C4-C3-C5	2.78	120.12	115.29
17	7	602	CLA	C3B-C4B-NB	2.78	112.81	109.21
17	9	609	CLA	CAC-C3C-C4C	2.79	128.76	124.83
17	b	841	CLA	CAC-C3C-C4C	2.79	128.76	124.83
17	b	804	CLA	CMC-C2C-C1C	2.79	129.25	125.02
17	b	802	CLA	C4-C3-C5	2.79	120.13	115.29
17	a	820	CLA	CMB-C2B-C3B	2.79	130.07	124.89
17	B	841	CLA	C4-C3-C5	2.79	120.13	115.29
17	9	603	CLA	CMC-C2C-C1C	2.79	129.26	125.02
20	a	851	BCR	C2-C1-C6	2.80	114.85	110.48
17	1	306	CLA	CAC-C3C-C4C	2.80	128.77	124.83
17	B	817	CLA	CMB-C2B-C3B	2.80	130.08	124.89
17	A	824	CLA	CAC-C3C-C4C	2.80	128.78	124.83
17	b	821	CLA	CAC-C3C-C4C	2.80	128.78	124.83
17	4	614	CLA	O2A-CGA-CBA	2.80	120.05	111.90
17	b	836	CLA	CMC-C2C-C1C	2.80	129.26	125.02
17	A	826	CLA	C3B-C4B-NB	2.80	112.83	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	816	CLA	C3B-C4B-NB	2.80	112.83	109.21
20	B	846	BCR	C29-C30-C25	2.80	114.86	110.48
17	1	308	CLA	C4-C3-C5	2.80	120.15	115.29
17	a	828	CLA	O2A-CGA-CBA	2.80	120.05	111.90
17	B	822	CLA	O2A-CGA-CBA	2.80	120.06	111.90
17	7	609	CLA	CAC-C3C-C4C	2.80	128.78	124.83
17	A	837	CLA	CAC-C3C-C4C	2.80	128.78	124.83
20	I	101	BCR	C2-C1-C6	2.80	114.86	110.48
17	A	808	CLA	CMC-C2C-C1C	2.81	129.27	125.02
17	A	825	CLA	CAC-C3C-C4C	2.81	128.79	124.83
17	b	826	CLA	C3B-C4B-NB	2.81	112.84	109.21
17	a	817	CLA	CAC-C3C-C4C	2.81	128.79	124.83
17	3	310	CLA	CAC-C3C-C4C	2.81	128.79	124.83
17	B	821	CLA	CAC-C3C-C4C	2.81	128.79	124.83
17	b	816	CLA	C3B-C4B-NB	2.81	112.84	109.21
17	a	840	CLA	O2A-CGA-CBA	2.81	120.09	111.90
17	L	203	CLA	C3B-C4B-NB	2.81	112.85	109.21
17	A	831	CLA	O2A-CGA-CBA	2.82	120.09	111.90
17	A	824	CLA	O2A-CGA-CBA	2.82	120.09	111.90
17	b	836	CLA	CAC-C3C-C4C	2.82	128.80	124.83
17	b	819	CLA	CAC-C3C-C4C	2.82	128.80	124.83
17	7	609	CLA	C3B-C4B-NB	2.82	112.85	109.21
25	4	619	LMG	O8-C28-C29	2.82	120.11	111.90
17	8	307	CLA	O2A-CGA-CBA	2.82	120.11	111.90
20	b	843	BCR	C29-C30-C25	2.82	114.89	110.48
17	a	802	CLA	C3B-C4B-NB	2.82	112.86	109.21
17	A	806	CLA	O2A-CGA-CBA	2.82	120.11	111.90
17	1	313	CLA	O2A-CGA-CBA	2.82	120.11	111.90
17	A	828	CLA	C3B-C4B-NB	2.82	112.86	109.21
17	a	815	CLA	C3B-C4B-NB	2.83	112.86	109.21
17	a	832	CLA	CAC-C3C-C4C	2.83	128.82	124.83
17	j	3002	CLA	CAC-C3C-C4C	2.83	128.82	124.83
17	b	809	CLA	O2A-CGA-CBA	2.83	120.13	111.90
17	8	308	CLA	CAC-C3C-C4C	2.83	128.82	124.83
17	A	827	CLA	C3B-C4B-NB	2.83	112.87	109.21
17	a	813	CLA	O2A-CGA-CBA	2.83	120.14	111.90
17	B	832	CLA	O2A-CGA-CBA	2.83	120.14	111.90
17	6	313	CLA	O2A-CGA-CBA	2.83	120.14	111.90
26	2	601	CHL	C4-C3-C5	2.83	120.20	115.29
20	2	617	BCR	C2-C1-C6	2.83	114.91	110.48
17	2	612	CLA	CAC-C3C-C4C	2.83	128.83	124.83
17	A	833	CLA	CMC-C2C-C1C	2.83	129.32	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	838	CLA	C3B-C4B-NB	2.84	112.88	109.21
17	6	305	CLA	CAC-C3C-C4C	2.84	128.83	124.83
17	9	602	CLA	C3B-C4B-NB	2.84	112.88	109.21
17	B	814	CLA	C3B-C4B-NB	2.84	112.88	109.21
17	b	824	CLA	C4-C3-C5	2.84	120.22	115.29
17	B	820	CLA	O2A-CGA-CBA	2.84	120.16	111.90
17	8	308	CLA	C3B-C4B-NB	2.84	112.88	109.21
20	B	847	BCR	C29-C30-C25	2.84	114.92	110.48
17	b	832	CLA	CAC-C3C-C4C	2.84	128.84	124.83
17	a	834	CLA	C4-C3-C5	2.84	120.22	115.29
17	b	833	CLA	C4-C3-C5	2.84	120.22	115.29
17	b	830	CLA	O2A-CGA-CBA	2.84	120.17	111.90
17	A	830	CLA	O2A-CGA-CBA	2.84	120.17	111.90
17	1	304	CLA	CAC-C3C-C4C	2.84	128.84	124.83
17	a	819	CLA	CAC-C3C-C4C	2.84	128.84	124.83
17	b	814	CLA	C3B-C4B-NB	2.84	112.89	109.21
17	A	811	CLA	O2A-CGA-CBA	2.85	120.18	111.90
17	a	806	CLA	CMC-C2C-C1C	2.85	129.34	125.02
17	b	814	CLA	O2A-CGA-CBA	2.85	120.18	111.90
17	A	823	CLA	O2A-CGA-CBA	2.85	120.18	111.90
17	7	602	CLA	CAC-C3C-C4C	2.85	128.85	124.83
17	a	830	CLA	CMC-C2C-C1C	2.85	129.34	125.02
17	6	310	CLA	C4-C3-C5	2.85	120.24	115.29
17	a	808	CLA	C4-C3-C5	2.85	120.24	115.29
17	4	609	CLA	C3B-C4B-NB	2.86	112.90	109.21
17	A	835	CLA	CAC-C3C-C4C	2.86	128.86	124.83
17	2	609	CLA	C3B-C4B-NB	2.86	112.90	109.21
17	A	813	CLA	O2A-CGA-CBA	2.86	120.21	111.90
17	A	818	CLA	O2A-CGA-CBA	2.86	120.21	111.90
17	a	832	CLA	O2A-CGA-CBA	2.86	120.22	111.90
17	A	835	CLA	O2A-CGA-CBA	2.86	120.22	111.90
17	a	816	CLA	C3B-C4B-NB	2.86	112.91	109.21
17	a	802	CLA	CMB-C2B-C3B	2.86	130.20	124.89
17	a	856	CLA	CMB-C2B-C3B	2.86	130.20	124.89
17	a	820	CLA	CAC-C3C-C4C	2.86	128.87	124.83
17	A	819	CLA	C3B-C4B-NB	2.86	112.91	109.21
17	8	302	CLA	CAC-C3C-C4C	2.86	128.87	124.83
17	B	803	CLA	O2A-CGA-CBA	2.87	120.24	111.90
17	B	832	CLA	CAC-C3C-C4C	2.87	128.87	124.83
17	6	314	CLA	CAC-C3C-C4C	2.87	128.88	124.83
17	B	830	CLA	O2A-CGA-CBA	2.87	120.25	111.90
17	a	846	CLA	O2A-CGA-CBA	2.87	120.25	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	831	CLA	CAC-C3C-C4C	2.87	128.88	124.83
17	k	1403	CLA	CAC-C3C-C4C	2.87	128.88	124.83
17	A	815	CLA	C3B-C4B-NB	2.87	112.92	109.21
19	6	320	LHG	O8-C23-C24	2.87	120.26	111.90
17	3	302	CLA	C3B-C4B-NB	2.87	112.93	109.21
17	6	311	CLA	C3B-C4B-NB	2.88	112.93	109.21
17	a	829	CLA	C3B-C4B-NB	2.88	112.93	109.21
17	1	303	CLA	C3B-C4B-NB	2.88	112.93	109.21
17	8	310	CLA	O2A-CGA-CBA	2.88	120.27	111.90
17	a	833	CLA	C4-C3-C5	2.88	120.28	115.29
17	b	832	CLA	C3B-C4B-NB	2.88	112.93	109.21
26	1	302	CHL	C4-C3-C5	2.88	120.29	115.29
17	a	807	CLA	C3B-C4B-NB	2.88	112.93	109.21
17	A	822	CLA	CAC-C3C-C4C	2.88	128.89	124.83
17	b	827	CLA	CMC-C2C-C1C	2.88	129.39	125.02
17	3	312	CLA	CAC-C3C-C4C	2.88	128.90	124.83
17	a	818	CLA	CMB-C2B-C3B	2.89	130.25	124.89
17	a	827	CLA	C3B-C4B-NB	2.89	112.94	109.21
17	A	808	CLA	CMB-C2B-C3B	2.89	130.25	124.89
17	8	303	CLA	CAC-C3C-C4C	2.89	128.90	124.83
25	G	102	LMG	O8-C28-C29	2.89	120.30	111.90
17	a	813	CLA	CAC-C3C-C4C	2.89	128.90	124.83
17	A	838	CLA	O2A-CGA-CBA	2.89	120.31	111.90
20	b	845	BCR	C8-C9-C10	2.89	123.38	118.94
17	b	824	CLA	CMC-C2C-C1C	2.89	129.40	125.02
17	b	816	CLA	CAC-C3C-C4C	2.89	128.91	124.83
17	b	816	CLA	O2A-CGA-CBA	2.89	120.32	111.90
17	3	302	CLA	CAC-C3C-C4C	2.90	128.91	124.83
17	B	830	CLA	C3B-C4B-NB	2.90	112.95	109.21
17	B	837	CLA	C3B-C4B-NB	2.90	112.95	109.21
17	6	310	CLA	O2A-CGA-CBA	2.90	120.33	111.90
17	8	302	CLA	O2A-CGA-CBA	2.90	120.34	111.90
17	A	845	CLA	O2A-CGA-CBA	2.90	120.34	111.90
17	a	833	CLA	C3B-C4B-NB	2.90	112.96	109.21
17	B	806	CLA	C3B-C4B-NB	2.90	112.96	109.21
17	3	309	CLA	C3B-C4B-NB	2.90	112.96	109.21
17	1	312	CLA	C4-C3-C5	2.90	120.32	115.29
17	a	828	CLA	C3B-C4B-NB	2.90	112.96	109.21
17	b	810	CLA	O2A-CGA-CBA	2.91	120.36	111.90
17	b	816	CLA	C4-C3-C5	2.91	120.33	115.29
17	a	804	CLA	O2A-CGA-CBA	2.91	120.36	111.90
17	6	316	CLA	CAC-C3C-C4C	2.91	128.93	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	832	CLA	O2A-CGA-CBA	2.91	120.36	111.90
17	A	833	CLA	C3B-C4B-NB	2.91	112.97	109.21
17	a	806	CLA	CAC-C3C-C4C	2.91	128.93	124.83
17	a	808	CLA	CMC-C2C-C1C	2.91	129.43	125.02
17	b	806	CLA	C3B-C4B-NB	2.91	112.97	109.21
17	b	830	CLA	CAC-C3C-C4C	2.91	128.94	124.83
17	b	823	CLA	C3B-C4B-NB	2.91	112.98	109.21
28	9	617	XAT	C18-C5-C4	2.91	117.62	114.28
17	A	810	CLA	C4-C3-C5	2.92	120.35	115.29
17	A	807	CLA	C3B-C4B-NB	2.92	112.98	109.21
17	l	203	CLA	C3B-C4B-NB	2.92	112.98	109.21
17	7	603	CLA	CAC-C3C-C4C	2.92	128.94	124.83
17	B	812	CLA	O2A-CGA-CBA	2.92	120.39	111.90
17	b	839	CLA	O2A-CGA-CBA	2.92	120.40	111.90
17	b	812	CLA	O2A-CGA-CBA	2.92	120.40	111.90
17	L	204	CLA	O2A-CGA-CBA	2.92	120.41	111.90
17	8	312	CLA	C3B-C4B-NB	2.93	112.99	109.21
17	A	808	CLA	C4-C3-C5	2.93	120.37	115.29
17	B	834	CLA	O2A-CGA-CBA	2.93	120.42	111.90
17	B	818	CLA	C3B-C4B-NB	2.93	113.00	109.21
17	b	817	CLA	C4-C3-C5	2.93	120.37	115.29
17	a	818	CLA	O2A-CGA-CBA	2.93	120.42	111.90
17	F	304	CLA	O2A-CGA-CBA	2.93	120.42	111.90
17	A	809	CLA	O2A-CGA-CBA	2.93	120.43	111.90
17	B	804	CLA	CMC-C2C-C1C	2.93	129.47	125.02
17	b	819	CLA	O2A-CGA-CBA	2.93	120.43	111.90
17	6	306	CLA	O2A-CGA-CBA	2.93	120.43	111.90
17	a	809	CLA	C3B-C4B-NB	2.93	113.00	109.21
17	b	818	CLA	CAC-C3C-C4C	2.93	128.97	124.83
17	b	822	CLA	O2A-CGA-CBA	2.93	120.44	111.90
17	8	307	CLA	C3B-C4B-NB	2.93	113.00	109.21
17	A	840	CLA	O2A-CGA-CBA	2.94	120.44	111.90
17	B	806	CLA	O2A-CGA-CBA	2.94	120.45	111.90
17	a	807	CLA	CMC-C2C-C1C	2.94	129.47	125.02
17	B	823	CLA	C3B-C4B-NB	2.94	113.01	109.21
17	1	312	CLA	O2A-CGA-CBA	2.94	120.45	111.90
17	a	811	CLA	O2A-CGA-CBA	2.94	120.45	111.90
17	b	826	CLA	O2A-CGA-CBA	2.94	120.45	111.90
17	2	603	CLA	C4-C3-C5	2.94	120.39	115.29
17	B	841	CLA	C3B-C4B-NB	2.94	113.02	109.21
17	9	612	CLA	O2A-CGA-CBA	2.94	120.47	111.90
17	B	832	CLA	C3B-C4B-NB	2.95	113.02	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	809	CLA	O2A-CGA-CBA	2.95	120.47	111.90
17	4	602	CLA	C3B-C4B-NB	2.95	113.02	109.21
17	A	814	CLA	O2A-CGA-CBA	2.95	120.48	111.90
26	1	307	CHL	O2A-CGA-CBA	2.95	120.48	111.90
17	B	836	CLA	O2A-CGA-CBA	2.95	120.48	111.90
17	a	844	CLA	CAC-C3C-C4C	2.95	128.99	124.83
17	b	818	CLA	C3B-C4B-NB	2.95	113.03	109.21
18	a	845	PQN	C14-C13-C15	2.95	120.41	115.29
17	a	844	CLA	O2A-CGA-CBA	2.95	120.49	111.90
26	9	607	CHL	O2A-CGA-CBA	2.95	120.49	111.90
26	9	606	CHL	O2A-CGA-CBA	2.95	120.50	111.90
28	3	317	XAT	C38-C25-C24	2.95	117.66	114.28
17	4	612	CLA	O2A-CGA-CBA	2.96	120.50	111.90
17	B	827	CLA	C3B-C4B-NB	2.96	113.03	109.21
17	a	843	CLA	O2A-CGA-CBA	2.96	120.50	111.90
17	a	829	CLA	CMC-C2C-C1C	2.96	129.51	125.02
17	b	836	CLA	O2A-CGA-CBA	2.96	120.51	111.90
26	9	607	CHL	O2D-CGD-CBD	2.96	118.42	111.20
17	B	807	CLA	C3B-C4B-NB	2.96	113.04	109.21
17	6	313	CLA	C4-C3-C5	2.96	120.42	115.29
17	A	804	CLA	C3B-C4B-NB	2.96	113.04	109.21
17	a	808	CLA	C3B-C4B-NB	2.96	113.04	109.21
17	a	844	CLA	CMC-C2C-C1C	2.96	129.51	125.02
17	F	304	CLA	C3B-C4B-NB	2.96	113.04	109.21
17	A	831	CLA	C4-C3-C5	2.96	120.43	115.29
17	3	315	CLA	C2C-C1C-NC	2.96	115.10	109.44
17	1	303	CLA	CAC-C3C-C4C	2.97	129.01	124.83
17	A	806	CLA	CAC-C3C-C4C	2.97	129.01	124.83
17	3	306	CLA	C3B-C4B-NB	2.97	113.05	109.21
17	A	812	CLA	O2A-CGA-CBA	2.97	120.54	111.90
17	A	843	CLA	CAC-C3C-C4C	2.97	129.02	124.83
17	9	609	CLA	C3B-C4B-NB	2.97	113.05	109.21
17	B	824	CLA	C4-C3-C5	2.97	120.44	115.29
17	b	823	CLA	CAC-C3C-C4C	2.98	129.03	124.83
24	B	850	DGD	O1G-C1A-C2A	2.98	120.56	111.90
17	7	612	CLA	O2A-CGA-CBA	2.98	120.56	111.90
17	b	838	CLA	CMB-C2B-C3B	2.98	130.42	124.89
17	7	608	CLA	C3B-C4B-NB	2.98	113.06	109.21
17	a	826	CLA	C3B-C4B-NB	2.98	113.06	109.21
17	A	823	CLA	C3B-C4B-NB	2.98	113.06	109.21
17	3	301	CLA	CAC-C3C-C4C	2.98	129.04	124.83
17	7	603	CLA	C3B-C4B-NB	2.98	113.07	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	842	CLA	C3B-C4B-NB	2.98	113.07	109.21
17	1	314	CLA	CAC-C3C-C4C	2.99	129.04	124.83
17	b	824	CLA	CAC-C3C-C4C	2.99	129.04	124.83
17	F	301	CLA	C3B-C4B-NB	2.99	113.07	109.21
17	B	831	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	1	306	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	a	831	CLA	O2A-CGA-CBA	2.99	120.61	111.90
17	b	841	CLA	C3B-C4B-NB	2.99	113.08	109.21
24	b	849	DGD	O1G-C1A-C2A	2.99	120.61	111.90
17	B	815	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	a	843	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	B	817	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	b	812	CLA	CAC-C3C-C4C	2.99	129.05	124.83
17	A	834	CLA	C4-C3-C5	2.99	120.48	115.29
17	A	816	CLA	C3B-C4B-NB	2.99	113.08	109.21
17	b	825	CLA	C3B-C4B-NB	2.99	113.08	109.21
19	3	319	LHG	O8-C23-C24	3.00	119.39	111.35
19	2	618	LHG	O8-C23-C24	3.00	120.62	111.90
17	a	839	CLA	C3B-C4B-NB	3.00	113.08	109.21
17	B	825	CLA	C3B-C4B-NB	3.00	113.09	109.21
17	B	835	CLA	C3B-C4B-NB	3.00	113.09	109.21
17	8	313	CLA	C2C-C1C-NC	3.00	115.17	109.44
17	3	303	CLA	O2A-CGA-CBA	3.00	120.63	111.90
17	A	822	CLA	C3B-C4B-NB	3.00	113.09	109.21
17	b	837	CLA	C3B-C4B-NB	3.00	113.09	109.21
17	B	816	CLA	O2A-CGA-CBA	3.00	120.63	111.90
17	4	611	CLA	O2A-CGA-CBA	3.00	120.64	111.90
17	b	803	CLA	O2A-CGA-CBA	3.00	120.64	111.90
17	a	812	CLA	C3B-C4B-NB	3.01	113.09	109.21
17	a	819	CLA	O2A-CGA-CBA	3.01	120.65	111.90
17	A	802	CLA	CMB-C2B-C3B	3.01	130.47	124.89
17	a	838	CLA	O2A-CGA-CBA	3.01	120.65	111.90
17	2	602	CLA	C3B-C4B-NB	3.01	113.10	109.21
17	b	822	CLA	C3B-C4B-NB	3.01	113.10	109.21
17	a	841	CLA	C3B-C4B-NB	3.01	113.10	109.21
17	B	833	CLA	C4-C3-C5	3.01	120.51	115.29
17	9	603	CLA	CAC-C3C-C4C	3.01	129.08	124.83
17	9	604	CLA	O2A-CGA-CBA	3.01	120.66	111.90
17	B	823	CLA	O2A-CGA-CBA	3.01	120.66	111.90
17	2	603	CLA	C3B-C4B-NB	3.01	113.11	109.21
17	B	812	CLA	CAC-C3C-C4C	3.01	129.08	124.83
17	B	821	CLA	C3B-C4B-NB	3.01	113.11	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	813	CLA	O2A-CGA-CBA	3.02	120.67	111.90
17	b	841	CLA	O2A-CGA-CBA	3.02	120.67	111.90
17	a	837	CLA	CAC-C3C-C4C	3.02	129.08	124.83
17	3	312	CLA	O2A-CGA-CBA	3.02	120.69	111.90
17	2	612	CLA	O2A-CGA-CBA	3.02	120.69	111.90
17	2	603	CLA	O2A-CGA-CBA	3.02	120.69	111.90
20	A	851	BCR	C38-C26-C27	3.02	119.19	113.45
17	B	805	CLA	C4-C3-C5	3.02	120.53	115.29
17	b	817	CLA	CAC-C3C-C4C	3.02	129.09	124.83
17	a	832	CLA	C3B-C4B-NB	3.03	113.12	109.21
17	a	829	CLA	CAC-C3C-C4C	3.03	129.10	124.83
17	B	818	CLA	O2A-CGA-CBA	3.03	120.70	111.90
17	7	604	CLA	O2A-CGA-CBA	3.03	120.70	111.90
19	A	847	LHG	O8-C23-C24	3.03	119.48	111.35
26	2	607	CHL	O2A-CGA-CBA	3.03	120.71	111.90
17	l	204	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	B	812	CLA	C3B-C4B-NB	3.03	113.13	109.21
26	7	607	CHL	O2A-CGA-CBA	3.03	120.72	111.90
17	a	834	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	L	204	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	A	826	CLA	C4-C3-C5	3.03	120.55	115.29
17	a	805	CLA	O2A-CGA-CBA	3.03	120.72	111.90
17	3	308	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	4	610	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	a	844	CLA	C4-C3-C5	3.03	120.55	115.29
17	A	842	CLA	O2A-CGA-CBA	3.03	120.73	111.90
17	A	834	CLA	O2A-CGA-CBA	3.03	120.73	111.90
17	b	810	CLA	C3B-C4B-NB	3.03	113.13	109.21
17	B	834	CLA	C3B-C4B-NB	3.04	113.14	109.21
26	2	606	CHL	O2A-CGA-CBA	3.04	120.74	111.90
17	a	803	CLA	CAC-C3C-C4C	3.04	129.12	124.83
17	B	813	CLA	C3B-C4B-NB	3.04	113.14	109.21
17	G	103	CLA	O2A-CGA-CBA	3.04	120.75	111.90
17	6	304	CLA	O2A-CGA-CBA	3.04	120.76	111.90
17	A	816	CLA	O2A-CGA-CBA	3.05	120.77	111.90
17	f	7002	CLA	C3B-C4B-NB	3.05	113.15	109.21
17	A	854	CLA	CMB-C2B-C3B	3.05	130.56	124.89
17	A	814	CLA	C3B-C4B-NB	3.05	113.16	109.21
17	a	822	CLA	C3B-C4B-NB	3.05	113.16	109.21
17	B	813	CLA	O2A-CGA-CBA	3.06	120.79	111.90
17	7	603	CLA	O2A-CGA-CBA	3.06	120.79	111.90
17	b	815	CLA	C3B-C4B-NB	3.06	113.16	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	813	CLA	C3B-C4B-NB	3.06	113.16	109.21
17	A	832	CLA	C3B-C4B-NB	3.06	113.16	109.21
17	A	825	CLA	O2A-CGA-CBA	3.06	120.81	111.90
17	A	838	CLA	C4-C3-C5	3.06	119.47	115.85
17	B	829	CLA	CAC-C3C-C4C	3.06	129.15	124.83
17	3	304	CLA	C3B-C4B-NB	3.06	113.17	109.21
17	b	807	CLA	O2A-CGA-CBA	3.07	120.82	111.90
17	b	836	CLA	CMB-C2B-C3B	3.07	130.58	124.89
17	4	604	CLA	O2A-CGA-CBA	3.07	120.83	111.90
17	B	810	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	6	312	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	8	304	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	7	612	CLA	CAC-C3C-C4C	3.07	129.16	124.83
17	k	1401	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	B	841	CLA	O2A-CGA-CBA	3.07	120.84	111.90
17	6	304	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	b	820	CLA	C3B-C4B-NB	3.07	113.18	109.21
17	B	841	CLA	CMC-C2C-C1C	3.08	129.68	125.02
17	A	814	CLA	CAC-C3C-C4C	3.08	129.17	124.83
17	A	803	CLA	C3B-C4B-NB	3.08	113.19	109.21
17	b	830	CLA	C3B-C4B-NB	3.08	113.19	109.21
17	G	104	CLA	C3B-C4B-NB	3.08	113.19	109.21
17	A	813	CLA	C3B-C4B-NB	3.08	113.19	109.21
17	a	835	CLA	C3B-C4B-NB	3.08	113.20	109.21
17	a	844	CLA	C3B-C4B-NB	3.08	113.20	109.21
17	6	307	CLA	C3B-C4B-NB	3.08	113.20	109.21
17	9	604	CLA	C3B-C4B-NB	3.08	113.20	109.21
17	2	604	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	B	838	CLA	O2A-CGA-CBA	3.09	120.88	111.90
17	1	309	CLA	O2A-CGA-CBA	3.09	120.88	111.90
17	J	3002	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	4	614	CLA	C3B-C4B-NB	3.09	113.20	109.21
26	4	607	CHL	O2A-CGA-CBA	3.09	120.89	111.90
17	b	829	CLA	CAC-C3C-C4C	3.09	129.19	124.83
17	3	309	CLA	O2A-CGA-CBA	3.09	120.89	111.90
17	4	604	CLA	CAC-C3C-C4C	3.09	129.19	124.83
17	B	828	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	A	829	CLA	C3B-C4B-NB	3.09	113.20	109.21
17	7	604	CLA	C3B-C4B-NB	3.09	113.21	109.21
17	B	833	CLA	O2A-CGA-CBA	3.09	120.89	111.90
17	B	816	CLA	CAC-C3C-C4C	3.09	129.19	124.83
17	b	838	CLA	O2A-CGA-CBA	3.09	120.90	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	303	CLA	C3B-C4B-NB	3.09	113.21	109.21
26	7	606	CHL	O2A-CGA-CBA	3.09	120.90	111.90
17	8	301	CLA	O2A-CGA-CBA	3.10	120.91	111.90
17	b	817	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	9	608	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	A	835	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	a	825	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	4	608	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	3	311	CLA	C3B-C4B-NB	3.10	113.22	109.21
26	2	605	CHL	O2D-CGD-CBD	3.10	118.77	111.20
17	f	7003	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	B	829	CLA	O2A-CGA-CBA	3.10	120.93	111.90
17	b	821	CLA	C3B-C4B-NB	3.10	113.22	109.21
17	3	308	CLA	O2A-CGA-CBA	3.10	120.93	111.90
17	b	807	CLA	C3B-C4B-NB	3.11	113.22	109.21
20	A	856	BCR	C38-C26-C27	3.11	119.35	113.45
17	b	834	CLA	O2A-CGA-CBA	3.11	120.94	111.90
17	6	309	CLA	C3B-C4B-NB	3.11	113.23	109.21
17	g	102	CLA	O2A-CGA-CBA	3.11	120.95	111.90
26	7	601	CHL	C4-C3-C5	3.11	120.68	115.29
17	8	308	CLA	O2A-CGA-CBA	3.11	120.95	111.90
17	B	834	CLA	CAC-C3C-C4C	3.11	129.22	124.83
17	B	817	CLA	C4-C3-C5	3.11	120.69	115.29
17	B	809	CLA	C3B-C4B-NB	3.11	113.23	109.21
17	B	840	CLA	O2A-CGA-CBA	3.11	120.96	111.90
17	b	805	CLA	C4-C3-C5	3.11	120.69	115.29
17	1	305	CLA	O2A-CGA-CBA	3.11	120.96	111.90
17	7	602	CLA	O2A-CGA-CBA	3.11	120.96	111.90
17	a	841	CLA	O2A-CGA-CBA	3.11	120.96	111.90
17	3	314	CLA	C3B-C4B-NB	3.11	113.24	109.21
17	2	611	CLA	O2A-CGA-CBA	3.12	120.97	111.90
17	7	611	CLA	O2A-CGA-CBA	3.12	120.97	111.90
17	6	315	CLA	O2A-CGA-CBA	3.12	120.97	111.90
17	A	836	CLA	C3B-C4B-NB	3.12	113.24	109.21
17	F	303	CLA	C3B-C4B-NB	3.12	113.24	109.21
18	B	842	PQN	C14-C13-C15	3.12	120.70	115.29
17	9	610	CLA	C3B-C4B-NB	3.12	113.25	109.21
17	a	806	CLA	O2A-CGA-CBA	3.12	120.98	111.90
17	a	804	CLA	CMB-C2B-C3B	3.12	130.69	124.89
17	3	311	CLA	O2A-CGA-CBA	3.12	120.99	111.90
17	4	604	CLA	C3B-C4B-NB	3.12	113.25	109.21
17	G	103	CLA	C3B-C4B-NB	3.12	113.25	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	604	CLA	O2A-CGA-CBA	3.13	120.99	111.90
17	b	804	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	7	613	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	1	311	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	A	828	CLA	O2A-CGA-CBA	3.13	121.00	111.90
17	B	805	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	A	845	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	A	842	CLA	C3B-C4B-NB	3.13	113.25	109.21
17	8	305	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	8	309	CLA	O2A-CGA-CBA	3.13	121.01	111.90
17	B	836	CLA	CMB-C2B-C3B	3.13	130.70	124.89
17	B	839	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	b	805	CLA	CAC-C3C-C4C	3.13	129.25	124.83
17	A	805	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	A	818	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	b	813	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	B	840	CLA	C3B-C4B-NB	3.13	113.26	109.21
17	b	828	CLA	C3B-C4B-NB	3.14	113.26	109.21
26	4	607	CHL	O2D-CGD-CBD	3.14	118.85	111.20
17	6	314	CLA	C3B-C4B-NB	3.14	113.27	109.21
17	B	808	CLA	C3B-C4B-NB	3.14	113.27	109.21
17	1	306	CLA	O2A-CGA-CBA	3.14	121.04	111.90
17	B	830	CLA	CAC-C3C-C4C	3.14	129.26	124.83
17	a	831	CLA	C3B-C4B-NB	3.14	113.27	109.21
17	b	834	CLA	C3B-C4B-NB	3.14	113.28	109.21
17	6	306	CLA	C3B-C4B-NB	3.14	113.28	109.21
17	B	837	CLA	O2A-CGA-CBA	3.15	121.05	111.90
17	B	820	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	a	836	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	2	608	CLA	O2A-CGA-CBA	3.15	121.06	111.90
17	3	305	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	j	3002	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	b	812	CLA	C3B-C4B-NB	3.15	113.28	109.21
17	A	812	CLA	C3B-C4B-NB	3.15	113.29	109.21
17	1	308	CLA	C3B-C4B-NB	3.15	113.29	109.21
17	2	613	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	B	822	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	1	310	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	4	613	CLA	C3B-C4B-NB	3.16	113.29	109.21
17	a	810	CLA	C3B-C4B-NB	3.16	113.29	109.21
20	a	853	BCR	C38-C26-C27	3.16	119.45	113.45
17	a	825	CLA	O2A-CGA-CBA	3.16	121.10	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	817	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	K	4002	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	a	846	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	6	304	CLA	CAC-C3C-C4C	3.16	129.29	124.83
17	B	833	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	A	819	CLA	O2A-CGA-CBA	3.16	121.11	111.90
17	a	805	CLA	C3B-C4B-NB	3.16	113.30	109.21
17	b	835	CLA	C3B-C4B-NB	3.17	113.30	109.21
17	b	818	CLA	O2A-CGA-CBA	3.17	121.11	111.90
17	b	829	CLA	O2A-CGA-CBA	3.17	121.12	111.90
17	g	102	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	b	809	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	4	602	CLA	O2A-CGA-CBA	3.17	121.12	111.90
17	A	801	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	B	804	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	K	4003	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	1	303	CLA	O2A-CGA-CBA	3.17	121.12	111.90
17	a	820	CLA	C3B-C4B-NB	3.17	113.31	109.21
20	b	844	BCR	C8-C9-C10	3.17	123.81	118.94
17	b	831	CLA	C3B-C4B-NB	3.17	113.31	109.21
17	a	834	CLA	O2A-CGA-CBA	3.17	121.13	111.90
17	1	308	CLA	O2A-CGA-CBA	3.17	121.13	111.90
28	8	315	XAT	O4-C5-C18	3.17	118.99	115.02
17	2	602	CLA	O2A-CGA-CBA	3.18	121.14	111.90
17	A	831	CLA	CAC-C3C-C4C	3.18	129.31	124.83
17	a	812	CLA	O2A-CGA-CBA	3.18	121.15	111.90
17	B	819	CLA	C3B-C4B-NB	3.18	113.32	109.21
17	9	613	CLA	C3B-C4B-NB	3.18	113.32	109.21
17	B	839	CLA	O2A-CGA-CBA	3.18	121.16	111.90
17	1	314	CLA	O2A-CGA-CBA	3.18	121.16	111.90
17	B	805	CLA	O2A-CGA-CBA	3.18	121.16	111.90
17	8	311	CLA	C3B-C4B-NB	3.18	113.33	109.21
17	9	612	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	9	614	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	1	305	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	A	843	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	2	612	CLA	C3B-C4B-NB	3.19	113.33	109.21
17	a	830	CLA	O2A-CGA-CBA	3.19	121.18	111.90
17	2	608	CLA	C3B-C4B-NB	3.19	113.33	109.21
20	B	844	BCR	C8-C9-C10	3.19	123.83	118.94
17	b	825	CLA	O2A-CGA-CBA	3.19	121.18	111.90
17	A	831	CLA	C3B-C4B-NB	3.19	113.33	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	834	CLA	C3B-C4B-NB	3.19	113.34	109.21
17	b	833	CLA	O2A-CGA-CBA	3.19	121.20	111.90
17	A	837	CLA	C3B-C4B-NB	3.20	113.34	109.21
26	9	605	CHL	C4-C3-C5	3.20	120.84	115.29
17	b	828	CLA	O2A-CGA-CBA	3.20	121.21	111.90
17	3	310	CLA	C3B-C4B-NB	3.20	113.35	109.21
17	1	315	CLA	C3B-C4B-NB	3.20	113.35	109.21
17	A	854	CLA	O2A-CGA-CBA	3.20	121.22	111.90
17	b	819	CLA	C3B-C4B-NB	3.21	113.35	109.21
17	B	807	CLA	O2A-CGA-CBA	3.21	121.23	111.90
17	L	202	CLA	C3B-C4B-NB	3.21	113.36	109.21
17	3	313	CLA	C3B-C4B-NB	3.21	113.36	109.21
18	A	844	PQN	C14-C13-C15	3.21	120.86	115.29
17	B	816	CLA	C4-C3-C5	3.21	120.86	115.29
17	b	839	CLA	C3B-C4B-NB	3.21	113.36	109.21
17	a	830	CLA	C3B-C4B-NB	3.21	113.37	109.21
17	A	840	CLA	C3B-C4B-NB	3.22	113.37	109.21
17	g	103	CLA	CAC-C3C-C4C	3.22	129.37	124.83
17	B	831	CLA	CAC-C3C-C4C	3.22	129.37	124.83
17	6	310	CLA	C3B-C4B-NB	3.22	113.37	109.21
26	8	306	CHL	O2D-CGD-CBD	3.22	119.05	111.20
17	2	611	CLA	C3B-C4B-NB	3.22	113.37	109.21
17	a	806	CLA	C3B-C4B-NB	3.22	113.38	109.21
17	b	817	CLA	O2A-CGA-CBA	3.23	121.29	111.90
17	A	830	CLA	C3B-C4B-NB	3.23	113.38	109.21
17	6	315	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	1	309	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	a	811	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	6	316	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	A	809	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	8	310	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	6	305	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	A	820	CLA	C3B-C4B-NB	3.23	113.39	109.21
17	g	103	CLA	C3B-C4B-NB	3.24	113.39	109.21
17	b	840	CLA	O2A-CGA-CBA	3.24	121.31	111.90
17	9	611	CLA	O2A-CGA-CBA	3.24	121.32	111.90
17	A	807	CLA	O2A-CGA-CBA	3.24	121.32	111.90
17	G	101	CLA	C3B-C4B-NB	3.24	113.39	109.21
17	A	811	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	a	823	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	a	837	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	3	312	CLA	C3B-C4B-NB	3.24	113.40	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	817	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	9	601	CLA	C3B-C4B-NB	3.24	113.40	109.21
17	3	301	CLA	C3B-C4B-NB	3.25	113.41	109.21
17	B	803	CLA	O2D-CGD-CBD	3.25	117.10	111.30
17	1	312	CLA	C3B-C4B-NB	3.25	113.41	109.21
17	b	824	CLA	C3B-C4B-NB	3.25	113.41	109.21
17	8	309	CLA	C3B-C4B-NB	3.25	113.42	109.21
17	4	601	CLA	C3B-C4B-NB	3.26	113.42	109.21
17	b	837	CLA	O2A-CGA-CBA	3.26	121.39	111.90
17	B	817	CLA	O2A-CGA-CBA	3.26	121.39	111.90
17	8	313	CLA	C3B-C4B-NB	3.26	112.97	110.11
