



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2018 – 08:44 PM EST

PDB ID : 5OY0
Title : Structure of synechocystis photosystem I trimer at 2.5A resolution
Authors : Nelson, N.; Malavath, T.; Caspy, I.
Deposited on : 2017-09-07
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
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) : rb-20030736

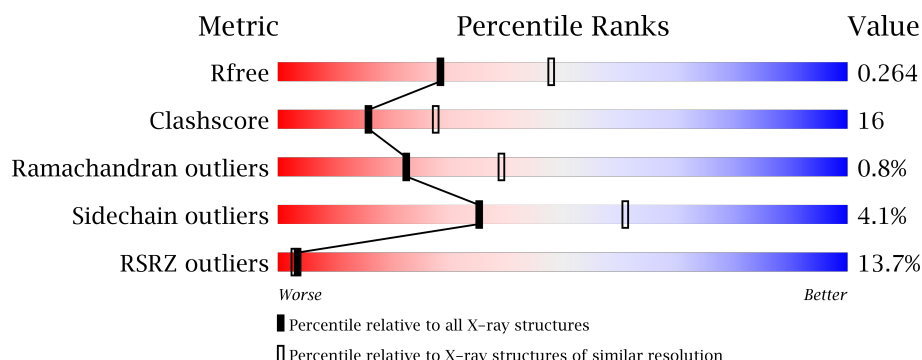
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



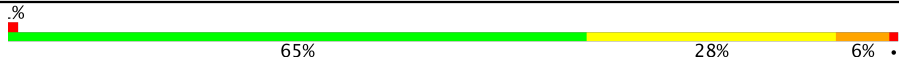

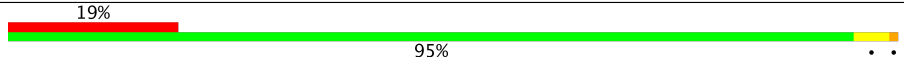
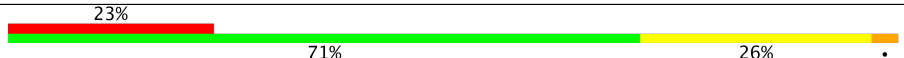
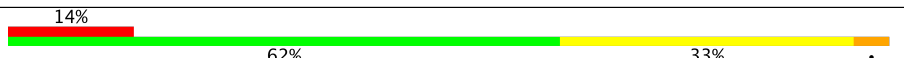
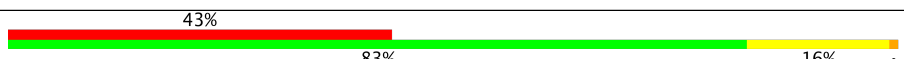
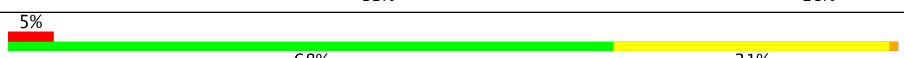

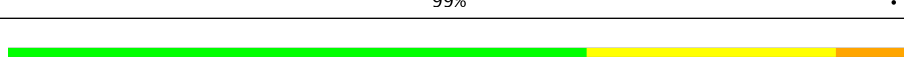

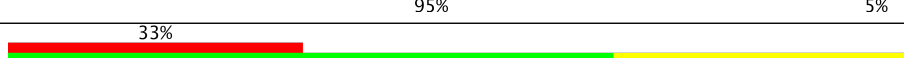

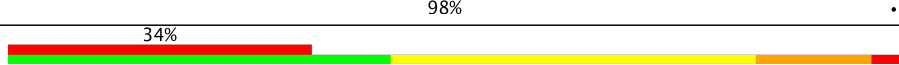
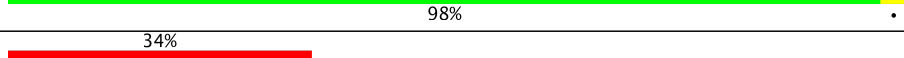


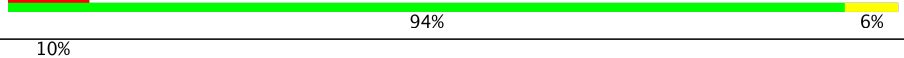

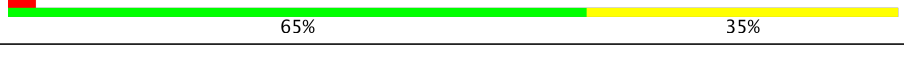
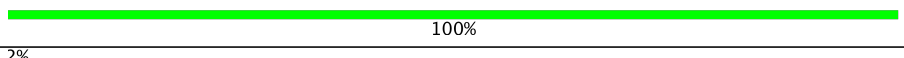
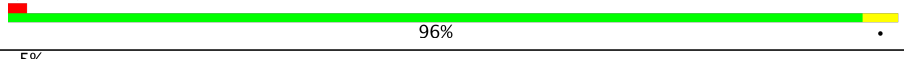
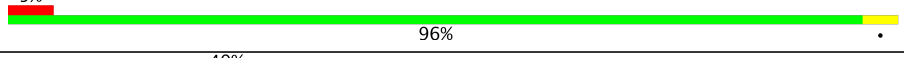
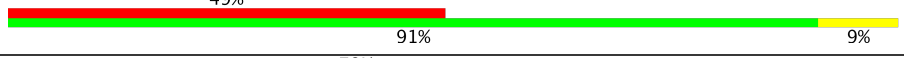


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	751	<div> <div>3%</div> <div>62%</div> <div>37%</div> <div>.</div> </div>
1	a	751	<div> <div>19%</div> <div>97%</div> <div>.</div> </div>
2	2	731	<div> <div>18%</div> <div>75%</div> <div>25%</div> <div>.</div> </div>
2	B	731	<div> <div>6%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>
3	3	80	<div> <div>29%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>

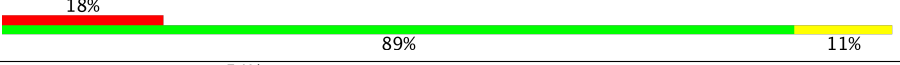


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Mol	Chain	Length	Quality of chain
3	C	80	
4	D	141	
4	d	141	
5	5	69	
5	E	69	
6	6	143	
6	F	143	
6	f	143	
7	I	40	
7	i	40	
8	7	40	
8	J	40	
8	j	40	
9	K	80	
10	L	157	
10	l	157	
11	9	31	
11	M	31	
11	m	31	
12	b	729	
13	c	81	
14	e	68	
15	k	78	
16	1	744	
17	4	140	

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Mol	Chain	Length	Quality of chain
18	h	38	
19	8	79	
20	0	154	

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
21	CLA	0	201	X	-	-	-
21	CLA	0	202	X	-	-	-
21	CLA	0	203	X	-	-	-
21	CLA	1	801	X	-	-	-
21	CLA	1	802	X	-	-	-
21	CLA	1	803	X	-	-	-
21	CLA	1	804	X	-	-	-
21	CLA	1	805	X	-	-	-
21	CLA	1	806	X	-	-	-
21	CLA	1	807	X	-	-	-
21	CLA	1	808	X	-	-	-
21	CLA	1	809	X	-	-	-
21	CLA	1	810	X	-	-	-
21	CLA	1	811	X	-	-	X
21	CLA	1	812	X	-	-	-
21	CLA	1	813	X	-	-	-
21	CLA	1	814	X	-	-	-
21	CLA	1	815	X	-	-	-
21	CLA	1	816	X	-	-	-
21	CLA	1	817	X	-	-	-
21	CLA	1	818	X	-	-	-
21	CLA	1	819	X	-	-	-
21	CLA	1	820	X	-	-	-
21	CLA	1	821	X	-	-	-
21	CLA	1	822	X	-	-	-
21	CLA	1	823	X	-	-	-
21	CLA	1	824	X	-	-	-
21	CLA	1	825	X	-	-	-
21	CLA	1	826	X	-	-	-
21	CLA	1	827	X	-	-	-
21	CLA	1	828	X	-	-	-
21	CLA	1	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	830	X	-	-	-
21	CLA	1	831	X	-	-	-
21	CLA	1	832	X	-	-	-
21	CLA	1	833	X	-	-	-
21	CLA	1	834	X	-	-	-
21	CLA	1	835	X	-	-	-
21	CLA	1	836	X	-	-	-
21	CLA	1	837	X	-	-	-
21	CLA	1	838	X	-	-	-
21	CLA	1	839	X	-	-	-
21	CLA	1	840	X	-	-	-
21	CLA	1	841	X	-	-	-
21	CLA	1	855	X	-	-	-
21	CLA	2	802	X	-	-	-
21	CLA	2	803	X	-	-	-
21	CLA	2	804	X	-	-	-
21	CLA	2	805	X	-	-	-
21	CLA	2	806	X	-	-	-
21	CLA	2	807	X	-	-	-
21	CLA	2	808	X	-	-	-
21	CLA	2	809	X	-	-	-
21	CLA	2	810	X	-	-	-
21	CLA	2	811	X	-	-	-
21	CLA	2	812	X	-	-	-
21	CLA	2	813	X	-	-	-
21	CLA	2	814	X	-	-	-
21	CLA	2	815	X	-	-	-
21	CLA	2	816	X	-	-	-
21	CLA	2	817	X	-	-	-
21	CLA	2	818	X	-	-	-
21	CLA	2	819	X	-	-	-
21	CLA	2	820	X	-	-	-
21	CLA	2	821	X	-	-	-
21	CLA	2	822	X	-	-	-
21	CLA	2	823	X	-	-	-
21	CLA	2	824	X	-	-	-
21	CLA	2	825	X	-	-	-
21	CLA	2	826	X	-	-	-
21	CLA	2	827	X	-	-	-
21	CLA	2	828	X	-	-	-
21	CLA	2	829	X	-	-	-
21	CLA	2	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	2	831	X	-	-	-
21	CLA	2	832	X	-	-	-
21	CLA	2	833	X	-	-	-
21	CLA	2	834	X	-	-	-
21	CLA	2	835	X	-	-	-
21	CLA	2	836	X	-	-	-
21	CLA	2	837	X	-	-	-
21	CLA	2	838	X	-	-	-
21	CLA	2	839	X	-	-	-
21	CLA	2	840	X	-	-	-
21	CLA	2	841	X	-	-	-
21	CLA	2	842	X	-	-	-
21	CLA	6	201	X	-	-	-
21	CLA	6	203	X	-	-	-
21	CLA	6	204	X	-	-	X
21	CLA	7	1101	X	-	-	-
21	CLA	7	1103	X	-	-	-
21	CLA	7	1104	X	-	-	X
21	CLA	7	1105	X	-	-	-
21	CLA	8	1401	X	-	-	-
21	CLA	8	1402	X	-	-	-
21	CLA	A	801	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	X
21	CLA	A	813	X	-	X	-
21	CLA	A	814	X	-	-	X
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	X	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	854	X	-	-	-
21	CLA	A	855	X	-	-	-
21	CLA	B	801	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	X
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	X
21	CLA	F	202	X	-	-	-
21	CLA	F	203	X	-	-	-
21	CLA	I	101	X	-	-	-
21	CLA	J	1101	X	-	-	-
21	CLA	J	1103	X	-	-	-
21	CLA	J	1105	X	-	-	-
21	CLA	J	1106	X	-	-	X
21	CLA	K	102	X	-	-	-
21	CLA	K	103	X	-	-	-
21	CLA	L	203	X	-	-	-
21	CLA	L	204	X	-	-	-
21	CLA	L	205	X	-	-	-
21	CLA	a	801	X	-	-	-
21	CLA	a	802	X	-	-	-
21	CLA	a	803	X	-	-	-
21	CLA	a	804	X	-	-	X
21	CLA	a	805	X	-	-	-
21	CLA	a	806	X	-	-	-
21	CLA	a	807	X	-	-	-
21	CLA	a	808	X	-	-	-
21	CLA	a	809	X	-	-	-
21	CLA	a	810	X	-	-	-
21	CLA	a	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	a	812	X	-	-	-
21	CLA	a	813	X	-	-	-
21	CLA	a	814	X	-	-	-
21	CLA	a	815	X	-	-	X
21	CLA	a	816	X	-	-	-
21	CLA	a	817	X	-	-	-
21	CLA	a	818	X	-	-	-
21	CLA	a	819	X	-	-	-
21	CLA	a	820	X	-	-	-
21	CLA	a	821	X	-	-	-
21	CLA	a	822	X	-	-	-
21	CLA	a	823	X	-	-	-
21	CLA	a	824	X	-	-	-
21	CLA	a	825	X	-	-	-
21	CLA	a	826	X	-	-	-
21	CLA	a	827	X	-	-	-
21	CLA	a	828	X	-	-	-
21	CLA	a	829	X	-	-	-
21	CLA	a	830	X	-	-	-
21	CLA	a	831	X	-	-	-
21	CLA	a	832	X	-	-	-
21	CLA	a	833	X	-	-	-
21	CLA	a	834	X	-	-	-
21	CLA	a	835	X	-	-	-
21	CLA	a	836	X	-	-	-
21	CLA	a	837	X	-	-	-
21	CLA	a	838	X	-	-	-
21	CLA	a	839	X	-	-	-
21	CLA	a	840	X	-	-	-
21	CLA	a	855	X	-	-	-
21	CLA	a	856	X	-	-	-
21	CLA	b	1801	X	-	-	-
21	CLA	b	1804	X	-	-	-
21	CLA	b	1805	X	-	-	-
21	CLA	b	1806	X	-	-	-
21	CLA	b	1807	X	-	-	-
21	CLA	b	1808	X	-	-	-
21	CLA	b	1809	X	-	-	-
21	CLA	b	1810	X	-	-	-
21	CLA	b	1811	X	-	-	-
21	CLA	b	1812	X	-	-	-
21	CLA	b	1813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	b	1814	X	-	-	-
21	CLA	b	1815	X	-	-	-
21	CLA	b	1816	X	-	-	-
21	CLA	b	1817	X	-	-	-
21	CLA	b	1818	X	-	-	-
21	CLA	b	1819	X	-	-	X
21	CLA	b	1820	X	-	-	-
21	CLA	b	1821	X	-	-	-
21	CLA	b	1822	X	-	-	-
21	CLA	b	1823	X	-	-	-
21	CLA	b	1824	X	-	-	-
21	CLA	b	1825	X	-	-	X
21	CLA	b	1826	X	-	-	X
21	CLA	b	1827	X	-	-	-
21	CLA	b	1828	X	-	-	-
21	CLA	b	1829	X	-	-	-
21	CLA	b	1830	X	-	-	-
21	CLA	b	1831	X	-	-	-
21	CLA	b	1832	X	-	-	-
21	CLA	b	1833	X	-	-	X
21	CLA	b	1834	X	-	-	-
21	CLA	b	1835	X	-	-	-
21	CLA	b	1836	X	-	-	X
21	CLA	b	1837	X	-	-	X
21	CLA	b	1838	X	-	-	-
21	CLA	b	1839	X	-	-	-
21	CLA	b	1840	X	-	-	-
21	CLA	b	1841	X	-	-	-
21	CLA	b	1842	X	-	-	-
21	CLA	b	1843	X	-	-	-
21	CLA	f	202	X	-	-	-
21	CLA	f	203	X	-	-	-
21	CLA	j	1101	X	-	-	-
21	CLA	j	1103	X	-	-	-
21	CLA	j	1104	X	-	-	-
21	CLA	j	1105	X	-	-	X
21	CLA	k	1401	X	-	-	-
21	CLA	k	1402	X	-	-	-
21	CLA	l	201	X	-	-	-
21	CLA	l	203	X	-	-	-
21	CLA	l	204	X	-	-	-
21	CLA	l	205	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	m	103	X	-	-	-
23	SF4	A	842	-	-	-	X
23	SF4	C	101	-	-	-	X
23	SF4	C	102	-	-	X	-
24	BCR	1	844	-	-	-	X
24	BCR	1	847	-	-	-	X
24	BCR	1	849	-	-	-	X
24	BCR	1	858	-	-	-	X
24	BCR	2	844	-	-	-	X
24	BCR	2	845	-	-	-	X
24	BCR	2	849	-	-	-	X
24	BCR	6	202	-	-	-	X
24	BCR	6	205	-	-	-	X
24	BCR	7	1102	-	-	-	X
24	BCR	8	1403	-	-	-	X
24	BCR	9	102	-	-	-	X
24	BCR	A	844	-	-	-	X
24	BCR	A	848	-	-	-	X
24	BCR	B	842	-	-	-	X
24	BCR	B	845	-	-	-	X
24	BCR	B	846	-	-	-	X
24	BCR	B	847	-	-	-	X
24	BCR	I	102	-	-	-	X
24	BCR	J	1102	-	-	-	X
24	BCR	a	846	-	-	-	X
24	BCR	a	847	-	-	-	X
24	BCR	a	859	-	-	-	X
24	BCR	b	1850	-	-	-	X
24	BCR	f	201	-	-	-	X
24	BCR	k	1403	-	-	-	X
24	BCR	l	207	-	-	-	X
25	LHG	1	852	-	-	-	X
25	LHG	2	851	-	-	-	X
25	LHG	9	101	-	-	-	X
25	LHG	B	851	-	-	-	X
25	LHG	B	855	-	-	-	X
25	LHG	L	210	-	-	-	X
25	LHG	M	7003	-	-	-	X
25	LHG	a	851	-	-	-	X
25	LHG	b	1802	-	-	-	X
25	LHG	l	208	-	-	-	X
25	LHG	l	209	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	LHG	m	101	-	-	-	X
26	LMG	0	206	-	-	-	X
26	LMG	1	851	-	-	-	X
26	LMG	1	853	-	-	-	X
26	LMG	2	852	-	-	-	X
26	LMG	A	850	-	-	-	X
26	LMG	A	852	-	-	-	X
26	LMG	B	850	-	-	-	X
26	LMG	K	101	-	-	-	X
26	LMG	a	850	-	-	-	X
26	LMG	a	852	-	-	-	X
26	LMG	b	1853	-	-	-	X
26	LMG	b	1855	-	-	-	X
27	ACT	A	853	-	-	-	X
27	ACT	M	7001	-	-	-	X
28	45D	2	854	-	-	-	X
29	CL	1	857	-	-	-	X
30	ECH	2	846	-	-	-	X
30	ECH	m	104	-	-	-	X
31	SQD	0	207	-	-	-	X
31	SQD	B	852	-	-	-	X
31	SQD	F	205	-	-	-	X
31	SQD	f	205	-	-	-	X
34	C7Z	2	855	-	-	-	X
35	LMT	J	1104	-	-	-	X
35	LMT	L	211	-	-	-	X
35	LMT	l	211	-	-	-	X
37	DGD	L	209	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 77117 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			5878	3847	1000	1003	28			
1	a	751	Total	C	N	O	S	0	0	0
			5878	3847	1000	1003	28			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			
8	j	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			
8	7	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	80	Total	C	N	O	S	0	1	0
			579	378	93	102	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	157	Total	C	N	O	S	0	0	0
			1178	766	191	218	3			
10	l	157	Total	C	N	O	S	0	0	0
			1178	766	191	218	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			
11	m	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			
11	9	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			

- Molecule 12 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	b	729	Total	C	N	O	S	0	0	0
			5770	3798	967	990	15			

- Molecule 13 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	c	81	Total	C	N	O	S	0	0	0
			608	374	104	118	12			

- Molecule 14 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	e	68	Total	C	N	O	0	0	0
			533	335	94	104			

- Molecule 15 is a protein called Photosystem I reaction center subunit Psak 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	k	78	Total	C	N	O	S	0	0	0
			559	366	90	98	5			