17	A	825	CLA	C3B-C4B-NB	3.27	113.43	109.21
19	a	848	LHG	O8-C23-C24	3.27	120.12	111.35
17	A	824	CLA	C4-C3-C5	3.27	119.72	115.85
17	b	840	CLA	C3B-C4B-NB	3.27	113.44	109.21
17	1	313	CLA	C3B-C4B-NB	3.27	113.44	109.21
17	B	810	CLA	O2A-CGA-CBA	3.27	121.42	111.90
17	B	826	CLA	O2A-CGA-CBA	3.27	121.42	111.90
17	7	603	CLA	C4-C3-C5	3.27	119.72	115.85
17	3	302	CLA	O2A-CGA-CBA	3.27	121.43	111.90
17	8	313	CLA	CHD-C4C-NC	3.28	128.36	124.50
17	a	842	CLA	O2A-CGA-CBA	3.28	121.43	111.90
25	4	620	LMG	O1-C1-C2	3.28	113.58	108.23
17	A	841	CLA	O2A-CGA-CBA	3.28	121.44	111.90
17	A	839	CLA	C3B-C4B-NB	3.28	113.45	109.21
17	2	609	CLA	O2A-CGA-CBA	3.28	121.45	111.90
17	7	612	CLA	C3B-C4B-NB	3.28	113.45	109.21
17	l	202	CLA	C3B-C4B-NB	3.28	113.45	109.21
17	b	805	CLA	O2A-CGA-CBA	3.28	121.45	111.90
17	A	806	CLA	C3B-C4B-NB	3.29	113.46	109.21
17	B	836	CLA	C3B-C4B-NB	3.29	113.46	109.21
17	4	609	CLA	O2A-CGA-CBA	3.29	121.47	111.90
17	B	802	CLA	C3B-C4B-NB	3.29	113.46	109.21
17	4	611	CLA	C3B-C4B-NB	3.29	113.47	109.21
17	4	612	CLA	C3B-C4B-NB	3.29	113.47	109.21
17	a	856	CLA	O2A-CGA-CBA	3.30	121.49	111.90
17	k	1402	CLA	C3B-C4B-NB	3.30	113.47	109.21
17	6	313	CLA	C3B-C4B-NB	3.30	113.48	109.21
17	B	802	CLA	O2A-CGA-CBA	3.30	121.51	111.90
17	b	833	CLA	C3B-C4B-NB	3.30	113.48	109.21
17	1	314	CLA	C3B-C4B-NB	3.30	113.48	109.21
17	A	801	CLA	O2A-CGA-CBA	3.31	121.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	824	CLA	C3B-C4B-NB	3.31	113.49	109.21
17	7	609	CLA	O2A-CGA-CBA	3.32	121.55	111.90
17	a	838	CLA	CMC-C2C-C1C	3.32	130.05	125.02
17	a	840	CLA	C3B-C4B-NB	3.32	113.50	109.21
17	4	603	CLA	C3B-C4B-NB	3.32	113.50	109.21
20	i	101	BCR	C29-C30-C25	3.32	115.67	110.48
17	A	810	CLA	C3B-C4B-NB	3.32	113.51	109.21
17	F	301	CLA	O2A-CGA-CBA	3.32	121.57	111.90
20	I	101	BCR	C29-C30-C25	3.32	115.68	110.48
17	A	824	CLA	C3B-C4B-NB	3.33	113.51	109.21
17	3	315	CLA	C3B-C4B-NB	3.33	113.02	110.11
17	a	821	CLA	C3B-C4B-NB	3.33	113.52	109.21
17	3	315	CLA	CHD-C4C-NC	3.33	128.42	124.50
17	b	829	CLA	C3B-C4B-NB	3.33	113.52	109.21
17	b	805	CLA	C3B-C4B-NB	3.33	113.52	109.21
17	9	611	CLA	C3B-C4B-NB	3.33	113.52	109.21
17	9	609	CLA	O2A-CGA-CBA	3.34	121.61	111.90
17	6	306	CLA	C4-C3-C5	3.34	119.80	115.85
17	1	304	CLA	C3B-C4B-NB	3.34	113.53	109.21
17	b	836	CLA	C3B-C4B-NB	3.34	113.53	109.21
17	b	802	CLA	O2A-CGA-CBA	3.35	121.64	111.90
17	a	802	CLA	O2D-CGD-CBD	3.35	117.28	111.30
17	7	611	CLA	C3B-C4B-NB	3.35	113.54	109.21
17	a	801	CLA	C3B-C4B-NB	3.35	113.54	109.21
17	a	802	CLA	O2A-CGA-CBA	3.35	121.65	111.90
17	a	804	CLA	C3B-C4B-NB	3.35	113.54	109.21
17	B	828	CLA	O2A-CGA-CBA	3.35	121.66	111.90
17	b	808	CLA	C3B-C4B-NB	3.36	113.55	109.21
28	4	617	XAT	O4-C5-C18	3.36	119.22	115.02
17	9	603	CLA	C3B-C4B-NB	3.36	113.55	109.21
17	6	311	CLA	O2A-CGA-CBA	3.37	121.70	111.90
17	B	808	CLA	O2A-CGA-CBA	3.38	121.73	111.90
17	9	602	CLA	O2A-CGA-CBA	3.38	121.74	111.90
17	B	813	CLA	CAC-C3C-C4C	3.39	129.60	124.83
17	A	802	CLA	O2D-CGD-CBD	3.39	117.36	111.30
17	1	310	CLA	O2A-CGA-CBA	3.40	121.78	111.90
26	2	607	CHL	O2D-CGD-CBD	3.40	119.49	111.20
17	a	842	CLA	O2D-CGD-CBD	3.40	117.37	111.30
26	7	605	CHL	O2D-CGD-CBD	3.40	119.50	111.20
17	A	821	CLA	C3B-C4B-NB	3.40	113.61	109.21
26	3	307	CHL	O2D-CGD-CBD	3.42	119.53	111.20
17	a	803	CLA	C3B-C4B-NB	3.42	113.63	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	k	1403	CLA	C3B-C4B-NB	3.42	113.63	109.21
26	7	607	CHL	O2D-CGD-CBD	3.44	119.61	111.20
17	B	825	CLA	O2A-CGA-CBA	3.46	121.96	111.90
17	b	838	CLA	C3B-C4B-NB	3.46	113.69	109.21
17	b	802	CLA	C3B-C4B-NB	3.47	113.69	109.21
17	A	805	CLA	O2A-CGA-CBA	3.47	122.00	111.90
28	3	317	XAT	O4-C5-C18	3.48	119.37	115.02
17	b	825	CLA	O2D-CGD-CBD	3.48	117.51	111.30
17	7	610	CLA	C3B-C4B-NB	3.48	113.72	109.21
26	4	606	CHL	CMD-C2D-C3D	3.49	123.11	114.27
25	6	302	LMG	O8-C28-C29	3.50	120.75	111.35
17	a	829	CLA	O2A-CGA-CBA	3.52	122.13	111.90
17	g	101	CLA	C3B-C4B-NB	3.52	113.76	109.21
17	8	302	CLA	C3B-C4B-NB	3.53	113.78	109.21
17	A	810	CLA	O2A-CGA-CBA	3.54	122.19	111.90
17	3	303	CLA	C3B-C4B-NB	3.55	113.80	109.21
17	B	829	CLA	C3B-C4B-NB	3.56	113.81	109.21
26	4	615	CHL	O2D-CGD-CBD	3.57	119.92	111.20
17	A	808	CLA	C3B-C4B-NB	3.58	113.84	109.21
17	a	810	CLA	O2A-CGA-CBA	3.59	122.34	111.90
17	b	813	CLA	CAC-C3C-C4C	3.59	129.89	124.83
17	a	824	CLA	C4-C3-C5	3.59	120.10	115.85
17	b	802	CLA	O2D-CGD-CBD	3.59	117.72	111.30
17	a	801	CLA	O2A-CGA-CBA	3.59	122.36	111.90
26	2	614	CHL	O2D-CGD-CBD	3.61	120.01	111.20
17	B	838	CLA	C3B-C4B-NB	3.63	113.90	109.21
17	2	610	CLA	C3B-C4B-NB	3.63	113.90	109.21
17	2	603	CLA	O2D-CGD-CBD	3.66	117.84	111.30
17	a	818	CLA	C3B-C4B-NB	3.66	113.94	109.21
17	B	802	CLA	O2D-CGD-CBD	3.67	117.86	111.30
17	a	825	CLA	O2D-CGD-CBD	3.67	117.86	111.30
26	6	308	CHL	O2D-CGD-CBD	3.70	120.23	111.20
28	9	617	XAT	O4-C5-C18	3.71	119.66	115.02
26	7	606	CHL	O2D-CGD-CBD	3.72	120.28	111.20
17	B	823	CLA	O2D-CGD-CBD	3.72	117.95	111.30
17	A	854	CLA	C3B-C4B-NB	3.73	114.03	109.21
17	b	832	CLA	O2A-CGA-CBA	3.74	122.77	111.90
24	B	850	DGD	O2G-C1B-C2B	3.74	119.31	111.55
26	1	307	CHL	O2D-CGD-CBD	3.74	120.33	111.20
25	G	102	LMG	O7-C10-C11	3.75	119.33	111.55
17	B	827	CLA	O2A-CGA-CBA	3.75	122.81	111.90
17	A	841	CLA	O2D-CGD-CBD	3.77	118.04	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	310	CLA	O2D-CGD-CBD	3.78	118.06	111.30
26	4	615	CHL	CMD-C2D-C3D	3.78	123.85	114.27
26	4	605	CHL	O2D-CGD-CBD	3.78	120.44	111.20
26	2	606	CHL	O2D-CGD-CBD	3.80	120.46	111.20
26	8	306	CHL	CMD-C2D-C3D	3.82	123.93	114.27
26	4	606	CHL	O2D-CGD-CBD	3.82	120.53	111.20
26	9	615	CHL	O2D-CGD-CBD	3.82	120.53	111.20
17	a	807	CLA	O2A-CGA-CBA	3.83	123.03	111.90
17	b	808	CLA	O2A-CGA-CBA	3.83	123.04	111.90
17	3	303	CLA	O2D-CGD-CBD	3.84	118.17	111.30
17	F	301	CLA	O2D-CGD-CBD	3.85	118.17	111.30
17	6	304	CLA	C3C-C4C-NC	3.85	114.11	110.21
17	B	806	CLA	O2D-CGD-CBD	3.86	118.19	111.30
17	B	835	CLA	O2D-CGD-CBD	3.86	118.20	111.30
26	7	614	CHL	O2D-CGD-CBD	3.86	120.62	111.20
17	1	309	CLA	O2D-CGD-CBD	3.86	118.20	111.30
26	9	605	CHL	CMD-C2D-C3D	3.87	124.05	114.27
26	9	607	CHL	CMD-C2D-C3D	3.87	124.06	114.27
17	B	825	CLA	O2D-CGD-CBD	3.87	118.21	111.30
26	9	605	CHL	O2D-CGD-CBD	3.87	120.64	111.20
26	2	605	CHL	CMD-C2D-C3D	3.87	124.06	114.27
26	6	308	CHL	CMD-C2D-C3D	3.87	124.07	114.27
26	7	614	CHL	CMD-C2D-C3D	3.88	124.10	114.27
26	4	605	CHL	CMD-C2D-C3D	3.89	124.11	114.27
26	1	307	CHL	CMD-C2D-C3D	3.89	124.12	114.27
25	4	620	LMG	O7-C10-C11	3.90	119.64	111.55
17	b	823	CLA	O2D-CGD-CBD	3.90	118.26	111.30
26	2	601	CHL	CMD-C2D-C3D	3.91	124.16	114.27
26	7	601	CHL	CMD-C2D-C3D	3.91	124.16	114.27
28	3	317	XAT	O24-C25-C38	3.91	119.92	115.02
25	9	619	LMG	O7-C10-C11	3.92	119.68	111.55
17	b	810	CLA	O2D-CGD-CBD	3.92	118.30	111.30
26	9	615	CHL	CMD-C2D-C3D	3.93	124.22	114.27
17	b	806	CLA	O2D-CGD-CBD	3.94	118.33	111.30
17	7	613	CLA	C3C-C4C-NC	3.94	114.20	110.21
25	6	302	LMG	O7-C10-C11	3.94	119.74	111.55
26	9	606	CHL	O2D-CGD-CBD	3.94	120.82	111.20
26	6	303	CHL	CMD-C2D-C3D	3.94	124.25	114.27
17	g	103	CLA	C3C-C4C-NC	3.95	114.22	110.21
26	9	606	CHL	CMD-C2D-C3D	3.96	124.28	114.27
26	3	307	CHL	CMD-C2D-C3D	3.96	124.30	114.27
19	2	618	LHG	O7-C7-C8	3.97	119.80	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	837	CLA	C3C-C4C-NC	3.97	114.23	110.21
26	2	606	CHL	CMD-C2D-C3D	3.97	124.33	114.27
17	a	856	CLA	C3B-C4B-NB	3.98	114.35	109.21
17	a	829	CLA	O2D-CGD-CBD	3.98	118.41	111.30
28	1	317	XAT	O24-C25-C38	3.98	120.00	115.02
17	1	314	CLA	C3C-C4C-NC	3.99	114.25	110.21
17	B	816	CLA	C3C-C4C-NC	3.99	114.25	110.21
17	8	308	CLA	O2D-CGD-CBD	3.99	118.43	111.30
17	A	811	CLA	C3C-C4C-NC	3.99	114.26	110.21
26	2	614	CHL	CMD-C2D-C3D	4.00	124.39	114.27
17	B	803	CLA	C3C-C4C-NC	4.02	114.28	110.21
17	2	602	CLA	C3C-C4C-NC	4.02	114.28	110.21
17	A	820	CLA	C3C-C4C-NC	4.02	114.28	110.21
17	7	609	CLA	C3C-C4C-NC	4.02	114.28	110.21
17	B	820	CLA	O2D-CGD-CBD	4.02	118.49	111.30
17	9	609	CLA	C3C-C4C-NC	4.03	114.29	110.21
17	b	808	CLA	C3C-C4C-NC	4.03	114.30	110.21
17	4	604	CLA	C3C-C4C-NC	4.03	114.30	110.21
17	1	310	CLA	O2D-CGD-CBD	4.04	118.52	111.30
26	7	605	CHL	CMD-C2D-C3D	4.04	124.50	114.27
17	b	817	CLA	C3C-C4C-NC	4.04	114.31	110.21
26	7	606	CHL	CMD-C2D-C3D	4.05	124.51	114.27
17	A	812	CLA	O2D-CGD-CBD	4.05	118.53	111.30
17	6	315	CLA	C3C-C4C-NC	4.05	114.32	110.21
17	B	829	CLA	C3C-C4C-NC	4.06	114.32	110.21
17	9	604	CLA	C3C-C4C-NC	4.06	114.33	110.21
17	a	802	CLA	C3C-C4C-NC	4.06	114.33	110.21
17	k	1403	CLA	C3C-C4C-NC	4.06	114.33	110.21
17	A	836	CLA	O2D-CGD-CBD	4.06	118.56	111.30
17	a	822	CLA	O2D-CGD-CBD	4.07	118.56	111.30
17	3	304	CLA	C3C-C4C-NC	4.07	114.33	110.21
17	1	305	CLA	C3C-C4C-NC	4.07	114.33	110.21
17	g	101	CLA	C3C-C4C-NC	4.07	114.33	110.21
19	1	319	LHG	O7-C7-C8	4.07	120.00	111.55
17	2	608	CLA	C3C-C4C-NC	4.07	114.34	110.21
17	4	609	CLA	C3C-C4C-NC	4.08	114.34	110.21
17	2	609	CLA	C3C-C4C-NC	4.08	114.34	110.21
17	1	304	CLA	C3C-C4C-NC	4.08	114.34	110.21
17	A	843	CLA	C3C-C4C-NC	4.08	114.35	110.21
28	2	616	XAT	O24-C25-C38	4.08	120.13	115.02
17	a	820	CLA	C3C-C4C-NC	4.09	114.35	110.21
19	6	301	LHG	O7-C7-C8	4.09	120.05	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	613	CLA	C3C-C4C-NC	4.09	114.36	110.21
17	A	813	CLA	C3C-C4C-NC	4.10	114.36	110.21
26	1	302	CHL	CMD-C2D-C3D	4.10	124.64	114.27
28	4	617	XAT	O24-C25-C38	4.10	120.16	115.02
17	A	822	CLA	O2D-CGD-CBD	4.10	118.63	111.30
17	4	612	CLA	C3C-C4C-NC	4.11	114.37	110.21
17	8	303	CLA	C3C-C4C-NC	4.11	114.37	110.21
17	b	819	CLA	C3C-C4C-NC	4.11	114.37	110.21
17	8	308	CLA	C3C-C4C-NC	4.11	114.37	110.21
17	8	309	CLA	C3C-C4C-NC	4.11	114.38	110.21
17	9	612	CLA	C3C-C4C-NC	4.12	114.39	110.21
17	B	822	CLA	C3C-C4C-NC	4.12	114.39	110.21
17	1	313	CLA	C3C-C4C-NC	4.13	114.39	110.21
17	A	833	CLA	C3C-C4C-NC	4.13	114.40	110.21
26	4	607	CHL	CMD-C2D-C3D	4.14	124.74	114.27
17	3	301	CLA	C3C-C4C-NC	4.14	114.40	110.21
17	L	202	CLA	C3C-C4C-NC	4.14	114.41	110.21
17	7	604	CLA	C3C-C4C-NC	4.14	114.41	110.21
17	4	609	CLA	O2D-CGD-CBD	4.14	118.70	111.30
17	6	311	CLA	C3C-C4C-NC	4.14	114.41	110.21
17	9	613	CLA	C3C-C4C-NC	4.14	114.41	110.21
17	2	604	CLA	C3C-C4C-NC	4.14	114.41	110.21
17	1	303	CLA	C3C-C4C-NC	4.14	114.41	110.21
26	7	607	CHL	CMD-C2D-C3D	4.15	124.76	114.27
17	4	602	CLA	C3C-C4C-NC	4.15	114.42	110.21
19	A	847	LHG	O7-C7-C8	4.15	120.18	111.55
17	b	828	CLA	O2D-CGD-CBD	4.15	118.72	111.30
17	2	610	CLA	C3C-C4C-NC	4.16	114.42	110.21
26	2	607	CHL	CMD-C2D-C3D	4.16	124.79	114.27
17	9	609	CLA	O2D-CGD-CBD	4.16	118.73	111.30
17	B	819	CLA	O2D-CGD-CBD	4.16	118.73	111.30
17	A	842	CLA	C3C-C4C-NC	4.16	114.43	110.21
17	8	304	CLA	C3C-C4C-NC	4.16	114.43	110.21
17	A	829	CLA	O2D-CGD-CBD	4.16	118.74	111.30
17	7	608	CLA	C3C-C4C-NC	4.16	114.43	110.21
17	3	308	CLA	O2D-CGD-CBD	4.17	118.74	111.30
17	B	834	CLA	C3C-C4C-NC	4.17	114.43	110.21
17	3	308	CLA	C3C-C4C-NC	4.17	114.44	110.21
17	B	810	CLA	C3C-C4C-NC	4.17	114.44	110.21
17	B	808	CLA	C3C-C4C-NC	4.17	114.44	110.21
17	A	817	CLA	C3C-C4C-NC	4.17	114.44	110.21
17	6	311	CLA	O2D-CGD-CBD	4.17	118.75	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	310	CLA	C3C-C4C-NC	4.17	114.44	110.21
17	8	301	CLA	C3C-C4C-NC	4.18	114.44	110.21
17	B	834	CLA	O2D-CGD-CBD	4.18	118.76	111.30
17	b	805	CLA	C3C-C4C-NC	4.18	114.44	110.21
17	L	204	CLA	C3C-C4C-NC	4.18	114.44	110.21
17	4	613	CLA	C3C-C4C-NC	4.18	114.44	110.21
17	9	601	CLA	C3C-C4C-NC	4.18	114.44	110.21
19	6	320	LHG	O7-C7-C8	4.18	120.23	111.55
17	A	835	CLA	C3C-C4C-NC	4.18	114.45	110.21
17	k	1402	CLA	C3C-C4C-NC	4.18	114.45	110.21
17	3	312	CLA	C3C-C4C-NC	4.18	114.45	110.21
17	8	310	CLA	C3C-C4C-NC	4.19	114.45	110.21
25	4	619	LMG	O7-C10-C11	4.19	120.24	111.55
17	6	309	CLA	O2D-CGD-CBD	4.19	118.79	111.30
17	a	820	CLA	O2D-CGD-CBD	4.19	118.79	111.30
17	a	827	CLA	O2D-CGD-CBD	4.19	118.79	111.30
17	1	309	CLA	C3C-C4C-NC	4.19	114.46	110.21
17	3	310	CLA	C3C-C4C-NC	4.19	114.46	110.21
26	1	302	CHL	O2D-CGD-CBD	4.19	121.44	111.20
17	6	305	CLA	C3C-C4C-NC	4.20	114.46	110.21
17	b	819	CLA	O2D-CGD-CBD	4.20	118.80	111.30
17	7	602	CLA	C3C-C4C-NC	4.20	114.47	110.21
17	b	840	CLA	O2D-CGD-CBD	4.20	118.81	111.30
28	8	315	XAT	O24-C25-C38	4.21	120.28	115.02
17	b	806	CLA	C3C-C4C-NC	4.21	114.47	110.21
17	6	313	CLA	C3C-C4C-NC	4.21	114.47	110.21
17	B	812	CLA	C3C-C4C-NC	4.21	114.47	110.21
17	A	813	CLA	O2D-CGD-CBD	4.21	118.82	111.30
17	A	822	CLA	C3C-C4C-NC	4.21	114.48	110.21
17	6	316	CLA	C3C-C4C-NC	4.21	114.48	110.21
17	b	816	CLA	C3C-C4C-NC	4.21	114.48	110.21
28	7	616	XAT	O24-C25-C38	4.22	120.30	115.02
17	b	812	CLA	C3C-C4C-NC	4.22	114.48	110.21
17	B	819	CLA	C3C-C4C-NC	4.22	114.48	110.21
17	F	303	CLA	O2D-CGD-CBD	4.22	118.84	111.30
17	8	307	CLA	O2D-CGD-CBD	4.22	118.84	111.30
17	b	838	CLA	C3C-C4C-NC	4.22	114.49	110.21
17	G	104	CLA	C3C-C4C-NC	4.22	114.49	110.21
17	b	814	CLA	C3C-C4C-NC	4.22	114.49	110.21
28	9	617	XAT	O24-C25-C38	4.22	120.30	115.02
17	1	308	CLA	O2D-CGD-CBD	4.22	118.84	111.30
17	b	830	CLA	C3C-C4C-NC	4.22	114.49	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	805	CLA	C3C-C4C-NC	4.22	114.49	110.21
17	B	822	CLA	O2D-CGD-CBD	4.23	118.85	111.30
17	3	302	CLA	C3C-C4C-NC	4.23	114.49	110.21
17	B	817	CLA	C3C-C4C-NC	4.23	114.50	110.21
17	f	7003	CLA	C3C-C4C-NC	4.23	114.50	110.21
17	2	612	CLA	C3C-C4C-NC	4.23	114.50	110.21
17	b	822	CLA	C3C-C4C-NC	4.24	114.51	110.21
17	7	608	CLA	O2D-CGD-CBD	4.24	118.88	111.30
17	B	804	CLA	C3C-C4C-NC	4.24	114.51	110.21
17	a	841	CLA	O2D-CGD-CBD	4.25	118.89	111.30
17	3	309	CLA	C3C-C4C-NC	4.25	114.51	110.21
17	b	841	CLA	C3C-C4C-NC	4.25	114.51	110.21
17	l	202	CLA	C3C-C4C-NC	4.25	114.51	110.21
17	a	834	CLA	C3C-C4C-NC	4.25	114.51	110.21
17	b	822	CLA	O2D-CGD-CBD	4.25	118.89	111.30
17	1	315	CLA	C3C-C4C-NC	4.25	114.52	110.21
17	F	304	CLA	C3C-C4C-NC	4.25	114.52	110.21
17	b	807	CLA	C3C-C4C-NC	4.25	114.52	110.21
17	b	835	CLA	C3C-C4C-NC	4.25	114.52	110.21
17	A	837	CLA	C3C-C4C-NC	4.25	114.52	110.21
17	4	610	CLA	C3C-C4C-NC	4.25	114.52	110.21
19	7	618	LHG	O7-C7-C8	4.25	120.39	111.55
17	7	612	CLA	C3C-C4C-NC	4.26	114.52	110.21
17	9	610	CLA	C3C-C4C-NC	4.26	114.52	110.21
17	b	839	CLA	O2D-CGD-CBD	4.26	118.91	111.30
17	a	812	CLA	C3C-C4C-NC	4.26	114.53	110.21
17	B	806	CLA	C3C-C4C-NC	4.26	114.53	110.21
17	8	305	CLA	C3C-C4C-NC	4.26	114.53	110.21
17	4	614	CLA	C3C-C4C-NC	4.26	114.53	110.21
19	a	848	LHG	O7-C7-C8	4.27	120.41	111.55
17	a	816	CLA	O2D-CGD-CBD	4.27	118.92	111.30
17	K	4002	CLA	C3C-C4C-NC	4.27	114.53	110.21
17	9	614	CLA	C3C-C4C-NC	4.27	114.53	110.21
17	8	307	CLA	C3C-C4C-NC	4.27	114.54	110.21
17	6	306	CLA	C3C-C4C-NC	4.27	114.54	110.21
17	a	836	CLA	O2D-CGD-CBD	4.27	118.93	111.30
17	b	823	CLA	C3C-C4C-NC	4.27	114.54	110.21
17	a	841	CLA	C3C-C4C-NC	4.27	114.54	110.21
19	A	846	LHG	O7-C7-C8	4.27	120.43	111.55
17	a	811	CLA	C3C-C4C-NC	4.28	114.55	110.21
17	b	818	CLA	C3C-C4C-NC	4.28	114.55	110.21
17	A	806	CLA	C3C-C4C-NC	4.28	114.55	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	309	CLA	O2D-CGD-CBD	4.28	118.96	111.30
17	A	824	CLA	C3C-C4C-NC	4.29	114.55	110.21
17	4	601	CLA	C3C-C4C-NC	4.29	114.55	110.21
26	6	303	CHL	O2D-CGD-CBD	4.29	121.67	111.20
17	b	829	CLA	C3C-C4C-NC	4.29	114.56	110.21
17	A	816	CLA	C3C-C4C-NC	4.29	114.56	110.21
17	7	610	CLA	C3C-C4C-NC	4.29	114.56	110.21
17	B	835	CLA	C3C-C4C-NC	4.30	114.56	110.21
17	a	813	CLA	C3C-C4C-NC	4.30	114.56	110.21
17	A	827	CLA	C3C-C4C-NC	4.30	114.56	110.21
17	A	809	CLA	C3C-C4C-NC	4.30	114.57	110.21
19	a	847	LHG	O7-C7-C8	4.30	120.48	111.55
17	7	603	CLA	C3C-C4C-NC	4.30	114.57	110.21
17	a	819	CLA	O2D-CGD-CBD	4.31	118.99	111.30
17	a	819	CLA	C3C-C4C-NC	4.31	114.57	110.21
17	g	101	CLA	O2D-CGD-CBD	4.31	119.00	111.30
17	a	844	CLA	C3C-C4C-NC	4.31	114.58	110.21
17	1	308	CLA	C3C-C4C-NC	4.31	114.58	110.21
17	6	307	CLA	C3C-C4C-NC	4.31	114.58	110.21
17	9	602	CLA	C3C-C4C-NC	4.32	114.58	110.21
17	6	314	CLA	C3C-C4C-NC	4.32	114.58	110.21
17	a	827	CLA	C3C-C4C-NC	4.32	114.58	110.21
17	3	311	CLA	C3C-C4C-NC	4.32	114.59	110.21
17	b	802	CLA	C3C-C4C-NC	4.32	114.59	110.21
17	B	833	CLA	C3C-C4C-NC	4.32	114.59	110.21
17	2	611	CLA	C3C-C4C-NC	4.32	114.59	110.21
17	J	3002	CLA	C3C-C4C-NC	4.32	114.59	110.21
17	B	837	CLA	C3C-C4C-NC	4.32	114.59	110.21
17	b	813	CLA	C3C-C4C-NC	4.33	114.59	110.21
17	G	101	CLA	C3C-C4C-NC	4.33	114.59	110.21
17	1	306	CLA	C3C-C4C-NC	4.33	114.60	110.21
17	a	822	CLA	C3C-C4C-NC	4.33	114.60	110.21
17	A	807	CLA	C3C-C4C-NC	4.34	114.60	110.21
17	B	841	CLA	C3C-C4C-NC	4.34	114.61	110.21
28	6	318	XAT	O4-C5-C18	4.34	120.45	115.02
17	B	840	CLA	C3C-C4C-NC	4.34	114.61	110.21
17	B	805	CLA	C3C-C4C-NC	4.35	114.61	110.21
17	a	809	CLA	C3C-C4C-NC	4.35	114.61	110.21
17	a	843	CLA	C3C-C4C-NC	4.35	114.62	110.21
17	B	811	CLA	C3C-C4C-NC	4.35	114.62	110.21
17	b	831	CLA	O2D-CGD-CBD	4.35	119.07	111.30
17	a	835	CLA	C3C-C4C-NC	4.35	114.62	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	849	DGD	O2G-C1B-C2B	4.35	120.59	111.55
17	2	603	CLA	C3C-C4C-NC	4.35	114.62	110.21
17	4	608	CLA	C3C-C4C-NC	4.35	114.62	110.21
17	A	810	CLA	O2D-CGD-CBD	4.36	119.08	111.30
17	A	806	CLA	O2D-CGD-CBD	4.36	119.09	111.30
17	A	830	CLA	O2D-CGD-CBD	4.36	119.09	111.30
17	A	845	CLA	C3C-C4C-NC	4.36	114.63	110.21
17	A	802	CLA	C3C-C4C-NC	4.36	114.63	110.21
17	B	830	CLA	C3C-C4C-NC	4.36	114.63	110.21
17	A	815	CLA	C3C-C4C-NC	4.36	114.63	110.21
17	A	812	CLA	C3C-C4C-NC	4.37	114.63	110.21
17	l	204	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	4	611	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	l	203	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	a	815	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	A	814	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	B	839	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	1	311	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	3	313	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	A	819	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	B	831	CLA	O2D-CGD-CBD	4.37	119.11	111.30
17	b	824	CLA	C3C-C4C-NC	4.37	114.64	110.21
17	g	102	CLA	C3C-C4C-NC	4.38	114.65	110.21
17	L	203	CLA	C3C-C4C-NC	4.38	114.65	110.21
17	A	839	CLA	C3C-C4C-NC	4.38	114.65	110.21
17	A	831	CLA	C3C-C4C-NC	4.38	114.65	110.21
17	A	825	CLA	C3C-C4C-NC	4.38	114.65	110.21
17	7	603	CLA	O2D-CGD-CBD	4.38	119.13	111.30
17	j	3002	CLA	C3C-C4C-NC	4.38	114.65	110.21
17	a	818	CLA	C3C-C4C-NC	4.39	114.66	110.21
17	3	305	CLA	C3C-C4C-NC	4.39	114.66	110.21
17	B	828	CLA	C3C-C4C-NC	4.39	114.66	110.21
17	k	1401	CLA	C3C-C4C-NC	4.39	114.66	110.21
17	A	811	CLA	O2D-CGD-CBD	4.39	119.14	111.30
17	b	803	CLA	C3C-C4C-NC	4.39	114.66	110.21
17	a	833	CLA	C3C-C4C-NC	4.39	114.66	110.21
17	F	301	CLA	C3C-C4C-NC	4.40	114.66	110.21
17	a	817	CLA	C3C-C4C-NC	4.40	114.67	110.21
17	G	103	CLA	O2D-CGD-CBD	4.40	119.16	111.30
17	A	808	CLA	C3C-C4C-NC	4.40	114.67	110.21
17	A	804	CLA	C3C-C4C-NC	4.40	114.67	110.21
17	b	828	CLA	C3C-C4C-NC	4.40	114.67	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	832	CLA	C3C-C4C-NC	4.40	114.67	110.21
17	4	608	CLA	O2D-CGD-CBD	4.40	119.17	111.30
17	B	809	CLA	O2D-CGD-CBD	4.41	119.17	111.30
17	2	609	CLA	O2D-CGD-CBD	4.41	119.17	111.30
17	a	846	CLA	C3C-C4C-NC	4.41	114.68	110.21
17	G	103	CLA	C3C-C4C-NC	4.41	114.68	110.21
17	9	608	CLA	O2D-CGD-CBD	4.41	119.18	111.30
17	B	828	CLA	O2D-CGD-CBD	4.41	119.18	111.30
17	3	303	CLA	C3C-C4C-NC	4.42	114.68	110.21
17	b	831	CLA	C3C-C4C-NC	4.42	114.69	110.21
17	A	801	CLA	C3C-C4C-NC	4.42	114.69	110.21
17	a	830	CLA	O2D-CGD-CBD	4.42	119.20	111.30
17	A	840	CLA	C3C-C4C-NC	4.42	114.69	110.21
17	8	302	CLA	C3C-C4C-NC	4.43	114.70	110.21
17	b	835	CLA	O2D-CGD-CBD	4.43	119.21	111.30
17	7	609	CLA	O2D-CGD-CBD	4.43	119.22	111.30
17	B	814	CLA	C3C-C4C-NC	4.43	114.70	110.21
17	F	304	CLA	O2D-CGD-CBD	4.44	119.23	111.30
17	a	840	CLA	C3C-C4C-NC	4.44	114.71	110.21
28	6	318	XAT	O24-C25-C38	4.44	120.58	115.02
17	a	804	CLA	C3C-C4C-NC	4.44	114.71	110.21
17	6	309	CLA	C3C-C4C-NC	4.44	114.71	110.21
17	a	812	CLA	O2D-CGD-CBD	4.44	119.23	111.30
17	9	611	CLA	C3C-C4C-NC	4.44	114.71	110.21
17	B	832	CLA	C3C-C4C-NC	4.44	114.71	110.21
17	f	7002	CLA	O2D-CGD-CBD	4.44	119.24	111.30
17	b	833	CLA	C3C-C4C-NC	4.44	114.71	110.21
17	7	611	CLA	C3C-C4C-NC	4.45	114.72	110.21
17	a	806	CLA	C3C-C4C-NC	4.45	114.72	110.21
17	4	611	CLA	O2D-CGD-CBD	4.45	119.25	111.30
17	4	603	CLA	C3C-C4C-NC	4.45	114.72	110.21
17	9	612	CLA	O2D-CGD-CBD	4.45	119.25	111.30
17	4	610	CLA	O2D-CGD-CBD	4.46	119.27	111.30
17	6	310	CLA	C3C-C4C-NC	4.46	114.73	110.21
17	F	303	CLA	C3C-C4C-NC	4.47	114.73	110.21
17	2	612	CLA	O2D-CGD-CBD	4.47	119.28	111.30
17	6	312	CLA	C3C-C4C-NC	4.47	114.74	110.21
17	K	4003	CLA	C3C-C4C-NC	4.47	114.74	110.21
17	b	820	CLA	C3C-C4C-NC	4.47	114.74	110.21
17	B	807	CLA	C3C-C4C-NC	4.47	114.74	110.21
17	A	838	CLA	C3C-C4C-NC	4.47	114.74	110.21
17	B	813	CLA	C3C-C4C-NC	4.48	114.75	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	9	603	CLA	C3C-C4C-NC	4.48	114.75	110.21
17	B	820	CLA	C3C-C4C-NC	4.48	114.75	110.21
17	A	832	CLA	C3C-C4C-NC	4.48	114.75	110.21
17	b	811	CLA	C3C-C4C-NC	4.48	114.75	110.21
19	1	301	LHG	O7-C7-C8	4.48	120.86	111.55
17	a	839	CLA	C3C-C4C-NC	4.48	114.75	110.21
17	B	831	CLA	C3C-C4C-NC	4.48	114.75	110.21
17	A	818	CLA	C3C-C4C-NC	4.48	114.75	110.21
17	a	844	CLA	O2D-CGD-CBD	4.49	119.31	111.30
17	8	311	CLA	O2D-CGD-CBD	4.49	119.31	111.30
17	B	809	CLA	C3C-C4C-NC	4.49	114.76	110.21
17	7	612	CLA	O2D-CGD-CBD	4.49	119.33	111.30
17	8	310	CLA	O2D-CGD-CBD	4.49	119.33	111.30
17	8	311	CLA	C3C-C4C-NC	4.49	114.76	110.21
17	B	818	CLA	C3C-C4C-NC	4.50	114.77	110.21
17	a	837	CLA	C3C-C4C-NC	4.50	114.77	110.21
17	a	810	CLA	C3C-C4C-NC	4.50	114.77	110.21
17	a	803	CLA	C3C-C4C-NC	4.50	114.77	110.21
17	8	302	CLA	O2D-CGD-CBD	4.50	119.34	111.30
17	a	825	CLA	C3C-C4C-NC	4.50	114.77	110.21
17	b	809	CLA	C3C-C4C-NC	4.50	114.77	110.21
17	a	823	CLA	C3C-C4C-NC	4.50	114.77	110.21
17	b	821	CLA	C3C-C4C-NC	4.50	114.77	110.21
17	A	823	CLA	C3C-C4C-NC	4.51	114.78	110.21
17	6	314	CLA	O2D-CGD-CBD	4.51	119.35	111.30
17	B	840	CLA	O2D-CGD-CBD	4.51	119.36	111.30
17	1	312	CLA	C3C-C4C-NC	4.51	114.78	110.21
17	b	804	CLA	C3C-C4C-NC	4.51	114.78	110.21
17	a	833	CLA	O2D-CGD-CBD	4.51	119.37	111.30
17	3	312	CLA	O2D-CGD-CBD	4.52	119.37	111.30
17	8	304	CLA	O2D-CGD-CBD	4.52	119.37	111.30
17	8	312	CLA	O2D-CGD-CBD	4.52	119.38	111.30
26	2	601	CHL	O2D-CGD-CBD	4.52	122.24	111.20
17	a	842	CLA	C3C-C4C-NC	4.52	114.79	110.21
17	b	834	CLA	C3C-C4C-NC	4.53	114.80	110.21
17	a	838	CLA	C3C-C4C-NC	4.53	114.80	110.21
17	a	824	CLA	C3C-C4C-NC	4.53	114.80	110.21
17	3	313	CLA	O2D-CGD-CBD	4.53	119.40	111.30
17	8	312	CLA	C3C-C4C-NC	4.54	114.81	110.21
17	2	608	CLA	O2D-CGD-CBD	4.54	119.41	111.30
17	B	815	CLA	C3C-C4C-NC	4.54	114.81	110.21
17	b	817	CLA	O2D-CGD-CBD	4.54	119.42	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	840	CLA	C3C-C4C-NC	4.55	114.82	110.21
17	B	839	CLA	O2D-CGD-CBD	4.55	119.43	111.30
17	1	313	CLA	O2D-CGD-CBD	4.55	119.43	111.30
17	a	810	CLA	O2D-CGD-CBD	4.55	119.44	111.30
17	3	315	CLA	C3C-C4C-NC	4.56	114.68	109.99
17	l	204	CLA	O2D-CGD-CBD	4.56	119.44	111.30
17	9	608	CLA	C3C-C4C-NC	4.56	114.83	110.21
17	f	7002	CLA	C3C-C4C-NC	4.56	114.83	110.21
17	A	805	CLA	C3C-C4C-NC	4.56	114.83	110.21
17	6	307	CLA	O2D-CGD-CBD	4.56	119.45	111.30
17	B	838	CLA	C3C-C4C-NC	4.56	114.83	110.21
17	b	815	CLA	C3C-C4C-NC	4.56	114.83	110.21
17	A	827	CLA	O2D-CGD-CBD	4.56	119.45	111.30
17	a	813	CLA	O2D-CGD-CBD	4.56	119.45	111.30
17	b	825	CLA	C3C-C4C-NC	4.56	114.83	110.21
17	B	825	CLA	C3C-C4C-NC	4.57	114.84	110.21
17	B	821	CLA	C3C-C4C-NC	4.57	114.84	110.21
17	8	313	CLA	C3C-C4C-NC	4.57	114.70	109.99
17	a	807	CLA	C3C-C4C-NC	4.57	114.84	110.21
17	3	306	CLA	C3C-C4C-NC	4.58	114.85	110.21
17	A	834	CLA	O2D-CGD-CBD	4.58	119.48	111.30
17	a	811	CLA	O2D-CGD-CBD	4.58	119.48	111.30
17	9	610	CLA	O2D-CGD-CBD	4.59	119.50	111.30
17	a	808	CLA	C3C-C4C-NC	4.59	114.86	110.21
17	a	814	CLA	C3C-C4C-NC	4.59	114.86	110.21
17	a	816	CLA	C3C-C4C-NC	4.60	114.88	110.21
17	B	824	CLA	C3C-C4C-NC	4.61	114.88	110.21
17	A	825	CLA	O2D-CGD-CBD	4.61	119.54	111.30
17	A	843	CLA	O2D-CGD-CBD	4.62	119.55	111.30
17	A	803	CLA	C3C-C4C-NC	4.62	114.89	110.21
17	a	826	CLA	C3C-C4C-NC	4.62	114.89	110.21
17	A	834	CLA	C3C-C4C-NC	4.63	114.90	110.21
17	3	314	CLA	C3C-C4C-NC	4.63	114.90	110.21
17	A	820	CLA	O2D-CGD-CBD	4.63	119.57	111.30
17	B	802	CLA	C3C-C4C-NC	4.63	114.91	110.21
17	B	810	CLA	O2D-CGD-CBD	4.64	119.58	111.30
17	A	841	CLA	C3C-C4C-NC	4.64	114.91	110.21
17	G	101	CLA	O2D-CGD-CBD	4.64	119.60	111.30
17	B	823	CLA	C3C-C4C-NC	4.65	114.92	110.21
17	4	612	CLA	O2D-CGD-CBD	4.65	119.60	111.30
17	a	808	CLA	O2D-CGD-CBD	4.65	119.61	111.30
17	B	811	CLA	O2D-CGD-CBD	4.65	119.61	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	842	CLA	O2D-CGD-CBD	4.66	119.63	111.30
17	A	808	CLA	O2D-CGD-CBD	4.67	119.64	111.30
17	b	834	CLA	O2D-CGD-CBD	4.67	119.65	111.30
17	A	828	CLA	C3C-C4C-NC	4.68	114.95	110.21
17	A	821	CLA	C3C-C4C-NC	4.68	114.96	110.21
17	a	801	CLA	C3C-C4C-NC	4.69	114.96	110.21
17	b	810	CLA	C3C-C4C-NC	4.69	114.96	110.21
17	b	809	CLA	O2D-CGD-CBD	4.70	119.69	111.30
17	b	826	CLA	C3C-C4C-NC	4.70	114.97	110.21
17	B	836	CLA	O2D-CGD-CBD	4.70	119.70	111.30
17	A	829	CLA	C3C-C4C-NC	4.70	114.97	110.21
17	a	805	CLA	O2D-CGD-CBD	4.71	119.71	111.30
17	A	833	CLA	O2D-CGD-CBD	4.71	119.72	111.30
17	A	816	CLA	O2D-CGD-CBD	4.71	119.72	111.30
17	7	610	CLA	O2D-CGD-CBD	4.71	119.72	111.30
17	8	305	CLA	O2D-CGD-CBD	4.72	119.72	111.30
17	a	836	CLA	C3C-C4C-NC	4.72	114.99	110.21
17	B	827	CLA	C3C-C4C-NC	4.72	114.99	110.21
17	b	836	CLA	C3C-C4C-NC	4.72	115.00	110.21
17	1	306	CLA	O2D-CGD-CBD	4.73	119.74	111.30
17	2	604	CLA	O2D-CGD-CBD	4.73	119.75	111.30
28	1	317	XAT	O4-C5-C18	4.73	120.94	115.02
17	B	836	CLA	C3C-C4C-NC	4.73	115.00	110.21
17	a	831	CLA	C3C-C4C-NC	4.73	115.01	110.21
17	a	829	CLA	C3C-C4C-NC	4.74	115.01	110.21
17	B	838	CLA	O2D-CGD-CBD	4.74	119.76	111.30
17	k	1402	CLA	O2D-CGD-CBD	4.74	119.76	111.30
17	a	803	CLA	O2D-CGD-CBD	4.74	119.77	111.30
28	7	616	XAT	O4-C5-C18	4.74	120.96	115.02
17	B	817	CLA	O2D-CGD-CBD	4.75	119.79	111.30
17	6	313	CLA	O2D-CGD-CBD	4.76	119.81	111.30
17	L	203	CLA	O2D-CGD-CBD	4.76	119.81	111.30
17	a	824	CLA	O2D-CGD-CBD	4.76	119.81	111.30
17	a	846	CLA	O2D-CGD-CBD	4.77	119.83	111.30
17	A	824	CLA	O2D-CGD-CBD	4.77	119.83	111.30
17	A	830	CLA	C3C-C4C-NC	4.78	115.06	110.21
17	g	102	CLA	O2D-CGD-CBD	4.79	119.86	111.30
17	a	830	CLA	C3C-C4C-NC	4.79	115.07	110.21
17	b	827	CLA	C3C-C4C-NC	4.80	115.07	110.21
17	A	817	CLA	O2D-CGD-CBD	4.80	119.88	111.30
17	a	806	CLA	O2D-CGD-CBD	4.81	119.89	111.30
17	7	611	CLA	O2D-CGD-CBD	4.81	119.90	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	839	CLA	C3C-C4C-NC	4.81	115.09	110.21
17	6	306	CLA	O2D-CGD-CBD	4.81	119.90	111.30
17	j	3002	CLA	O2D-CGD-CBD	4.82	119.91	111.30
26	7	601	CHL	O2D-CGD-CBD	4.82	122.95	111.20
17	B	812	CLA	O2D-CGD-CBD	4.83	119.92	111.30
17	3	314	CLA	O2D-CGD-CBD	4.83	119.94	111.30
17	A	810	CLA	C3C-C4C-NC	4.84	115.11	110.21
17	a	834	CLA	O2D-CGD-CBD	4.84	119.94	111.30
17	a	832	CLA	C3C-C4C-NC	4.84	115.11	110.21
17	L	204	CLA	O2D-CGD-CBD	4.84	119.95	111.30
17	4	604	CLA	O2D-CGD-CBD	4.84	119.95	111.30
17	2	610	CLA	O2D-CGD-CBD	4.84	119.95	111.30
17	b	812	CLA	O2D-CGD-CBD	4.84	119.96	111.30
17	3	306	CLA	O2D-CGD-CBD	4.85	119.96	111.30
17	a	821	CLA	C3C-C4C-NC	4.85	115.12	110.21
17	A	838	CLA	O2D-CGD-CBD	4.85	119.97	111.30
17	a	817	CLA	O2D-CGD-CBD	4.85	119.97	111.30
17	a	815	CLA	O2D-CGD-CBD	4.86	119.98	111.30
17	G	104	CLA	O2D-CGD-CBD	4.86	119.98	111.30
17	A	826	CLA	C3C-C4C-NC	4.86	115.14	110.21
17	B	827	CLA	O2D-CGD-CBD	4.87	120.00	111.30
17	6	312	CLA	O2D-CGD-CBD	4.87	120.00	111.30
17	2	611	CLA	O2D-CGD-CBD	4.87	120.01	111.30
17	1	312	CLA	O2D-CGD-CBD	4.89	120.03	111.30
17	A	836	CLA	C3C-C4C-NC	4.89	115.16	110.21
17	7	613	CLA	O2D-CGD-CBD	4.89	120.04	111.30
17	7	604	CLA	O2D-CGD-CBD	4.89	120.05	111.30
17	a	856	CLA	C3C-C4C-NC	4.90	115.17	110.21
17	A	819	CLA	O2D-CGD-CBD	4.93	120.11	111.30
17	a	832	CLA	O2D-CGD-CBD	4.93	120.11	111.30
17	A	803	CLA	O2D-CGD-CBD	4.93	120.11	111.30
17	2	602	CLA	O2D-CGD-CBD	4.94	120.12	111.30
17	L	202	CLA	O2D-CGD-CBD	4.94	120.13	111.30
17	6	316	CLA	O2D-CGD-CBD	4.95	120.15	111.30
17	b	838	CLA	O2D-CGD-CBD	4.96	120.16	111.30
28	2	616	XAT	O4-C5-C18	4.96	121.23	115.02
17	3	311	CLA	O2D-CGD-CBD	4.97	120.18	111.30
17	b	832	CLA	O2D-CGD-CBD	4.97	120.18	111.30
17	9	611	CLA	O2D-CGD-CBD	4.98	120.20	111.30
17	J	3002	CLA	O2D-CGD-CBD	4.99	120.21	111.30
17	1	305	CLA	O2D-CGD-CBD	5.00	120.23	111.30
17	1	315	CLA	O2D-CGD-CBD	5.00	120.23	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	305	CLA	O2D-CGD-CBD	5.00	120.24	111.30
17	b	826	CLA	O2D-CGD-CBD	5.01	120.25	111.30
17	b	827	CLA	O2D-CGD-CBD	5.02	120.28	111.30
17	6	305	CLA	O2D-CGD-CBD	5.03	120.28	111.30
17	1	304	CLA	O2D-CGD-CBD	5.03	120.28	111.30
17	B	826	CLA	C3C-C4C-NC	5.03	115.31	110.21
17	4	602	CLA	O2D-CGD-CBD	5.03	120.29	111.30
17	3	302	CLA	O2D-CGD-CBD	5.05	120.31	111.30
17	6	304	CLA	O2D-CGD-CBD	5.05	120.32	111.30
17	A	854	CLA	C3C-C4C-NC	5.05	115.33	110.21
17	8	309	CLA	O2D-CGD-CBD	5.06	120.35	111.30
17	B	814	CLA	O2D-CGD-CBD	5.07	120.37	111.30
17	b	816	CLA	O2D-CGD-CBD	5.08	120.37	111.30
17	a	807	CLA	O2D-CGD-CBD	5.08	120.37	111.30
17	a	837	CLA	O2D-CGD-CBD	5.08	120.37	111.30
17	a	828	CLA	C3C-C4C-NC	5.09	115.37	110.21
17	A	821	CLA	O2D-CGD-CBD	5.10	120.41	111.30
17	8	301	CLA	O2D-CGD-CBD	5.10	120.42	111.30
17	a	804	CLA	O2D-CGD-CBD	5.12	120.44	111.30
17	B	832	CLA	O2D-CGD-CBD	5.13	120.46	111.30
17	9	603	CLA	O2D-CGD-CBD	5.13	120.46	111.30
17	A	801	CLA	O2D-CGD-CBD	5.13	120.46	111.30
17	f	7003	CLA	O2D-CGD-CBD	5.13	120.47	111.30
17	B	813	CLA	O2D-CGD-CBD	5.13	120.47	111.30
17	A	815	CLA	O2D-CGD-CBD	5.14	120.48	111.30
17	4	614	CLA	O2D-CGD-CBD	5.14	120.48	111.30
17	1	311	CLA	O2D-CGD-CBD	5.14	120.49	111.30
17	9	613	CLA	O2D-CGD-CBD	5.14	120.49	111.30
17	B	818	CLA	O2D-CGD-CBD	5.15	120.50	111.30
17	K	4003	CLA	O2D-CGD-CBD	5.15	120.50	111.30
17	b	836	CLA	O2D-CGD-CBD	5.15	120.51	111.30
17	4	613	CLA	O2D-CGD-CBD	5.15	120.51	111.30
17	l	202	CLA	O2D-CGD-CBD	5.17	120.54	111.30
17	B	805	CLA	O2D-CGD-CBD	5.19	120.57	111.30
17	B	807	CLA	O2D-CGD-CBD	5.19	120.57	111.30
17	a	823	CLA	O2D-CGD-CBD	5.19	120.58	111.30
17	3	304	CLA	O2D-CGD-CBD	5.20	120.58	111.30
17	b	807	CLA	O2D-CGD-CBD	5.21	120.61	111.30
17	B	815	CLA	O2D-CGD-CBD	5.21	120.62	111.30
17	9	614	CLA	O2D-CGD-CBD	5.23	120.64	111.30
17	B	826	CLA	O2D-CGD-CBD	5.23	120.64	111.30
17	b	820	CLA	O2D-CGD-CBD	5.24	120.66	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	k	1401	CLA	O2D-CGD-CBD	5.25	120.68	111.30
17	9	604	CLA	O2D-CGD-CBD	5.25	120.69	111.30
17	B	816	CLA	O2D-CGD-CBD	5.26	120.69	111.30
17	A	837	CLA	O2D-CGD-CBD	5.27	120.72	111.30
26	7	601	CHL	C3B-C4B-NB	5.27	112.74	103.55
17	A	832	CLA	O2D-CGD-CBD	5.28	120.73	111.30
17	b	805	CLA	O2D-CGD-CBD	5.28	120.74	111.30
17	b	821	CLA	O2D-CGD-CBD	5.28	120.74	111.30
17	B	833	CLA	O2D-CGD-CBD	5.29	120.76	111.30
17	a	814	CLA	O2D-CGD-CBD	5.29	120.76	111.30
17	b	813	CLA	O2D-CGD-CBD	5.31	120.79	111.30
17	1	314	CLA	O2D-CGD-CBD	5.31	120.79	111.30
17	1	303	CLA	O2D-CGD-CBD	5.32	120.80	111.30
17	a	843	CLA	O2D-CGD-CBD	5.33	120.82	111.30
17	a	801	CLA	O2D-CGD-CBD	5.35	120.85	111.30
17	4	603	CLA	O2D-CGD-CBD	5.35	120.87	111.30
17	6	315	CLA	O2D-CGD-CBD	5.36	120.87	111.30
17	A	845	CLA	O2D-CGD-CBD	5.37	120.89	111.30
17	a	821	CLA	O2D-CGD-CBD	5.37	120.90	111.30
17	g	103	CLA	O2D-CGD-CBD	5.37	120.90	111.30
17	7	602	CLA	O2D-CGD-CBD	5.38	120.91	111.30
17	K	4002	CLA	O2D-CGD-CBD	5.39	120.93	111.30
17	A	823	CLA	O2D-CGD-CBD	5.41	120.96	111.30
17	b	811	CLA	O2D-CGD-CBD	5.41	120.97	111.30
17	a	828	CLA	O2D-CGD-CBD	5.42	120.98	111.30
17	b	814	CLA	O2D-CGD-CBD	5.44	121.02	111.30
17	B	824	CLA	O2D-CGD-CBD	5.44	121.02	111.30
17	l	203	CLA	O2D-CGD-CBD	5.45	121.05	111.30
26	2	607	CHL	C3B-C4B-NB	5.46	113.07	103.55
17	a	838	CLA	O2D-CGD-CBD	5.46	121.06	111.30
26	1	302	CHL	C3B-C4B-NB	5.47	113.09	103.55
17	3	301	CLA	O2D-CGD-CBD	5.47	121.08	111.30
17	B	830	CLA	O2D-CGD-CBD	5.49	121.11	111.30
26	4	606	CHL	C3B-C4B-NB	5.49	113.12	103.55
17	b	818	CLA	O2D-CGD-CBD	5.51	121.14	111.30
26	7	605	CHL	C3B-C4B-NB	5.52	113.17	103.55
26	2	601	CHL	C3B-C4B-NB	5.52	113.18	103.55
17	B	814	CLA	C2C-C1C-NC	5.52	114.02	110.22
17	b	833	CLA	O2D-CGD-CBD	5.53	121.18	111.30
26	4	615	CHL	C3B-C4B-NB	5.53	113.19	103.55
26	8	306	CHL	C3B-C4B-NB	5.55	113.23	103.55
17	2	613	CLA	O2D-CGD-CBD	5.57	121.25	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	605	CHL	C3B-C4B-NB	5.57	113.27	103.55
26	6	303	CHL	C3B-C4B-NB	5.58	113.27	103.55
17	a	840	CLA	O2D-CGD-CBD	5.58	121.27	111.30
17	9	601	CLA	O2D-CGD-CBD	5.59	121.29	111.30
26	7	607	CHL	C3B-C4B-NB	5.59	113.30	103.55
26	2	605	CHL	C3B-C4B-NB	5.60	113.31	103.55
17	A	807	CLA	O2D-CGD-CBD	5.60	121.32	111.30
26	4	607	CHL	C3B-C4B-NB	5.63	113.36	103.55
26	9	615	CHL	C3B-C4B-NB	5.63	113.36	103.55
17	A	814	CLA	O2D-CGD-CBD	5.63	121.37	111.30
17	B	821	CLA	O2D-CGD-CBD	5.65	121.40	111.30
17	9	602	CLA	O2D-CGD-CBD	5.66	121.42	111.30
26	9	607	CHL	C3B-C4B-NB	5.66	113.42	103.55
26	6	308	CHL	C3B-C4B-NB	5.66	113.42	103.55
17	b	830	CLA	O2D-CGD-CBD	5.67	121.44	111.30
17	a	838	CLA	C2C-C1C-NC	5.67	114.12	110.22
26	2	606	CHL	C3B-C4B-NB	5.67	113.44	103.55
17	7	609	CLA	C2C-C1C-NC	5.68	114.13	110.22
26	1	307	CHL	C3B-C4B-NB	5.68	113.45	103.55
26	7	606	CHL	C3B-C4B-NB	5.69	113.47	103.55
26	9	606	CHL	C3B-C4B-NB	5.69	113.48	103.55
17	A	839	CLA	O2D-CGD-CBD	5.70	121.48	111.30
17	9	602	CLA	C2C-C1C-NC	5.70	114.14	110.22
17	8	303	CLA	O2D-CGD-CBD	5.71	121.50	111.30
17	A	828	CLA	O2D-CGD-CBD	5.71	121.50	111.30
17	2	609	CLA	C2C-C1C-NC	5.71	114.15	110.22
26	4	605	CHL	C3B-C4B-NB	5.71	113.51	103.55
17	b	814	CLA	C2C-C1C-NC	5.73	114.16	110.22
17	a	809	CLA	O2D-CGD-CBD	5.74	121.55	111.30
17	k	1403	CLA	O2D-CGD-CBD	5.74	121.56	111.30
17	A	826	CLA	O2D-CGD-CBD	5.74	121.56	111.30
17	4	601	CLA	O2D-CGD-CBD	5.75	121.57	111.30
17	a	839	CLA	O2D-CGD-CBD	5.75	121.58	111.30
17	3	309	CLA	C2C-C1C-NC	5.76	114.18	110.22
17	b	803	CLA	C2C-C1C-NC	5.76	114.18	110.22
17	B	803	CLA	C2C-C1C-NC	5.76	114.18	110.22
28	7	616	XAT	O4-C5-C4	5.77	117.51	113.33
17	8	301	CLA	C2C-C1C-NC	5.77	114.19	110.22
17	a	835	CLA	O2D-CGD-CBD	5.78	121.64	111.30
26	3	307	CHL	C3B-C4B-NB	5.79	113.64	103.55
26	2	614	CHL	C3B-C4B-NB	5.79	113.64	103.55
17	A	809	CLA	O2D-CGD-CBD	5.79	121.65	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	308	CLA	C2C-C1C-NC	5.79	114.21	110.22
17	6	311	CLA	C2C-C1C-NC	5.80	114.21	110.22
17	A	802	CLA	C2C-C1C-NC	5.81	114.22	110.22
17	a	818	CLA	O2D-CGD-CBD	5.81	121.68	111.30
17	b	824	CLA	O2D-CGD-CBD	5.82	121.69	111.30
26	7	614	CHL	C3B-C4B-NB	5.82	113.69	103.55
17	l	203	CLA	C2C-C1C-NC	5.83	114.23	110.22
17	A	827	CLA	C2C-C1C-NC	5.83	114.23	110.22
17	A	828	CLA	C2C-C1C-NC	5.85	114.24	110.22
17	B	837	CLA	O2D-CGD-CBD	5.87	121.79	111.30
17	A	818	CLA	O2D-CGD-CBD	5.87	121.80	111.30
17	A	804	CLA	O2D-CGD-CBD	5.88	121.81	111.30
17	A	840	CLA	O2D-CGD-CBD	5.90	121.84	111.30
17	B	804	CLA	O2D-CGD-CBD	5.90	121.85	111.30
17	4	609	CLA	C2C-C1C-NC	5.90	114.28	110.22
17	b	837	CLA	O2D-CGD-CBD	5.91	121.85	111.30
17	a	819	CLA	C2C-C1C-NC	5.92	114.30	110.22
26	4	605	CHL	C4B-CHC-C1C	5.94	125.03	112.37
17	4	602	CLA	C2C-C1C-NC	5.94	114.31	110.22
17	B	841	CLA	O2D-CGD-CBD	5.94	121.92	111.30
17	7	602	CLA	C2C-C1C-NC	5.95	114.32	110.22
17	b	806	CLA	C2C-C1C-NC	5.95	114.32	110.22
26	8	306	CHL	C4B-CHC-C1C	5.96	125.08	112.37
17	l	306	CLA	C2C-C1C-NC	5.96	114.32	110.22
17	b	841	CLA	O2D-CGD-CBD	6.00	122.02	111.30
17	a	843	CLA	C2C-C1C-NC	6.00	114.35	110.22
17	B	841	CLA	C2C-C1C-NC	6.01	114.36	110.22
17	B	825	CLA	C2C-C1C-NC	6.02	114.36	110.22
17	b	815	CLA	O2D-CGD-CBD	6.03	122.07	111.30
17	a	827	CLA	C2C-C1C-NC	6.03	114.37	110.22
17	B	829	CLA	O2D-CGD-CBD	6.03	122.08	111.30
17	b	825	CLA	C2C-C1C-NC	6.04	114.38	110.22
17	9	609	CLA	C2C-C1C-NC	6.05	114.39	110.22
26	4	607	CHL	C4B-CHC-C1C	6.05	125.27	112.37
17	a	826	CLA	O2D-CGD-CBD	6.06	122.12	111.30
17	a	814	CLA	C2C-C1C-NC	6.06	114.39	110.22
17	a	833	CLA	C2C-C1C-NC	6.07	114.39	110.22
26	6	308	CHL	C4B-CHC-C1C	6.07	125.30	112.37
17	L	203	CLA	C2C-C1C-NC	6.07	114.40	110.22
26	7	607	CHL	CMB-C2B-C3B	6.07	127.82	113.69
17	3	302	CLA	C2C-C1C-NC	6.08	114.40	110.22
17	8	307	CLA	C2C-C1C-NC	6.08	114.41	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	815	CLA	C2C-C1C-NC	6.09	114.41	110.22
17	1	303	CLA	C2C-C1C-NC	6.09	114.41	110.22
17	a	831	CLA	O2D-CGD-CBD	6.10	122.19	111.30
26	9	605	CHL	C4B-CHC-C1C	6.10	125.37	112.37
17	b	832	CLA	C2C-C1C-NC	6.10	114.42	110.22
17	b	841	CLA	C2C-C1C-NC	6.11	114.43	110.22
17	A	841	CLA	C2C-C1C-NC	6.11	114.43	110.22
17	A	835	CLA	O2D-CGD-CBD	6.12	122.23	111.30
17	a	809	CLA	C2C-C1C-NC	6.12	114.43	110.22
17	a	802	CLA	C2C-C1C-NC	6.12	114.43	110.22
17	a	808	CLA	C2C-C1C-NC	6.14	114.45	110.22
17	A	838	CLA	C2C-C1C-NC	6.14	114.45	110.22
26	6	303	CHL	C4B-CHC-C1C	6.16	125.49	112.37
17	B	806	CLA	C2C-C1C-NC	6.16	114.46	110.22
17	B	832	CLA	C2C-C1C-NC	6.17	114.47	110.22
17	b	822	CLA	C2C-C1C-NC	6.17	114.47	110.22
26	4	606	CHL	C4B-CHC-C1C	6.18	125.53	112.37
26	1	307	CHL	C4B-CHC-C1C	6.18	125.54	112.37
17	A	831	CLA	O2D-CGD-CBD	6.18	122.35	111.30
17	3	315	CLA	C2D-C1D-ND	6.20	115.53	110.14
17	A	806	CLA	C2C-C1C-NC	6.21	114.49	110.22
17	B	826	CLA	C2C-C1C-NC	6.21	114.49	110.22
26	2	605	CHL	C4B-CHC-C1C	6.21	125.60	112.37
17	2	602	CLA	C2C-C1C-NC	6.23	114.51	110.22
26	1	302	CHL	C4B-CHC-C1C	6.23	125.65	112.37
17	a	856	CLA	O2D-CGD-CBD	6.24	122.45	111.30
17	a	807	CLA	C2C-C1C-NC	6.24	114.51	110.22
26	9	607	CHL	C4B-CHC-C1C	6.24	125.67	112.37
17	B	808	CLA	O2D-CGD-CBD	6.24	122.45	111.30
17	b	827	CLA	C2C-C1C-NC	6.24	114.52	110.22
17	1	310	CLA	C2C-C1C-NC	6.25	114.52	110.22
17	B	813	CLA	C2C-C1C-NC	6.26	114.53	110.22
28	2	616	XAT	O4-C5-C4	6.26	117.87	113.33
17	b	829	CLA	O2D-CGD-CBD	6.26	122.49	111.30
17	b	810	CLA	C2C-C1C-NC	6.27	114.53	110.22
26	3	307	CHL	C4B-CHC-C1C	6.27	125.73	112.37
17	8	313	CLA	C2D-C1D-ND	6.28	115.60	110.14
26	2	607	CHL	C4B-CHC-C1C	6.28	125.75	112.37
17	A	815	CLA	C2C-C1C-NC	6.29	114.55	110.22
17	a	806	CLA	C2C-C1C-NC	6.30	114.56	110.22
17	b	828	CLA	C2C-C1C-NC	6.31	114.56	110.22
28	1	317	XAT	O4-C5-C4	6.31	117.91	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	605	CHL	C4B-CHC-C1C	6.31	125.82	112.37
17	A	819	CLA	C2C-C1C-NC	6.31	114.56	110.22
26	7	614	CHL	C4B-CHC-C1C	6.32	125.84	112.37
26	4	607	CHL	CMB-C2B-C3B	6.32	128.39	113.69
17	A	809	CLA	C2C-C1C-NC	6.32	114.57	110.22
17	3	308	CLA	C2C-C1C-NC	6.33	114.58	110.22
17	B	837	CLA	C2C-C1C-NC	6.34	114.58	110.22
17	a	816	CLA	C2C-C1C-NC	6.34	114.58	110.22
17	b	808	CLA	O2D-CGD-CBD	6.34	122.64	111.30
26	7	607	CHL	C4B-CHC-C1C	6.36	125.92	112.37
17	a	844	CLA	C2C-C1C-NC	6.36	114.60	110.22
17	B	824	CLA	C2C-C1C-NC	6.36	114.60	110.22
17	a	828	CLA	C2C-C1C-NC	6.37	114.60	110.22
26	6	303	CHL	CMB-C2B-C3B	6.37	128.51	113.69
26	4	615	CHL	C4B-CHC-C1C	6.37	125.95	112.37
17	A	833	CLA	C2C-C1C-NC	6.38	114.61	110.22
17	L	204	CLA	C2C-C1C-NC	6.38	114.61	110.22
26	9	615	CHL	C4B-CHC-C1C	6.39	125.99	112.37
26	2	601	CHL	C4B-CHC-C1C	6.39	126.00	112.37
17	A	805	CLA	O2D-CGD-CBD	6.40	122.73	111.30
17	b	826	CLA	C2C-C1C-NC	6.40	114.62	110.22
17	a	804	CLA	C2C-C1C-NC	6.40	114.62	110.22
17	A	826	CLA	C2C-C1C-NC	6.40	114.62	110.22
17	A	842	CLA	C2C-C1C-NC	6.40	114.63	110.22
17	G	104	CLA	C2C-C1C-NC	6.40	114.63	110.22
17	B	827	CLA	C2C-C1C-NC	6.41	114.63	110.22
17	b	837	CLA	C2C-C1C-NC	6.41	114.63	110.22
17	b	813	CLA	C2C-C1C-NC	6.41	114.63	110.22
17	A	820	CLA	C2C-C1C-NC	6.42	114.64	110.22
17	A	854	CLA	O2D-CGD-CBD	6.42	122.77	111.30
17	b	830	CLA	C2C-C1C-NC	6.43	114.64	110.22
17	a	841	CLA	C2C-C1C-NC	6.43	114.65	110.22
17	B	822	CLA	C2C-C1C-NC	6.44	114.65	110.22
26	2	606	CHL	C4B-CHC-C1C	6.44	126.09	112.37
17	9	604	CLA	C2C-C1C-NC	6.44	114.65	110.22
17	B	805	CLA	C2C-C1C-NC	6.45	114.66	110.22
17	6	304	CLA	C2C-C1C-NC	6.45	114.66	110.22
26	7	601	CHL	C4B-CHC-C1C	6.46	126.13	112.37
17	A	805	CLA	C2C-C1C-NC	6.46	114.67	110.22
26	4	605	CHL	CMB-C2B-C3B	6.46	128.72	113.69
17	B	830	CLA	C2C-C1C-NC	6.46	114.67	110.22
26	2	614	CHL	C4B-CHC-C1C	6.46	126.14	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	824	CLA	C2C-C1C-NC	6.46	114.67	110.22
26	9	606	CHL	C4B-CHC-C1C	6.47	126.16	112.37
17	a	834	CLA	C2C-C1C-NC	6.47	114.67	110.22
26	2	601	CHL	CMB-C2B-C3B	6.48	128.78	113.69
26	1	302	CHL	CMB-C2B-C3B	6.49	128.78	113.69
17	l	204	CLA	C2C-C1C-NC	6.49	114.69	110.22
17	b	823	CLA	C2C-C1C-NC	6.49	114.69	110.22
17	a	826	CLA	C2C-C1C-NC	6.49	114.69	110.22
17	a	812	CLA	C2C-C1C-NC	6.51	114.70	110.22
17	B	810	CLA	C2C-C1C-NC	6.51	114.70	110.22
17	B	835	CLA	C2C-C1C-NC	6.51	114.70	110.22
26	7	606	CHL	C4B-CHC-C1C	6.51	126.25	112.37
17	A	829	CLA	C2C-C1C-NC	6.51	114.70	110.22
17	B	833	CLA	C2C-C1C-NC	6.52	114.71	110.22
17	7	608	CLA	C2C-C1C-NC	6.52	114.71	110.22
17	B	802	CLA	C2C-C1C-NC	6.53	114.71	110.22
26	9	605	CHL	CMB-C2B-C3B	6.53	128.89	113.69
17	B	807	CLA	C2C-C1C-NC	6.54	114.72	110.22
17	b	804	CLA	O2D-CGD-CBD	6.54	122.99	111.30
17	B	816	CLA	C2C-C1C-NC	6.55	114.72	110.22
17	1	305	CLA	C2C-C1C-NC	6.55	114.73	110.22
17	8	304	CLA	C2C-C1C-NC	6.55	114.73	110.22
17	B	823	CLA	C2C-C1C-NC	6.55	114.73	110.22
17	B	817	CLA	C2C-C1C-NC	6.55	114.73	110.22
17	b	807	CLA	C2C-C1C-NC	6.56	114.73	110.22
17	8	303	CLA	C2C-C1C-NC	6.56	114.73	110.22
26	9	607	CHL	CMB-C2B-C3B	6.56	128.95	113.69
17	B	840	CLA	C2C-C1C-NC	6.56	114.74	110.22
17	G	103	CLA	C2C-C1C-NC	6.56	114.74	110.22
17	A	807	CLA	C2C-C1C-NC	6.57	114.74	110.22
26	7	605	CHL	CMB-C2B-C3B	6.57	128.97	113.69
17	b	836	CLA	C2C-C1C-NC	6.57	114.74	110.22
17	B	831	CLA	C2C-C1C-NC	6.57	114.74	110.22
17	6	307	CLA	C2C-C1C-NC	6.58	114.75	110.22
17	8	313	CLA	C2B-C1B-NB	6.58	115.87	110.11
17	9	603	CLA	C2C-C1C-NC	6.58	114.75	110.22
17	3	315	CLA	C2B-C1B-NB	6.58	115.88	110.11
17	a	829	CLA	C2C-C1C-NC	6.59	114.75	110.22
17	b	820	CLA	C2C-C1C-NC	6.59	114.75	110.22
17	4	610	CLA	C2C-C1C-NC	6.59	114.75	110.22
17	A	814	CLA	C2C-C1C-NC	6.59	114.75	110.22
17	A	801	CLA	C2C-C1C-NC	6.59	114.76	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	839	CLA	C2C-C1C-NC	6.59	114.76	110.22
17	k	1401	CLA	C2C-C1C-NC	6.60	114.76	110.22
17	2	613	CLA	C2C-C1C-NC	6.60	114.76	110.22
17	a	805	CLA	C2C-C1C-NC	6.60	114.76	110.22
17	b	804	CLA	C2C-C1C-NC	6.61	114.77	110.22
28	3	317	XAT	O24-C25-C24	6.61	118.13	113.33
17	F	304	CLA	C2C-C1C-NC	6.61	114.77	110.22
17	a	822	CLA	C2C-C1C-NC	6.62	114.77	110.22
17	B	811	CLA	C2C-C1C-NC	6.62	114.77	110.22
17	B	828	CLA	C2C-C1C-NC	6.62	114.77	110.22
17	A	812	CLA	C2C-C1C-NC	6.62	114.77	110.22
17	B	836	CLA	C2C-C1C-NC	6.62	114.77	110.22
17	b	802	CLA	C2C-C1C-NC	6.62	114.78	110.22
26	2	607	CHL	CMB-C2B-C3B	6.62	129.10	113.69
26	2	614	CHL	CMB-C2B-C3B	6.62	129.10	113.69
26	8	306	CHL	CMB-C2B-C3B	6.63	129.10	113.69
17	A	818	CLA	C2C-C1C-NC	6.63	114.78	110.22
17	f	7002	CLA	C2C-C1C-NC	6.63	114.78	110.22
17	3	304	CLA	C2C-C1C-NC	6.63	114.78	110.22
17	b	811	CLA	C2C-C1C-NC	6.63	114.78	110.22
26	7	601	CHL	CMB-C2B-C3B	6.63	129.12	113.69
17	2	612	CLA	C2C-C1C-NC	6.63	114.78	110.22
17	B	812	CLA	C2C-C1C-NC	6.64	114.79	110.22
17	9	610	CLA	C2C-C1C-NC	6.64	114.79	110.22
26	3	307	CHL	CMB-C2B-C3B	6.64	129.13	113.69
17	a	835	CLA	C2C-C1C-NC	6.65	114.80	110.22
17	b	808	CLA	C2C-C1C-NC	6.65	114.80	110.22
17	A	811	CLA	C2C-C1C-NC	6.66	114.80	110.22
17	6	316	CLA	C2C-C1C-NC	6.66	114.80	110.22
17	b	812	CLA	C2C-C1C-NC	6.66	114.80	110.22
26	7	606	CHL	CMB-C2B-C3B	6.66	129.18	113.69
17	1	308	CLA	C2C-C1C-NC	6.66	114.80	110.22
17	a	831	CLA	C2C-C1C-NC	6.67	114.81	110.22
17	A	822	CLA	C2C-C1C-NC	6.67	114.81	110.22
17	A	830	CLA	C2C-C1C-NC	6.67	114.81	110.22
17	4	614	CLA	C2C-C1C-NC	6.67	114.81	110.22
26	7	614	CHL	CMB-C2B-C3B	6.67	129.22	113.69
17	4	603	CLA	C2C-C1C-NC	6.68	114.81	110.22
17	3	306	CLA	C2C-C1C-NC	6.68	114.81	110.22
17	g	103	CLA	C2C-C1C-NC	6.69	114.82	110.22
17	a	820	CLA	C2C-C1C-NC	6.69	114.82	110.22
17	6	309	CLA	C2C-C1C-NC	6.69	114.82	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	604	CLA	C2C-C1C-NC	6.69	114.82	110.22
26	2	605	CHL	CMB-C2B-C3B	6.70	129.27	113.69
17	a	830	CLA	C2C-C1C-NC	6.70	114.83	110.22
17	A	804	CLA	C2C-C1C-NC	6.70	114.83	110.22
17	a	823	CLA	C2C-C1C-NC	6.70	114.83	110.22
26	9	606	CHL	CMB-C2B-C3B	6.71	129.29	113.69
17	a	810	CLA	C2C-C1C-NC	6.71	114.84	110.22
26	2	606	CHL	CMB-C2B-C3B	6.71	129.30	113.69
28	8	315	XAT	O24-C25-C24	6.71	118.20	113.33
28	4	617	XAT	O24-C25-C24	6.72	118.21	113.33
17	2	611	CLA	C2C-C1C-NC	6.72	114.84	110.22
17	A	823	CLA	C2C-C1C-NC	6.72	114.84	110.22
17	B	815	CLA	C2C-C1C-NC	6.72	114.85	110.22
17	A	840	CLA	C2C-C1C-NC	6.73	114.85	110.22
17	7	613	CLA	C2C-C1C-NC	6.73	114.85	110.22
17	B	804	CLA	C2C-C1C-NC	6.73	114.85	110.22
26	4	615	CHL	CMB-C2B-C3B	6.73	129.35	113.69
17	b	833	CLA	C2C-C1C-NC	6.73	114.85	110.22
17	b	817	CLA	C2C-C1C-NC	6.73	114.85	110.22
17	1	315	CLA	C2C-C1C-NC	6.74	114.86	110.22
17	b	835	CLA	C2C-C1C-NC	6.75	114.86	110.22
17	4	604	CLA	C2C-C1C-NC	6.75	114.86	110.22
17	G	101	CLA	C2C-C1C-NC	6.75	114.86	110.22
17	3	301	CLA	C2C-C1C-NC	6.75	114.87	110.22
17	7	604	CLA	C2C-C1C-NC	6.76	114.87	110.22
17	A	816	CLA	C2C-C1C-NC	6.76	114.87	110.22
17	l	202	CLA	C2C-C1C-NC	6.77	114.88	110.22
17	A	813	CLA	C2C-C1C-NC	6.78	114.88	110.22
17	k	1402	CLA	C2C-C1C-NC	6.78	114.88	110.22
17	B	834	CLA	C2C-C1C-NC	6.78	114.88	110.22
17	9	614	CLA	C2C-C1C-NC	6.78	114.89	110.22
26	1	307	CHL	CMB-C2B-C3B	6.78	129.47	113.69
17	1	311	CLA	C2C-C1C-NC	6.78	114.89	110.22
17	7	612	CLA	C2C-C1C-NC	6.78	114.89	110.22
17	7	603	CLA	C2C-C1C-NC	6.79	114.89	110.22
17	K	4002	CLA	C2C-C1C-NC	6.79	114.89	110.22
17	B	839	CLA	C2C-C1C-NC	6.79	114.89	110.22
17	9	613	CLA	C2C-C1C-NC	6.79	114.89	110.22
26	6	308	CHL	CMB-C2B-C3B	6.80	129.50	113.69
17	b	815	CLA	C2C-C1C-NC	6.81	114.90	110.22
17	B	820	CLA	C2C-C1C-NC	6.81	114.90	110.22
17	b	809	CLA	C2C-C1C-NC	6.81	114.91	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	831	CLA	C2C-C1C-NC	6.81	114.91	110.22
26	9	615	CHL	CMB-C2B-C3B	6.82	129.55	113.69
17	f	7003	CLA	C2C-C1C-NC	6.82	114.91	110.22
17	6	313	CLA	C2C-C1C-NC	6.82	114.91	110.22
17	j	3002	CLA	C2C-C1C-NC	6.83	114.92	110.22
17	8	309	CLA	C2C-C1C-NC	6.83	114.92	110.22
28	6	318	XAT	O24-C25-C24	6.83	118.28	113.33
17	b	839	CLA	C2C-C1C-NC	6.84	114.92	110.22
17	4	613	CLA	C2C-C1C-NC	6.85	114.93	110.22
17	2	603	CLA	C2C-C1C-NC	6.85	114.94	110.22
17	4	611	CLA	C2C-C1C-NC	6.85	114.94	110.22
17	3	305	CLA	C2C-C1C-NC	6.86	114.94	110.22
17	a	842	CLA	C2C-C1C-NC	6.86	114.94	110.22
17	A	839	CLA	C2C-C1C-NC	6.86	114.94	110.22
17	A	835	CLA	C2C-C1C-NC	6.86	114.94	110.22
17	B	809	CLA	C2C-C1C-NC	6.86	114.94	110.22
17	9	612	CLA	C2C-C1C-NC	6.86	114.94	110.22
17	4	601	CLA	C2C-C1C-NC	6.87	114.94	110.22
17	6	314	CLA	C2C-C1C-NC	6.87	114.94	110.22
17	9	601	CLA	C2C-C1C-NC	6.88	114.95	110.22
17	3	311	CLA	C2C-C1C-NC	6.88	114.95	110.22
28	6	318	XAT	O4-C5-C4	6.88	118.32	113.33
17	1	313	CLA	C2C-C1C-NC	6.89	114.96	110.22
17	b	816	CLA	C2C-C1C-NC	6.89	114.96	110.22
17	g	102	CLA	C2C-C1C-NC	6.89	114.96	110.22
17	A	843	CLA	C2C-C1C-NC	6.89	114.96	110.22
17	b	805	CLA	C2C-C1C-NC	6.89	114.96	110.22
17	b	838	CLA	C2C-C1C-NC	6.90	114.97	110.22
17	F	303	CLA	C2C-C1C-NC	6.91	114.97	110.22
17	8	310	CLA	C2C-C1C-NC	6.91	114.97	110.22
17	6	315	CLA	C2C-C1C-NC	6.91	114.97	110.22
17	B	808	CLA	C2C-C1C-NC	6.91	114.97	110.22
17	4	612	CLA	C2C-C1C-NC	6.91	114.97	110.22
17	1	309	CLA	C2C-C1C-NC	6.91	114.98	110.22
17	3	312	CLA	C2C-C1C-NC	6.92	114.98	110.22
17	a	825	CLA	C2C-C1C-NC	6.92	114.98	110.22
17	B	818	CLA	C2C-C1C-NC	6.92	114.98	110.22
17	1	312	CLA	C2C-C1C-NC	6.93	114.98	110.22
17	6	306	CLA	C2C-C1C-NC	6.93	114.98	110.22
17	4	608	CLA	C2C-C1C-NC	6.93	114.99	110.22
17	A	810	CLA	C2C-C1C-NC	6.93	114.99	110.22
17	3	310	CLA	C2C-C1C-NC	6.93	114.99	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	811	CLA	C2C-C1C-NC	6.94	114.99	110.22
28	9	617	XAT	O24-C25-C24	6.95	118.37	113.33
17	1	314	CLA	C2C-C1C-NC	6.95	115.00	110.22
17	A	808	CLA	C2C-C1C-NC	6.95	115.00	110.22
17	a	813	CLA	C2C-C1C-NC	6.95	115.00	110.22
17	A	845	CLA	C2C-C1C-NC	6.96	115.01	110.22
26	4	606	CHL	CMB-C2B-C3B	6.96	129.89	113.69
17	A	837	CLA	C2C-C1C-NC	6.96	115.01	110.22
17	a	801	CLA	C2C-C1C-NC	6.97	115.01	110.22
17	9	611	CLA	C2C-C1C-NC	6.97	115.02	110.22
17	L	202	CLA	C2C-C1C-NC	6.98	115.02	110.22
17	a	840	CLA	C2C-C1C-NC	6.98	115.03	110.22
17	8	305	CLA	C2C-C1C-NC	6.99	115.03	110.22
17	2	608	CLA	C2C-C1C-NC	7.00	115.03	110.22
17	7	611	CLA	C2C-C1C-NC	7.00	115.03	110.22
17	a	846	CLA	C2C-C1C-NC	7.00	115.03	110.22
17	6	305	CLA	C2C-C1C-NC	7.00	115.04	110.22
17	F	301	CLA	C2C-C1C-NC	7.00	115.04	110.22
17	6	310	CLA	C2C-C1C-NC	7.01	115.04	110.22
17	A	832	CLA	C2C-C1C-NC	7.01	115.04	110.22
17	J	3002	CLA	C2C-C1C-NC	7.02	115.05	110.22
17	b	840	CLA	C2C-C1C-NC	7.03	115.06	110.22
17	b	818	CLA	C2C-C1C-NC	7.04	115.06	110.22
17	A	831	CLA	C2C-C1C-NC	7.04	115.06	110.22
17	k	1403	CLA	C2C-C1C-NC	7.05	115.07	110.22
17	8	311	CLA	C2C-C1C-NC	7.06	115.07	110.22
17	a	824	CLA	C2C-C1C-NC	7.06	115.08	110.22
17	6	312	CLA	C2C-C1C-NC	7.06	115.08	110.22
17	A	817	CLA	C2C-C1C-NC	7.06	115.08	110.22
17	b	834	CLA	C2C-C1C-NC	7.07	115.08	110.22
17	b	819	CLA	C2C-C1C-NC	7.08	115.09	110.22
17	K	4003	CLA	C2C-C1C-NC	7.08	115.09	110.22
17	9	608	CLA	C2C-C1C-NC	7.08	115.09	110.22
17	B	838	CLA	C2C-C1C-NC	7.09	115.10	110.22
17	b	821	CLA	C2C-C1C-NC	7.10	115.11	110.22
17	8	312	CLA	C2C-C1C-NC	7.12	115.12	110.22
17	2	610	CLA	C2C-C1C-NC	7.13	115.12	110.22
17	A	803	CLA	C2C-C1C-NC	7.14	115.14	110.22
17	a	832	CLA	C2C-C1C-NC	7.15	115.14	110.22
17	B	821	CLA	C2C-C1C-NC	7.15	115.14	110.22
17	A	824	CLA	C2C-C1C-NC	7.16	115.15	110.22
17	3	313	CLA	C2C-C1C-NC	7.16	115.15	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	314	CLA	C2C-C1C-NC	7.17	115.15	110.22
17	B	819	CLA	C2C-C1C-NC	7.17	115.16	110.22
28	9	617	XAT	O4-C5-C4	7.18	118.54	113.33
17	1	304	CLA	C2C-C1C-NC	7.18	115.16	110.22
17	7	610	CLA	C2C-C1C-NC	7.19	115.16	110.22
17	g	101	CLA	C2C-C1C-NC	7.21	115.18	110.22
17	a	818	CLA	C2C-C1C-NC	7.24	115.20	110.22
17	A	825	CLA	C2C-C1C-NC	7.26	115.22	110.22
17	a	837	CLA	C2C-C1C-NC	7.31	115.25	110.22
17	A	854	CLA	C2C-C1C-NC	7.39	115.31	110.22
17	A	834	CLA	C2C-C1C-NC	7.40	115.31	110.22
17	3	303	CLA	C2C-C1C-NC	7.41	115.32	110.22
17	a	817	CLA	C2C-C1C-NC	7.43	115.33	110.22
17	a	836	CLA	C2C-C1C-NC	7.48	115.36	110.22
17	8	302	CLA	C2C-C1C-NC	7.50	115.38	110.22
17	a	821	CLA	C2C-C1C-NC	7.55	115.42	110.22
28	7	616	XAT	O24-C25-C24	7.61	118.85	113.33
17	A	836	CLA	C2C-C1C-NC	7.64	115.48	110.22
17	a	803	CLA	C2C-C1C-NC	7.64	115.48	110.22
17	A	821	CLA	C2C-C1C-NC	7.69	115.51	110.22
17	a	856	CLA	C2C-C1C-NC	7.73	115.54	110.22
17	b	829	CLA	C2C-C1C-NC	7.77	115.57	110.22
17	B	829	CLA	C2C-C1C-NC	7.77	115.57	110.22
28	2	616	XAT	O24-C25-C24	7.86	119.03	113.33
28	1	317	XAT	O24-C25-C24	7.99	119.13	113.33
17	8	313	CLA	C3D-C4D-ND	8.02	117.11	110.14
17	3	315	CLA	C3D-C4D-ND	8.14	117.22	110.14
28	3	317	XAT	O4-C5-C4	8.73	119.66	113.33
28	8	315	XAT	O4-C5-C4	8.74	119.67	113.33
28	4	617	XAT	O4-C5-C4	8.79	119.70	113.33