- Molecule 16 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1	744	Total	C	N	O	S	0	0	0
			5826	3814	993	992	27			

- Molecule 17 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	140	Total	C	N	O	S	0	0	0
			1094	692	189	210	3			

- Molecule 18 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	h	38	Total	C	N	O	S	0	0	0
			298	202	42	51	3			

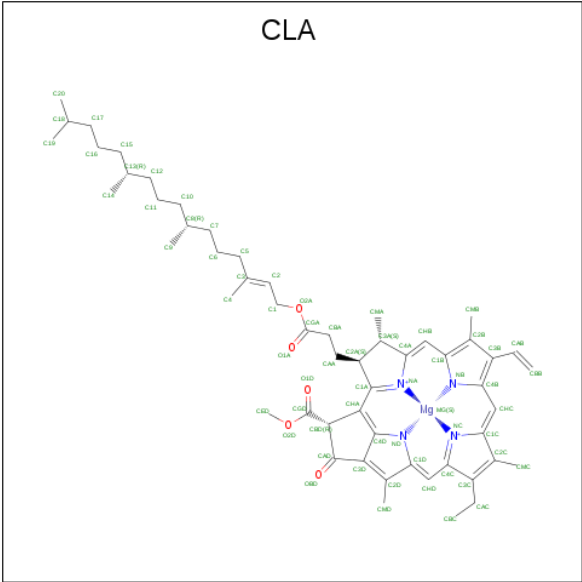
- Molecule 19 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	8	79	Total	C	N	O	S	0	0	0
			565	369	91	100	5			

- Molecule 20 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	0	154	Total	C	N	O	S	0	0	0
			1156	753	188	213	2			

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	I	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	K	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	K	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	f	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	f	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	j	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	j	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	j	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	j	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	k	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	k	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
21	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	m	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
21	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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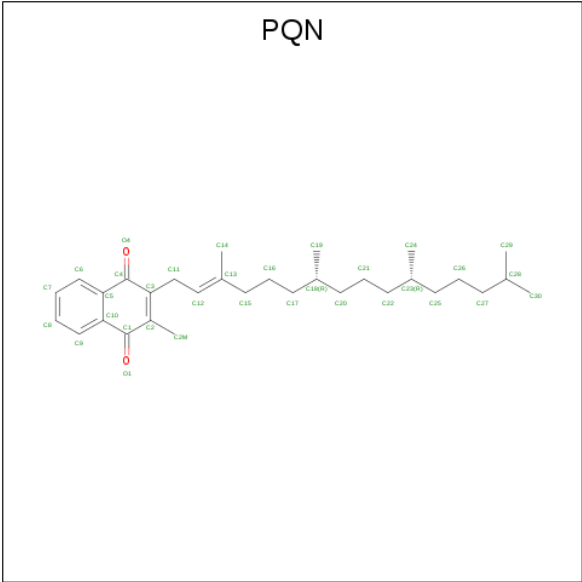
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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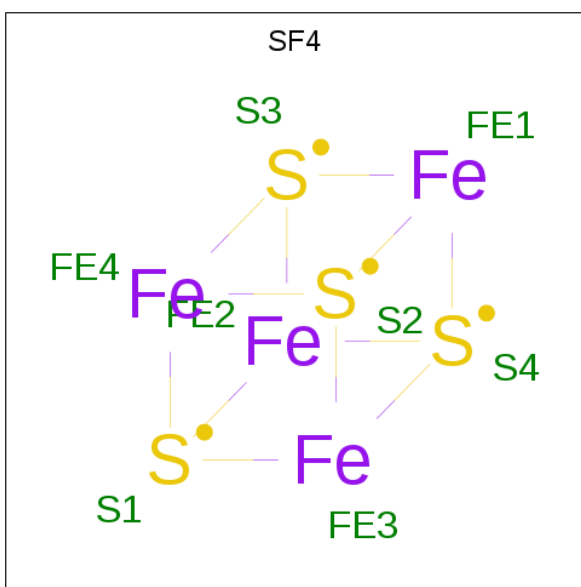
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	6	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
21	6	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
21	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	7	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
21	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



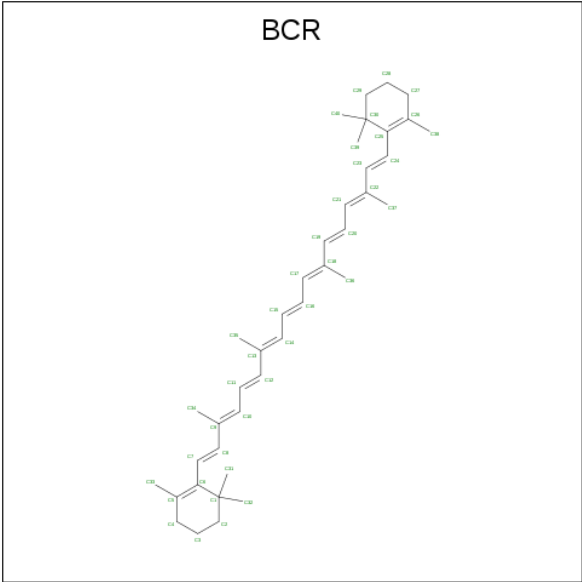
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			33	31	2		
22	B	1	Total	C	O	0	0
			33	31	2		
22	a	1	Total	C	O	0	0
			33	31	2		
22	b	1	Total	C	O	0	0
			33	31	2		
22	1	1	Total	C	O	0	0
			33	31	2		
22	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	Fe	S	0	0
			8	4	4		
23	C	1	Total	Fe	S	0	0
			8	4	4		
23	C	1	Total	Fe	S	0	0
			8	4	4		
23	a	1	Total	Fe	S	0	0
			8	4	4		
23	c	1	Total	Fe	S	0	0
			8	4	4		
23	c	1	Total	Fe	S	0	0
			8	4	4		
23	1	1	Total	Fe	S	0	0
			8	4	4		
23	3	1	Total	Fe	S	0	0
			8	4	4		
23	3	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	L	1	Total C 40 40	0	0
24	L	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	i	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0

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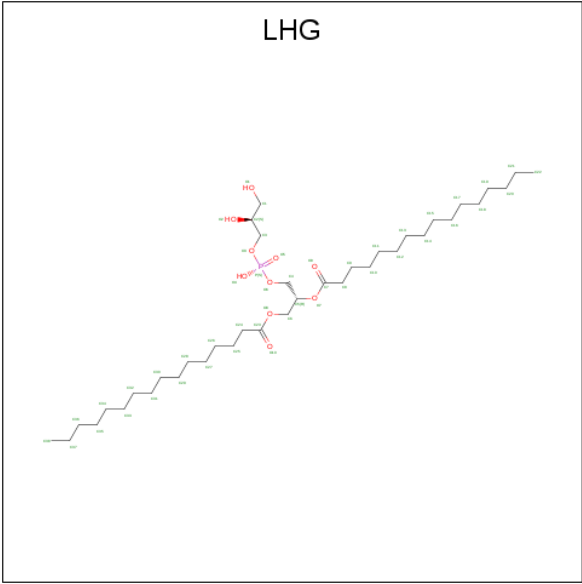
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	2	1	Total C 40 40	0	0
24	6	1	Total C 40 40	0	0
24	6	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	7	1	Total C 40 40	0	0
24	8	1	Total C 40 40	0	0
24	0	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	0	1	Total C 40 40	0	0
24	9	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



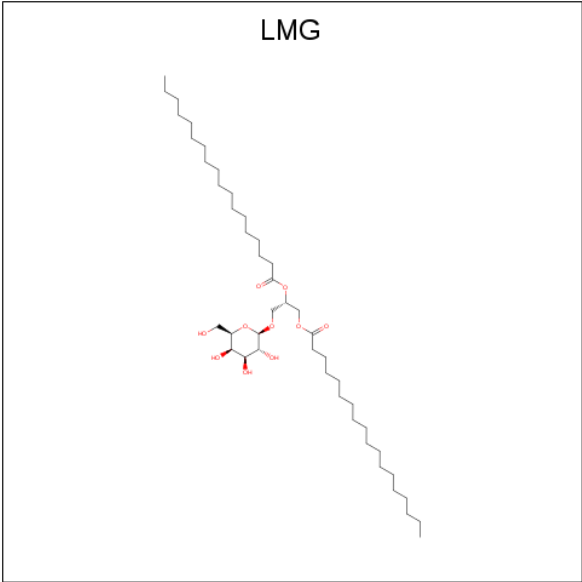
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	I	1	Total C O P 49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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	L	1	Total	C	O	P	0	0
			49	38	10	1		
25	M	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	a	1	Total	C	O	P	0	0
			49	38	10	1		
25	b	1	Total	C	O	P	0	0
			49	38	10	1		
25	b	1	Total	C	O	P	0	0
			49	38	10	1		
25	b	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	l	1	Total	C	O	P	0	0
			49	38	10	1		
25	m	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	1	1	Total	C	O	P	0	0
			49	38	10	1		
25	2	1	Total	C	O	P	0	0
			49	38	10	1		
25	2	1	Total	C	O	P	0	0
			49	38	10	1		
25	6	1	Total	C	O	P	0	0
			12	5	6	1		
25	9	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



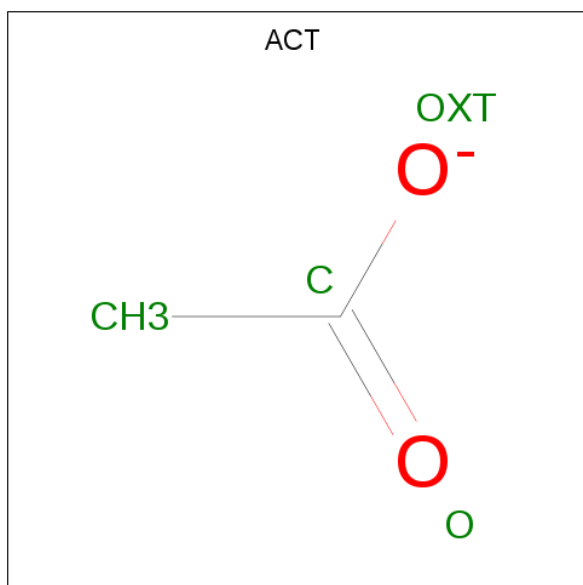
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			50	40	10		
26	A	1	Total	C	O	0	0
			48	38	10		
26	B	1	Total	C	O	0	0
			55	45	10		
26	B	1	Total	C	O	0	0
			55	45	10		
26	K	1	Total	C	O	0	0
			55	45	10		
26	K	1	Total	C	O	0	0
			55	45	10		
26	a	1	Total	C	O	0	0
			50	40	10		
26	a	1	Total	C	O	0	0
			55	45	10		
26	b	1	Total	C	O	0	0
			55	45	10		
26	b	1	Total	C	O	0	0
			55	45	10		
26	b	1	Total	C	O	0	0
			55	45	10		
26	1	1	Total	C	O	0	0
			50	40	10		
26	1	1	Total	C	O	0	0
			55	45	10		
26	2	1	Total	C	O	0	0
			55	45	10		

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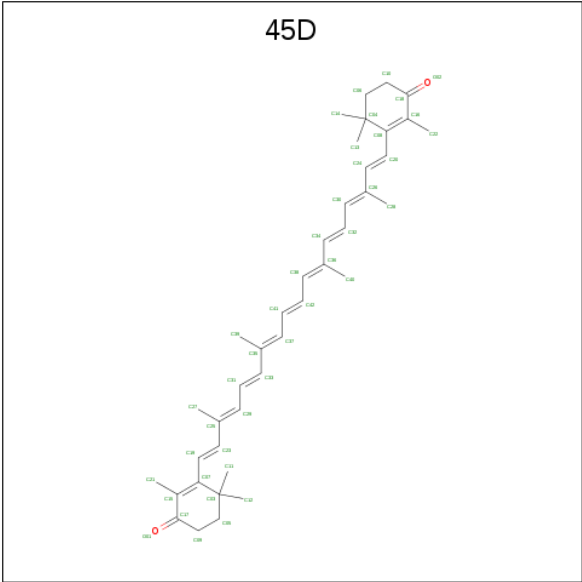
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	2	1	Total	C	O	0	0
			55	45	10		
26	0	1	Total	C	O	0	0
			55	45	10		

- Molecule 27 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			4	2	2		
27	D	1	Total	C	O	0	0
			4	2	2		
27	M	1	Total	C	O	0	0
			4	2	2		
27	a	1	Total	C	O	0	0
			4	2	2		

- Molecule 28 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).

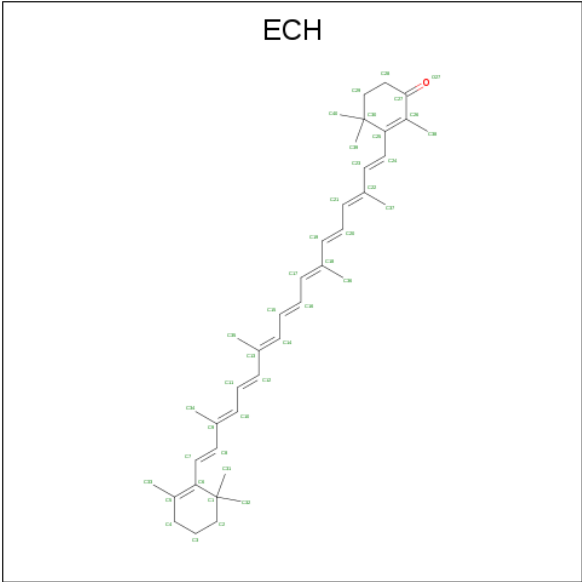


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			42	40	2		
28	2	1	Total	C	O	0	0
			42	40	2		

- Molecule 29 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

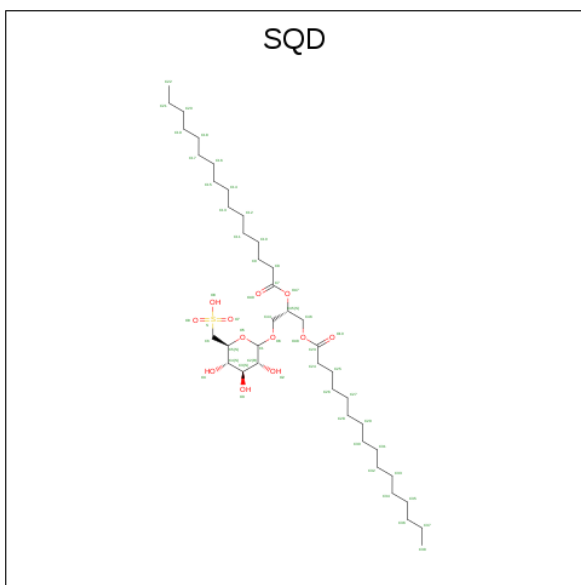
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	1	1	Total	Cl	0	0
			1	1		
29	A	1	Total	Cl	0	0
			1	1		
29	a	1	Total	Cl	0	0
			1	1		

- Molecule 30 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			41	40	1		
30	M	1	Total	C	O	0	0
			41	40	1		
30	a	1	Total	C	O	0	0
			41	40	1		
30	b	1	Total	C	O	0	0
			41	40	1		
30	l	1	Total	C	O	0	0
			41	40	1		
30	m	1	Total	C	O	0	0
			41	40	1		
30	2	1	Total	C	O	0	0
			41	40	1		

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	S	0	0
			54	41	12	1		
31	F	1	Total	C	O	S	0	0
			54	41	12	1		
31	L	1	Total	C	O	S	0	0
			51	38	12	1		
31	b	1	Total	C	O	S	0	0
			54	41	12	1		
31	f	1	Total	C	O	S	0	0
			54	41	12	1		
31	m	1	Total	C	O	S	0	0
			54	41	12	1		
31	0	1	Total	C	O	S	0	0
			54	41	12	1		

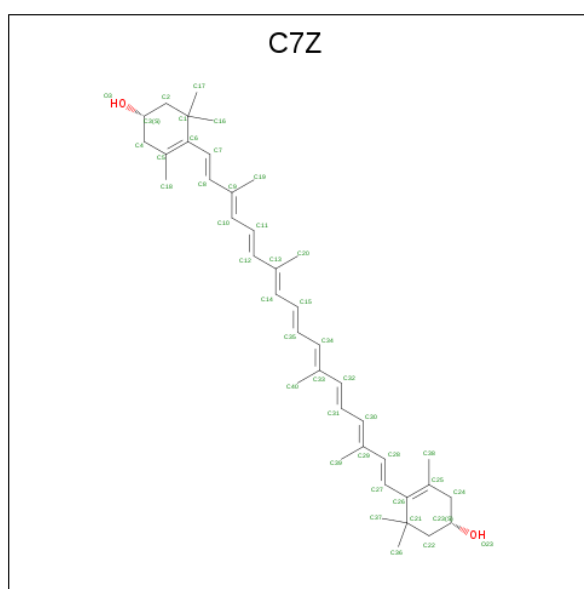
- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	l	1	Total	Ca	0	0
			1	1		
32	B	1	Total	Ca	0	0
			1	1		
32	L	2	Total	Ca	0	0
			2	2		
32	b	1	Total	Ca	0	0
			1	1		
32	2	1	Total	Ca	0	0
			1	1		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

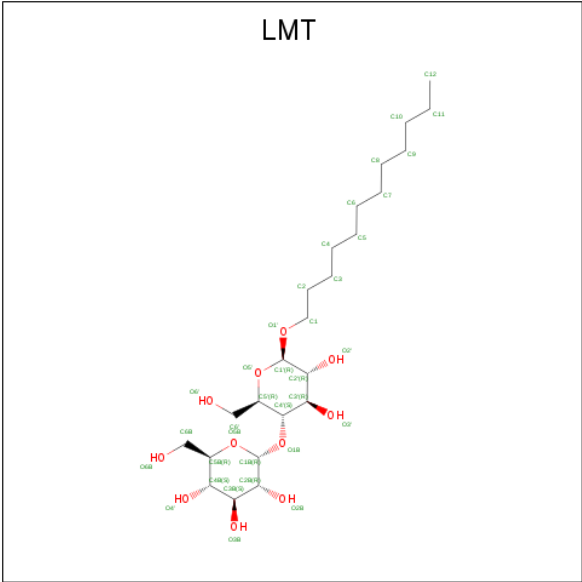
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Mg	0	0
			1	1		
33	b	1	Total	Mg	0	0
			1	1		

- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C₄₀H₅₆O₂).