All (824) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	9	609	CLA	NC
17	9	609	CLA	ND
17	9	609	CLA	NA
17	a	812	CLA	NC
17	a	812	CLA	ND
17	a	812	CLA	NA
17	A	803	CLA	ND
17	6	313	CLA	NC

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Mol	Chain	Res	Type	Atom
17	6	313	CLA	ND
17	6	313	CLA	NA
17	B	805	CLA	NC
17	B	805	CLA	ND
17	B	805	CLA	NA
17	3	314	CLA	ND
17	3	314	CLA	NA
17	a	828	CLA	NC
17	a	828	CLA	ND
17	a	828	CLA	NA
17	A	815	CLA	NC
17	A	815	CLA	ND
17	A	815	CLA	NA
17	a	856	CLA	ND
17	A	831	CLA	NC
17	A	831	CLA	ND
17	A	831	CLA	NA
17	2	604	CLA	NC
17	2	604	CLA	ND
17	2	604	CLA	NA
17	b	835	CLA	NC
17	b	835	CLA	ND
17	b	835	CLA	NA
17	3	305	CLA	NC
17	3	305	CLA	ND
17	3	305	CLA	NA
17	a	809	CLA	NC
17	a	809	CLA	ND
17	a	809	CLA	NA
17	a	836	CLA	NC
17	a	836	CLA	ND
17	a	836	CLA	NA
17	A	808	CLA	NC
17	A	808	CLA	ND
17	A	808	CLA	NA
17	a	831	CLA	NC
17	a	831	CLA	ND
17	a	831	CLA	NA
17	A	806	CLA	NC
17	A	806	CLA	ND
17	A	806	CLA	NA
17	f	7003	CLA	NA

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Mol	Chain	Res	Type	Atom
17	b	840	CLA	NC
17	b	840	CLA	ND
17	b	840	CLA	NA
17	A	811	CLA	NC
17	A	811	CLA	ND
17	A	811	CLA	NA
17	A	826	CLA	NC
17	A	826	CLA	ND
17	A	826	CLA	NA
17	a	825	CLA	NC
17	a	825	CLA	ND
17	a	825	CLA	NA
17	A	833	CLA	NC
17	A	833	CLA	ND
17	A	833	CLA	NA
17	7	608	CLA	NC
17	7	608	CLA	ND
17	7	608	CLA	NA
26	4	605	CHL	C8
17	4	602	CLA	NC
17	4	602	CLA	ND
17	4	602	CLA	NA
17	6	305	CLA	NC
17	6	305	CLA	ND
17	6	305	CLA	NA
17	B	827	CLA	ND
17	A	845	CLA	NC
17	A	845	CLA	ND
17	A	845	CLA	NA
17	a	819	CLA	NC
17	a	819	CLA	ND
17	a	819	CLA	NA
17	4	601	CLA	NC
17	4	601	CLA	ND
17	4	601	CLA	NA
17	a	824	CLA	NC
17	a	824	CLA	ND
17	a	824	CLA	NA
17	b	816	CLA	NC
17	b	816	CLA	ND
17	b	816	CLA	NA
17	a	818	CLA	NC