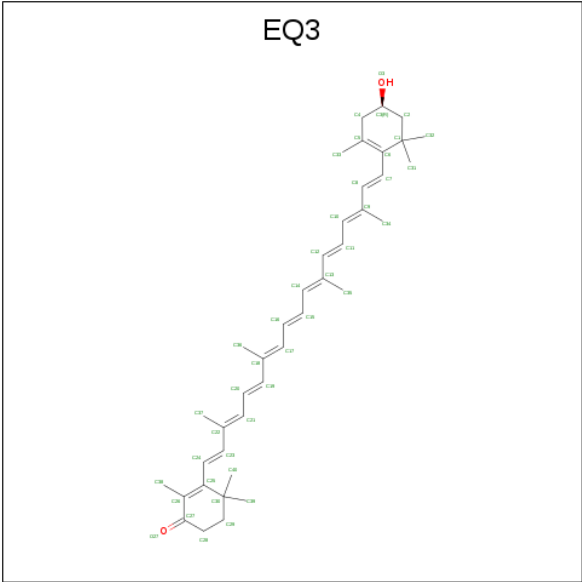
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			42	40	2		
34	F	1	Total	C	O	0	0
			42	40	2		
34	b	1	Total	C	O	0	0
			42	40	2		
34	2	1	Total	C	O	0	0
			42	40	2		

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



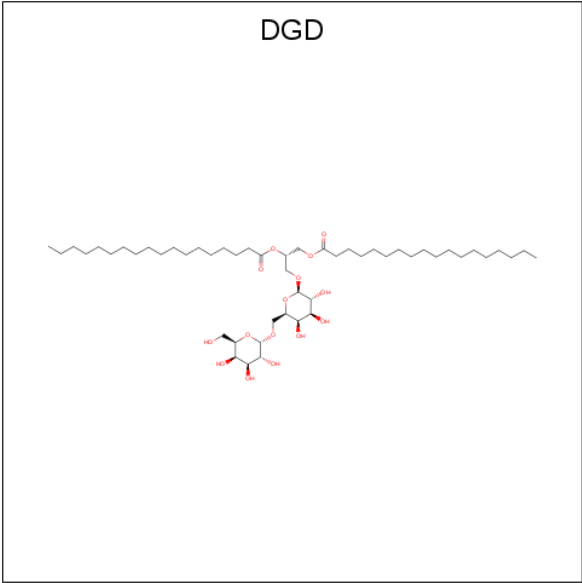
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	J	1	Total	C	O	0	0
			35	24	11		
35	L	1	Total	C	O	0	0
			35	24	11		
35	1	1	Total	C	O	0	0
			35	24	11		
35	1	1	Total	C	O	0	0
			35	24	11		
35	0	1	Total	C	O	0	0
			35	24	11		

- Molecule 36 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: C₄₀H₅₄O₂).



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

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	L	1	Total	C	O	0	0
			66	51	15		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	186	Total O 186 186	0	0
38	B	114	Total O 114 114	0	0
38	C	48	Total O 48 48	0	0
38	D	57	Total O 57 57	0	0
38	E	16	Total O 16 16	0	0
38	F	8	Total O 8 8	0	0
38	I	6	Total O 6 6	0	0
38	J	4	Total O 4 4	0	0
38	K	9	Total O 9 9	0	0
38	L	46	Total O 46 46	0	0
38	M	3	Total O 3 3	0	0
38	a	39	Total O 39 39	0	0
38	b	141	Total O 141 141	0	0
38	c	13	Total O 13 13	0	0
38	d	15	Total O 15 15	0	0
38	e	4	Total O 4 4	0	0
38	f	10	Total O 10 10	0	0
38	i	7	Total O 7 7	0	0
38	j	5	Total O 5 5	0	0
38	l	20	Total O 20 20	0	0
38	m	8	Total O 8 8	0	0
38	1	37	Total O 37 37	0	0

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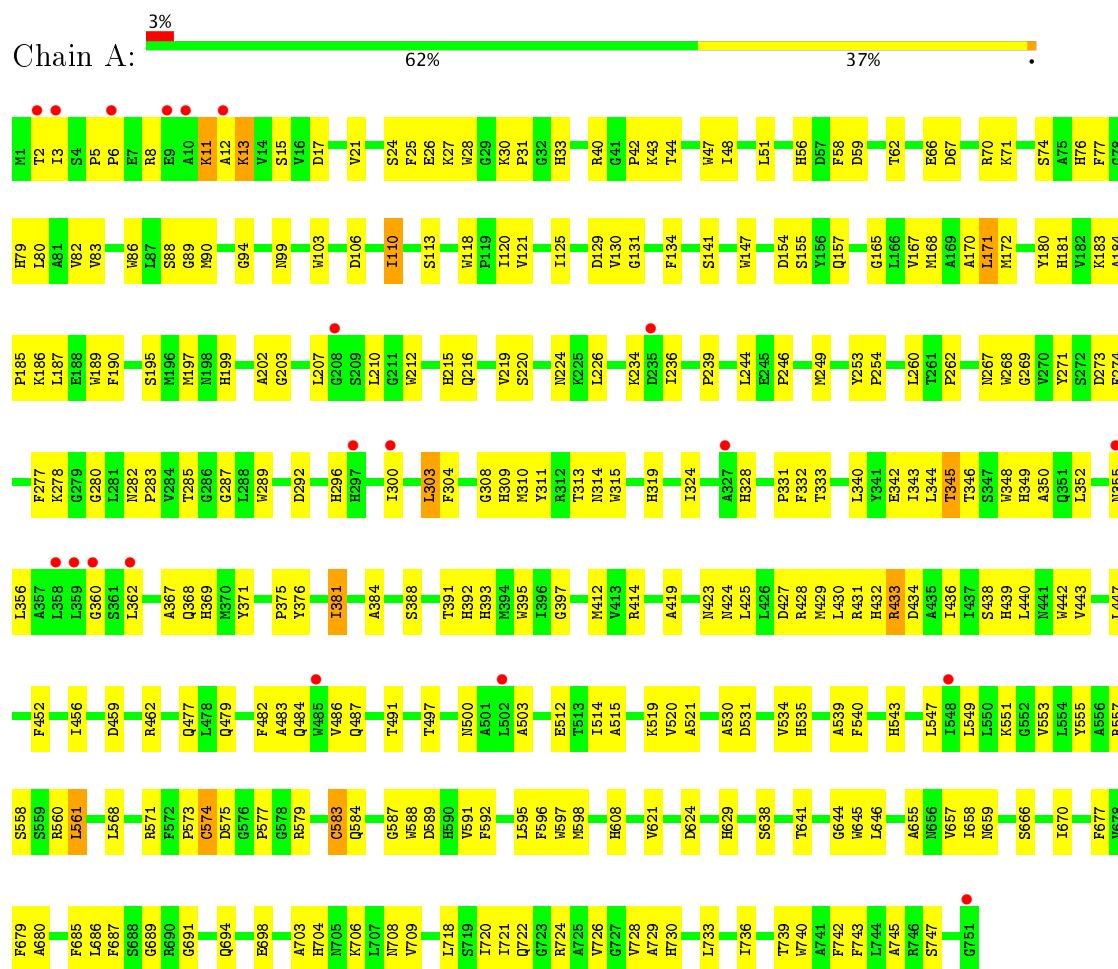
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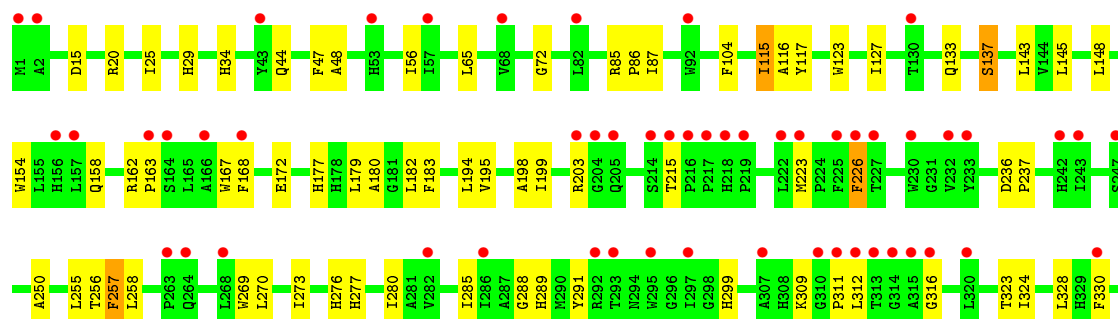
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	2	24	Total 24	O 24	0	0
38	3	11	Total 11	O 11	0	0
38	4	13	Total 13	O 13	0	0
38	5	4	Total 4	O 4	0	0
38	6	1	Total 1	O 1	0	0
38	h	3	Total 3	O 3	0	0
38	7	1	Total 1	O 1	0	0
38	8	2	Total 2	O 2	0	0
38	0	33	Total 33	O 33	0	0
38	9	1	Total 1	O 1	0	0

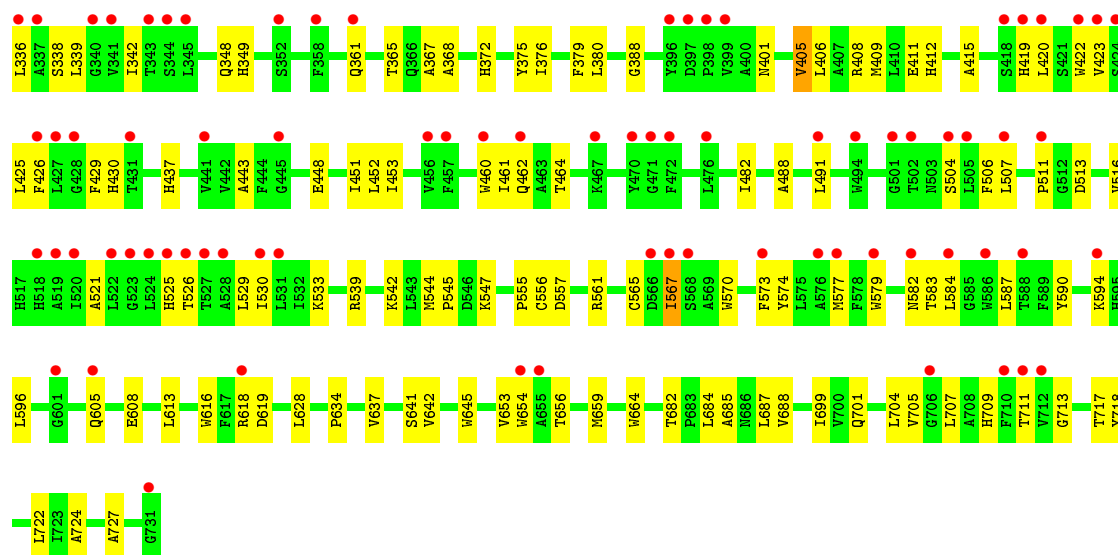
3 Residue-property plots

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



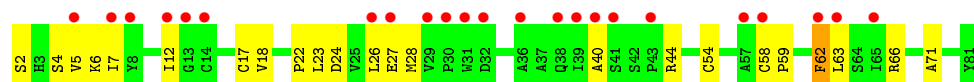




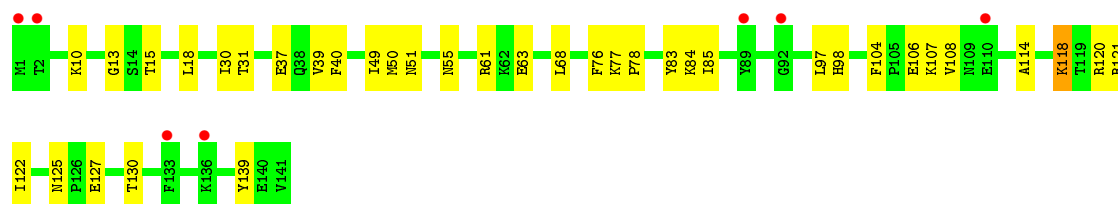
- Molecule 3: Photosystem I iron-sulfur center



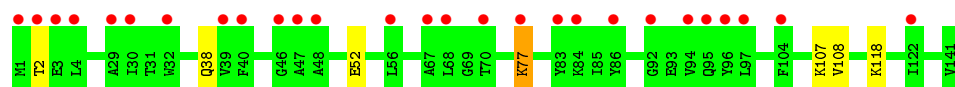
- Molecule 3: Photosystem I iron-sulfur center



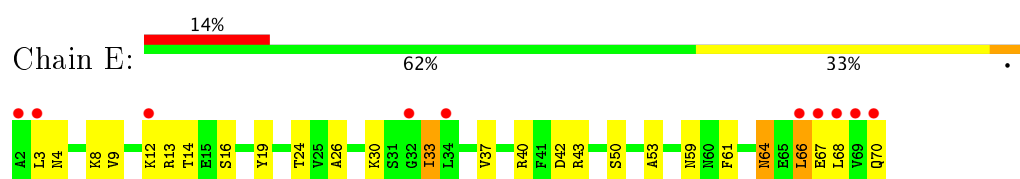
- Molecule 4: Photosystem I reaction center subunit II



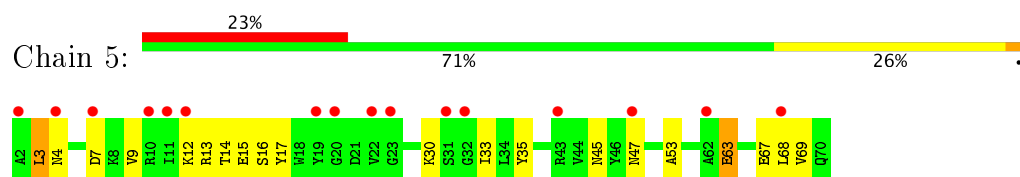
- Molecule 4: Photosystem I reaction center subunit II



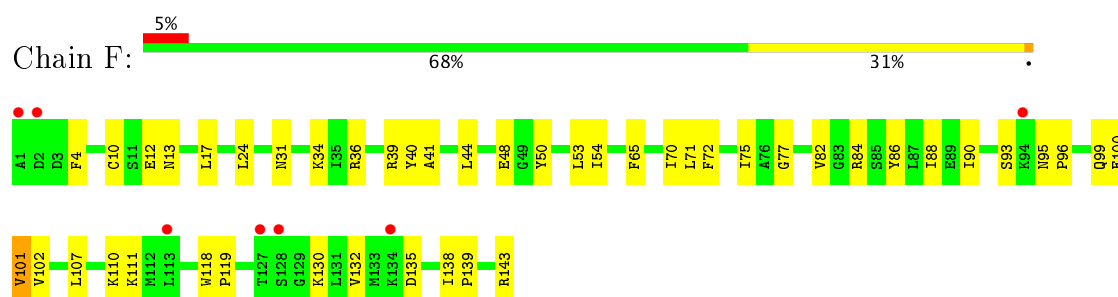
- Molecule 5: Photosystem I reaction center subunit IV



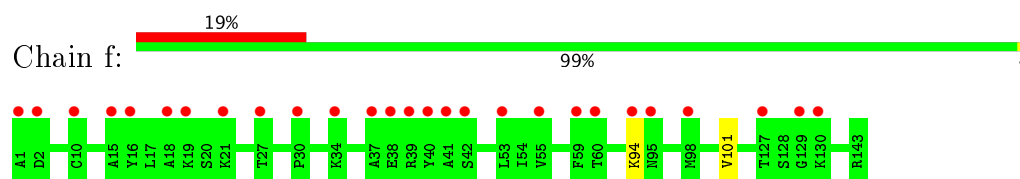
- Molecule 5: Photosystem I reaction center subunit IV



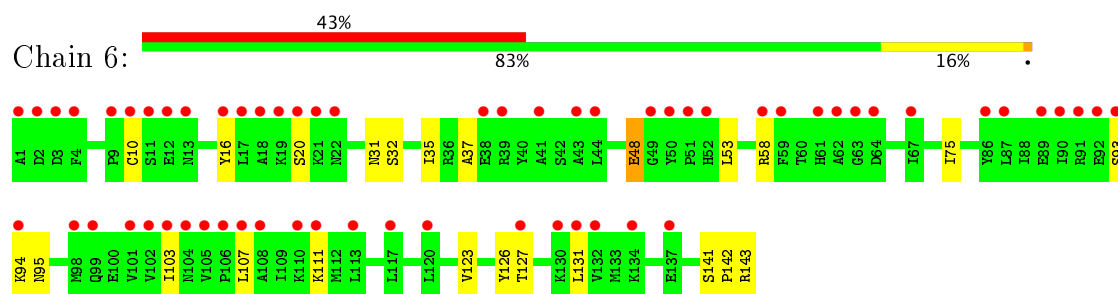
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



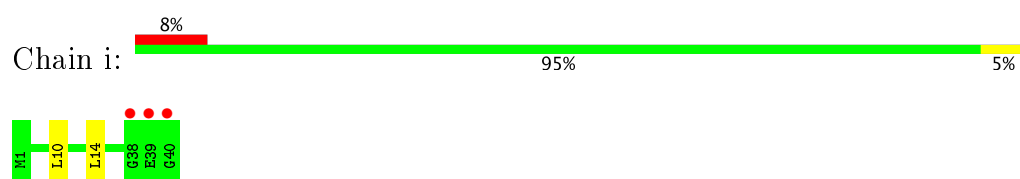
- Molecule 6: Photosystem I reaction center subunit III



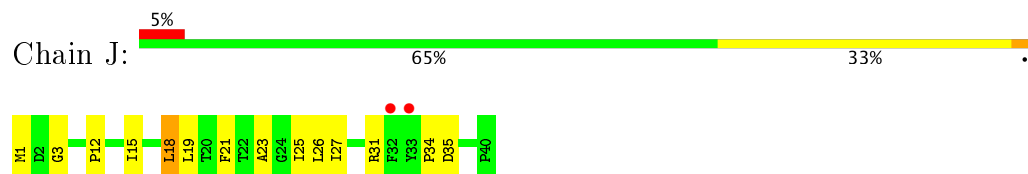
- Molecule 7: Photosystem I reaction center subunit VIII



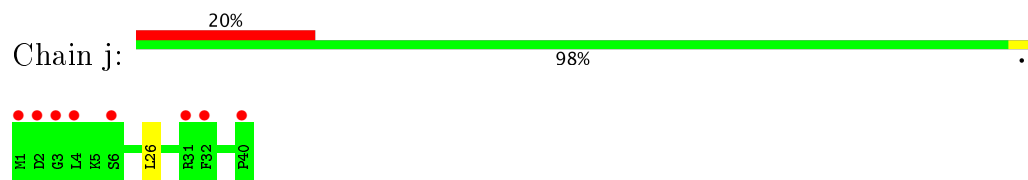
- Molecule 7: Photosystem I reaction center subunit VIII



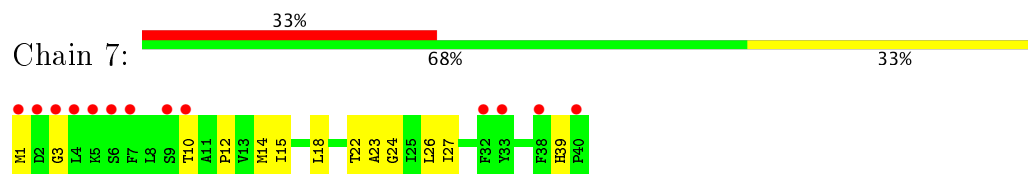
- Molecule 8: Photosystem I reaction center subunit IX



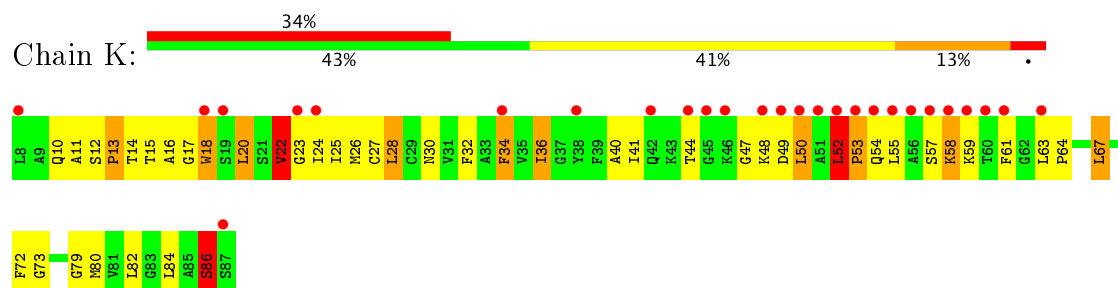
- Molecule 8: Photosystem I reaction center subunit IX



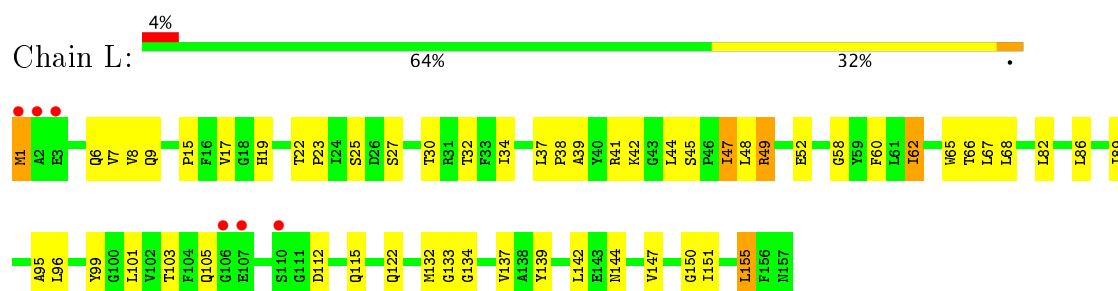
- Molecule 8: Photosystem I reaction center subunit IX



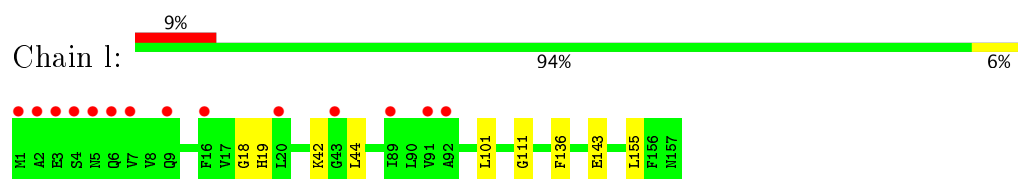
- Molecule 9: Photosystem I reaction center subunit PsaK 2



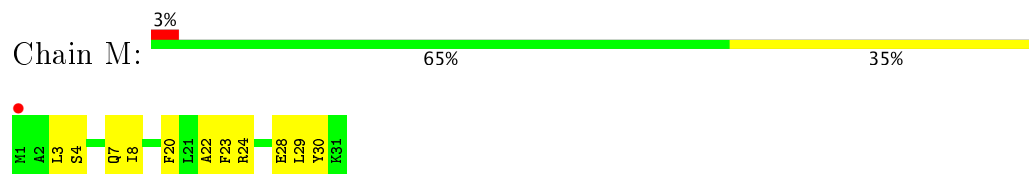
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII

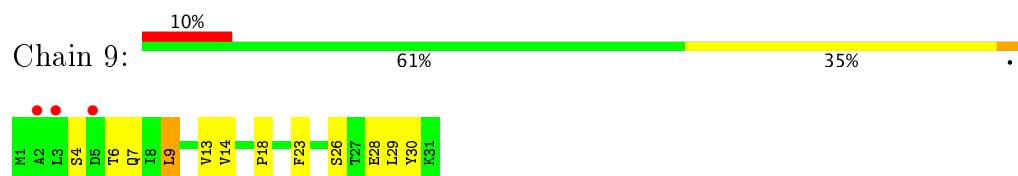


- Molecule 11: Photosystem I reaction center subunit XII

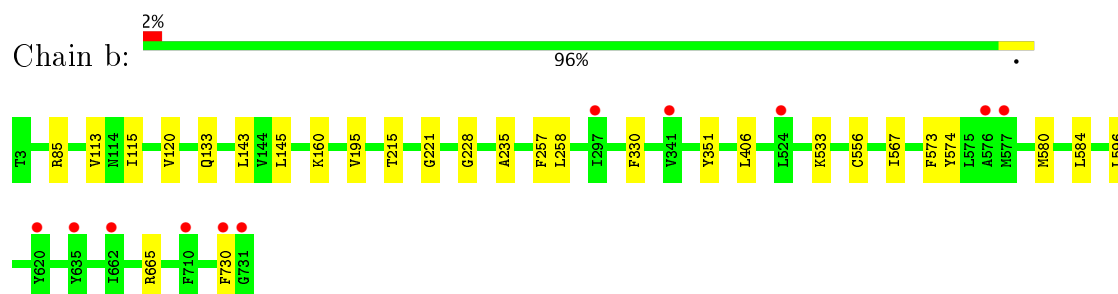


There are no outlier residues recorded for this chain.

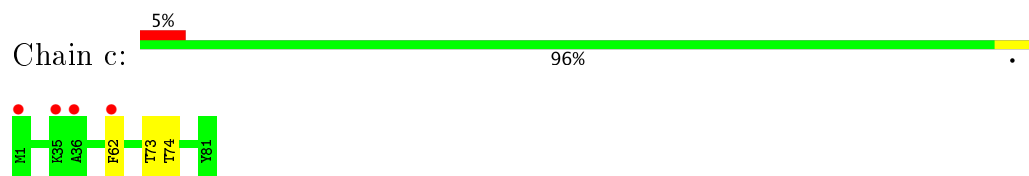
- Molecule 11: Photosystem I reaction center subunit XII



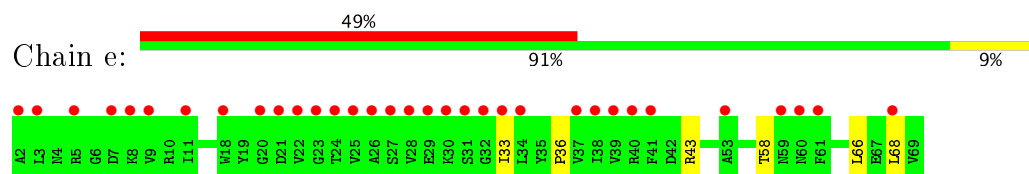
- Molecule 12: Photosystem I P700 chlorophyll a apoprotein A2



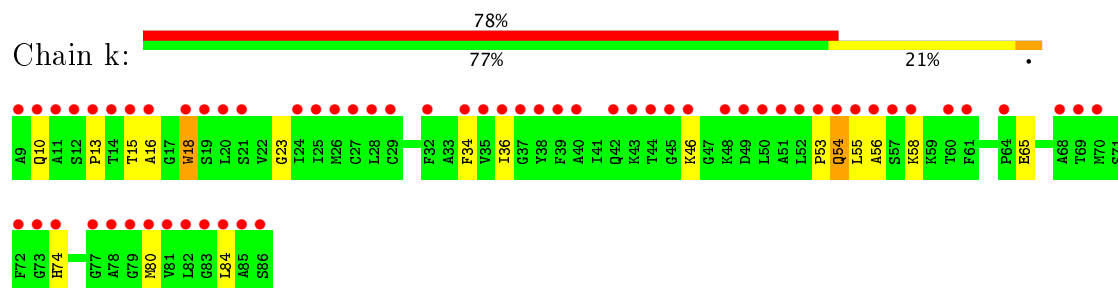
- Molecule 13: Photosystem I iron-sulfur center



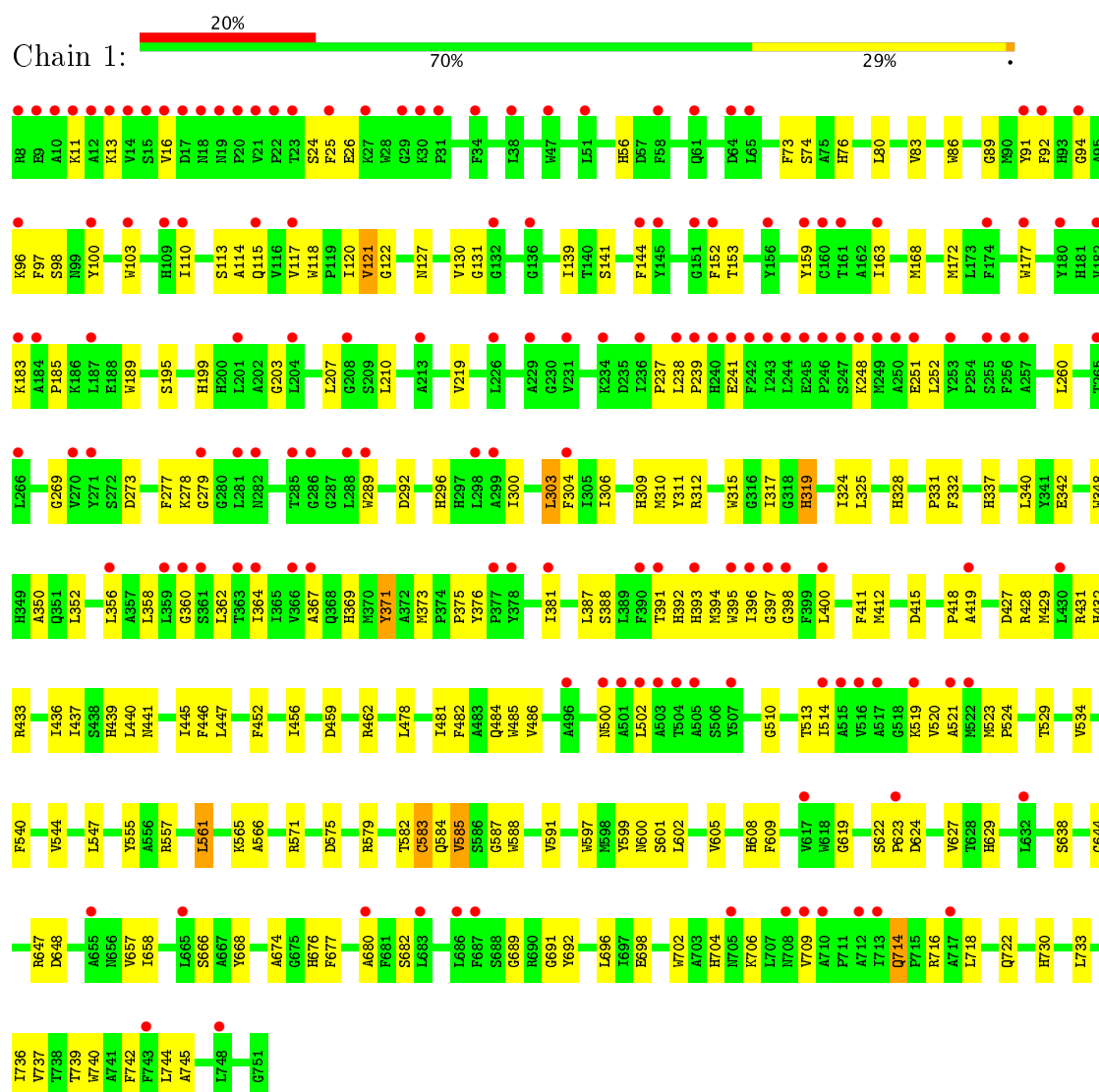
- Molecule 14: Photosystem I reaction center subunit IV



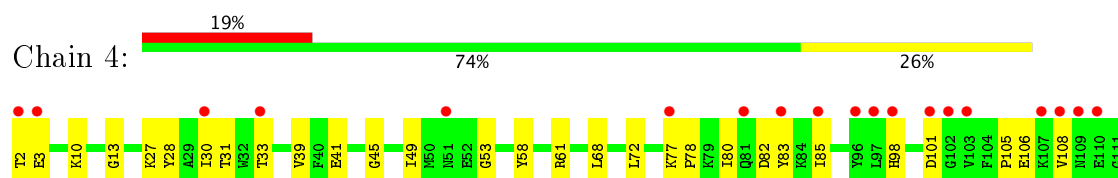
- Molecule 15: Photosystem I reaction center subunit PsaK 2

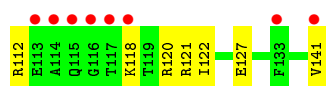


- Molecule 16: Photosystem I P700 chlorophyll a apoprotein A1

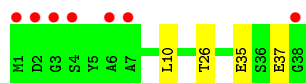
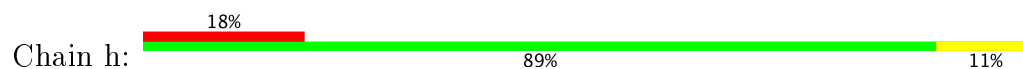


- Molecule 17: Photosystem I reaction center subunit II

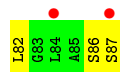
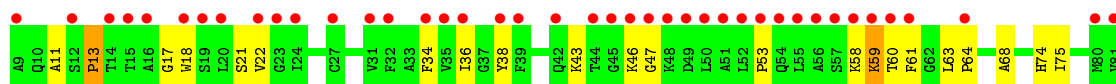




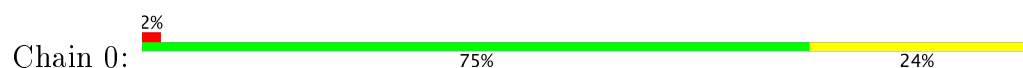
- Molecule 18: Photosystem I reaction center subunit VIII



- Molecule 19: Photosystem I reaction center subunit PsaK 2



- Molecule 20: Photosystem I reaction center subunit XI



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	212.17Å 137.62Å 225.09Å 90.00° 116.74° 90.00°	Depositor
Resolution (Å)	49.48 – 2.50 49.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.48-2.50) 99.4 (49.48-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_2947: ???)	Depositor
R, R_{free}	0.228 , 0.264 0.227 , 0.264	Depositor DCC
R_{free} test set	7879 reflections (1.99%)	DCC
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	77117	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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, MG, C7Z, DGD, CL, SF4, LMT, CLA, PQN, ECH, BCR, ACT, LMG, 45D, EQ3, CA, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/6078	0.46	0/8284
1	a	0.27	0/6078	0.42	0/8284
2	2	0.26	0/5994	0.41	0/8195
2	B	0.33	0/5994	0.45	2/8195 (0.0%)
3	3	0.24	0/610	0.45	0/826
3	C	0.37	1/610 (0.2%)	0.56	1/826 (0.1%)
4	D	0.29	0/1126	0.49	0/1517
4	d	0.26	0/1126	0.48	0/1517
5	5	0.25	0/552	0.39	0/745
5	E	0.26	0/552	0.44	0/745
6	6	0.25	0/1143	0.40	0/1553
6	F	0.26	0/1143	0.43	0/1553
6	f	0.25	0/1143	0.40	0/1553
7	I	0.26	0/322	0.43	0/438
7	i	0.26	0/322	0.44	0/438
8	7	0.27	0/328	0.42	0/443
8	J	0.28	0/328	0.46	0/443
8	j	0.26	0/328	0.42	0/443
9	K	0.29	0/590	0.53	0/797
10	L	0.28	0/1208	0.47	0/1640
10	l	0.27	0/1208	0.43	0/1640
11	9	0.25	0/241	0.55	1/326 (0.3%)
11	M	0.27	0/241	0.41	0/326
11	m	0.27	0/241	0.39	0/326
12	b	0.31	0/5981	0.46	1/8178 (0.0%)
13	c	0.26	0/618	0.49	0/836
14	e	0.26	0/542	0.42	0/733
15	k	0.28	0/570	0.45	0/770
16	1	0.26	0/6024	0.41	0/8209
17	4	0.26	0/1118	0.45	0/1507
18	h	0.26	0/309	0.43	0/421
19	8	0.27	0/576	0.46	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	0	0.28	0/1186	0.43	0/1611
All	All	0.29	1/54430 (0.0%)	0.44	5/74096 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	17	CYS	CB-SG	5.38	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	665	ARG	N-CA-C	7.42	131.03	111.00
2	B	587	LEU	CA-CB-CG	6.99	131.38	115.30
2	B	665	ARG	N-CA-C	6.41	128.31	111.00
11	9	9	LEU	CA-CB-CG	6.23	129.62	115.30
3	C	17	CYS	CA-CB-SG	5.76	124.37	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	52	LEU	Peptide

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	5878	0	5743	305	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5878	0	5743	0	0
2	2	5783	0	5565	158	0
2	B	5783	0	5564	195	0
3	3	600	0	589	16	0
3	C	600	0	582	29	0
4	D	1102	0	1101	28	0
4	d	1102	0	1101	0	0
5	5	543	0	525	11	0
5	E	543	0	525	21	0
6	6	1113	0	1108	13	0
6	F	1113	0	1108	44	0
6	f	1113	0	1108	0	0
7	I	311	0	304	18	0
7	i	311	0	304	0	0
8	7	319	0	328	13	0
8	J	319	0	328	17	0
8	j	319	0	328	0	0
9	K	579	0	601	54	0
10	L	1178	0	1150	56	0
10	l	1178	0	1150	0	0
11	9	238	0	260	11	0
11	M	238	0	260	12	0
11	m	238	0	260	0	0
12	b	5770	0	5547	0	0
13	c	608	0	596	0	0
14	e	533	0	517	0	0
15	k	559	0	581	0	0
16	1	5826	0	5688	198	0
17	4	1094	0	1089	26	0
18	h	298	0	295	0	0
19	8	565	0	586	16	0
20	0	1156	0	1127	36	0
21	0	195	0	216	20	0
21	1	2522	0	2556	210	0
21	2	2306	0	2180	191	0
21	6	155	0	138	15	0
21	7	194	0	162	16	0
21	8	91	0	64	7	0
21	A	2706	0	2964	443	0
21	B	2527	0	2702	226	0
21	F	130	0	143	16	0
21	I	65	0	71	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	J	260	0	286	35	0
21	K	130	0	144	13	0
21	L	195	0	215	30	0
21	a	2588	0	2684	0	0
21	b	2629	0	2861	0	0
21	f	115	0	111	0	0
21	j	250	0	263	0	0
21	k	99	0	77	0	0
21	l	260	0	287	0	0
21	m	65	0	72	0	0
22	1	33	0	46	5	0
22	2	33	0	46	4	0
22	A	33	0	46	7	0
22	B	33	0	46	2	0
22	a	33	0	46	0	0
22	b	33	0	46	0	0
23	1	8	0	0	0	0
23	3	16	0	0	1	0
23	A	8	0	0	0	0
23	C	16	0	0	6	0
23	a	8	0	0	0	0
23	c	16	0	0	0	0
24	0	80	0	110	8	0
24	1	320	0	440	42	0
24	2	200	0	275	25	0
24	6	80	0	110	8	0
24	7	40	0	55	7	0
24	8	40	0	55	3	0
24	9	40	0	56	5	0
24	A	240	0	330	54	0
24	B	200	0	275	39	0
24	F	40	0	55	7	0
24	I	40	0	55	6	0
24	J	80	0	110	22	0
24	K	40	0	55	4	0
24	L	80	0	110	13	0
24	a	280	0	384	0	0
24	b	200	0	275	0	0
24	f	80	0	110	0	0
24	h	40	0	55	0	0
24	i	40	0	55	0	0
24	j	40	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	k	40	0	55	0	0
24	l	80	0	110	0	0
25	1	98	0	148	7	0
25	2	98	0	148	9	0
25	6	12	0	9	1	0
25	9	49	0	74	4	0
25	A	98	0	148	24	0
25	B	245	0	370	19	0
25	I	98	0	148	8	0
25	L	49	0	74	5	0
25	M	49	0	74	2	0
25	a	147	0	222	0	0
25	b	147	0	222	0	0
25	l	147	0	222	0	0
25	m	49	0	74	0	0
26	0	55	0	86	4	0
26	1	105	0	159	5	0
26	2	110	0	172	11	0
26	A	98	0	142	13	0
26	B	110	0	172	9	0
26	K	110	0	172	16	0
26	a	105	0	159	0	0
26	b	165	0	258	0	0
27	A	4	0	3	1	0
27	D	4	0	3	0	0
27	M	4	0	3	0	0
27	a	4	0	3	0	0
28	2	42	0	52	8	0
28	A	42	0	52	5	0
29	1	1	0	0	0	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	2	41	0	54	2	0
30	B	41	0	54	3	0
30	M	41	0	54	2	0
30	a	41	0	54	0	0
30	b	41	0	54	0	0
30	l	41	0	54	0	0
30	m	41	0	54	0	0
31	0	54	0	77	2	0
31	B	54	0	77	6	0
31	F	54	0	77	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	L	51	0	68	3	0
31	b	54	0	77	0	0
31	f	54	0	77	0	0
31	m	54	0	77	0	0
32	2	1	0	0	0	0
32	B	1	0	0	0	0
32	L	2	0	0	0	0
32	b	1	0	0	0	0
32	l	1	0	0	0	0
33	B	1	0	0	0	0
33	b	1	0	0	0	0
34	2	42	0	0	0	0
34	B	42	0	0	0	0
34	F	42	0	0	0	0
34	b	42	0	0	0	0
35	0	35	0	45	4	0
35	1	35	0	46	0	0
35	J	35	0	45	0	0
35	L	35	0	45	2	0
35	l	35	0	45	0	0
36	L	42	0	0	0	0
37	L	66	0	96	5	0
38	0	33	0	0	1	0
38	1	37	0	0	5	0
38	2	24	0	0	1	0
38	3	11	0	0	0	0
38	4	13	0	0	0	0
38	5	4	0	0	0	0
38	6	1	0	0	0	0
38	7	1	0	0	0	0
38	8	2	0	0	0	0
38	9	1	0	0	1	0
38	A	186	0	0	6	0
38	B	114	0	0	1	0
38	C	48	0	0	0	0
38	D	57	0	0	0	0
38	E	16	0	0	5	0
38	F	8	0	0	2	0
38	I	6	0	0	1	0
38	J	4	0	0	0	0
38	K	9	0	0	1	0
38	L	46	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	M	3	0	0	0	0
38	a	39	0	0	0	0
38	b	141	0	0	0	0
38	c	13	0	0	0	0
38	d	15	0	0	0	0
38	e	4	0	0	0	0
38	f	10	0	0	0	0
38	h	3	0	0	0	0
38	i	7	0	0	0	0
38	j	5	0	0	0	0
38	l	20	0	0	0	0
38	m	8	0	0	0	0
All	All	77117	0	77922	2082	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 16.