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Mol	Chain	Res	Type	Atom
17	a	818	CLA	ND
17	a	818	CLA	NA
17	1	309	CLA	NC
17	1	309	CLA	ND
17	1	309	CLA	NA
17	A	854	CLA	ND
17	b	818	CLA	NC
17	b	818	CLA	ND
17	b	818	CLA	NA
17	A	827	CLA	NC
17	A	827	CLA	ND
17	A	827	CLA	NA
17	1	306	CLA	NC
17	1	306	CLA	ND
17	1	306	CLA	NA
26	6	303	CHL	C8
17	j	3002	CLA	NC
17	j	3002	CLA	ND
17	j	3002	CLA	NA
17	3	303	CLA	NA
17	3	303	CLA	NC
17	3	303	CLA	ND
17	9	611	CLA	NC
17	9	611	CLA	ND
17	9	611	CLA	NA
17	A	824	CLA	NC
17	A	824	CLA	ND
17	A	824	CLA	NA
17	1	315	CLA	NC
17	1	315	CLA	ND
17	1	315	CLA	NA
17	2	613	CLA	NC
17	2	613	CLA	ND
17	2	613	CLA	NA
17	1	305	CLA	NC
17	1	305	CLA	ND
17	1	305	CLA	NA
17	A	825	CLA	NC
17	A	825	CLA	ND
17	A	825	CLA	NA
17	b	836	CLA	NC
17	b	836	CLA	ND

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Mol	Chain	Res	Type	Atom
17	b	836	CLA	NA
17	g	102	CLA	NC
17	g	102	CLA	ND
17	g	102	CLA	NA
17	A	828	CLA	NC
17	A	828	CLA	ND
17	A	828	CLA	NA
17	b	813	CLA	NC
17	b	813	CLA	ND
17	b	813	CLA	NA
17	b	834	CLA	NC
17	b	834	CLA	ND
17	b	834	CLA	NA
17	a	820	CLA	NC
17	a	820	CLA	ND
17	a	820	CLA	NA
17	A	801	CLA	CBD
17	A	801	CLA	NC
17	A	801	CLA	ND
17	A	801	CLA	NA
17	b	815	CLA	NC
17	b	815	CLA	ND
17	b	815	CLA	NA
17	B	819	CLA	ND
17	B	819	CLA	NA
17	4	604	CLA	NC
17	4	604	CLA	ND
17	4	604	CLA	NA
17	B	818	CLA	ND
17	B	818	CLA	NA
17	a	827	CLA	NC
17	a	827	CLA	ND
17	a	827	CLA	NA
17	f	7002	CLA	NC
17	f	7002	CLA	ND
17	f	7002	CLA	NA
17	3	311	CLA	NC
17	3	311	CLA	ND
17	3	311	CLA	NA
17	b	821	CLA	NC
17	b	821	CLA	ND
17	b	821	CLA	NA

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Mol	Chain	Res	Type	Atom
17	b	809	CLA	NC
17	b	809	CLA	ND
17	b	809	CLA	NA
17	a	835	CLA	NC
17	a	835	CLA	ND
17	a	835	CLA	NA
17	b	838	CLA	NC
17	b	838	CLA	ND
17	b	838	CLA	NA
17	2	611	CLA	NC
17	2	611	CLA	ND
17	2	611	CLA	NA
17	B	824	CLA	NC
17	B	824	CLA	NA
17	B	841	CLA	NC
17	B	841	CLA	ND
17	B	841	CLA	NA
17	3	308	CLA	NC
17	3	308	CLA	ND
17	3	308	CLA	NA
17	b	810	CLA	NC
17	b	810	CLA	ND
17	b	810	CLA	NA
17	a	834	CLA	NC
17	a	834	CLA	ND
17	a	834	CLA	NA
17	a	814	CLA	NC
17	a	814	CLA	ND
17	a	814	CLA	NA
17	a	839	CLA	NC
17	a	839	CLA	ND
17	a	839	CLA	NA
17	b	822	CLA	NC
17	b	822	CLA	ND
17	b	822	CLA	NA
17	a	817	CLA	ND
17	a	817	CLA	NA
17	A	814	CLA	NC
17	A	814	CLA	ND
17	A	814	CLA	NA
17	1	312	CLA	NC
17	1	312	CLA	ND

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Mol	Chain	Res	Type	Atom
17	1	312	CLA	NA
17	7	610	CLA	NC
17	7	610	CLA	ND
17	7	610	CLA	NA
17	a	837	CLA	ND
17	a	837	CLA	NA
17	A	834	CLA	ND
17	A	834	CLA	NA
17	a	811	CLA	NC
17	a	811	CLA	ND
17	a	811	CLA	NA
17	A	836	CLA	NC
17	A	836	CLA	ND
17	A	836	CLA	NA
17	8	304	CLA	NC
17	8	304	CLA	ND
17	8	304	CLA	NA
17	B	806	CLA	NC
17	B	806	CLA	ND
17	B	806	CLA	NA
17	B	821	CLA	NC
17	B	821	CLA	ND
17	B	821	CLA	NA
17	8	305	CLA	NC
17	8	305	CLA	ND
17	8	305	CLA	NA
17	b	802	CLA	NC
17	b	802	CLA	ND
17	L	203	CLA	NC
17	L	203	CLA	ND
17	L	203	CLA	NA
17	B	811	CLA	NC
17	B	811	CLA	ND
17	B	811	CLA	NA
17	b	839	CLA	NC
17	b	839	CLA	ND
17	b	839	CLA	NA
17	9	612	CLA	NC
17	9	612	CLA	ND
17	9	612	CLA	NA
17	6	315	CLA	NC
17	6	315	CLA	ND

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Mol	Chain	Res	Type	Atom
17	6	315	CLA	NA
17	B	823	CLA	NC
17	B	823	CLA	ND
17	B	823	CLA	NA
17	1	308	CLA	NC
17	1	308	CLA	ND
17	1	308	CLA	NA
17	a	844	CLA	NC
17	a	844	CLA	ND
17	a	844	CLA	NA
17	4	609	CLA	NC
17	4	609	CLA	ND
17	4	609	CLA	NA
17	B	826	CLA	NC
17	B	826	CLA	ND
17	B	826	CLA	NA
17	9	608	CLA	NC
17	9	608	CLA	ND
17	9	608	CLA	NA
17	B	839	CLA	NC
17	B	839	CLA	ND
17	B	839	CLA	NA
17	A	842	CLA	NC
17	A	842	CLA	ND
17	A	842	CLA	NA
17	B	820	CLA	NC
17	B	820	CLA	ND
17	B	820	CLA	NA
17	9	603	CLA	NA
17	9	603	CLA	NC
17	9	603	CLA	ND
17	L	204	CLA	NC
17	L	204	CLA	ND
17	L	204	CLA	NA
17	B	825	CLA	NC
17	B	825	CLA	ND
17	B	825	CLA	NA
17	A	810	CLA	NC
17	A	810	CLA	ND
17	A	810	CLA	NA
17	2	602	CLA	NC
17	2	602	CLA	ND

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Mol	Chain	Res	Type	Atom
17	2	602	CLA	NA
17	1	203	CLA	NC
17	1	203	CLA	ND
17	1	203	CLA	NA
17	6	316	CLA	NC
17	6	316	CLA	ND
17	6	316	CLA	NA
17	A	838	CLA	NC
17	A	838	CLA	ND
17	A	838	CLA	NA
17	3	309	CLA	NC
17	3	309	CLA	ND
17	3	309	CLA	NA
17	A	819	CLA	NC
17	A	819	CLA	ND
17	A	819	CLA	NA
17	F	303	CLA	NC
17	F	303	CLA	ND
17	F	303	CLA	NA
17	B	810	CLA	NC
17	B	810	CLA	ND
17	B	810	CLA	NA
17	A	835	CLA	NC
17	A	835	CLA	ND
17	A	835	CLA	NA
17	3	306	CLA	NC
17	3	306	CLA	ND
17	3	306	CLA	NA
17	b	814	CLA	NC
17	b	814	CLA	ND
17	b	814	CLA	NA
17	1	313	CLA	NC
17	1	313	CLA	ND
17	1	313	CLA	NA
17	b	826	CLA	NC
17	b	826	CLA	ND
17	b	826	CLA	NA
17	b	829	CLA	NC
17	b	829	CLA	ND
17	b	829	CLA	NA
17	k	1402	CLA	NC
17	k	1402	CLA	ND