All (2082) 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)
21:A:813:CLA:HAB	24:A:844:BCR:H14C	1.41	1.03
21:2:825:CLA:HAB	21:2:832:CLA:HMD2	1.44	0.97
21:B:823:CLA:HAB	21:B:830:CLA:HMD2	1.48	0.96
21:1:809:CLA:HBB1	24:7:1102:BCR:HC8	1.48	0.94
1:A:56:HIS:HB2	21:A:830:CLA:HBA1	38.21	0.92
1:A:86:TRP:HA	21:A:807:CLA:HBB2	14.87	0.90
9:K:80:MET:HE2	26:K:105:LMG:H222	1.55	0.89
21:F:202:CLA:HMA1	21:J:1103:CLA:H91	3.08	0.86
24:1:856:BCR:H362	21:2:803:CLA:H42	1.57	0.86
8:J:31:ARG:HD3	24:J:1107:BCR:H312	1.58	0.85
21:A:831:CLA:HMA2	10:L:22:THR:HG21	27.48	0.83
21:A:830:CLA:HMA2	10:L:22:THR:HG21	1.60	0.82
1:A:56:HIS:HB2	21:A:829:CLA:HBA1	1.61	0.82
21:B:812:CLA:H101	21:B:820:CLA:H2	1.62	0.81
21:2:808:CLA:HMB2	21:2:831:CLA:HBB2	1.61	0.81
21:A:832:CLA:HMA2	10:L:68:LEU:HB3	1.61	0.81
1:A:269:GLY:H	9:K:13:PRO:HG3	1.55	0.81
21:A:827:CLA:HED1	21:A:833:CLA:HAB	30.86	0.80
16:1:76:HIS:HB3	21:1:813:CLA:HED2	1.63	0.80
21:B:835:CLA:H52	21:F:203:CLA:HBB2	1.62	0.80
16:1:388:SER:HB3	21:1:828:CLA:HMA1	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:809:CLA:HBB1	24:J:1102:BCR:HC8	42.94	0.79
2:B:160:LYS:H	2:B:160:LYS:HE3	5.77	0.79
16:1:86:TRP:HA	21:1:807:CLA:HBB2	1.63	0.78
22:A:841:PQN:H201	21:J:1101:CLA:H12	1.65	0.77
21:A:808:CLA:HBB1	24:J:1102:BCR:HC8	1.64	0.77
10:L:41:ARG:O	10:L:49:ARG:NH2	2.18	0.77
16:1:118:TRP:HE1	24:1:849:BCR:H332	1.50	0.77
16:1:348:TRP:HB3	21:1:805:CLA:HAC1	1.67	0.76
21:2:827:CLA:HBA1	21:2:828:CLA:HED2	1.66	0.76
21:A:811:CLA:H102	26:K:101:LMG:H252	1.68	0.76
24:2:847:BCR:H21C	24:2:849:BCR:H402	1.66	0.76
11:9:4:SER:HB3	11:9:7:GLN:HB2	1.66	0.76
21:1:831:CLA:HMA2	20:0:22:THR:HG21	1.65	0.76
21:1:839:CLA:H43	21:2:834:CLA:HAA2	1.68	0.76
21:A:839:CLA:H41	8:J:18:LEU:HD23	1.66	0.76
1:A:315:TRP:HA	9:K:47:GLY:HA2	1.68	0.75
21:1:803:CLA:H152	24:2:848:BCR:H11C	1.69	0.75
21:A:836:CLA:HBC1	26:A:850:LMG:H391	5.48	0.75
22:A:841:PQN:H262	21:J:1101:CLA:HMA2	1.68	0.75
21:A:828:CLA:H161	24:J:1102:BCR:H14C	33.75	0.75
1:A:362:LEU:HD11	21:A:818:CLA:H71	1.69	0.74
21:A:823:CLA:HBB2	25:A:851:LHG:HC82	1.68	0.74
21:A:804:CLA:H72	24:A:845:BCR:H24C	1.70	0.74
5:E:12:LYS:HD2	5:E:67:GLU:HB2	1.69	0.74
1:A:388:SER:HB3	21:A:828:CLA:HMA1	7.33	0.73
2:2:15:ASP:HB3	2:2:20:ARG:HB2	1.69	0.73
1:A:706:LYS:NZ	6:F:135:ASP:OD1	3.07	0.73
21:A:827:CLA:H52	28:A:856:45D:H221	1.71	0.73
21:2:837:CLA:HMB1	21:2:837:CLA:HBB1	1.71	0.73
1:A:103:TRP:HA	1:A:110:ILE:HG21	1.72	0.73
2:2:642:VAL:HG22	21:2:811:CLA:HAC1	1.71	0.72
21:2:826:CLA:HMA2	21:2:826:CLA:H11	1.71	0.72
21:A:823:CLA:H43	24:A:846:BCR:H19C	1.71	0.72
21:1:855:CLA:HBB1	21:1:855:CLA:H93	1.70	0.72
16:1:113:SER:HB2	16:1:130:VAL:HG11	1.72	0.72
21:A:837:CLA:H122	24:A:846:BCR:H23C	1.70	0.72
25:B:849:LHG:H122	25:B:849:LHG:H272	1.71	0.72
21:1:805:CLA:H51	21:1:813:CLA:H12	1.71	0.72
16:1:103:TRP:HA	16:1:110:ILE:HG21	1.72	0.72
21:A:831:CLA:HMA1	24:I:102:BCR:H292	1.71	0.72
9:K:34:PHE:HE2	21:K:103:CLA:H42	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:856:BCR:H271	21:2:834:CLA:HHB	1.71	0.72
25:1:852:LHG:H121	25:1:852:LHG:H262	1.70	0.71
21:A:806:CLA:HHC	21:A:806:CLA:HBB1	1.71	0.71
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.77	0.71
21:7:1101:CLA:HBD	21:7:1101:CLA:HBA2	1.72	0.71
1:A:500:ASN:HB2	21:A:834:CLA:HED2	1.87	0.71
16:1:739:THR:HG23	21:1:828:CLA:HBB2	1.73	0.71
24:1:856:BCR:H282	24:6:202:BCR:H14C	1.73	0.71
21:2:809:CLA:H152	21:2:810:CLA:H191	1.73	0.71
21:2:833:CLA:HBD	25:6:206:LHG:HC2	1.71	0.71
1:A:40:ARG:HH21	1:A:43:LYS:HG3	1.54	0.71
2:2:336:LEU:HD21	21:2:831:CLA:HBB1	1.72	0.71
21:A:855:CLA:HBB1	21:A:855:CLA:HMB1	1.76	0.71
21:2:802:CLA:H2	21:0:202:CLA:H43	1.71	0.71
20:0:133:GLY:HA3	24:0:205:BCR:H383	1.71	0.71
21:A:804:CLA:HMC1	25:A:849:LHG:H181	15.79	0.71
21:B:806:CLA:HBB1	21:B:806:CLA:HMB1	1.73	0.71
21:B:834:CLA:HBB1	21:B:834:CLA:HHC	1.72	0.70
21:B:830:CLA:HBC1	24:B:847:BCR:H21C	1.73	0.70
2:2:718:TYR:HB2	21:2:804:CLA:HED3	1.74	0.70
21:1:817:CLA:H72	21:8:1401:CLA:HMD3	1.72	0.70
3:C:58:CYS:HA	23:C:102:SF4:S4	2.30	0.70
21:B:829:CLA:H191	24:B:846:BCR:H10C	1.74	0.70
6:F:100:GLU:OE2	38:F:301:HOH:O	21.47	0.70
21:1:805:CLA:H142	24:1:846:BCR:H372	1.73	0.70
21:1:836:CLA:HBB1	21:1:836:CLA:HMB1	1.73	0.70
21:B:838:CLA:H18	24:I:102:BCR:H362	1.74	0.70
21:1:831:CLA:HBB2	21:1:838:CLA:HMC2	1.74	0.69
21:2:832:CLA:HBB1	21:2:832:CLA:HHC	1.73	0.69
21:1:855:CLA:HMA2	28:2:854:45D:H132	1.74	0.69
21:1:833:CLA:HMA2	20:0:68:LEU:HB3	1.74	0.69
21:A:814:CLA:HHC	24:A:844:BCR:H14C	9.09	0.69
2:B:4:LYS:HE3	7:I:38:GLY:HA3	1.73	0.69
21:1:839:CLA:HBB1	21:1:839:CLA:HHC	1.75	0.69
16:1:315:TRP:HA	19:8:47:GLY:HA2	1.74	0.69
1:A:388:SER:HB3	21:A:827:CLA:HMA1	1.72	0.69
16:1:207:LEU:HD21	21:1:820:CLA:HMC1	1.74	0.69
16:1:13:LYS:HB2	21:1:812:CLA:HED1	1.75	0.69
21:1:837:CLA:HBC1	26:1:851:LMG:H391	1.74	0.69
21:B:809:CLA:H121	21:B:827:CLA:H171	1.73	0.69
21:J:1101:CLA:HBB1	24:J:1107:BCR:H292	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:813:CLA:C3B	24:A:844:BCR:H12C	2.23	0.69
21:A:838:CLA:H111	21:A:838:CLA:HAB	1.74	0.69
9:K:23:GLY:HA2	9:K:27[B]:CYS:HB2	1.75	0.69
6:F:24:LEU:O	6:F:36:ARG:NH2	2.26	0.69
2:B:154:TRP:CD1	11:M:28:GLU:HG3	2.55	0.69
16:1:210:LEU:HD11	24:1:844:BCR:H10C	1.74	0.68
21:A:803:CLA:HBB1	21:A:803:CLA:HMB1	1.84	0.68
1:A:332:PHE:HB2	25:A:851:LHG:HC41	1.77	0.68
21:A:805:CLA:H51	21:A:813:CLA:H12	30.70	0.68
21:L:203:CLA:HAB	38:L:319:HOH:O	11.15	0.68
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.74	0.68
2:B:312:LEU:HB2	25:B:849:LHG:HC42	1.76	0.68
21:A:806:CLA:H151	21:A:829:CLA:HBB2	26.17	0.68
21:A:838:CLA:H43	21:B:832:CLA:HAA2	1.76	0.68
4:D:31:THR:O	4:D:83:TYR:HA	2.16	0.68
20:0:41:ARG:HB3	20:0:44:LEU:HD22	1.75	0.68
21:1:804:CLA:HBB1	21:1:804:CLA:HMB1	1.75	0.68
21:B:835:CLA:HMB1	21:B:835:CLA:HBB1	1.76	0.68
21:2:828:CLA:HBB1	21:2:835:CLA:HMA2	1.74	0.68
21:2:829:CLA:HBC3	26:2:850:LMG:H441	1.76	0.68
3:3:27:GLU:HG3	3:3:44:ARG:HH22	1.58	0.68
21:K:102:CLA:HMB3	26:K:105:LMG:H442	1.76	0.68
2:2:180:ALA:HB2	2:2:288:GLY:HA3	1.76	0.67
5:5:12:LYS:HD2	5:5:67:GLU:HG3	1.76	0.67
1:A:90:MET:HE3	21:A:807:CLA:HBA2	1.75	0.67
31:B:852:SQD:H262	21:1:841:CLA:H52	1.76	0.67
2:2:461:ILE:HD11	21:2:837:CLA:H2	1.75	0.67
1:A:736:ILE:HG21	21:A:828:CLA:HMC2	14.64	0.67
16:1:303:LEU:HD22	21:1:821:CLA:HMC1	1.76	0.67
21:1:814:CLA:HBA2	24:1:845:BCR:H342	1.77	0.67
21:1:806:CLA:H151	21:1:829:CLA:HBB2	1.77	0.67
16:1:83:VAL:HG12	21:1:805:CLA:H92	1.76	0.67
1:A:86:TRP:HA	21:A:806:CLA:HBB2	1.75	0.67
24:1:858:BCR:H391	8:7:12:PRO:HB2	1.76	0.67
21:A:820:CLA:HMB1	21:A:820:CLA:HBB1	1.74	0.67
21:A:835:CLA:H193	25:A:851:LHG:H262	1.74	0.67
2:B:16:PRO:HG3	3:C:74:THR:HG22	5.62	0.67
1:A:691:GLY:HA3	2:B:567:ILE:HG12	2.05	0.67
21:B:802:CLA:H42	10:L:34:ILE:HD11	1.75	0.67
24:L:207:BCR:H282	24:L:207:BCR:H292	2.42	0.67
4:D:118:LYS:NZ	4:D:139:TYR:O	2.35	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:582:ASN:HB2	21:2:803:CLA:HBC2	1.77	0.67
1:A:348:TRP:HB3	21:A:804:CLA:HAC1	1.77	0.66
1:A:433:ARG:HG3	1:A:555:TYR:CZ	2.29	0.66
21:A:814:CLA:HBA2	24:A:844:BCR:H342	19.63	0.66
16:1:737:VAL:HG22	24:1:856:BCR:HC21	1.76	0.66
1:A:292:ASP:HB3	21:A:817:CLA:HMA1	1.77	0.66
2:2:579:TRP:CH2	21:2:803:CLA:HAB	2.31	0.66
1:A:629:HIS:NE2	38:A:904:HOH:O	2.28	0.66
2:B:223:MET:HB2	26:K:105:LMG:H122	141.81	0.66
21:1:824:CLA:H43	24:1:847:BCR:H19C	1.77	0.66
21:A:831:CLA:HAB	21:A:837:CLA:CBB	24.30	0.66
1:A:195:SER:O	1:A:199:HIS:ND1	2.47	0.66
1:A:315:TRP:HB3	9:K:64:PRO:HB3	1.92	0.66
10:L:133:GLY:HA3	24:L:207:BCR:H383	2.19	0.66
28:A:856:45D:H191	21:J:1103:CLA:HMC2	1.78	0.66
9:K:79:GLY:O	38:K:201:HOH:O	2.13	0.66
4:D:77:LYS:HB2	4:D:78:PRO:HD3	1.77	0.66
21:1:830:CLA:HMB1	21:1:830:CLA:HBB1	1.78	0.66
25:B:858:LHG:H241	21:1:841:CLA:HMD2	1.76	0.66
21:B:815:CLA:HBB1	21:B:815:CLA:HHC	1.76	0.66
2:B:72:GLY:HA2	2:B:87:ILE:HG13	4.60	0.66
6:F:86:TYR:O	6:F:90:ILE:HG13	1.96	0.66
1:A:584:GLN:HB3	1:A:589:ASP:HB3	2.04	0.65
3:C:5:VAL:HG22	3:C:67:VAL:HG22	1.97	0.65
21:1:822:CLA:HMD2	24:1:844:BCR:H24C	1.77	0.65
2:B:117:TYR:HA	2:B:365:THR:HG22	1.78	0.65
21:B:808:CLA:H152	26:0:206:LMG:H242	1.78	0.65
21:1:806:CLA:H43	21:1:830:CLA:H51	1.79	0.65
1:A:207:LEU:HD13	24:A:845:BCR:H10C	1.78	0.65
1:A:433:ARG:HH21	1:A:555:TYR:HA	1.61	0.65
21:A:802:CLA:HMA1	21:A:802:CLA:H51	2.00	0.65
1:A:482:PHE:HB3	21:A:835:CLA:H42	1.79	0.65
21:B:802:CLA:H12	21:L:204:CLA:H93	1.78	0.65
16:1:117:VAL:HB	16:1:127:ASN:HD21	1.62	0.65
21:A:854:CLA:HMB1	21:A:854:CLA:HBB1	1.77	0.65
9:K:53:PRO:HG2	24:K:104:BCR:H282	1.78	0.65
21:L:205:CLA:HMB1	21:L:205:CLA:HBB1	2.20	0.65
21:A:824:CLA:HMB3	25:A:851:LHG:HC2	14.80	0.65
21:A:831:CLA:HBB2	21:A:837:CLA:HMC2	22.37	0.65
21:B:825:CLA:HMA1	24:B:845:BCR:H14C	1.79	0.65
21:I:101:CLA:HBC3	24:I:102:BCR:C21	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:811:CLA:HBB1	21:A:811:CLA:HMB1	4.70	0.65
21:B:822:CLA:HBD	21:B:822:CLA:HBA1	1.78	0.65
8:J:12:PRO:HB2	24:J:1107:BCR:H381	1.78	0.65
21:1:820:CLA:HBB1	21:1:820:CLA:HMB1	1.77	0.64
5:5:9:VAL:HG12	5:5:68:LEU:HA	1.78	0.64
1:A:203:GLY:HA3	21:A:813:CLA:HBB1	12.51	0.64
10:L:44:LEU:O	10:L:49:ARG:NH1	2.90	0.64
10:L:62:ILE:HD11	10:L:82:LEU:HA	1.79	0.64
16:1:317:ILE:HD13	19:8:68:ALA:HB2	1.79	0.64
21:B:822:CLA:HBB1	21:B:822:CLA:HHC	1.79	0.64
21:A:833:CLA:H142	21:K:102:CLA:H172	1.77	0.64
9:K:23:GLY:HA2	9:K:27[A]:CYS:HB3	1.77	0.64
21:7:1105:CLA:HBB1	21:7:1105:CLA:HMB1	1.79	0.64
2:B:539:ARG:NH1	4:D:127:GLU:OE1	2.31	0.64
16:1:398:GLY:HA3	16:1:602:LEU:HD11	1.78	0.64
21:1:829:CLA:H51	24:1:846:BCR:H23C	1.79	0.64
1:A:89:GLY:HA3	21:A:807:CLA:HBB1	12.71	0.64
2:B:339:LEU:HD12	2:B:342:ILE:HD11	1.79	0.64
21:B:831:CLA:HBB1	21:B:831:CLA:HMB1	1.78	0.64
17:4:77:LYS:HB2	17:4:78:PRO:HD3	1.79	0.64
1:A:304:PHE:HZ	21:A:818:CLA:H121	1.61	0.64
2:2:608:GLU:HG2	6:6:48:GLU:HG2	1.78	0.64
21:2:833:CLA:HBB1	21:2:833:CLA:HHC	1.80	0.64
2:B:127:ILE:HG21	21:B:814:CLA:HMA3	1.80	0.64
5:E:64:ASN:OD1	5:E:64:ASN:N	2.28	0.64
24:1:845:BCR:H291	21:8:1402:CLA:HMC3	1.79	0.63
2:2:488:ALA:HB3	2:2:491:LEU:HD13	1.80	0.63
1:A:207:LEU:HB3	24:A:845:BCR:H12C	1.78	0.63
10:L:67:LEU:HG	21:L:205:CLA:HMA1	1.92	0.63
21:A:824:CLA:H42	21:A:828:CLA:H193	1.79	0.63
21:B:804:CLA:H151	24:B:846:BCR:H16C	1.79	0.63
21:2:834:CLA:HBB1	21:2:834:CLA:HHC	1.81	0.63
21:A:831:CLA:HMD3	21:A:836:CLA:H141	1.80	0.63