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Mol	Chain	Res	Type	Atom
17	k	1402	CLA	NA
17	B	808	CLA	NC
17	B	808	CLA	ND
17	B	808	CLA	NA
17	b	833	CLA	NC
17	b	833	CLA	ND
17	b	833	CLA	NA
17	6	306	CLA	NC
17	6	306	CLA	ND
17	6	306	CLA	NA
17	1	310	CLA	NC
17	1	310	CLA	ND
17	1	310	CLA	NA
17	a	842	CLA	NC
17	a	842	CLA	ND
17	a	842	CLA	NA
17	6	304	CLA	NC
17	6	304	CLA	ND
17	6	304	CLA	NA
26	7	601	CHL	C8
17	B	840	CLA	NC
17	B	840	CLA	NA
17	A	813	CLA	NC
17	A	813	CLA	ND
17	A	813	CLA	NA
17	A	816	CLA	NC
17	A	816	CLA	ND
17	A	816	CLA	NA
17	A	823	CLA	NC
17	A	823	CLA	ND
17	A	823	CLA	NA
17	B	809	CLA	NC
17	B	809	CLA	ND
17	B	809	CLA	NA
17	L	202	CLA	NC
17	L	202	CLA	ND
17	L	202	CLA	NA
17	G	103	CLA	NC
17	G	103	CLA	ND
17	G	103	CLA	NA
17	A	809	CLA	NC
17	A	809	CLA	ND

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Mol	Chain	Res	Type	Atom
17	A	809	CLA	NA
17	b	830	CLA	NC
17	b	830	CLA	ND
17	b	830	CLA	NA
17	B	832	CLA	NC
17	B	832	CLA	ND
17	B	832	CLA	NA
17	B	802	CLA	NC
17	B	802	CLA	ND
17	8	308	CLA	NC
17	8	308	CLA	ND
17	8	308	CLA	NA
17	F	301	CLA	NC
17	F	301	CLA	ND
17	F	301	CLA	NA
17	G	104	CLA	NC
17	G	104	CLA	ND
17	G	104	CLA	NA
17	A	821	CLA	NC
17	A	821	CLA	ND
17	A	821	CLA	NA
17	b	841	CLA	NC
17	b	841	CLA	ND
17	b	841	CLA	NA
17	A	805	CLA	NC
17	A	805	CLA	ND
17	A	805	CLA	NA
17	2	608	CLA	NC
17	2	608	CLA	ND
17	2	608	CLA	NA
17	B	831	CLA	NC
17	B	831	CLA	ND
17	B	831	CLA	NA
17	a	821	CLA	NC
17	a	821	CLA	ND
17	a	821	CLA	NA
17	B	828	CLA	NC
17	B	828	CLA	ND
17	B	828	CLA	NA
17	a	826	CLA	NA
17	a	826	CLA	NC
17	a	826	CLA	ND

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Mol	Chain	Res	Type	Atom
17	l	202	CLA	NC
17	l	202	CLA	ND
17	l	202	CLA	NA
17	9	602	CLA	NC
17	9	602	CLA	ND
17	9	602	CLA	NA
17	a	815	CLA	NC
17	a	815	CLA	ND
17	a	815	CLA	NA
17	a	833	CLA	NC
17	a	833	CLA	ND
17	a	833	CLA	NA
17	A	818	CLA	NC
17	A	818	CLA	ND
17	A	818	CLA	NA
17	A	812	CLA	NC
17	A	812	CLA	ND
17	A	812	CLA	NA
17	A	841	CLA	NC
17	A	841	CLA	ND
17	A	841	CLA	NA
17	b	827	CLA	NC
17	b	827	CLA	ND
17	2	612	CLA	NC
17	2	612	CLA	ND
17	2	612	CLA	NA
17	A	832	CLA	ND
17	A	832	CLA	NA
17	3	301	CLA	NC
17	3	301	CLA	ND
17	3	301	CLA	NA
17	k	1401	CLA	NC
17	k	1401	CLA	ND
17	k	1401	CLA	NA
17	A	822	CLA	NC
17	A	822	CLA	ND
17	A	822	CLA	NA
17	g	101	CLA	NC
17	g	101	CLA	NA
17	7	609	CLA	NC
17	7	609	CLA	ND
17	7	609	CLA	NA

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Mol	Chain	Res	Type	Atom
17	6	309	CLA	NC
17	6	309	CLA	ND
17	6	309	CLA	NA
17	B	833	CLA	NC
17	B	833	CLA	ND
17	B	833	CLA	NA
17	B	836	CLA	NC
17	B	836	CLA	ND
17	B	836	CLA	NA
17	A	837	CLA	NC
17	A	837	CLA	ND
17	A	837	CLA	NA
17	B	822	CLA	NC
17	B	822	CLA	ND
17	B	822	CLA	NA
17	4	610	CLA	NC
17	4	610	CLA	ND
17	4	610	CLA	NA
17	B	813	CLA	NC
17	B	813	CLA	ND
17	B	813	CLA	NA
17	B	830	CLA	NC
17	B	830	CLA	ND
17	B	830	CLA	NA
17	J	3002	CLA	NC
17	J	3002	CLA	ND
17	J	3002	CLA	NA
17	2	610	CLA	NC
17	2	610	CLA	ND
17	B	815	CLA	NC
17	B	815	CLA	ND
17	B	815	CLA	NA
17	a	840	CLA	ND
17	a	840	CLA	NA
17	B	834	CLA	NC
17	B	834	CLA	ND
17	B	834	CLA	NA
17	7	602	CLA	NC
17	7	602	CLA	ND
17	7	602	CLA	NA
17	A	804	CLA	NC
17	A	804	CLA	ND

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Mol	Chain	Res	Type	Atom
17	A	804	CLA	NA
17	b	811	CLA	NC
17	b	811	CLA	ND
17	b	811	CLA	NA
17	4	613	CLA	NC
17	4	613	CLA	ND
17	4	613	CLA	NA
17	6	307	CLA	NC
17	6	307	CLA	ND
17	6	307	CLA	NA
17	a	822	CLA	NC
17	a	822	CLA	ND
17	a	822	CLA	NA
17	9	604	CLA	NC
17	9	604	CLA	ND
17	9	604	CLA	NA
17	7	611	CLA	NC
17	7	611	CLA	ND
17	7	611	CLA	NA
17	8	303	CLA	NC
17	8	303	CLA	ND
17	8	303	CLA	NA
17	l	204	CLA	NC
17	l	204	CLA	ND
17	l	204	CLA	NA
17	a	810	CLA	NC
17	a	810	CLA	ND
17	a	810	CLA	NA
17	4	612	CLA	NC
17	4	612	CLA	ND
17	4	612	CLA	NA
17	3	315	CLA	NC
17	3	315	CLA	ND
17	3	315	CLA	NA
17	b	803	CLA	NC
17	b	803	CLA	ND
17	b	803	CLA	NA
17	6	312	CLA	NC
17	6	312	CLA	ND
17	6	312	CLA	NA
17	b	824	CLA	NC
17	b	824	CLA	ND

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Mol	Chain	Res	Type	Atom
17	b	824	CLA	NA
17	6	310	CLA	NC
17	6	310	CLA	ND
17	6	310	CLA	NA
17	2	603	CLA	NC
17	2	603	CLA	ND
17	2	603	CLA	NA
17	2	609	CLA	NC
17	2	609	CLA	ND
17	2	609	CLA	NA
17	B	835	CLA	NC
17	B	835	CLA	ND
17	B	835	CLA	NA
17	K	4002	CLA	NC
17	K	4002	CLA	ND
17	K	4002	CLA	NA
17	F	304	CLA	NC
17	F	304	CLA	ND
17	F	304	CLA	NA
17	a	823	CLA	NC
17	a	823	CLA	ND
17	a	823	CLA	NA
17	b	823	CLA	NC
17	b	823	CLA	ND
17	b	823	CLA	NA
17	a	830	CLA	NC
17	a	830	CLA	ND
17	a	830	CLA	NA
17	b	831	CLA	ND
17	b	831	CLA	NA
17	b	819	CLA	NC
17	b	819	CLA	ND
17	b	819	CLA	NA
17	b	828	CLA	NC
17	b	828	CLA	ND
17	b	828	CLA	NA
17	A	802	CLA	NC
17	A	802	CLA	ND
17	A	802	CLA	NA
17	4	611	CLA	NC
17	4	611	CLA	ND
17	4	611	CLA	NA

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Mol	Chain	Res	Type	Atom
17	b	832	CLA	NC
17	b	832	CLA	ND
17	b	832	CLA	NA
17	b	837	CLA	NC
17	b	837	CLA	ND
17	b	837	CLA	NA
17	B	816	CLA	NC
17	B	816	CLA	ND
17	B	816	CLA	NA
26	2	601	CHL	C8
17	b	806	CLA	NC
17	b	806	CLA	ND
17	b	806	CLA	NA
17	a	838	CLA	NC
17	a	838	CLA	ND
17	a	838	CLA	NA
17	A	820	CLA	NC
17	A	820	CLA	ND
17	A	820	CLA	NA
17	b	808	CLA	NC
17	b	808	CLA	ND
17	b	808	CLA	NA
17	b	825	CLA	NC
17	b	825	CLA	ND
17	b	825	CLA	NA
17	b	817	CLA	NC
17	b	817	CLA	ND
17	b	817	CLA	NA
17	g	103	CLA	NC
17	g	103	CLA	ND
17	g	103	CLA	NA
17	B	812	CLA	NC
17	B	812	CLA	ND
17	B	812	CLA	NA
17	1	303	CLA	NC
17	1	303	CLA	ND
17	1	303	CLA	NA
17	9	610	CLA	NC
17	9	610	CLA	ND
17	9	610	CLA	NA
17	a	803	CLA	ND
17	a	832	CLA	ND

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Mol	Chain	Res	Type	Atom
17	a	832	CLA	NA
17	G	101	CLA	NC
17	G	101	CLA	ND
17	G	101	CLA	NA
17	B	804	CLA	NC
17	B	804	CLA	ND
17	B	804	CLA	NA
17	6	311	CLA	NC
17	6	311	CLA	ND
17	6	311	CLA	NA
17	8	309	CLA	NC
17	8	309	CLA	ND
17	8	309	CLA	NA
17	1	314	CLA	NC
17	1	314	CLA	NA
17	B	803	CLA	NC
17	B	803	CLA	NA
17	B	803	CLA	ND
17	b	804	CLA	NC
17	b	804	CLA	ND
17	b	804	CLA	NA
17	3	310	CLA	NC
17	3	310	CLA	ND
17	3	310	CLA	NA
17	a	841	CLA	NC
17	a	841	CLA	ND
17	a	841	CLA	NA
17	7	604	CLA	NC
17	7	604	CLA	ND
17	7	604	CLA	NA
17	A	807	CLA	NC
17	A	807	CLA	ND
17	A	807	CLA	NA
17	a	843	CLA	NC
17	a	843	CLA	ND
17	a	843	CLA	NA
17	8	311	CLA	ND
17	8	311	CLA	NA
17	9	614	CLA	NC
17	9	614	CLA	ND
17	9	614	CLA	NA
17	9	613	CLA	NC

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Mol	Chain	Res	Type	Atom
17	9	613	CLA	ND
17	9	613	CLA	NA
17	B	838	CLA	ND
17	B	838	CLA	NA
17	7	613	CLA	NC
17	7	613	CLA	NA
17	k	1403	CLA	NC
17	k	1403	CLA	ND
17	k	1403	CLA	NA
17	a	801	CLA	CBD
17	a	801	CLA	NC
17	a	801	CLA	ND
17	a	801	CLA	NA
17	b	812	CLA	NC
17	b	812	CLA	ND
17	b	812	CLA	NA
17	b	807	CLA	NC
17	b	807	CLA	ND
17	b	807	CLA	NA
17	4	608	CLA	NC
17	4	608	CLA	ND
17	4	608	CLA	NA
17	a	804	CLA	NC
17	a	804	CLA	ND
17	a	804	CLA	NA
17	3	313	CLA	NC
17	3	313	CLA	ND
17	3	313	CLA	NA
17	A	839	CLA	NC
17	A	839	CLA	ND
17	A	839	CLA	NA
17	3	304	CLA	NC
17	3	304	CLA	ND
17	3	304	CLA	NA
17	1	311	CLA	NC
17	1	311	CLA	ND
17	1	311	CLA	NA
17	A	817	CLA	NC
17	A	817	CLA	NA
17	a	829	CLA	ND
17	A	840	CLA	NC
17	A	840	CLA	ND

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Mol	Chain	Res	Type	Atom
17	A	840	CLA	NA
17	a	802	CLA	NC
17	a	802	CLA	ND
17	a	802	CLA	NA
17	A	843	CLA	NC
17	A	843	CLA	ND
17	A	843	CLA	NA
17	a	808	CLA	NC
17	a	808	CLA	ND
17	a	808	CLA	NA
17	a	813	CLA	NC
17	a	813	CLA	ND
17	a	813	CLA	NA
17	A	830	CLA	NC
17	A	830	CLA	ND
17	A	830	CLA	NA
17	B	817	CLA	NC
17	B	817	CLA	ND
17	B	817	CLA	NA
17	a	806	CLA	NC
17	a	806	CLA	ND
17	a	806	CLA	NA
17	8	310	CLA	NC
17	8	310	CLA	ND
17	8	310	CLA	NA
17	7	612	CLA	NC
17	7	612	CLA	ND
17	7	612	CLA	NA
17	9	601	CLA	NC
17	9	601	CLA	ND
17	9	601	CLA	NA
17	a	805	CLA	NC
17	a	805	CLA	ND
17	a	805	CLA	NA
17	b	805	CLA	NC
17	b	805	CLA	ND
17	b	805	CLA	NA
17	A	829	CLA	NC
17	A	829	CLA	ND
17	8	313	CLA	NC
17	8	313	CLA	ND
17	8	313	CLA	NA

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Mol	Chain	Res	Type	Atom
26	9	605	CHL	C8
26	1	302	CHL	C8
17	6	314	CLA	NC
17	6	314	CLA	ND
17	6	314	CLA	NA
17	3	302	CLA	NC
17	3	302	CLA	ND
17	3	302	CLA	NA
17	a	816	CLA	NC
17	a	816	CLA	ND
17	a	816	CLA	NA
17	8	312	CLA	ND
17	8	312	CLA	NA
17	B	814	CLA	NC
17	B	814	CLA	ND
17	B	814	CLA	NA
17	1	304	CLA	NC
17	1	304	CLA	ND
17	1	304	CLA	NA
17	a	846	CLA	NC
17	a	846	CLA	ND
17	a	846	CLA	NA
17	a	807	CLA	NC
17	a	807	CLA	ND
17	a	807	CLA	NA
17	B	829	CLA	NC
17	B	829	CLA	ND
17	B	829	CLA	NA
17	b	820	CLA	NC
17	b	820	CLA	ND
17	b	820	CLA	NA
17	4	614	CLA	NC
17	4	614	CLA	ND
17	4	614	CLA	NA
17	B	837	CLA	NC
17	B	837	CLA	ND
17	B	837	CLA	NA
17	4	603	CLA	NA
17	4	603	CLA	NC
17	4	603	CLA	ND
17	8	301	CLA	NC
17	8	301	CLA	ND

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Mol	Chain	Res	Type	Atom
17	8	301	CLA	NA
17	B	807	CLA	ND
17	B	807	CLA	NA
17	3	312	CLA	NC
17	3	312	CLA	ND
17	3	312	CLA	NA
17	K	4003	CLA	NC
17	K	4003	CLA	ND
17	K	4003	CLA	NA
17	8	302	CLA	NA
17	8	302	CLA	NC
17	8	302	CLA	ND
17	8	307	CLA	NC
17	8	307	CLA	ND
17	8	307	CLA	NA
17	7	603	CLA	NC
17	7	603	CLA	ND
17	7	603	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	7	601	CHL	OMC-CMC-C2C-C1C
26	6	303	CHL	OMC-CMC-C2C-C1C

There are no ring outliers.

267 monomers are involved in 1072 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	302	CHL	11	0
17	1	303	CLA	3	0
17	1	304	CLA	5	0
17	1	306	CLA	4	0
26	1	307	CHL	2	0
17	1	308	CLA	5	0
17	1	309	CLA	4	0
17	1	310	CLA	2	0
17	1	311	CLA	2	0
17	1	312	CLA	2	0
17	1	313	CLA	8	0
17	1	314	CLA	3	0
17	1	315	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	316	LUT	8	0
28	1	317	XAT	7	0
20	1	318	BCR	4	0
19	1	319	LHG	3	0
27	1	320	LUT	3	0
26	2	601	CHL	8	0
17	2	602	CLA	6	0
17	2	603	CLA	3	0
17	2	604	CLA	8	0
26	2	605	CHL	1	0
26	2	606	CHL	1	0
26	2	607	CHL	5	0
17	2	608	CLA	3	0
17	2	609	CLA	6	0
17	2	610	CLA	1	0
17	2	611	CLA	5	0
17	2	612	CLA	2	0
17	2	613	CLA	3	0
26	2	614	CHL	3	0
27	2	615	LUT	6	0
28	2	616	XAT	6	0
20	2	617	BCR	12	0
19	2	618	LHG	3	0
17	3	301	CLA	2	0
17	3	302	CLA	10	0
17	3	303	CLA	5	0
17	3	304	CLA	4	0
17	3	305	CLA	1	0
17	3	306	CLA	4	0
17	3	308	CLA	5	0
17	3	309	CLA	6	0
17	3	311	CLA	2	0
17	3	312	CLA	3	0
17	3	313	CLA	1	0
17	3	314	CLA	3	0
27	3	316	LUT	7	0
28	3	317	XAT	5	0
20	3	318	BCR	3	0
19	3	319	LHG	1	0
17	4	601	CLA	3	0
17	4	602	CLA	3	0
17	4	603	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	4	604	CLA	3	0
26	4	605	CHL	2	0
26	4	606	CHL	4	0
26	4	607	CHL	4	0
17	4	608	CLA	7	0
17	4	609	CLA	8	0
17	4	610	CLA	6	0
17	4	611	CLA	3	0
17	4	613	CLA	3	0
17	4	614	CLA	1	0
26	4	615	CHL	1	0
27	4	616	LUT	5	0
28	4	617	XAT	5	0
20	4	618	BCR	9	0
25	4	619	LMG	4	0
25	4	620	LMG	4	0
25	6	302	LMG	3	0
26	6	303	CHL	9	0
17	6	304	CLA	4	0
17	6	305	CLA	4	0
17	6	306	CLA	3	0
17	6	307	CLA	4	0
26	6	308	CHL	3	0
17	6	309	CLA	1	0
17	6	310	CLA	2	0
17	6	311	CLA	4	0
17	6	312	CLA	1	0
17	6	313	CLA	3	0
17	6	314	CLA	5	0
17	6	315	CLA	3	0
17	6	316	CLA	1	0
27	6	317	LUT	9	0
28	6	318	XAT	8	0
20	6	319	BCR	7	0
19	6	320	LHG	5	0
27	6	321	LUT	5	0
26	7	601	CHL	5	0
17	7	602	CLA	6	0
17	7	604	CLA	6	0
26	7	605	CHL	5	0
26	7	606	CHL	2	0
26	7	607	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	7	608	CLA	5	0
17	7	609	CLA	8	0
17	7	611	CLA	2	0
17	7	612	CLA	4	0
17	7	613	CLA	2	0
26	7	614	CHL	3	0
27	7	615	LUT	9	0
28	7	616	XAT	6	0
20	7	617	BCR	14	0
19	7	618	LHG	2	0
17	8	301	CLA	6	0
17	8	302	CLA	2	0
17	8	303	CLA	3	0
17	8	304	CLA	1	0
17	8	305	CLA	2	0
26	8	306	CHL	3	0
17	8	307	CLA	6	0
17	8	308	CLA	6	0
17	8	309	CLA	3	0
17	8	310	CLA	1	0
17	8	311	CLA	1	0
17	8	312	CLA	2	0
27	8	314	LUT	7	0
28	8	315	XAT	7	0
20	8	316	BCR	7	0
17	9	601	CLA	3	0
17	9	602	CLA	5	0
17	9	603	CLA	1	0
17	9	604	CLA	4	0
26	9	605	CHL	4	0
26	9	606	CHL	3	0
26	9	607	CHL	4	0
17	9	608	CLA	8	0
17	9	609	CLA	6	0
17	9	610	CLA	2	0
17	9	611	CLA	5	0
17	9	612	CLA	1	0
17	9	614	CLA	4	0
26	9	615	CHL	1	0
27	9	616	LUT	5	0
28	9	617	XAT	8	0
20	9	618	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	9	619	LMG	2	0
17	A	801	CLA	7	0
17	A	802	CLA	7	0
17	A	803	CLA	10	0
17	A	804	CLA	11	0
17	A	805	CLA	5	0
17	A	806	CLA	13	0
17	A	807	CLA	13	0
17	A	808	CLA	4	0
17	A	809	CLA	12	0
17	A	810	CLA	8	0
17	A	811	CLA	8	0
17	A	812	CLA	10	0
17	A	813	CLA	6	0
17	A	814	CLA	7	0
17	A	815	CLA	3	0
17	A	816	CLA	6	0
17	A	817	CLA	1	0
17	A	818	CLA	9	0
17	A	819	CLA	6	0
17	A	820	CLA	8	0
17	A	821	CLA	3	0
17	A	822	CLA	6	0
17	A	823	CLA	2	0
17	A	824	CLA	4	0
17	A	825	CLA	7	0
17	A	826	CLA	8	0
17	A	827	CLA	6	0
17	A	828	CLA	3	0
17	A	829	CLA	17	0
17	A	830	CLA	9	0
17	A	831	CLA	11	0
17	A	832	CLA	4	0
17	A	833	CLA	9	0
17	A	834	CLA	10	0
17	A	835	CLA	8	0
17	A	836	CLA	4	0
17	A	837	CLA	3	0
17	A	838	CLA	3	0
17	A	839	CLA	11	0
17	A	840	CLA	6	0
17	A	841	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	842	CLA	12	0
17	A	843	CLA	18	0
18	A	844	PQN	5	0
17	A	845	CLA	3	0
19	A	846	LHG	4	0
19	A	847	LHG	3	0
20	A	848	BCR	4	0
20	A	849	BCR	7	0
20	A	850	BCR	5	0
20	A	851	BCR	9	0
20	A	852	BCR	9	0
17	A	854	CLA	7	0
20	A	856	BCR	5	0
20	B	801	BCR	6	0
17	B	802	CLA	9	0
17	B	803	CLA	7	0
17	B	804	CLA	6	0
17	B	805	CLA	5	0
17	B	806	CLA	11	0
17	B	807	CLA	7	0
17	B	808	CLA	8	0
17	B	809	CLA	6	0
17	B	810	CLA	6	0
17	B	811	CLA	6	0
17	B	812	CLA	5	0
17	B	813	CLA	11	0
17	B	814	CLA	4	0
17	B	815	CLA	8	0
17	B	816	CLA	7	0
17	B	817	CLA	7	0
17	B	818	CLA	7	0
17	B	819	CLA	4	0
17	B	820	CLA	2	0
17	B	821	CLA	1	0
17	B	822	CLA	4	0
17	B	823	CLA	5	0
17	B	824	CLA	10	0
17	B	825	CLA	12	0
17	B	826	CLA	3	0
17	B	827	CLA	10	0
17	B	828	CLA	6	0
17	B	829	CLA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	830	CLA	6	0
17	B	831	CLA	10	0
17	B	832	CLA	10	0
17	B	833	CLA	7	0
17	B	834	CLA	2	0
17	B	835	CLA	1	0
17	B	836	CLA	10	0
17	B	837	CLA	8	0
17	B	838	CLA	8	0
17	B	839	CLA	14	0
17	B	840	CLA	9	0
17	B	841	CLA	9	0
18	B	842	PQN	2	0
20	B	843	BCR	8	0
20	B	844	BCR	8	0
20	B	845	BCR	8	0
20	B	846	BCR	10	0
20	B	847	BCR	5	0
20	B	848	BCR	5	0
23	B	849	LMT	2	0
24	B	850	DGD	2	0
17	F	301	CLA	4	0
22	F	302	HTG	2	0
17	F	303	CLA	3	0
17	F	304	CLA	4	0
20	F	305	BCR	6	0
17	G	101	CLA	3	0
25	G	102	LMG	2	0
17	G	103	CLA	5	0
17	G	104	CLA	4	0
20	G	105	BCR	5	0
20	I	101	BCR	7	0
17	J	3002	CLA	2	0
20	J	3003	BCR	6	0
20	K	4001	BCR	4	0
17	K	4002	CLA	3	0
17	K	4003	CLA	3	0
20	K	4004	BCR	2	0
20	L	201	BCR	4	0
17	L	202	CLA	7	0
17	L	203	CLA	7	0
17	L	204	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	205	BCR	5	0
20	L	206	BCR	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	742/742 (100%)	0.17	32 (4%) 36 26	42, 58, 91, 169	0
1	a	742/742 (100%)	0.11	31 (4%) 37 26	36, 48, 81, 140	0
2	B	733/733 (100%)	0.34	66 (9%) 10 5	42, 56, 80, 121	0
2	b	733/733 (100%)	0.24	51 (6%) 17 10	36, 55, 86, 139	0
3	C	80/80 (100%)	0.16	5 (6%) 21 13	50, 62, 77, 96	0
3	c	80/80 (100%)	-0.18	0 100 100	44, 55, 72, 88	0
4	D	141/141 (100%)	0.38	11 (7%) 14 7	53, 71, 103, 163	0
4	d	140/141 (99%)	0.29	5 (3%) 43 32	45, 61, 92, 132	0
5	E	63/64 (98%)	0.96	14 (22%) 1 1	51, 77, 115, 127	0
5	e	63/64 (98%)	-0.08	1 (1%) 72 65	51, 78, 96, 119	0
6	F	151/151 (100%)	0.25	13 (8%) 11 6	50, 69, 98, 126	0
6	f	151/151 (100%)	0.15	8 (5%) 27 18	49, 73, 101, 132	0
7	G	95/95 (100%)	0.25	4 (4%) 37 26	60, 79, 103, 127	0
7	g	95/95 (100%)	0.45	12 (12%) 4 2	62, 83, 123, 171	0
8	H	90/90 (100%)	0.41	10 (11%) 6 3	61, 83, 116, 127	0
8	h	90/90 (100%)	-0.07	3 (3%) 47 36	51, 70, 100, 111	0
9	I	29/30 (96%)	-0.22	1 (3%) 46 34	53, 65, 87, 117	0
9	i	30/30 (100%)	-0.20	1 (3%) 47 36	48, 56, 80, 129	0
10	J	39/39 (100%)	0.00	3 (7%) 14 8	51, 62, 97, 100	0
10	j	39/39 (100%)	0.27	3 (7%) 14 8	48, 65, 95, 100	0
11	K	45/84 (53%)	1.75	16 (35%) 0 0	92, 111, 131, 143	0
11	k	46/84 (54%)	0.88	5 (10%) 6 3	68, 86, 126, 134	0
12	L	153/153 (100%)	0.24	15 (9%) 8 4	56, 80, 120, 143	0
12	l	151/153 (98%)	-0.32	0 100 100	42, 60, 87, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	195/195 (100%)	0.57	33 (16%) 2 1	61, 87, 119, 136	0
13	6	195/195 (100%)	0.60	30 (15%) 2 1	74, 114, 164, 176	0
14	2	206/206 (100%)	1.23	57 (27%) 1 0	67, 97, 133, 188	0
14	7	206/206 (100%)	0.64	30 (14%) 3 1	61, 89, 122, 158	0
15	3	218/218 (100%)	0.81	39 (17%) 2 1	62, 96, 133, 155	0
15	8	217/218 (99%)	0.38	24 (11%) 6 3	56, 81, 112, 142	0
16	4	196/196 (100%)	0.83	40 (20%) 1 1	61, 85, 115, 160	0
16	9	196/196 (100%)	0.46	22 (11%) 6 3	65, 97, 134, 155	0
All	All	6350/6434 (98%)	0.34	585 (9%) 10 5	36, 68, 116, 188	0