2:B:195:VAL:HG22	2:B:254:ILE:HB	2.62	0.63
21:B:819:CLA:HBB1	21:B:824:CLA:H121	1.80	0.63
21:B:830:CLA:H93	25:B:849:LHG:H101	1.81	0.63
2:B:461:ILE:HD11	21:B:835:CLA:H2	1.80	0.63
21:0:202:CLA:HMA1	21:0:203:CLA:HBC1	1.79	0.63
21:1:803:CLA:H162	21:2:811:CLA:HMB2	1.81	0.63
2:2:255:LEU:HD11	21:2:817:CLA:HBC1	1.80	0.63
28:2:854:45D:C32	21:0:202:CLA:HAB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:815:CLA:H172	24:2:845:BCR:H271	1.80	0.63
6:F:86:TYR:CE2	6:F:90:ILE:HD11	2.34	0.63
16:1:309:HIS:CD2	24:1:844:BCR:H19C	2.34	0.62
21:2:841:CLA:HBA2	24:2:848:BCR:H352	1.80	0.62
17:4:30:ILE:HD11	17:4:83:TYR:HB2	1.81	0.62
1:A:447:LEU:HB3	1:A:540:PHE:HB2	2.17	0.62
2:B:513:ASP:OD2	2:B:594:LYS:NZ	2.44	0.62
16:1:696:LEU:HD21	21:1:802:CLA:HED2	1.81	0.62
21:1:803:CLA:HMB1	21:1:803:CLA:HBB1	1.80	0.62
1:A:76:HIS:HB3	21:A:813:CLA:HED2	27.14	0.62
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.87	0.62
3:C:13:GLY:O	3:C:38:GLN:NE2	2.29	0.62
4:D:10:LYS:HB2	4:D:49:ILE:HB	1.99	0.62
21:2:830:CLA:H51	24:2:845:BCR:H23C	1.81	0.62
2:B:420:LEU:HD13	2:B:529:LEU:HA	1.82	0.62
6:F:101:VAL:HG12	6:F:102:VAL:HG23	1.81	0.62
21:2:802:CLA:HBB1	21:2:802:CLA:HMB1	1.81	0.62
21:2:811:CLA:H142	26:2:850:LMG:H222	1.81	0.62
21:L:203:CLA:HMB1	21:L:203:CLA:HBB1	2.09	0.62
24:6:202:BCR:H10C	21:6:203:CLA:C3B	2.29	0.62
21:A:828:CLA:HBB1	21:A:828:CLA:HMB1	1.86	0.62
21:A:830:CLA:HBB1	21:A:830:CLA:HMB1	2.07	0.62
26:A:850:LMG:H322	26:A:850:LMG:HC91	1.82	0.62
5:E:13:ARG:NH1	38:E:101:HOH:O	2.31	0.62
30:M:7002:ECH:H33B	35:0:208:LMT:H81	1.82	0.62
9:K:50:LEU:HD22	9:K:52:LEU:HA	1.82	0.62
21:2:842:CLA:HMB3	25:2:851:LHG:HC81	1.82	0.62
1:A:33:HIS:NE2	21:A:810:CLA:O1A	2.31	0.62
21:A:824:CLA:H43	24:A:847:BCR:H363	20.90	0.62
2:B:174:ARG:HB2	21:B:813:CLA:HBC2	1.81	0.62
21:2:803:CLA:HMA1	21:2:804:CLA:H202	1.82	0.62
21:A:816:CLA:H101	21:K:102:CLA:HHH	1.82	0.62
21:A:821:CLA:HBB1	21:A:821:CLA:HMB1	1.82	0.62
8:J:1:MET:HG3	8:J:3:GLY:H	1.63	0.62
21:1:821:CLA:HMB1	21:1:821:CLA:HBB1	1.82	0.62
2:2:375:TYR:HA	2:2:584:LEU:HD13	1.82	0.62
2:2:582:ASN:OD1	38:2:901:HOH:O	2.16	0.62
21:A:820:CLA:H71	24:A:847:BCR:H12C	1.82	0.62
16:1:575:ASP:OD2	16:1:579:ARG:NH2	2.33	0.61
2:2:324:ILE:HD12	21:2:826:CLA:HMC2	1.81	0.61
3:3:58:CYS:O	5:5:47:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:202:BCR:H12C	21:6:203:CLA:CAB	2.30	0.61
6:6:58:ARG:HA	21:6:204:CLA:HMD3	1.82	0.61
21:B:820:CLA:HMC2	21:B:820:CLA:H121	1.82	0.61
2:2:44:GLN:OE1	2:2:162:ARG:NH2	2.31	0.61
9:K:10:GLN:NE2	9:K:11:ALA:O	2.32	0.61
16:1:571:ARG:NH1	21:1:830:CLA:O1D	2.33	0.61
2:2:203:ARG:HD3	2:2:250:ALA:HB1	1.83	0.61
24:1:856:BCR:H23C	21:7:1103:CLA:HMC2	1.81	0.61
21:6:204:CLA:HBB1	21:6:204:CLA:HMB1	1.81	0.61
1:A:571:ARG:NH1	21:A:830:CLA:O1D	31.31	0.61
21:A:805:CLA:H42	25:A:849:LHG:H261	1.81	0.61
17:4:121:ARG:HD3	5:5:13:ARG:HH11	1.65	0.61
16:1:482:PHE:HB3	21:1:836:CLA:H11	1.81	0.61
16:1:523:MET:HE1	16:1:627:VAL:HG11	1.82	0.61
16:1:56:HIS:HB2	21:1:830:CLA:HBA1	1.82	0.61
1:A:670:ILE:HG23	21:A:855:CLA:H62	50.33	0.61
7:I:29:LEU:HB3	31:L:208:SQD:H241	48.16	0.61
16:1:584:GLN:HG3	2:2:664:TRP:HB2	1.83	0.61
1:A:500:ASN:HB3	21:A:817:CLA:HED2	20.10	0.61
2:2:237:PRO:HB3	2:2:256:THR:HG21	1.82	0.61
3:3:17:CYS:HB2	3:3:54:CYS:HB2	1.83	0.61
21:B:820:CLA:HBB1	24:B:842:BCR:H14C	1.83	0.61
1:A:303:LEU:HD22	21:A:821:CLA:HMC1	6.68	0.60
1:A:170:ALA:HB2	24:A:848:BCR:H381	1.82	0.60
21:1:839:CLA:HMA2	21:2:833:CLA:HMB3	1.84	0.60
21:A:820:CLA:H141	24:A:844:BCR:H292	43.28	0.60
21:B:802:CLA:H141	37:L:209:DGD:HBN2	1.83	0.60
21:B:829:CLA:HBB1	21:B:829:CLA:HMB1	1.83	0.60
16:1:433:ARG:HA	16:1:436:ILE:HD12	1.83	0.60
2:2:545:PRO:HB3	6:6:142:PRO:HG2	1.83	0.60
21:A:825:CLA:HBA1	21:A:829:CLA:H191	34.61	0.60
21:B:801:CLA:HMB1	21:B:801:CLA:HBB1	1.82	0.60
21:B:817:CLA:HBD	21:B:826:CLA:HAB	1.84	0.60
21:1:829:CLA:H2	24:1:846:BCR:H392	1.83	0.60
21:1:824:CLA:HMA1	21:1:841:CLA:HAB	1.82	0.60
6:6:141:SER:O	6:6:143:ARG:NH1	2.35	0.60
21:A:835:CLA:HBB1	21:A:835:CLA:HMB1	1.82	0.60
21:B:807:CLA:H43	26:B:848:LMG:H321	1.81	0.60
21:B:825:CLA:HMB1	21:B:825:CLA:HBB1	1.83	0.60
21:A:840:CLA:H143	21:J:1101:CLA:H192	1.84	0.60
21:B:818:CLA:H101	21:B:824:CLA:H41	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:37:LEU:HD22	21:L:204:CLA:HBD	1.91	0.60
10:L:23:PRO:HB3	25:L:210:LHG:HC5	1.82	0.60
16:1:622:SER:O	16:1:624:ASP:N	2.33	0.60
1:A:168:MET:HE2	21:A:813:CLA:H151	1.84	0.60
21:A:829:CLA:HMB1	21:A:829:CLA:HBB1	1.84	0.60
21:A:836:CLA:HBB2	21:A:837:CLA:HBC3	1.83	0.60
19:8:59:LYS:HD2	24:8:1403:BCR:H383	1.84	0.60
2:2:48:ALA:HB3	11:9:29:LEU:HD21	1.84	0.59
37:L:209:DGD:HB81	35:L:211:LMT:H82	1.84	0.59
37:L:209:DGD:O4D	37:L:209:DGD:O5D	2.09	0.59
21:1:835:CLA:HHC	21:1:835:CLA:HBB1	1.84	0.59
21:2:805:CLA:H111	24:2:848:BCR:H362	1.84	0.59
21:A:833:CLA:HMD2	21:A:834:CLA:HBB1	4.10	0.59
1:A:677:PHE:HE1	21:A:854:CLA:HMB2	1.67	0.59
21:2:834:CLA:H203	24:6:205:BCR:H17C	1.84	0.59
21:A:828:CLA:HMC1	25:A:849:LHG:H381	14.70	0.59
2:B:665:ARG:O	2:B:665:ARG:HG2	2.33	0.59
21:K:102:CLA:HBB1	21:K:102:CLA:HMB1	1.84	0.59
16:1:26:GLU:HA	8:7:3:GLY:HA3	1.84	0.59
21:2:820:CLA:HBB2	21:2:826:CLA:H193	1.84	0.59
16:1:269:GLY:H	19:8:13:PRO:HG3	1.68	0.59
21:A:826:CLA:HMB1	21:A:826:CLA:HBB1	1.85	0.59
2:B:276:HIS:HB2	21:B:817:CLA:C1B	2.33	0.59
6:6:107:LEU:O	6:6:111:LYS:HG2	2.03	0.59
21:2:806:CLA:H12	11:9:26:SER:HB3	1.84	0.59
21:A:835:CLA:H93	26:A:852:LMG:H371	6.00	0.59
5:E:13:ARG:HH21	5:E:59:ASN:HD21	4.32	0.59
25:I:103:LHG:O1	25:I:103:LHG:O3	2.16	0.59
2:2:104:PHE:CZ	2:2:642:VAL:HG23	2.37	0.59
21:A:819:CLA:HAB	21:A:819:CLA:H152	1.84	0.59
21:A:835:CLA:H171	25:A:851:LHG:H211	1.85	0.59
6:F:138:ILE:O	38:F:301:HOH:O	2.17	0.59
10:L:8:VAL:HG13	10:L:22:THR:HG22	2.03	0.59
21:1:839:CLA:HED2	2:2:422:TRP:HB2	1.83	0.59
2:2:87:ILE:HA	2:2:115:ILE:HA	1.85	0.59
21:2:818:CLA:HMD2	26:2:852:LMG:H171	1.85	0.59
21:A:813:CLA:HBA2	24:A:844:BCR:H342	1.85	0.59
21:A:833:CLA:H203	24:A:846:BCR:H21C	1.84	0.59
21:A:834:CLA:H151	21:A:834:CLA:H42	1.85	0.59
21:B:812:CLA:H18	21:B:820:CLA:HMA1	1.84	0.59
21:B:818:CLA:HBB2	21:B:824:CLA:H203	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:39:ALA:HB2	21:L:204:CLA:HMD1	1.85	0.59
10:L:99:TYR:O	10:L:103:THR:HG23	2.03	0.59
24:F:201:BCR:H12C	21:F:202:CLA:CAB	2.32	0.59
8:J:26:LEU:HD23	24:J:1102:BCR:HC7	1.85	0.59
21:B:829:CLA:H142	26:B:848:LMG:H211	1.84	0.59
22:B:841:PQN:H292	24:L:206:BCR:H343	1.84	0.59
25:M:7003:LHG:H241	25:M:7003:LHG:H112	1.85	0.59
21:1:820:CLA:H193	24:1:845:BCR:H372	1.85	0.58
24:L:207:BCR:H393	20:0:132:MET:HB3	9.22	0.58
16:1:740:TRP:NE1	21:1:828:CLA:O1A	2.36	0.58
2:B:312:LEU:HD11	21:B:840:CLA:HED1	1.84	0.58
21:B:802:CLA:O1A	10:L:25:SER:HA	2.03	0.58
20:0:44:LEU:HG	20:0:48:LEU:HD23	1.85	0.58
1:A:646:LEU:HD23	2:B:629:ILE:HD11	6.50	0.58
4:D:37:GLU:HG2	4:D:51:ASN:HA	3.65	0.58
17:4:72:LEU:HB3	17:4:80:ILE:HB	1.84	0.58
11:9:23:PHE:HE1	25:9:101:LHG:H112	1.68	0.58
1:A:333:THR:HG21	1:A:425:LEU:HD23	3.57	0.58
2:B:409:MET:HG3	24:B:847:BCR:H402	1.84	0.58
21:2:819:CLA:HBC3	21:2:826:CLA:H192	1.85	0.58
1:A:207:LEU:HD21	21:A:819:CLA:HMC1	1.85	0.58
21:1:818:CLA:H71	21:1:835:CLA:HMA2	1.84	0.58
21:I:101:CLA:HED2	10:L:65:TRP:CD1	2.38	0.58
16:1:666:SER:HB2	2:2:443:ALA:HB1	1.86	0.58
21:2:832:CLA:HBA2	25:2:851:LHG:H241	1.84	0.58
1:A:655:ALA:O	1:A:659:ASN:ND2	2.31	0.58
21:A:802:CLA:HBA2	2:B:425:LEU:HD12	1.88	0.58
21:A:819:CLA:H8	21:A:819:CLA:HAB	5.73	0.58
16:1:86:TRP:HE1	21:1:808:CLA:HBA1	1.68	0.58
2:2:406:LEU:HG	21:2:825:CLA:HBC1	1.86	0.58
24:2:844:BCR:HC31	30:2:846:ECH:H32A	1.85	0.58
1:A:189:TRP:CZ2	21:A:809:CLA:HMA1	2.39	0.58
22:A:841:PQN:H212	21:J:1101:CLA:H92	2.55	0.58
1:A:477:GLN:H	26:A:850:LMG:HC72	1.69	0.58
16:1:195:SER:O	16:1:199:HIS:ND1	2.25	0.58
21:2:811:CLA:H122	25:9:101:LHG:H381	1.84	0.58
21:8:1401:CLA:HMB1	21:8:1401:CLA:HBB1	1.84	0.58
21:A:819:CLA:H172	21:A:827:CLA:H51	44.03	0.58
6:F:44:LEU:HD12	6:F:54:ILE:HD11	2.25	0.58
2:2:462:GLN:HG2	2:2:506:PHE:HD1	1.70	0.57
2:2:590:TYR:HA	2:2:616:TRP:HH2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:840:CLA:H161	8:7:23:ALA:HB2	1.86	0.57
21:A:819:CLA:HBB1	21:A:819:CLA:HMB1	2.23	0.57
21:A:820:CLA:H8	24:A:846:BCR:H11C	1.85	0.57
16:1:412:MET:O	16:1:557:ARG:HD3	2.03	0.57
16:1:292:ASP:HB3	21:1:818:CLA:HMA1	1.85	0.57
6:6:93:SER:O	6:6:95:ASN:N	2.34	0.57
1:A:303:LEU:HD22	21:A:820:CLA:HMC1	1.85	0.57
1:A:15:SER:HB2	1:A:186:LYS:HD2	2.10	0.57
21:B:822:CLA:CBB	21:B:840:CLA:HBB1	2.34	0.57
10:L:96:LEU:HG	24:L:206:BCR:H24C	1.86	0.57
2:2:336:LEU:HD21	21:2:831:CLA:CBB	2.34	0.57
28:2:854:45D:H133	21:0:202:CLA:H52	1.86	0.57
2:B:712:VAL:HG22	26:B:848:LMG:H432	1.87	0.57
16:1:456:ILE:HG22	21:1:833:CLA:HBC2	1.86	0.57
21:1:828:CLA:HMB1	21:1:828:CLA:HBB1	1.86	0.57
2:2:420:LEU:HD13	2:2:529:LEU:HA	1.86	0.57
1:A:77:PHE:CE1	21:A:810:CLA:HBB1	17.15	0.57
21:B:835:CLA:H93	21:B:836:CLA:H42	1.86	0.57
2:B:653:VAL:HG22	21:B:839:CLA:HMB3	1.85	0.57
21:B:801:CLA:H152	24:B:846:BCR:H11C	1.84	0.57
24:A:843:BCR:H11C	24:K:104:BCR:H333	1.87	0.57
2:2:25:ILE:HA	21:2:806:CLA:HMD3	1.85	0.57
2:2:167:TRP:CE2	21:2:815:CLA:HBC3	2.39	0.57
26:2:852:LMG:H402	26:2:852:LMG:H453	1.85	0.57
16:1:534:VAL:HG11	16:1:608:HIS:CG	2.40	0.57
2:2:415:ALA:O	2:2:419:HIS:ND1	2.31	0.57
2:2:577:MET:HG3	2:2:707:LEU:HD21	1.86	0.57
2:2:72:GLY:HA2	2:2:87:ILE:HG13	1.86	0.57
21:2:813:CLA:H2	21:2:814:CLA:C1D	2.35	0.57
1:A:433:ARG:NH2	1:A:558:SER:O	2.38	0.57
1:A:348:TRP:HB3	21:A:805:CLA:HAC1	21.71	0.57
2:B:367:ALA:HB1	2:B:722:LEU:HD11	2.03	0.57
21:B:828:CLA:H8	24:B:843:BCR:H21C	1.85	0.57
21:6:201:CLA:H2	8:7:15:ILE:HB	1.85	0.57
21:A:839:CLA:H143	21:J:1101:CLA:H192	13.40	0.57
16:1:306:ILE:HG12	24:1:844:BCR:H362	1.87	0.57
21:2:806:CLA:HMA2	11:9:29:LEU:HB3	1.87	0.57
21:1:813:CLA:HBA2	21:1:825:CLA:H43	1.85	0.57
16:1:520:VAL:HG21	16:1:523:MET:HE3	1.88	0.56
2:B:312:LEU:HD22	31:F:205:SQD:H121	13.41	0.56
21:B:811:CLA:H172	21:B:814:CLA:H111	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:716:ARG:NH2	5:5:45:ASN:O	2.38	0.56
21:1:813:CLA:H203	24:1:846:BCR:H11C	1.86	0.56
21:1:840:CLA:H143	21:7:1101:CLA:H192	1.86	0.56
21:2:821:CLA:CMD	21:2:823:CLA:HAB	2.34	0.56
3:C:26:LEU:HA	3:C:41:SER:O	2.08	0.56
16:1:561:LEU:HD22	16:1:579:ARG:HD2	1.87	0.56
1:A:212:TRP:NE1	21:A:819:CLA:O1D	26.94	0.56
2:B:564:THR:HB	2:B:567:ILE:HG13	2.27	0.56