All (585) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	3	259	ASN	8.7
9	i	2	ILE	8.2
15	8	121	LEU	7.2
5	E	2	GLY	7.0
14	2	121	ILE	6.8
16	9	122	ASN	6.7
15	3	121	LEU	6.7
16	9	118	ILE	6.5
13	6	166	TYR	6.5
7	g	63	PRO	6.2
14	2	257	THR	6.2
15	8	120	GLY	6.1
13	6	163	PRO	5.9
14	2	256	PHE	5.8
14	7	256	PHE	5.6
14	2	139	THR	5.6
13	6	168	LYS	5.5
15	3	122	ILE	5.4
14	2	179	THR	5.3
13	1	98	TYR	5.3
15	3	219	LEU	5.3
14	2	177	LYS	5.2
13	6	167	SER	5.1
14	2	189	LEU	5.1
5	E	3	PRO	5.0
6	F	188	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
5	E	4	LYS	5.0
15	3	128	LEU	5.0
14	7	53	ASP	5.0
16	4	138	SER	4.9
13	6	158	GLY	4.9
7	g	64	VAL	4.9
14	2	133	GLN	4.9
7	g	59	LYS	4.8
14	2	128	TYR	4.8
12	L	152	PHE	4.8
13	6	164	LEU	4.8
15	8	178	LYS	4.8
16	4	195	ALA	4.8
16	9	174	GLN	4.8
13	1	99	GLY	4.8
15	3	255	ALA	4.7
6	F	186	ASP	4.6
15	8	122	ILE	4.6
14	2	175	ASN	4.6
16	9	119	GLY	4.6
16	4	132	GLU	4.5
2	B	734	GLY	4.5
13	1	121	PRO	4.5
16	4	237	ILE	4.5
15	3	258	VAL	4.5
16	4	88	LEU	4.5
16	9	120	ILE	4.5
2	b	214	ASP	4.4
6	f	188	LYS	4.4
11	K	55	PHE	4.4
13	6	161	PHE	4.4
1	a	502	THR	4.4
14	7	202	GLN	4.3
4	D	75	ASP	4.2
16	9	132	GLU	4.2
16	9	133	GLU	4.2
1	a	516	GLY	4.2
2	b	110	LEU	4.2
13	6	165	GLY	4.2
2	B	714	SER	4.2
2	B	377	TYR	4.2
13	1	114	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
16	9	123	VAL	4.1
14	2	120	GLY	4.1
13	1	96	LEU	4.1
16	4	134	TYR	4.1
6	F	137	LEU	4.1
12	L	155	TYR	4.1
15	3	178	LYS	4.1
14	7	193	PRO	4.1
14	2	178	LEU	4.1
11	K	20	PHE	4.0
15	3	256	ASP	4.0
13	1	97	GLY	4.0
14	2	134	GLU	4.0
1	A	644	GLN	4.0
2	B	214	ASP	4.0
11	K	63	CYS	4.0
14	2	135	TYR	4.0
13	1	115	ALA	3.9
13	6	219	HIS	3.9
15	3	115	TYR	3.9
13	6	216	ASP	3.9
14	7	70	SER	3.9
16	4	243	ASN	3.8
14	2	68	ASP	3.8
16	9	164	GLY	3.8
15	3	123	PRO	3.8
1	a	35	ALA	3.8
16	4	235	GLN	3.8
1	a	36	LYS	3.8
15	8	119	VAL	3.8
11	K	62	ALA	3.8
16	9	121	ILE	3.8
2	b	303	TYR	3.8
1	A	516	GLY	3.8
11	K	60	THR	3.8
16	4	131	LYS	3.8
13	1	147	MET	3.7
8	H	81	TYR	3.7
7	g	60	SER	3.7
6	F	135	TYR	3.7
14	2	85	ASP	3.7
15	3	125	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
16	4	241	TRP	3.7
13	6	157	PRO	3.7
16	4	181	GLU	3.7
10	J	37	LEU	3.7
2	B	474	PHE	3.6
16	9	192	LEU	3.6
13	6	215	ALA	3.6
15	3	186	LYS	3.6
1	a	30	SER	3.6
15	3	51	LEU	3.6
2	b	282	PHE	3.6
13	1	109	ALA	3.6
15	3	254	VAL	3.6
14	2	87	GLU	3.6
11	K	17	LEU	3.6
5	E	25	VAL	3.6
2	b	346	SER	3.5
11	k	53	ALA	3.5
14	2	122	LEU	3.5
15	8	207	PHE	3.5
2	B	379	ALA	3.5
8	H	75	SER	3.5
13	6	218	TRP	3.5
2	B	659	THR	3.5
13	6	217	PRO	3.5
2	b	583	MET	3.5
4	D	188	PHE	3.5
2	B	380	GLY	3.5
14	2	132	GLU	3.5
2	b	379	ALA	3.4
2	B	381	PHE	3.4
13	6	169	ASP	3.4
14	2	181	THR	3.4
2	b	474	PHE	3.4
2	B	213	LEU	3.4
2	b	342	GLY	3.4
5	E	57	LEU	3.4
16	4	133	GLU	3.4
7	g	41	LEU	3.4
2	B	580	VAL	3.4
15	3	220	LYS	3.4
14	2	182	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
8	H	134	GLN	3.3
2	b	344	ILE	3.3
2	B	583	MET	3.3
14	2	255	ALA	3.3
14	2	131	GLY	3.3
15	3	174	GLY	3.3
2	b	584	LEU	3.3
16	4	205	ILE	3.3
2	B	713	PHE	3.3
15	3	207	PHE	3.3
7	G	1	GLU	3.3
11	K	57	LEU	3.3
2	b	345	THR	3.3
1	a	517	GLY	3.3
2	b	580	VAL	3.3
6	F	189	LYS	3.3
10	j	2	ARG	3.3
6	f	224	GLU	3.3
16	4	242	HIS	3.3
2	b	482	ASN	3.3
11	k	2	PHE	3.3
13	1	116	THR	3.3
2	b	317	ARG	3.3
14	2	231	TYR	3.3
5	E	37	PRO	3.3
16	9	165	SER	3.3
8	h	58	PHE	3.3
16	4	199	GLU	3.3
15	3	257	PRO	3.3
14	2	198	SER	3.2
14	2	136	PHE	3.2
1	a	501	GLY	3.2
1	a	519	ASP	3.2
6	F	147	LEU	3.2
11	K	77	GLY	3.2
13	1	167	SER	3.2
2	B	709	GLY	3.2
14	2	137	THR	3.2
2	B	585	ASN	3.2
2	B	588	GLY	3.2
13	6	111	PRO	3.2
14	7	125	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
12	L	47	LEU	3.2
13	6	156	TYR	3.2
6	f	189	LYS	3.2
2	B	587	ILE	3.2
2	B	206	TYR	3.2
16	9	206	ALA	3.1
14	7	134	GLU	3.1
8	H	140	PRO	3.1
1	a	551	VAL	3.1
1	a	627	THR	3.1
2	b	213	LEU	3.1
13	6	173	LEU	3.1
11	K	18	MET	3.1
5	E	23	GLY	3.1
2	B	584	LEU	3.1
14	2	176	ASN	3.1
15	3	260	ASN	3.1
16	4	236	HIS	3.1
15	3	126	THR	3.1
6	F	158	GLU	3.1
2	B	664	LEU	3.1
15	8	115	TYR	3.1
14	7	221	ALA	3.1
1	A	339	THR	3.1
2	B	378	ILE	3.1
16	4	123	VAL	3.0
16	4	83	GLU	3.0
14	7	175	ASN	3.0
2	B	581	PHE	3.0
11	K	78	LEU	3.0
4	d	73	GLU	3.0
14	2	168	ASN	3.0
16	9	125	LYS	3.0
5	E	60	ILE	3.0
14	7	110	ILE	3.0
14	2	127	TRP	3.0
1	a	494	ASN	3.0
15	3	124	GLN	3.0
6	F	141	SER	3.0
2	B	717	TYR	2.9
1	A	631	GLN	2.9
13	6	162	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
15	8	259	ASN	2.9
2	B	589	TRP	2.9
5	E	28	VAL	2.9
2	B	82	PHE	2.9
6	F	136	GLY	2.9
14	2	76	GLY	2.9
15	3	116	LEU	2.9
15	3	145	TRP	2.9
13	6	66	PRO	2.9
13	6	159	GLY	2.9
13	6	170	PRO	2.9
16	4	85	PRO	2.9
2	b	380	GLY	2.9
15	3	59	LEU	2.9
16	4	164	GLY	2.9
1	A	529	LEU	2.9
2	B	712	HIS	2.9
1	A	607	ASN	2.9
11	K	59	ASP	2.9
12	L	29	ILE	2.9
1	a	208	ALA	2.9
10	j	1	MET	2.9
2	B	662	MET	2.9
13	1	203	GLY	2.9
12	L	41	THR	2.9
15	3	138	PRO	2.9
1	A	111	ASN	2.9
6	f	222	ASN	2.8
16	4	230	PHE	2.8
13	6	123	PRO	2.8
12	L	149	TRP	2.8
15	3	142	TYR	2.8
13	1	160	ALA	2.8
4	D	70	THR	2.8
15	8	247	TYR	2.8
7	g	35	VAL	2.8
2	B	591	THR	2.8
7	g	92	GLY	2.8
8	H	58	PHE	2.8
15	3	247	TYR	2.8
12	L	27	PRO	2.8
2	B	344	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	b	586	THR	2.8
3	C	39	ILE	2.8
2	B	454	LEU	2.8
16	4	177	LEU	2.8
2	b	714	SER	2.8
11	k	71	GLY	2.8
2	B	346	SER	2.8
8	h	79	SER	2.8
2	B	215	VAL	2.8
15	8	126	THR	2.8
2	b	235	GLN	2.8
2	b	340	SER	2.8
5	E	38	VAL	2.8
14	7	255	ALA	2.8
15	8	249	ASN	2.7
14	2	66	TRP	2.7
13	6	155	LYS	2.7
14	7	124	THR	2.7
13	1	52	PRO	2.7
1	a	498	LEU	2.7
12	L	156	VAL	2.7
2	B	374	HIS	2.7
6	f	135	TYR	2.7
13	1	204	THR	2.7
14	2	234	THR	2.7
13	1	120	ASN	2.7
1	a	713	LYS	2.7
6	f	227	ASP	2.7
16	4	86	GLU	2.7
11	K	15	THR	2.7
8	H	137	LYS	2.7
11	k	54	GLY	2.7
14	7	249	HIS	2.7
14	2	232	THR	2.7
13	1	144	GLN	2.7
14	2	52	PRO	2.7
1	A	734	GLY	2.7
15	3	111	ILE	2.7
7	g	55	VAL	2.7
12	L	122	GLU	2.7
14	7	71	LEU	2.7
2	B	577	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	155	TYR	2.7
16	4	115	PHE	2.7
16	9	96	LEU	2.7
4	D	126	PRO	2.7
5	E	5	ARG	2.7
6	F	154	ARG	2.7
1	A	28	LYS	2.6
1	A	110	LEU	2.6
1	a	714	LEU	2.6
16	9	175	TYR	2.6
2	B	343	VAL	2.6
2	B	345	THR	2.6
2	b	318	GLY	2.6
10	j	6	THR	2.6
8	H	101	LEU	2.6
14	7	128	TYR	2.6
14	7	135	TYR	2.6
15	8	128	LEU	2.6
15	8	179	GLN	2.6
2	B	210	ASN	2.6
2	B	482	ASN	2.6
8	H	79	SER	2.6
12	L	78	GLN	2.6
15	3	151	LEU	2.6
13	1	125	GLY	2.6
9	I	2	ILE	2.6
14	7	84	SER	2.6
15	3	222	VAL	2.6
15	8	174	GLY	2.6
2	B	458	ILE	2.6
13	1	119	GLY	2.6
7	G	55	VAL	2.6
7	g	94	ASP	2.6
16	4	167	ASN	2.6
14	2	54	ARG	2.6
13	1	56	GLY	2.6
15	8	116	LEU	2.6
14	2	226	TRP	2.6
16	4	202	GLU	2.6
16	9	131	LYS	2.6
8	h	60	LEU	2.5
11	K	19	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
11	K	56	THR	2.5
6	f	77	ASP	2.5
16	4	62	SER	2.5
14	2	190	TRP	2.5
10	J	38	ILE	2.5
2	b	481	THR	2.5
7	g	58	LEU	2.5
7	G	54	TYR	2.5
1	A	689	SER	2.5
2	B	340	SER	2.5
15	3	118	LYS	2.5
13	6	149	LYS	2.5
2	B	579	ALA	2.5
14	2	201	PRO	2.5
1	a	715	LYS	2.5
13	6	194	PHE	2.5
14	7	66	TRP	2.5
14	2	188	GLY	2.5
1	A	365	LEU	2.5
16	4	75	GLY	2.5
1	A	210	LEU	2.5
2	b	527	LEU	2.5
13	1	122	VAL	2.5
16	4	239	ASP	2.5
12	L	31	TRP	2.5
15	8	124	GLN	2.5
1	A	480	THR	2.5
2	b	157	LEU	2.5
1	A	471	GLY	2.4
13	6	67	ALA	2.4
1	A	213	LEU	2.4
16	4	120	ILE	2.4
2	B	715	VAL	2.4
2	b	343	VAL	2.4
14	7	123	ASN	2.4
14	2	199	ALA	2.4
2	b	305	LEU	2.4
16	9	189	PHE	2.4
15	8	123	PRO	2.4
1	a	450	CYS	2.4
16	4	84	ASP	2.4
15	3	223	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	710	LEU	2.4
4	d	82	ILE	2.4
2	b	384	THR	2.4
15	8	245	GLY	2.4
1	A	517	GLY	2.4
1	a	367	SER	2.4
14	2	160	ASP	2.4
7	G	26	PHE	2.4
14	2	247	PRO	2.4
16	4	201	LYS	2.4
1	A	604	TRP	2.4
4	D	105	ASP	2.4
14	2	74	ASP	2.4
2	B	660	GLY	2.4
1	a	444	SER	2.4
2	B	710	LEU	2.4
2	b	375	HIS	2.3
15	3	127	ALA	2.3
3	C	41	SER	2.3
1	a	27	ILE	2.3
12	L	28	LEU	2.3
1	A	214	GLY	2.3
4	D	153	GLN	2.3
14	2	245	ALA	2.3
2	B	32	GLU	2.3
2	B	718	ILE	2.3
15	3	250	LEU	2.3
3	C	27	GLU	2.3
14	7	127	TRP	2.3
2	B	282	PHE	2.3
4	d	112	PHE	2.3
14	2	67	LEU	2.3
14	2	129	THR	2.3
16	4	67	THR	2.3
2	b	186	SER	2.3
15	3	120	GLY	2.3
1	A	505	PRO	2.3
2	B	384	THR	2.3
1	a	366	GLY	2.3
1	a	210	LEU	2.3
1	a	548	THR	2.3
2	B	663	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
16	4	165	SER	2.3
2	B	711	VAL	2.3
8	H	78	PRO	2.3
12	L	151	TYR	2.3
1	A	681	GLY	2.3
2	B	342	GLY	2.3
5	e	5	ARG	2.3
2	b	585	ASN	2.3
14	7	52	PRO	2.3
14	7	201	PRO	2.3
16	9	191	PRO	2.3
1	A	212	GLY	2.3
1	A	738	TYR	2.3
1	a	209	GLY	2.3
7	g	40	GLY	2.3
15	8	180	TYR	2.3
7	g	50	ARG	2.3
2	b	525	LEU	2.3
14	7	130	ALA	2.3
13	6	46	TYR	2.3
1	a	28	LYS	2.3
2	B	487	ASN	2.2
2	b	187	SER	2.2
2	b	281	ALA	2.2
14	2	250	ALA	2.2
15	8	189	GLY	2.2
13	6	117	TYR	2.2
2	b	320	LYS	2.2
2	B	339	ALA	2.2
13	1	159	GLY	2.2
15	8	177	GLY	2.2
2	B	453	ILE	2.2
2	B	582	TRP	2.2
11	k	7	THR	2.2
2	B	347	LEU	2.2
3	C	26	LEU	2.2
16	4	233	LEU	2.2
2	b	587	ILE	2.2
2	B	529	THR	2.2
2	B	586	THR	2.2
13	1	118	LEU	2.2
14	2	248	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
15	3	132	GLN	2.2
4	D	169	LYS	2.2
1	A	519	ASP	2.2
2	b	313	GLY	2.2
2	b	475	ASP	2.2
1	A	87	SER	2.2
2	b	579	ALA	2.2
1	a	46	LYS	2.2
15	8	138	PRO	2.2
2	b	377	TYR	2.2
2	b	109	ALA	2.2
13	1	211	ALA	2.2
2	b	341	LEU	2.2
2	B	530	THR	2.2
2	b	300	SER	2.2
16	4	238	SER	2.2
2	b	526	GLY	2.2
2	b	347	LEU	2.2
15	3	139	ALA	2.2
11	K	11	MET	2.2
14	2	203	LYS	2.2
2	B	525	LEU	2.1
11	K	61	LEU	2.1
14	7	68	ASP	2.1
14	7	111	PHE	2.1
3	C	38	GLN	2.1
4	d	151	LYS	2.1
13	1	152	GLU	2.1
16	9	225	THR	2.1
12	L	154	LEU	2.1
13	1	127	LEU	2.1
13	6	114	GLN	2.1
14	2	251	THR	2.1
1	a	690	LEU	2.1
14	7	203	LYS	2.1
2	B	382	ILE	2.1
16	4	136	ALA	2.1
2	B	375	HIS	2.1
8	H	55	SER	2.1
13	1	117	TYR	2.1
14	7	237	ILE	2.1
1	a	447	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
14	7	198	SER	2.1
1	A	384	TYR	2.1
15	8	205	LEU	2.1
5	E	29	ASP	2.1
5	E	7	ALA	2.1
13	1	181	ILE	2.1
1	A	404	GLY	2.1
13	1	165	GLY	2.1
14	2	239	ASN	2.1
4	D	76	PRO	2.1
4	D	168	PRO	2.1
14	2	55	PRO	2.1
4	d	182	GLN	2.1
6	F	111	ASP	2.1
16	4	65	TYR	2.1
2	b	382	ILE	2.1
2	B	716	GLY	2.1
13	1	218	TRP	2.1
1	a	135	ASP	2.1
16	4	64	GLY	2.1
13	1	123	PRO	2.1
14	2	115	PHE	2.1
14	2	254	ALA	2.1
15	3	243	GLY	2.1
2	B	504	ASN	2.1
13	1	128	PRO	2.1
6	F	155	HIS	2.0
2	b	480	SER	2.0
12	L	5	GLN	2.0
15	8	217	LEU	2.0
14	7	126	SER	2.0
1	A	175	ALA	2.0
1	a	214	GLY	2.0
2	b	184	GLY	2.0
2	b	530	THR	2.0
4	D	185	GLY	2.0
1	A	174	PHE	2.0
6	F	138	LEU	2.0
14	2	119	LEU	2.0
16	4	234	LEU	2.0
2	B	526	GLY	2.0
5	E	27	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
16	9	228	GLY	2.0
13	1	194	PHE	2.0
14	2	53	ASP	2.0
2	B	634	GLY	2.0
1	A	685	VAL	2.0
1	A	176	GLY	2.0
16	9	241	TRP	2.0
2	b	711	VAL	2.0
1	A	90	PHE	2.0
10	J	32	PHE	2.0
1	a	520	LEU	2.0
6	f	107	LEU	2.0
14	7	204	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
20	BCR	2	617	40/40	0.67	0.77	20.87	125,133,163,164	0
27	LUT	6	321	42/42	0.75	0.49	7.93	107,113,133,134	0
20	BCR	7	617	40/40	0.70	0.63	7.51	112,119,127,128	0
20	BCR	L	206	40/40	0.48	0.80	6.13	146,151,156,156	0
17	CLA	A	824	51/65	0.84	0.38	6.02	77,89,118,118	0
20	BCR	1	206	40/40	0.77	0.52	5.60	77,82,93,93	0
17	CLA	6	316	46/65	0.82	0.30	5.14	152,162,171,203	0
19	LHG	6	320	49/49	0.89	0.32	4.34	90,100,111,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	BCR	a	852	40/40	0.86	0.33	4.33	40,62,120,120	0
17	CLA	g	102	50/65	0.92	0.33	4.18	92,107,123,124	0
22	HTG	f	7001	19/19	0.86	0.33	3.92	49,104,107,108	0
17	CLA	3	301	46/65	0.80	0.78	3.83	142,149,154,175	0
20	BCR	K	4004	40/40	0.49	0.62	3.56	94,115,138,138	0
20	BCR	A	850	40/40	0.84	0.30	3.53	53,72,112,112	0
17	CLA	A	845	52/65	0.85	0.41	3.49	90,115,146,149	0
20	BCR	6	319	40/40	0.82	0.47	3.10	104,124,138,140	0
17	CLA	l	202	65/65	0.87	0.40	2.83	57,88,111,113	0
20	BCR	1	318	40/40	0.77	0.50	2.72	94,105,126,127	0
20	BCR	4	618	40/40	0.85	0.30	2.63	79,86,89,90	0
17	CLA	a	824	51/65	0.91	0.23	2.51	61,74,91,93	0
19	LHG	1	319	49/49	0.90	0.27	2.49	77,84,109,109	0
18	PQN	B	842	33/33	0.94	0.44	2.43	46,56,63,63	0
20	BCR	l	205	40/40	0.93	0.24	2.34	39,46,52,54	0
17	CLA	B	809	65/65	0.93	0.23	2.23	41,50,81,82	0
17	CLA	9	609	60/65	0.91	0.37	2.19	72,93,107,108	0
20	BCR	9	618	40/40	0.90	0.29	2.14	86,92,100,101	0
27	LUT	7	615	42/42	0.88	0.47	2.06	72,83,97,98	0
20	BCR	B	844	40/40	0.87	0.28	2.02	50,53,85,87	0
17	CLA	a	811	65/65	0.93	0.20	2.01	42,59,94,96	0
17	CLA	A	811	65/65	0.94	0.26	1.99	54,69,89,90	0
17	CLA	a	809	65/65	0.95	0.20	1.98	36,39,53,57	0
20	BCR	A	856	40/40	0.81	0.25	1.91	65,71,85,85	0
20	BCR	g	104	40/40	0.86	0.40	1.83	57,102,117,118	0
20	BCR	K	4001	40/40	0.59	0.41	1.75	91,94,96,96	0
20	BCR	L	205	40/40	0.92	0.21	1.72	51,61,70,71	0
20	BCR	8	316	40/40	0.87	0.36	1.69	66,71,88,90	0
17	CLA	7	611	52/65	0.91	0.33	1.66	87,104,123,126	0
17	CLA	G	103	50/65	0.91	0.23	1.66	61,80,91,93	0
27	LUT	1	320	42/42	0.87	0.22	1.64	71,79,90,91	0
17	CLA	a	819	65/65	0.93	0.22	1.60	38,54,96,99	0
27	LUT	8	314	42/42	0.91	0.39	1.56	57,73,82,84	0
20	BCR	G	105	40/40	0.85	0.30	1.53	63,71,83,83	0
20	BCR	A	849	40/40	0.93	0.44	1.50	54,62,83,84	0
17	CLA	1	309	65/65	0.86	0.25	1.50	71,79,106,108	0
28	XAT	3	317	44/44	0.87	0.26	1.47	61,74,100,101	0
28	XAT	8	315	44/44	0.90	0.23	1.47	64,69,80,83	0
20	BCR	B	848	40/40	0.94	0.33	1.45	40,45,51,52	0
19	LHG	a	848	27/49	0.73	0.33	1.44	74,95,125,127	0
17	CLA	a	816	50/65	0.93	0.23	1.44	43,52,94,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	BCR	j	3004	40/40	0.88	0.24	1.44	56,71,82,84	0
17	CLA	8	310	55/65	0.92	0.33	1.44	74,88,99,104	0
17	CLA	2	608	50/65	0.91	0.18	1.42	65,69,108,111	0
25	LMG	6	302	40/55	0.75	0.34	1.41	116,148,163,164	0
17	CLA	K	4002	45/65	0.76	0.46	1.41	115,123,125,154	0
17	CLA	8	311	45/65	0.89	0.34	1.40	100,110,122,161	0
27	LUT	9	616	42/42	0.89	0.38	1.39	68,79,103,104	0
17	CLA	9	614	47/65	0.94	0.23	1.38	62,75,97,99	0
17	CLA	a	846	52/65	0.88	0.32	1.37	86,102,115,140	0
19	LHG	2	618	37/49	0.94	0.30	1.31	80,91,127,130	0
17	CLA	7	603	51/65	0.95	0.19	1.30	52,60,97,98	0
18	PQN	A	844	33/33	0.96	0.24	1.26	42,45,57,58	0
17	CLA	1	308	65/65	0.92	0.37	1.22	57,92,120,121	0
17	CLA	B	808	65/65	0.95	0.25	1.19	41,45,70,73	0
20	BCR	I	101	40/40	0.90	0.23	1.14	54,60,65,65	0
20	BCR	j	3003	40/40	0.92	0.22	1.11	42,52,59,61	0
17	CLA	B	810	65/65	0.92	0.22	1.10	59,77,84,86	0
17	CLA	A	835	65/65	0.92	0.23	1.10	58,67,75,81	0
17	CLA	G	104	46/65	0.93	0.31	1.09	70,93,100,111	0
17	CLA	B	807	65/65	0.93	0.21	1.07	51,66,113,117	0
22	HTG	j	3001	19/19	0.93	0.37	1.07	61,71,80,84	0
28	XAT	6	318	44/44	0.92	0.24	1.04	71,81,94,95	0
17	CLA	b	832	65/65	0.93	0.22	1.04	36,55,70,79	0
17	CLA	a	829	65/65	0.95	0.23	1.04	35,41,56,58	0
17	CLA	A	809	65/65	0.95	0.19	1.03	44,51,63,65	0
26	CHL	2	601	61/66	0.92	0.32	1.02	68,99,113,115	0
17	CLA	b	811	54/65	0.88	0.29	1.02	50,74,114,114	0
17	CLA	B	827	65/65	0.92	0.40	1.02	49,61,78,80	0
17	CLA	b	834	65/65	0.93	0.21	1.02	61,74,105,106	0
17	CLA	B	839	65/65	0.93	0.25	1.02	53,60,69,72	0
17	CLA	7	608	50/65	0.91	0.20	1.01	60,65,93,96	0
27	LUT	4	616	42/42	0.85	0.31	0.99	71,90,94,95	0
26	CHL	9	615	43/66	0.87	0.34	0.98	90,144,147,148	0
26	CHL	7	614	43/66	0.92	0.29	0.97	105,120,127,139	0
25	LMG	4	619	44/55	0.80	0.35	0.95	82,92,103,104	0
17	CLA	3	303	50/65	0.95	0.21	0.94	60,67,75,76	0
17	CLA	6	310	65/65	0.89	0.25	0.91	80,90,121,126	0
17	CLA	7	609	60/65	0.93	0.27	0.90	64,86,97,97	0
17	CLA	4	603	46/65	0.95	0.19	0.89	54,62,69,72	0
17	CLA	A	814	65/65	0.92	0.31	0.88	50,59,67,68	0
17	CLA	a	833	65/65	0.94	0.25	0.88	39,46,98,102	0
17	CLA	6	307	42/65	0.91	0.27	0.88	112,126,137,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	CLA	6	314	60/65	0.93	0.23	0.87	66,109,124,125	0
17	CLA	A	837	45/65	0.86	0.28	0.86	84,95,103,165	0
17	CLA	4	614	50/65	0.94	0.20	0.85	60,68,90,91	0
20	BCR	B	846	40/40	0.91	0.23	0.84	49,53,70,70	0
20	BCR	3	318	40/40	0.92	0.23	0.83	77,83,105,108	0
17	CLA	B	838	47/65	0.95	0.30	0.83	43,48,65,68	0
20	BCR	b	844	40/40	0.83	0.32	0.83	52,67,91,93	0
27	LUT	2	615	42/42	0.90	0.27	0.82	77,84,89,89	0
17	CLA	B	817	59/65	0.91	0.22	0.79	46,53,59,64	0
17	CLA	7	613	43/65	0.93	0.23	0.79	73,78,82,86	0
28	XAT	7	616	44/44	0.89	0.33	0.78	57,64,73,74	0
17	CLA	B	805	65/65	0.93	0.25	0.77	45,47,53,60	0
17	CLA	L	202	65/65	0.84	0.37	0.76	83,111,131,132	0
17	CLA	A	843	65/65	0.94	0.26	0.74	48,64,79,81	0
20	BCR	k	1404	40/40	0.87	0.26	0.71	49,89,103,104	0
27	LUT	6	317	42/42	0.66	0.43	0.70	86,93,118,120	0
28	XAT	1	317	44/44	0.93	0.21	0.69	63,68,93,96	0
17	CLA	1	313	65/65	0.92	0.21	0.69	81,88,108,112	0
20	BCR	B	847	40/40	0.90	0.31	0.68	44,49,52,53	0
24	DGD	b	849	66/66	0.86	0.27	0.68	41,64,90,91	0
24	DGD	B	850	66/66	0.80	0.33	0.68	52,71,93,102	0
17	CLA	a	808	65/65	0.95	0.20	0.67	54,63,86,87	0
17	CLA	B	819	65/65	0.96	0.23	0.67	46,53,80,83	0
17	CLA	b	827	65/65	0.95	0.28	0.67	40,53,83,83	0
17	CLA	g	101	41/65	0.86	0.21	0.66	146,164,166,167	0
17	CLA	8	308	50/65	0.91	0.33	0.64	75,81,87,88	0
20	BCR	a	849	40/40	0.87	0.26	0.62	56,63,75,76	0
26	CHL	9	607	51/66	0.92	0.27	0.60	67,77,98,99	0
17	CLA	a	842	65/65	0.94	0.21	0.60	47,59,96,98	0
25	LMG	9	619	50/55	0.84	0.28	0.59	68,88,96,98	0
17	CLA	A	806	65/65	0.91	0.29	0.59	46,51,59,59	0
17	CLA	B	840	65/65	0.93	0.33	0.59	41,50,72,78	0
17	CLA	B	824	65/65	0.91	0.27	0.58	48,53,70,74	0
20	BCR	B	843	40/40	0.91	0.23	0.57	54,64,72,72	0
17	CLA	B	803	65/65	0.94	0.33	0.57	39,50,61,68	0
19	LHG	1	301	23/49	0.95	0.20	0.57	63,84,93,94	0
20	BCR	l	201	40/40	0.93	0.21	0.57	38,46,54,54	0
17	CLA	A	823	49/65	0.89	0.25	0.56	66,79,104,105	0
20	BCR	A	851	40/40	0.88	0.28	0.56	43,66,78,79	0
17	CLA	7	604	60/65	0.87	0.34	0.55	92,101,106,109	0
17	CLA	a	843	65/65	0.95	0.24	0.55	35,39,60,65	0
19	LHG	a	847	49/49	0.96	0.21	0.55	35,41,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	BCR	L	201	40/40	0.94	0.18	0.55	51,59,72,73	0
17	CLA	2	612	65/65	0.90	0.32	0.55	70,93,113,118	0
20	BCR	b	846	40/40	0.92	0.22	0.54	48,56,76,77	0
17	CLA	b	810	65/65	0.95	0.17	0.54	39,49,59,62	0
17	CLA	k	1401	45/65	0.88	0.34	0.54	75,83,94,96	0
17	CLA	b	837	65/65	0.95	0.21	0.53	46,57,69,70	0
26	CHL	6	308	47/66	0.92	0.23	0.53	103,135,146,149	0
17	CLA	A	801	65/65	0.94	0.27	0.52	40,44,49,53	0
17	CLA	B	832	65/65	0.95	0.23	0.52	43,48,73,76	0
17	CLA	a	813	54/65	0.93	0.19	0.51	43,51,60,70	0
17	CLA	k	1402	46/65	0.90	0.26	0.50	62,78,100,106	0
17	CLA	6	306	51/65	0.92	0.24	0.49	118,123,130,131	0
17	CLA	A	834	65/65	0.90	0.24	0.48	49,60,71,75	0
28	XAT	9	617	44/44	0.85	0.23	0.48	72,81,97,98	0
20	BCR	A	848	40/40	0.89	0.32	0.47	50,59,95,95	0
17	CLA	B	818	60/65	0.91	0.26	0.47	45,50,57,61	0
17	CLA	a	814	65/65	0.94	0.24	0.46	39,47,64,67	0
20	BCR	b	801	40/40	0.92	0.20	0.46	36,43,52,55	0
17	CLA	K	4003	46/65	0.83	0.29	0.44	81,119,128,130	0
25	LMG	4	620	44/55	0.69	0.42	0.43	89,97,111,113	0
17	CLA	b	817	59/65	0.92	0.24	0.43	56,59,67,68	0
17	CLA	a	840	65/65	0.92	0.32	0.42	36,41,87,89	0
17	CLA	A	819	65/65	0.95	0.21	0.42	54,65,117,120	0
26	CHL	2	606	48/66	0.86	0.45	0.41	89,97,105,107	0
17	CLA	4	604	50/65	0.90	0.30	0.40	75,84,111,114	0
17	CLA	A	829	65/65	0.95	0.23	0.39	42,46,55,58	0
17	CLA	a	806	65/65	0.95	0.21	0.39	37,39,49,51	0
17	CLA	A	830	65/65	0.95	0.28	0.39	45,53,58,61	0
20	BCR	F	305	40/40	0.95	0.20	0.39	46,51,58,60	0
17	CLA	A	804	65/65	0.92	0.23	0.38	46,58,70,71	0
17	CLA	9	603	46/65	0.95	0.17	0.38	62,64,77,78	0
17	CLA	b	809	65/65	0.94	0.20	0.38	39,50,72,75	0
26	CHL	6	303	61/66	0.93	0.20	0.38	78,91,102,103	0
17	CLA	f	7003	55/65	0.93	0.24	0.37	68,87,121,122	0
17	CLA	6	311	60/65	0.91	0.46	0.37	81,99,115,116	0
20	BCR	b	845	40/40	0.88	0.24	0.36	46,67,106,106	0
17	CLA	A	841	65/65	0.95	0.19	0.36	44,50,55,60	0
28	XAT	4	617	44/44	0.93	0.19	0.36	63,72,87,88	0
17	CLA	l	203	65/65	0.93	0.20	0.35	40,51,71,73	0
17	CLA	B	834	65/65	0.90	0.21	0.35	46,58,90,90	0
17	CLA	b	833	58/65	0.93	0.20	0.35	48,63,77,78	0
17	CLA	8	301	60/65	0.96	0.17	0.34	56,64,68,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	CLA	9	612	56/65	0.91	0.24	0.34	68,77,89,92	0
17	CLA	6	315	55/65	0.93	0.28	0.34	105,114,131,131	0
20	BCR	a	851	40/40	0.95	0.32	0.34	37,53,66,67	0
17	CLA	3	313	45/65	0.87	0.41	0.32	85,97,102,106	0
17	CLA	a	839	65/65	0.93	0.24	0.32	36,43,65,69	0
17	CLA	B	828	65/65	0.95	0.29	0.31	43,48,58,61	0
17	CLA	A	803	65/65	0.95	0.27	0.31	39,44,54,59	0
17	CLA	2	604	60/65	0.88	0.34	0.31	100,111,118,119	0
17	CLA	3	302	60/65	0.88	0.20	0.31	67,79,85,95	0
17	CLA	A	826	65/65	0.93	0.23	0.29	47,57,65,66	0
26	CHL	7	606	48/66	0.90	0.29	0.29	71,87,104,105	0
17	CLA	a	810	65/65	0.95	0.19	0.29	44,59,94,95	0
20	BCR	f	7004	40/40	0.93	0.20	0.28	55,62,66,66	0
17	CLA	7	612	65/65	0.94	0.24	0.27	56,66,87,89	0
17	CLA	9	602	60/65	0.94	0.18	0.27	60,67,74,86	0
17	CLA	4	609	60/65	0.88	0.31	0.26	69,86,106,111	0
17	CLA	a	841	65/65	0.95	0.21	0.26	55,62,65,67	0
17	CLA	2	610	41/65	0.90	0.21	0.26	80,94,108,110	0
17	CLA	B	811	54/65	0.90	0.21	0.26	58,74,103,104	0
17	CLA	b	839	65/65	0.96	0.18	0.25	38,44,50,53	0
17	CLA	9	608	50/65	0.94	0.18	0.25	72,78,103,105	0
17	CLA	B	841	65/65	0.94	0.19	0.25	49,56,63,68	0
22	HTG	F	302	19/19	0.84	0.32	0.24	43,98,105,107	0
17	CLA	4	608	50/65	0.94	0.17	0.24	56,66,76,86	0
17	CLA	a	835	65/65	0.96	0.19	0.24	36,43,48,49	0
17	CLA	F	303	45/65	0.95	0.20	0.23	51,60,71,76	0
28	XAT	2	616	44/44	0.92	0.25	0.23	69,79,86,87	0
17	CLA	F	301	65/65	0.94	0.19	0.23	48,55,83,87	0
17	CLA	A	818	65/65	0.92	0.22	0.23	58,71,95,97	0
20	BCR	B	801	40/40	0.95	0.21	0.22	43,46,54,55	0
17	CLA	A	813	54/65	0.93	0.21	0.22	60,68,77,95	0
17	CLA	L	203	65/65	0.91	0.23	0.21	64,74,87,89	0
17	CLA	B	802	65/65	0.92	0.30	0.20	40,44,50,52	0
17	CLA	b	818	60/65	0.95	0.28	0.20	44,47,53,56	0
17	CLA	B	813	65/65	0.91	0.23	0.20	47,51,54,55	0
17	CLA	b	807	65/65	0.91	0.22	0.19	42,51,102,104	0
17	CLA	B	820	50/65	0.95	0.20	0.19	53,69,95,100	0
17	CLA	1	303	65/65	0.90	0.24	0.19	60,67,83,90	0
17	CLA	B	837	65/65	0.94	0.23	0.18	49,55,61,65	0
18	PQN	a	845	33/33	0.96	0.22	0.18	35,48,54,58	0
17	CLA	b	802	65/65	0.95	0.24	0.17	36,41,45,52	0
17	CLA	3	308	50/65	0.94	0.21	0.16	76,86,93,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	CLA	b	820	50/65	0.91	0.21	0.16	65,72,77,82	0
17	CLA	b	835	45/65	0.93	0.16	0.16	86,92,94,96	0
17	CLA	b	815	55/65	0.92	0.28	0.15	62,78,93,94	0
17	CLA	B	821	46/65	0.88	0.23	0.15	51,60,72,80	0
17	CLA	A	816	50/65	0.95	0.20	0.15	52,70,108,108	0
17	CLA	6	304	65/65	0.94	0.20	0.15	66,79,104,106	0
27	LUT	3	316	42/42	0.92	0.25	0.15	74,78,97,99	0
17	CLA	b	812	55/65	0.91	0.22	0.14	59,70,103,104	0
17	CLA	b	828	65/65	0.96	0.29	0.14	41,47,56,56	0
17	CLA	B	822	55/65	0.93	0.23	0.13	48,58,82,83	0
18	PQN	b	842	33/33	0.96	0.22	0.13	36,41,49,50	0
17	CLA	a	826	65/65	0.94	0.22	0.13	39,43,48,56	0
17	CLA	b	813	65/65	0.94	0.23	0.12	44,57,67,69	0
17	CLA	a	818	65/65	0.95	0.21	0.12	45,53,81,83	0
20	BCR	a	850	40/40	0.96	0.23	0.12	39,48,79,81	0
26	CHL	7	605	43/66	0.87	0.27	0.11	85,89,93,99	0
17	CLA	1	314	55/65	0.89	0.23	0.11	78,93,105,110	0
17	CLA	B	814	65/65	0.91	0.20	0.10	50,57,80,82	0
17	CLA	1	310	60/65	0.90	0.25	0.10	63,80,90,92	0
17	CLA	b	836	60/65	0.94	0.23	0.10	43,53,106,107	0
17	CLA	a	834	65/65	0.94	0.24	0.10	37,44,48,50	0
17	CLA	6	309	46/65	0.90	0.30	0.10	92,99,106,137	0
17	CLA	A	802	65/65	0.95	0.29	0.10	41,45,51,53	0
17	CLA	a	815	45/65	0.94	0.19	0.10	41,54,63,63	0
17	CLA	B	826	65/65	0.95	0.28	0.09	44,50,56,64	0
17	CLA	9	604	50/65	0.89	0.23	0.09	105,116,125,126	0
17	CLA	b	830	50/65	0.90	0.21	0.09	46,59,70,74	0
17	CLA	b	840	65/65	0.94	0.23	0.09	36,41,59,67	0
17	CLA	A	832	50/65	0.90	0.24	0.06	52,70,98,99	0
17	CLA	a	804	65/65	0.91	0.21	0.06	36,52,71,73	0
17	CLA	a	825	55/65	0.96	0.18	0.06	39,44,58,68	0
17	CLA	A	820	65/65	0.94	0.22	0.06	46,50,57,58	0
22	HTG	J	3001	19/19	0.85	0.18	0.05	73,76,78,82	0
17	CLA	B	823	60/65	0.92	0.20	0.05	46,57,84,84	0
17	CLA	A	815	45/65	0.95	0.19	0.04	54,59,65,70	0
26	CHL	7	607	51/66	0.94	0.20	0.04	64,70,92,98	0
17	CLA	A	831	65/65	0.93	0.21	0.03	43,52,59,61	0
17	CLA	B	816	55/65	0.93	0.20	0.03	60,67,73,91	0
17	CLA	A	854	65/65	0.95	0.31	0.03	40,44,57,59	0
17	CLA	8	307	50/65	0.96	0.18	0.02	52,65,91,93	0
17	CLA	A	833	65/65	0.93	0.22	0.02	54,61,101,102	0
17	CLA	B	825	65/65	0.92	0.35	0.01	42,50,83,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	CLA	4	601	46/65	0.92	0.20	0.00	84,92,95,111	0
17	CLA	a	817	45/65	0.92	0.20	-0.01	64,73,78,79	0
17	CLA	J	3002	42/65	0.91	0.17	-0.01	92,105,119,148	0
17	CLA	4	610	55/65	0.89	0.28	-0.01	72,88,94,122	0
17	CLA	A	805	55/65	0.90	0.23	-0.01	45,54,89,89	0
17	CLA	a	802	65/65	0.95	0.27	-0.03	35,42,56,62	0
17	CLA	A	827	65/65	0.92	0.27	-0.04	40,60,97,98	0
17	CLA	B	829	65/65	0.89	0.26	-0.05	42,50,76,77	0
17	CLA	2	609	60/65	0.88	0.23	-0.05	73,87,98,101	0
19	LHG	A	847	27/49	0.83	0.26	-0.06	68,88,113,113	0
26	CHL	2	614	43/66	0.88	0.33	-0.06	116,134,143,145	0
26	CHL	1	302	61/66	0.94	0.21	-0.06	64,74,101,105	0
17	CLA	b	805	65/65	0.94	0.21	-0.06	42,45,52,58	0
17	CLA	9	613	45/65	0.91	0.20	-0.07	87,105,115,137	0
17	CLA	7	602	65/65	0.91	0.20	-0.08	62,70,88,93	0
17	CLA	b	826	65/65	0.95	0.27	-0.11	48,55,59,62	0
17	CLA	a	856	65/65	0.94	0.26	-0.11	36,41,56,59	0
17	CLA	A	808	65/65	0.92	0.18	-0.11	52,61,113,115	0
17	CLA	a	828	65/65	0.95	0.22	-0.11	37,44,67,72	0
17	CLA	a	805	55/65	0.94	0.18	-0.11	38,43,76,78	0
17	CLA	a	820	65/65	0.98	0.20	-0.12	38,43,48,50	0
17	CLA	B	804	45/65	0.94	0.18	-0.12	44,50,68,77	0
25	LMG	G	102	44/55	0.83	0.21	-0.12	72,95,110,113	0
20	BCR	b	847	40/40	0.91	0.24	-0.12	40,49,69,70	0
26	CHL	4	605	56/66	0.91	0.26	-0.12	69,88,96,102	0
17	CLA	a	831	65/65	0.96	0.19	-0.13	36,43,54,56	0
17	CLA	a	807	65/65	0.95	0.22	-0.13	35,41,50,54	0
17	CLA	B	830	50/65	0.94	0.17	-0.13	45,56,75,75	0
17	CLA	B	836	60/65	0.92	0.22	-0.13	43,46,97,97	0
17	CLA	b	841	65/65	0.88	0.20	-0.14	64,80,92,94	0
17	CLA	2	603	65/65	0.94	0.16	-0.14	64,72,106,108	0
17	CLA	b	814	65/65	0.90	0.18	-0.14	47,55,69,71	0
17	CLA	2	602	65/65	0.93	0.22	-0.15	66,73,80,83	0
17	CLA	b	829	65/65	0.93	0.23	-0.15	39,54,67,69	0
17	CLA	a	801	65/65	0.96	0.21	-0.15	35,39,44,46	0
17	CLA	A	836	50/65	0.92	0.18	-0.16	60,73,80,86	0
17	CLA	A	810	65/65	0.93	0.19	-0.16	43,51,85,89	0
17	CLA	a	844	65/65	0.96	0.23	-0.16	38,49,59,64	0
17	CLA	b	824	65/65	0.88	0.27	-0.16	45,51,69,72	0
17	CLA	b	808	65/65	0.95	0.18	-0.16	39,47,53,59	0
17	CLA	B	806	65/65	0.94	0.26	-0.17	43,52,60,64	0
20	BCR	B	845	40/40	0.90	0.18	-0.18	47,63,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	CLA	a	832	50/65	0.94	0.20	-0.18	41,54,78,83	0
17	CLA	6	312	41/65	0.92	0.20	-0.19	90,102,109,129	0
17	CLA	A	817	45/65	0.92	0.22	-0.19	66,75,86,92	0
26	CHL	2	607	51/66	0.93	0.22	-0.20	66,75,117,118	0
17	CLA	8	302	50/65	0.95	0.16	-0.20	46,54,73,74	0
17	CLA	A	828	65/65	0.94	0.22	-0.21	49,61,79,84	0
17	CLA	b	821	46/65	0.93	0.18	-0.21	58,69,90,118	0
17	CLA	a	838	51/65	0.95	0.19	-0.21	36,40,63,68	0
26	CHL	3	307	47/66	0.95	0.17	-0.21	72,77,94,97	0
17	CLA	G	101	45/65	0.93	0.21	-0.21	74,79,85,89	0
20	BCR	J	3003	40/40	0.92	0.21	-0.21	45,54,67,68	0
17	CLA	1	305	52/65	0.92	0.23	-0.22	76,101,105,108	0
17	CLA	b	816	55/65	0.93	0.19	-0.22	57,65,72,75	0
20	BCR	b	843	40/40	0.93	0.20	-0.23	54,60,68,69	0
19	LHG	A	846	49/49	0.94	0.21	-0.25	44,49,58,59	0
17	CLA	b	831	49/65	0.91	0.23	-0.25	51,55,71,71	0
17	CLA	a	823	49/65	0.92	0.18	-0.26	60,67,102,104	0
17	CLA	a	830	65/65	0.97	0.21	-0.26	36,40,47,49	0
17	CLA	3	309	50/65	0.91	0.23	-0.28	76,95,104,107	0
17	CLA	a	803	65/65	0.96	0.22	-0.28	35,38,50,53	0
17	CLA	a	812	65/65	0.93	0.23	-0.28	47,59,70,77	0
17	CLA	b	806	65/65	0.95	0.26	-0.28	39,43,52,65	0
17	CLA	B	812	55/65	0.95	0.21	-0.28	53,62,106,107	0
19	LHG	7	618	37/49	0.90	0.25	-0.29	83,95,102,104	0
17	CLA	b	823	60/65	0.92	0.23	-0.30	50,60,92,94	0
17	CLA	8	303	45/65	0.92	0.26	-0.31	75,92,99,133	0
17	CLA	A	807	65/65	0.96	0.27	-0.31	44,47,58,69	0
21	SF4	A	853	8/8	0.99	0.18	-0.31	43,44,48,51	0
17	CLA	9	601	46/65	0.93	0.18	-0.32	81,91,95,110	0
26	CHL	7	601	61/66	0.93	0.20	-0.33	62,74,93,95	0
17	CLA	8	304	42/65	0.93	0.18	-0.33	59,72,78,80	0
17	CLA	b	838	47/65	0.95	0.22	-0.34	38,44,54,64	0
17	CLA	2	611	52/65	0.94	0.17	-0.34	68,83,119,128	0
17	CLA	b	804	45/65	0.96	0.14	-0.34	42,52,68,75	0
17	CLA	a	836	50/65	0.91	0.17	-0.35	42,54,73,74	0
17	CLA	4	602	60/65	0.92	0.19	-0.35	54,67,73,74	0
17	CLA	j	3002	42/65	0.91	0.15	-0.35	91,94,96,97	0
17	CLA	a	821	45/65	0.94	0.19	-0.35	51,62,70,87	0
26	CHL	8	306	47/66	0.94	0.21	-0.36	60,64,79,84	0
26	CHL	2	605	43/66	0.86	0.27	-0.37	77,89,100,106	0
17	CLA	g	103	46/65	0.90	0.28	-0.37	87,99,103,116	0
17	CLA	B	815	60/65	0.89	0.22	-0.38	60,72,100,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	CHL	4	606	51/66	0.90	0.21	-0.38	71,81,109,110	0
17	CLA	k	1403	46/65	0.85	0.21	-0.39	89,95,103,110	0
17	CLA	L	204	50/65	0.92	0.19	-0.41	76,84,109,109	0
17	CLA	4	613	45/65	0.91	0.25	-0.42	92,103,108,160	0
17	CLA	a	837	45/65	0.93	0.18	-0.43	57,65,74,77	0
17	CLA	l	204	50/65	0.93	0.18	-0.43	46,59,100,104	0
17	CLA	A	842	65/65	0.95	0.23	-0.44	42,45,56,65	0
27	LUT	1	316	42/42	0.92	0.19	-0.44	69,74,100,101	0
20	BCR	A	852	40/40	0.96	0.23	-0.45	42,44,49,50	0
17	CLA	f	7002	45/65	0.96	0.16	-0.45	54,59,76,77	0
17	CLA	B	833	58/65	0.93	0.18	-0.46	43,52,79,80	0
21	SF4	C	101	8/8	0.99	0.14	-0.47	47,49,53,57	0
17	CLA	A	839	65/65	0.92	0.19	-0.49	54,60,80,83	0
17	CLA	A	822	65/65	0.95	0.20	-0.50	49,67,76,79	0
20	BCR	a	854	40/40	0.97	0.20	-0.51	35,40,47,47	0
17	CLA	8	305	47/65	0.95	0.15	-0.51	61,71,78,79	0
17	CLA	A	812	65/65	0.90	0.21	-0.51	49,63,74,82	0
17	CLA	a	827	65/65	0.95	0.27	-0.52	35,41,82,85	0
17	CLA	b	822	55/65	0.93	0.16	-0.52	46,60,80,83	0
21	SF4	a	855	8/8	0.98	0.20	-0.53	37,37,43,43	0
17	CLA	4	612	56/65	0.91	0.19	-0.54	63,78,87,88	0
17	CLA	A	821	45/65	0.93	0.21	-0.54	69,74,88,109	0
17	CLA	1	315	46/65	0.93	0.15	-0.55	76,87,93,132	0
26	CHL	1	307	48/66	0.91	0.19	-0.56	75,95,109,110	0
26	CHL	4	607	51/66	0.93	0.20	-0.56	57,73,82,85	0
17	CLA	b	819	65/65	0.94	0.24	-0.57	50,57,92,95	0
17	CLA	A	840	65/65	0.95	0.23	-0.58	48,55,95,96	0
17	CLA	b	803	65/65	0.97	0.27	-0.60	35,40,47,49	0
17	CLA	1	311	41/65	0.95	0.17	-0.61	67,74,81,82	0
26	CHL	4	615	43/66	0.92	0.19	-0.62	61,74,87,89	0
21	SF4	c	101	8/8	0.99	0.16	-0.63	41,46,54,56	0
26	CHL	9	606	51/66	0.92	0.19	-0.64	86,106,118,119	0
20	BCR	a	853	40/40	0.93	0.26	-0.65	44,48,66,67	0
17	CLA	1	306	52/65	0.92	0.17	-0.65	90,99,109,111	0
17	CLA	A	838	51/65	0.95	0.17	-0.65	45,60,67,68	0
17	CLA	F	304	55/65	0.90	0.21	-0.67	52,69,95,95	0
17	CLA	B	831	49/65	0.96	0.18	-0.68	45,53,62,65	0
17	CLA	b	825	65/65	0.92	0.32	-0.70	38,55,82,83	0
19	LHG	6	301	23/49	0.93	0.15	-0.71	67,101,110,111	0
26	CHL	9	605	56/66	0.92	0.18	-0.71	80,94,97,126	0
17	CLA	3	304	45/65	0.90	0.21	-0.71	109,122,133,162	0
17	CLA	A	825	55/65	0.93	0.16	-0.74	58,67,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	BCR	b	848	40/40	0.94	0.20	-0.76	37,42,45,47	0
17	CLA	B	835	45/65	0.92	0.17	-0.81	57,66,70,72	0
21	SF4	c	102	8/8	0.99	0.12	-0.82	41,50,62,77	0
17	CLA	3	306	47/65	0.94	0.18	-0.87	67,79,90,91	0
17	CLA	a	822	65/65	0.95	0.17	-0.91	42,46,53,57	0
17	CLA	3	312	55/65	0.93	0.15	-0.91	86,107,114,117	0
17	CLA	3	305	42/65	0.93	0.20	-0.93	67,78,84,90	0
17	CLA	7	610	41/65	0.95	0.19	-1.23	74,82,94,99	0
17	CLA	9	610	41/65	0.95	0.25	-1.25	99,103,113,114	0
21	SF4	C	102	8/8	0.99	0.09	-1.70	51,62,72,84	0
17	CLA	2	613	43/65	0.88	0.23	-2.46	80,88,94,95	0
17	CLA	6	305	65/65	0.89	0.23	-	83,87,104,110	0
17	CLA	8	313	25/65	0.83	0.28	-	102,110,116,146	0
17	CLA	3	311	52/65	0.89	0.41	-	129,142,154,157	0
22	HTG	A	855	19/19	0.96	0.15	-	68,72,74,75	0
17	CLA	4	611	52/65	0.91	0.28	-	71,88,123,125	0
17	CLA	9	611	52/65	0.90	0.36	-	76,89,102,103	0
17	CLA	1	312	52/65	0.93	0.20	-	70,76,99,100	0
19	LHG	3	319	20/49	0.79	0.50	-	152,157,193,194	0
17	CLA	8	309	52/65	0.61	0.51	-	155,164,169,259	0
17	CLA	3	315	25/65	0.87	0.26	-	112,115,121,157	0
17	CLA	3	314	46/65	0.92	0.18	-	73,78,101,103	0
17	CLA	6	313	52/65	0.88	0.23	-	83,94,119,120	0
22	HTG	a	857	19/19	0.93	0.25	-	53,70,79,81	0
17	CLA	8	312	46/65	0.95	0.15	-	57,66,99,103	0
20	BCR	i	101	40/40	0.93	0.17	-	36,45,49,50	0
17	CLA	1	304	65/65	0.94	0.21	-	63,70,95,97	0
17	CLA	3	310	37/65	0.82	0.63	-	179,186,191,221	0
23	LMT	B	849	35/35	0.80	0.33	-	80,97,102,103	0

6.5 Other polymers ⓘ

There are no such residues in this entry.