2:B:719:ALA:HB2	21:B:827:CLA:HBB1	1.86	0.56
21:B:813:CLA:H151	21:B:828:CLA:HMD2	1.87	0.56
5:E:8:LYS:HD3	5:E:24:THR:HG22	1.88	0.56
10:L:47:ILE:HG12	10:L:122:GLN:HB3	1.87	0.56
16:1:332:PHE:O	16:1:428:ARG:NH1	2.38	0.56
19:8:47:GLY:HA3	19:8:64:PRO:HG3	1.87	0.56
1:A:59:ASP:OD2	1:A:349:HIS:NE2	2.42	0.56
20:0:153:ARG:HH12	35:0:208:LMT:H6D	1.70	0.56
21:2:840:CLA:H51	21:2:841:CLA:H121	1.88	0.56
1:A:733:LEU:HD22	21:A:839:CLA:HMA1	20.76	0.56
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.88	0.56
21:F:202:CLA:HMB1	21:F:202:CLA:HBB1	2.00	0.56
6:F:71:LEU:HD11	21:J:1103:CLA:H122	4.14	0.56
16:1:440:LEU:HG	16:1:547:LEU:HB2	1.88	0.56
24:1:844:BCR:H361	19:8:75:ILE:HD11	1.86	0.56
21:A:816:CLA:H72	21:K:102:CLA:HMD3	1.86	0.56
2:B:167:TRP:CZ2	21:B:811:CLA:HMA1	2.40	0.56
21:L:203:CLA:HBA1	24:L:207:BCR:H363	1.85	0.56
16:1:25:PHE:HB2	8:7:1:MET:HG2	1.88	0.56
2:2:349:HIS:HB3	21:2:819:CLA:HED2	1.88	0.56
21:2:839:CLA:H43	24:2:847:BCR:H10C	1.88	0.56
1:A:332:PHE:O	1:A:428:ARG:NH1	2.81	0.56
2:2:86:PRO:O	2:2:116:ALA:N	2.34	0.56
21:7:1101:CLA:HBB1	21:7:1101:CLA:HHC	1.87	0.56
21:B:816:CLA:HBD	21:B:816:CLA:HBA1	1.88	0.56
21:B:827:CLA:H161	26:B:848:LMG:H272	1.86	0.56
1:A:367:ALA:HB2	1:A:393:HIS:HB2	1.86	0.56
2:B:441:VAL:HG22	2:B:449:LYS:HE3	1.87	0.56
16:1:356:LEU:HD21	21:1:830:CLA:HAB	1.88	0.56
21:1:855:CLA:HMA3	2:2:682:THR:HG21	1.87	0.56
1:A:375:PRO:HB3	21:A:819:CLA:HMA2	34.32	0.56
21:A:830:CLA:H8	21:L:204:CLA:H141	1.87	0.56
16:1:177:TRP:HB2	21:1:811:CLA:HMC3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:THR:HG23	1:A:287:GLY:H	4.97	0.56
21:B:816:CLA:CHD	21:B:817:CLA:HBB2	2.36	0.56
21:A:831:CLA:H91	21:B:839:CLA:H93	1.89	0.56
16:1:481:ILE:HG23	26:1:853:LMG:HC91	1.88	0.55
1:A:355:ASN:ND2	21:A:805:CLA:OBD	19.33	0.55
21:A:839:CLA:HAA1	21:J:1101:CLA:H43	1.88	0.55
1:A:726:VAL:O	1:A:730:HIS:ND1	4.29	0.55
21:A:812:CLA:H41	21:A:820:CLA:H42	22.88	0.55
21:A:827:CLA:HMB1	21:A:827:CLA:HBB1	1.87	0.55
2:B:304:ILE:O	2:B:308:HIS:ND1	2.61	0.55
6:F:31:ASN:HA	6:F:34:LYS:HE3	1.87	0.55
21:L:203:CLA:HMB1	24:L:207:BCR:H11C	4.80	0.55
21:1:809:CLA:CAB	21:7:1103:CLA:HMD2	2.36	0.55
2:2:257:PHE:CD2	21:2:819:CLA:HBB1	2.42	0.55
21:1:809:CLA:HAB	21:7:1103:CLA:HMD2	1.88	0.55
1:A:376:TYR:CE2	21:A:828:CLA:HED2	2.42	0.55
2:B:372:HIS:HB2	21:B:827:CLA:CHB	2.36	0.55
2:B:104:PHE:CZ	2:B:642:VAL:HG23	5.18	0.55
21:B:808:CLA:H71	24:I:102:BCR:HC32	1.89	0.55
1:A:216:GLN:HA	1:A:220:SER:HB2	1.92	0.55
1:A:42:PRO:HB3	1:A:47:TRP:CD2	2.62	0.55
21:A:831:CLA:HAB	21:A:837:CLA:HBB2	24.76	0.55
2:B:461:ILE:O	2:B:464:THR:OG1	2.15	0.55
2:B:460:TRP:HE1	2:B:474:VAL:HG21	1.80	0.55
21:B:819:CLA:H43	21:B:826:CLA:H111	1.89	0.55
21:B:817:CLA:H91	21:B:833:CLA:H42	1.87	0.55
16:1:296:HIS:HB2	21:1:818:CLA:C1B	2.36	0.55
21:A:854:CLA:HBC2	2:B:582:ASN:HB2	1.87	0.55
6:F:88:ILE:HG21	6:F:130:LYS:HZ1	2.20	0.55
21:1:823:CLA:H92	21:1:823:CLA:H41	1.89	0.55
1:A:588:TRP:CD1	21:A:830:CLA:HMD1	27.37	0.55
6:6:103:ILE:HG13	21:6:201:CLA:H11	1.88	0.55
2:B:173:SER:O	2:B:177:HIS:ND1	2.28	0.55
21:B:835:CLA:HMB2	21:B:837:CLA:HED1	1.89	0.55
6:F:90:ILE:HG22	6:F:96:PRO:HA	1.87	0.55
11:M:4:SER:HB3	11:M:7:GLN:HG3	1.88	0.55
2:2:123:TRP:O	2:2:127:ILE:HG12	2.06	0.55
2:2:154:TRP:CD1	11:9:28:GLU:HG3	2.41	0.55
21:A:807:CLA:H71	24:J:1102:BCR:H372	1.89	0.55
21:A:826:CLA:HED1	21:A:833:CLA:HAB	1.89	0.55
21:A:803:CLA:H11	2:B:648:LEU:HD23	52.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:613:LEU:HD13	21:2:803:CLA:HMA2	1.88	0.55
1:A:157:GLN:NE2	21:A:814:CLA:O1D	18.53	0.55
21:A:820:CLA:HBA1	21:A:824:CLA:C3B	2.37	0.55
2:B:178:HIS:HA	2:B:182:LEU:HB3	2.24	0.55
2:B:405:VAL:O	2:B:409:MET:HG2	2.09	0.55
5:E:19:TYR:HB2	38:E:106:HOH:O	2.07	0.55
21:A:828:CLA:H152	21:A:855:CLA:H202	52.67	0.55
2:B:226:PHE:HZ	21:B:815:CLA:H52	1.71	0.55
21:B:824:CLA:HMA2	21:B:824:CLA:H2	1.89	0.55
1:A:224:ASN:ND2	38:A:903:HOH:O	26.55	0.54
1:A:268:TRP:O	1:A:271:TYR:HB2	2.50	0.54
2:B:3:THR:HG21	2:B:20:ARG:HD2	1.89	0.54
2:B:402:LYS:HA	31:F:205:SQD:H372	2.83	0.54
4:D:121:ARG:HD2	5:E:13:ARG:HD3	2.92	0.54
16:1:237:PRO:HG3	16:1:248:LYS:HE2	1.87	0.54
21:1:824:CLA:HAB	21:1:831:CLA:HMD2	1.89	0.54
3:3:24:ASP:OD2	17:4:98:HIS:ND1	2.36	0.54
1:A:262:PRO:HA	1:A:267:ASN:HB3	2.33	0.54
21:A:821:CLA:H142	24:A:847:BCR:HC8	34.13	0.54
2:B:262:HIS:HE1	2:B:264:GLN:HB3	1.73	0.54
6:F:72:PHE:HB2	24:F:201:BCR:H321	1.89	0.54
20:0:92:ALA:HB1	24:0:204:BCR:H401	1.90	0.54
2:2:684:LEU:HB2	28:2:854:45D:H102	1.90	0.54
16:1:561:LEU:HD13	16:1:582:THR:HG22	1.90	0.54
21:1:855:CLA:H61	21:2:840:CLA:H43	1.90	0.54
21:1:832:CLA:H111	21:2:841:CLA:H71	1.89	0.54
17:4:33:THR:OG1	17:4:82:ASP:OD2	2.19	0.54
1:A:26:GLU:HA	8:J:3:GLY:HA3	1.97	0.54
1:A:429:MET:HA	1:A:432:HIS:CE1	2.92	0.54
1:A:462:ARG:NE	38:A:905:HOH:O	36.66	0.54
1:A:260:LEU:HD11	21:A:814:CLA:HBA2	1.90	0.54
9:K:32:PHE:O	9:K:36:ILE:HG23	2.07	0.54
16:1:367:ALA:HB2	16:1:393:HIS:HB2	1.88	0.54
6:F:93:SER:O	6:F:95:ASN:N	2.40	0.54
2:B:1:MET:N	7:I:37:GLU:OE1	2.40	0.54
22:A:841:PQN:H303	21:J:1101:CLA:H172	1.90	0.54
10:L:23:PRO:HA	10:L:27:SER:HB3	2.15	0.54
21:F:202:CLA:H13	21:J:1105:CLA:HMC3	1.90	0.54
8:7:24:GLY:HA3	21:7:1104:CLA:HBB1	1.88	0.54
21:A:836:CLA:HMC2	21:A:836:CLA:H112	2.76	0.54
21:B:833:CLA:H111	21:B:834:CLA:H2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:557:ASP:OD2	2:2:561:ARG:NH2	2.32	0.54
21:A:802:CLA:HMB1	21:A:802:CLA:HBB1	1.89	0.54
21:A:817:CLA:O1D	21:A:818:CLA:HMA1	2.08	0.54
21:L:204:CLA:HMA1	21:L:205:CLA:HBC1	1.90	0.54
21:2:825:CLA:CAB	21:2:832:CLA:HMD2	2.29	0.54
1:A:296:HIS:HB2	21:A:818:CLA:C1B	6.84	0.54
21:A:809:CLA:H12	24:J:1102:BCR:H17C	41.50	0.54
2:B:169:LYS:NZ	2:B:326:ASN:OD1	2.41	0.54
5:5:13:ARG:O	5:5:15:GLU:N	2.41	0.54
1:A:296:HIS:HB2	21:A:817:CLA:C1B	2.38	0.54
21:A:831:CLA:HAA2	10:L:8:VAL:HG21	28.22	0.54
2:2:408:ARG:O	2:2:412:HIS:ND1	2.41	0.53
31:B:852:SQD:H301	31:B:852:SQD:H132	1.90	0.53
21:1:805:CLA:HBA2	21:1:813:CLA:HED1	1.90	0.53
1:A:113:SER:HB2	1:A:130:VAL:HG11	2.20	0.53
1:A:561:LEU:HD22	1:A:579:ARG:HD2	2.52	0.53
1:A:729:ALA:HA	25:A:849:LHG:H341	3.14	0.53
2:B:317:HIS:HB3	2:B:320:LEU:HD12	1.89	0.53
21:B:807:CLA:H143	21:B:828:CLA:HBB2	1.90	0.53
3:C:18:VAL:HG22	3:C:26:LEU:HB2	1.90	0.53
1:A:118:TRP:HB3	24:J:1107:BCR:HC21	1.90	0.53
2:2:488:ALA:HB2	21:2:836:CLA:HED3	1.89	0.53
24:F:201:BCR:HC31	21:J:1103:CLA:HBA2	1.91	0.53
21:2:808:CLA:H43	26:2:850:LMG:H321	1.90	0.53
1:A:645:TRP:HB3	21:A:801:CLA:H101	2.58	0.53
1:A:736:ILE:HG21	21:A:827:CLA:HMC2	1.90	0.53
21:A:827:CLA:HMB2	21:A:833:CLA:H43	31.01	0.53
1:A:419:ALA:HA	4:D:39:VAL:HG11	1.91	0.53
21:B:825:CLA:H92	21:B:837:CLA:H41	1.88	0.53
4:D:37:GLU:HA	4:D:50:MET:O	2.17	0.53
16:1:733:LEU:HD22	21:1:840:CLA:HMA1	1.90	0.53
2:2:258:LEU:HD23	2:2:258:LEU:H	1.74	0.53
1:A:319:HIS:NE2	21:A:823:CLA:OBD	12.05	0.53
21:A:822:CLA:HBD	21:A:822:CLA:HBA1	1.89	0.53
2:2:587:LEU:HD21	21:2:837:CLA:HBB2	1.91	0.53
1:A:726:VAL:HG13	1:A:730:HIS:CE1	3.29	0.53
2:B:313:THR:OG1	25:B:849:LHG:O6	2.27	0.53
3:C:52:LYS:NZ	3:C:67:VAL:O	2.54	0.53
6:F:132:VAL:HG11	31:F:205:SQD:H3	2.62	0.53
7:I:26:THR:HG22	25:I:103:LHG:H172	1.91	0.53
1:A:442:TRP:HH2	21:A:836:CLA:H141	4.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:840:CLA:HBA1	21:B:840:CLA:HED2	1.89	0.53
1:A:439:HIS:O	1:A:443:VAL:HG23	2.08	0.53
21:A:820:CLA:H102	21:A:823:CLA:H93	1.90	0.53
2:B:324:ILE:HD12	21:B:824:CLA:HMC2	1.91	0.53
20:0:153:ARG:NH1	35:0:208:LMT:H6D	2.24	0.53
21:1:833:CLA:H51	28:2:854:45D:H411	1.89	0.53
21:1:802:CLA:H122	21:1:840:CLA:HMC2	1.91	0.53
2:2:584:LEU:HD23	2:2:587:LEU:HD22	1.91	0.53
11:9:14:VAL:O	11:9:18:PRO:HD2	2.09	0.53
1:A:333:THR:OG1	25:A:851:LHG:O4	2.55	0.53
21:A:813:CLA:H13	21:A:813:CLA:H52	1.91	0.52
20:0:39:ALA:HB2	21:0:202:CLA:HMD1	1.91	0.52
21:1:821:CLA:H41	24:1:848:BCR:H16C	1.91	0.52
21:2:813:CLA:H62	24:2:845:BCR:H333	1.90	0.52
1:A:574:CYS:HB3	1:A:583:CYS:HA	1.90	0.52
1:A:86:TRP:HE1	21:A:808:CLA:HBA1	14.28	0.52
21:A:803:CLA:HMA2	21:A:810:CLA:HMD2	1.91	0.52
16:1:168:MET:O	16:1:172:MET:HG2	2.09	0.52
1:A:456:ILE:HG22	21:A:832:CLA:HBC2	1.90	0.52
1:A:587:GLY:O	1:A:591:VAL:HG23	2.25	0.52
21:A:808:CLA:HMC3	21:A:809:CLA:HMD2	47.82	0.52
24:A:846:BCR:H402	25:L:210:LHG:H181	1.91	0.52
2:B:256:THR:HA	21:B:816:CLA:HED1	1.90	0.52
5:E:8:LYS:HB2	5:E:70:GLN:HA	1.92	0.52
2:2:133:GLN:O	2:2:137:SER:OG	2.27	0.52
2:2:276:HIS:HB2	21:2:819:CLA:CHB	2.40	0.52
24:9:102:BCR:H403	24:9:102:BCR:H23C	1.92	0.52
21:A:819:CLA:H8	21:A:819:CLA:CAB	5.52	0.52
21:B:816:CLA:H18	24:B:842:BCR:H21C	1.91	0.52
21:1:821:CLA:H111	24:1:847:BCR:H12C	1.91	0.52
21:1:828:CLA:H161	24:7:1102:BCR:H14C	1.91	0.52
1:A:304:PHE:HE1	21:A:820:CLA:HAB	1.74	0.52
1:A:331:PRO:HG2	21:A:840:CLA:HED2	49.11	0.52
1:A:539:ALA:O	1:A:543:HIS:ND1	2.47	0.52
21:J:1105:CLA:HBC3	21:J:1105:CLA:H93	1.91	0.52
2:2:236:ASP:OD1	2:2:236:ASP:N	2.43	0.52
2:B:254:ILE:HG13	2:B:255:LEU:HG	1.92	0.52
9:K:20:LEU:O	9:K:25:ILE:HG12	2.09	0.52
24:A:843:BCR:H401	9:K:41:ILE:HD11	2.85	0.52
21:1:820:CLA:H203	24:1:846:BCR:H332	1.92	0.52
2:2:544:MET:SD	2:2:567:ILE:HG21	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:840:CLA:HBB2	22:2:843:PQN:H141	1.91	0.52
17:4:30:ILE:HG21	17:4:68:LEU:HD23	1.91	0.52
1:A:262:PRO:HG2	1:A:271:TYR:CZ	4.06	0.52
1:A:79:HIS:CD2	21:A:805:CLA:HMA1	7.05	0.52
21:A:821:CLA:HMD2	24:A:843:BCR:H24C	1.91	0.52
2:B:101:VAL:O	2:B:105:THR:HG23	5.10	0.52
16:1:677:PHE:CG	24:1:856:BCR:H363	2.45	0.52
21:1:855:CLA:H192	20:0:61:LEU:HD21	1.91	0.52
21:2:805:CLA:HMA2	21:2:805:CLA:H12	1.92	0.52
21:2:810:CLA:H111	21:2:810:CLA:H2	1.92	0.52
2:2:409:MET:HE2	24:2:849:BCR:H271	1.92	0.52
1:A:120:ILE:HG13	1:A:121:VAL:HG13	1.92	0.52
2:B:374:GLN:HB3	2:B:584:LEU:HD21	2.21	0.52
6:F:107:LEU:O	6:F:111:LYS:HG2	2.19	0.52
2:2:637:VAL:HG13	2:2:641:SER:HB2	1.91	0.52
17:4:10:LYS:HB2	17:4:49:ILE:HB	1.92	0.52
1:A:21:VAL:O	1:A:181:HIS:ND1	2.42	0.52
21:A:834:CLA:HBA1	21:A:834:CLA:CHA	2.40	0.52
2:B:371:THR:HG23	2:B:588:THR:HG21	2.14	0.52
1:A:438:SER:HB2	2:B:678:ALA:HB2	2.12	0.52
21:1:820:CLA:H151	24:1:845:BCR:H24C	1.91	0.52
21:2:806:CLA:H93	24:9:102:BCR:H11C	1.91	0.52
17:4:72:LEU:HD22	17:4:80:ILE:HD12	1.92	0.52
1:A:531:ASP:O	1:A:535:HIS:ND1	2.45	0.52
1:A:657:VAL:HG22	1:A:745:ALA:HB3	1.91	0.52
4:D:127:GLU:HB2	4:D:130:THR:HG23	2.20	0.52
21:1:834:CLA:HMB3	21:1:836:CLA:HED3	1.92	0.51
2:2:349:HIS:ND1	21:2:819:CLA:OBD	2.42	0.51
1:A:207:LEU:HD22	24:A:844:BCR:H361	2.07	0.51
21:A:821:CLA:H152	21:A:831:CLA:HBC1	44.91	0.51
1:A:484:GLN:HB3	26:A:852:LMG:HC5	1.92	0.51
21:B:816:CLA:H111	26:B:850:LMG:H453	1.91	0.51
21:0:201:CLA:HMB2	24:0:205:BCR:H11C	1.91	0.51
16:1:74:SER:HB2	21:1:811:CLA:HAC2	1.92	0.51
3:C:62:PHE:CE2	4:D:122:ILE:HG21	2.91	0.51
4:D:120:ARG:NH1	4:D:125:ASN:OD1	2.43	0.51
7:I:10:LEU:O	7:I:14:LEU:HB2	2.17	0.51
21:1:824:CLA:HMA1	21:1:841:CLA:CAB	2.40	0.51
2:2:312:LEU:HB2	25:2:851:LHG:HC42	1.91	0.51
2:B:372:HIS:HB2	21:B:827:CLA:C1B	2.40	0.51
2:B:408:ARG:HD3	21:B:830:CLA:OBD	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:38:PRO:HG3	10:L:52:GLU:CD	2.31	0.51
21:A:811:CLA:H71	26:K:101:LMG:H261	1.92	0.51
21:A:839:CLA:H161	8:J:23:ALA:HB2	12.59	0.51
21:A:813:CLA:C4B	24:A:844:BCR:H12C	2.40	0.51
2:B:48:ALA:HB3	11:M:29:LEU:HD21	1.98	0.51
21:B:802:CLA:HMB1	21:B:802:CLA:HBB1	1.92	0.51
21:A:838:CLA:H2	8:J:15:ILE:HB	14.73	0.51
9:K:22:VAL:HG21	21:K:103:CLA:H171	1.93	0.51
2:2:713:GLY:O	2:2:717:THR:HG22	2.11	0.51
1:A:360:GLY:HA2	1:A:397:GLY:HA2	2.08	0.51
21:A:803:CLA:HMC3	21:A:805:CLA:HED2	1.92	0.51
21:A:808:CLA:HBA1	21:A:808:CLA:HBD	1.91	0.51
21:A:832:CLA:H162	21:L:204:CLA:HMB2	1.92	0.51
2:B:385:PHE:HB3	2:B:531:LEU:HB3	1.92	0.51
21:B:803:CLA:O2D	21:B:803:CLA:HAA2	2.11	0.51
21:B:830:CLA:HHC	21:B:830:CLA:HBB1	1.91	0.51
21:B:823:CLA:HMB3	21:B:840:CLA:HAB	1.93	0.51
10:L:6:GLN:O	10:L:9:GLN:NE2	3.34	0.51
16:1:278:LYS:HG2	16:1:502:LEU:HD12	1.93	0.51
21:A:840:CLA:H41	2:2:148:LEU:HD23	129.55	0.51
21:2:827:CLA:H11	21:2:839:CLA:HBD	1.91	0.51
1:A:483:ALA:HA	21:A:835:CLA:HBA1	2.30	0.51
21:2:830:CLA:H122	30:2:846:ECH:H37A	1.93	0.51
1:A:94:GLY:HA3	1:A:147:TRP:CH2	2.69	0.51
1:A:74:SER:OG	1:A:180:TYR:HB2	2.11	0.51
1:A:28:TRP:CZ2	21:A:804:CLA:H11	24.35	0.51
24:A:845:BCR:H23C	24:A:845:BCR:H383	2.89	0.51
21:B:819:CLA:H43	24:B:847:BCR:H363	1.91	0.51
21:B:835:CLA:H111	25:B:849:LHG:H382	1.93	0.51
20:0:36:ASN:HB3	21:0:201:CLA:HAC1	1.93	0.51
16:1:141:SER:HB2	21:1:829:CLA:HMA2	1.93	0.51
2:2:342:ILE:HG21	21:2:826:CLA:H42	1.91	0.51
21:A:802:CLA:O2A	2:B:425:LEU:HA	2.10	0.51
21:A:803:CLA:H141	21:A:808:CLA:H161	1.92	0.51
21:A:818:CLA:H62	21:A:834:CLA:HMA2	16.47	0.51
2:B:718:TYR:HB2	21:B:803:CLA:HED3	1.92	0.51
4:D:61:ARG:NH1	4:D:63:GLU:OE1	2.42	0.51
16:1:120:ILE:HG12	16:1:121:VAL:HG13	1.92	0.51
2:2:426:PHE:O	2:2:430:HIS:ND1	2.31	0.51
2:2:521:ALA:O	2:2:525:HIS:ND1	2.42	0.51
1:A:342:GLU:N	1:A:342:GLU:OE1	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:814:CLA:H202	21:A:814:CLA:H43	12.65	0.51
21:A:840:CLA:H162	24:J:1102:BCR:H11C	1.92	0.51
9:K:13:PRO:O	9:K:15:THR:N	4.67	0.51
16:1:400:LEU:HD21	21:1:806:CLA:H142	1.92	0.51
2:2:461:ILE:O	2:2:464:THR:OG1	2.25	0.51
21:2:840:CLA:HMC2	24:2:848:BCR:H381	1.92	0.51
21:1:808:CLA:H8	24:7:1102:BCR:H372	1.92	0.51
19:8:74:HIS:CE1	24:8:1403:BCR:H14C	2.46	0.51
21:A:804:CLA:HMC3	21:A:829:CLA:HMA1	1.93	0.51
1:A:462:ARG:NH1	2:B:634:PRO:HA	2.91	0.51
21:B:822:CLA:HMC2	24:B:847:BCR:HC8	1.92	0.51
16:1:428:ARG:O	16:1:432:HIS:ND1	2.37	0.50
2:2:285:ILE:O	2:2:289:HIS:ND1	2.44	0.50
21:A:802:CLA:H2	21:A:802:CLA:HMA2	2.20	0.50
21:A:806:CLA:O2D	21:A:806:CLA:HBA2	5.97	0.50
6:F:10:CYS:HB2	6:F:41:ALA:HA	2.10	0.50
16:1:373:MET:HE3	21:1:827:CLA:HHC	1.93	0.50
16:1:94:GLY:O	16:1:98:SER:OG	2.29	0.50
1:A:596:PHE:HZ	1:A:686:LEU:HD21	2.32	0.50
1:A:718:LEU:HD11	21:A:839:CLA:HMD3	17.74	0.50
2:B:160:LYS:CE	2:B:160:LYS:H	5.33	0.50
2:B:545:PRO:HD2	3:C:62:PHE:CE1	2.46	0.50
3:C:62:PHE:HZ	3:C:66:ARG:HH21	1.76	0.50
9:K:20:LEU:HA	9:K:24:ILE:HD12	1.92	0.50
21:1:833:CLA:OBD	38:1:901:HOH:O	2.19	0.50
1:A:685:PHE:HA	22:A:841:PQN:H9	2.12	0.50
2:B:87:ILE:HA	2:B:115:ILE:HA	2.65	0.50
25:I:103:LHG:H121	11:M:23:PHE:HE1	1.76	0.50
16:1:657:VAL:HG22	16:1:745:ALA:HB3	1.93	0.50
16:1:740:TRP:HD1	21:1:828:CLA:HMB2	1.77	0.50
1:A:447:LEU:HD21	21:A:836:CLA:CAB	2.42	0.50
21:B:827:CLA:CGA	21:B:827:CLA:H3A	2.41	0.50
21:B:832:CLA:HBB1	21:B:832:CLA:HHC	1.92	0.50
3:C:35:LYS:N	5:E:33:ILE:HD11	2.40	0.50
2:2:372:HIS:HB2	21:2:829:CLA:C1B	2.42	0.50
21:B:814:CLA:H122	21:B:828:CLA:H193	1.93	0.50
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.94	0.50
10:L:17:VAL:O	10:L:19:HIS:N	2.61	0.50
20:0:64:PRO:HA	21:0:203:CLA:HBB1	1.93	0.50
21:1:817:CLA:C1D	21:1:818:CLA:HBB2	2.42	0.50
16:1:691:GLY:HA3	2:2:567:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:56:ILE:HG12	24:9:102:BCR:H343	1.94	0.50
2:2:195:VAL:HG21	21:2:817:CLA:HBC3	1.92	0.50
21:2:820:CLA:HBB2	21:2:826:CLA:C19	2.41	0.50
21:2:837:CLA:HMB2	21:2:839:CLA:HED1	1.93	0.50
1:A:729:ALA:HA	25:A:849:LHG:H342	1.93	0.50
21:A:825:CLA:HMB1	21:A:825:CLA:HBB1	1.94	0.50
1:A:588:TRP:CD1	21:A:829:CLA:HMD1	2.46	0.50
21:B:836:CLA:H11	21:B:837:CLA:HMD1	1.94	0.50
9:K:34:PHE:CE2	21:K:103:CLA:H42	2.40	0.50
9:K:30:ASN:HA	9:K:73:GLY:HA3	2.18	0.50
10:L:58:GLY:HA2	10:L:89:ILE:HD11	1.94	0.50
16:1:500:ASN:HB3	21:1:817:CLA:HED2	1.93	0.50
2:2:653:VAL:HG22	21:2:841:CLA:HMB3	1.93	0.50
1:A:428:ARG:HD3	21:A:830:CLA:OBD	2.12	0.50
21:A:808:CLA:H12	24:J:1102:BCR:H17C	1.93	0.50
21:A:825:CLA:H42	21:A:829:CLA:H193	37.76	0.50
2:B:104:PHE:HZ	2:B:642:VAL:HG23	4.51	0.50
20:0:32:THR:O	20:0:36:ASN:ND2	2.36	0.50
22:1:842:PQN:H241	21:7:1101:CLA:HAA1	1.94	0.50
21:A:805:CLA:H61	21:A:829:CLA:HBC3	1.94	0.50
16:1:310:MET:O	16:1:319:HIS:N	2.44	0.50
16:1:375:PRO:HB3	21:1:819:CLA:HMA2	1.92	0.50
26:1:853:LMG:O8	26:1:853:LMG:O2	2.23	0.50
1:A:447:LEU:HD21	21:A:836:CLA:HAB	1.93	0.50
24:A:843:BCR:H282	9:K:36:ILE:HD11	1.94	0.50
2:2:117:TYR:HA	2:2:365:THR:HG22	1.94	0.49
6:6:20:SER:HB2	6:6:37:ALA:HB1	1.94	0.49
1:A:689:GLY:HA3	2:B:565:CYS:HB2	1.93	0.49
21:A:823:CLA:HAC2	21:A:823:CLA:H111	9.63	0.49
21:A:854:CLA:H152	28:A:856:45D:H381	1.93	0.49
2:B:659:MET:HB2	21:B:804:CLA:C1C	2.42	0.49
2:B:655:ALA:C	21:B:804:CLA:HAB	2.33	0.49
1:A:118:TRP:CE3	24:J:1107:BCR:H323	2.46	0.49
16:1:706:LYS:HE2	21:2:833:CLA:HED2	1.93	0.49
21:2:803:CLA:H201	24:7:1102:BCR:H16C	1.93	0.49
21:2:818:CLA:C1D	21:2:819:CLA:HBB2	2.42	0.49
21:A:813:CLA:OBD	38:A:902:HOH:O	2.19	0.49
21:B:809:CLA:O1A	21:B:827:CLA:HBD	2.11	0.49
21:B:815:CLA:C4B	24:B:842:BCR:HC21	2.42	0.49
21:B:839:CLA:HMB2	24:B:846:BCR:H14C	1.94	0.49
5:E:13:ARG:O	5:E:14:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:84:LEU:HD12	26:K:105:LMG:H331	1.93	0.49
21:L:203:CLA:C1B	21:L:204:CLA:HED1	2.42	0.49
2:B:154:TRP:NE1	11:M:28:GLU:HG3	2.47	0.49
21:B:805:CLA:HMA2	11:M:29:LEU:HB3	1.94	0.49
16:1:486:VAL:HG21	21:1:836:CLA:H12	1.94	0.49
1:A:5:PRO:HG2	1:A:183:LYS:HE3	1.95	0.49
2:B:349:HIS:HB3	21:B:817:CLA:HED2	1.94	0.49
21:B:827:CLA:H193	26:B:848:LMG:H251	1.94	0.49
5:E:16:SER:HB3	38:E:106:HOH:O	2.11	0.49
26:K:105:LMG:H172	26:K:105:LMG:H311	1.92	0.49
20:0:38:PRO:HG3	20:0:52:GLU:OE2	2.12	0.49
16:1:121:VAL:HB	21:7:1103:CLA:HMD1	1.94	0.49
19:8:17:GLY:HA2	19:8:21:SER:HB3	1.94	0.49
2:B:181:GLY:HA3	21:B:813:CLA:HBB1	1.94	0.49
21:A:854:CLA:H11	2:B:613:LEU:HD12	1.94	0.49
31:B:852:SQD:H331	31:B:852:SQD:H161	1.94	0.49
3:C:27:GLU:OE2	3:C:44:ARG:NH1	2.59	0.49
2:B:361:GLN:OE1	2:B:361:GLN:N	2.59	0.49
21:B:825:CLA:HHB	24:B:845:BCR:H16C	1.94	0.49
10:L:96:LEU:HD21	24:L:206:BCR:H383	2.14	0.49
16:1:394:MET:HE3	16:1:602:LEU:HD22	1.95	0.49
2:2:688:VAL:HG13	20:0:99:TYR:CE1	2.48	0.49
24:2:847:BCR:C21	24:2:849:BCR:H402	2.41	0.49
16:1:431:ARG:NH1	17:4:13:GLY:O	2.43	0.49
2:B:225:PHE:HB2	2:B:233:TYR:HE2	1.78	0.49
5:E:26:ALA:HB2	5:E:40:ARG:HE	3.61	0.49
21:A:809:CLA:CHB	24:J:1102:BCR:H12C	42.68	0.49
16:1:597:TRP:CH2	21:1:803:CLA:HAB	2.48	0.49
21:2:827:CLA:H43	21:2:838:CLA:HBA1	1.95	0.49
1:A:324:ILE:O	1:A:328:HIS:ND1	2.54	0.49
1:A:658:ILE:HD12	2:B:618:ARG:HG3	1.95	0.49
21:A:805:CLA:H101	21:A:827:CLA:HBC1	1.95	0.49
21:A:824:CLA:CHA	21:A:824:CLA:HBA1	4.79	0.49
24:A:843:BCR:H23C	9:K:72:PHE:HB2	1.94	0.49
21:0:201:CLA:CMB	24:0:205:BCR:H11C	2.42	0.49
16:1:657:VAL:HG21	16:1:742:PHE:HA	1.93	0.49
16:1:452:PHE:HE1	21:1:803:CLA:HMA1	1.77	0.49
21:2:808:CLA:H162	21:2:830:CLA:HBB2	1.94	0.49
1:A:202:ALA:HB2	1:A:308:GLY:HA3	1.95	0.49
1:A:219:VAL:HG13	1:A:239:PRO:HB3	2.00	0.49
21:A:823:CLA:HBA1	21:A:823:CLA:CHA	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:HB2	21:A:827:CLA:CHB	2.43	0.49
2:B:618:ARG:HA	2:B:622:TRP:HB3	2.18	0.49
16:1:16:VAL:HG12	16:1:185:PRO:HA	1.94	0.49
16:1:736:ILE:HG21	21:1:828:CLA:HMC2	1.94	0.49
21:1:826:CLA:O1A	21:1:836:CLA:HMA1	2.13	0.49
21:2:810:CLA:CAD	21:2:829:CLA:HBA1	2.43	0.49
21:2:810:CLA:HMB2	21:2:810:CLA:H142	1.94	0.49
21:2:827:CLA:O1A	21:2:837:CLA:HMA1	2.13	0.49
1:A:423:ASN:OD1	1:A:431:ARG:NH2	2.45	0.49
21:A:833:CLA:H41	21:A:833:CLA:H62	1.50	0.49
1:A:597:TRP:HE1	21:B:804:CLA:C1D	2.25	0.49
2:2:177:HIS:ND1	21:2:815:CLA:HMC2	2.28	0.49
21:1:833:CLA:H72	28:2:854:45D:H381	1.94	0.49
6:6:126:TYR:HB2	6:6:131:LEU:HD23	1.95	0.49
1:A:110:ILE:HG13	1:A:131:GLY:HA3	3.19	0.49
1:A:381:ILE:HG13	1:A:519:LYS:HE3	1.94	0.49
6:F:88:ILE:HG21	6:F:130:LYS:NZ	2.52	0.49
20:0:150:GLY:HA2	20:0:155:LEU:HD22	1.95	0.48
16:1:324:ILE:O	16:1:328:HIS:ND1	2.46	0.48
16:1:600:ASN:OD1	38:1:902:HOH:O	2.20	0.48
1:A:315:TRP:HZ3	21:A:811:CLA:HMA1	1.78	0.48
21:A:801:CLA:H162	21:A:801:CLA:H122	2.30	0.48
21:A:822:CLA:H112	21:A:822:CLA:H93	1.72	0.48
1:A:482:PHE:HB3	21:A:835:CLA:H11	1.95	0.48
2:B:526:THR:HG21	2:B:579:TRP:CE2	2.48	0.48
16:1:118:TRP:CE2	24:1:858:BCR:HC41	2.48	0.48
16:1:92:PHE:CZ	16:1:96:LYS:HD2	2.47	0.48
21:2:802:CLA:H61	21:2:802:CLA:H41	1.56	0.48
8:7:12:PRO:HA	8:7:15:ILE:HG22	1.94	0.48
21:B:805:CLA:HMC3	21:B:807:CLA:HED2	1.95	0.48
2:B:388:GLY:HA2	24:B:845:BCR:H393	1.95	0.48
9:K:86:SER:HA	26:K:105:LMG:H391	1.94	0.48
10:L:150:GLY:HA2	10:L:155:LEU:HD22	1.94	0.48
21:A:831:CLA:HBA1	10:L:22:THR:HB	27.44	0.48
21:1:811:CLA:H91	21:1:811:CLA:H142	1.95	0.48
21:1:822:CLA:H152	21:8:1401:CLA:HMC2	1.95	0.48
16:1:98:SER:HB2	16:1:144:PHE:HZ	1.78	0.48
21:2:827:CLA:HMA1	24:2:847:BCR:C14	2.43	0.48
21:A:803:CLA:H52	21:A:810:CLA:H13	1.94	0.48
1:A:577:PRO:HB3	2:B:556:CYS:SG	2.74	0.48
21:B:823:CLA:NC	24:B:847:BCR:H19C	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:843:BCR:C11	24:K:104:BCR:H333	2.42	0.48
16:1:376:TYR:CE2	21:1:829:CLA:HED2	2.48	0.48
2:2:223:MET:HA	2:2:226:PHE:HB2	1.96	0.48
2:2:628:LEU:HD12	2:2:724:ALA:HB3	1.96	0.48
2:2:557:ASP:CG	3:3:66:ARG:HH12	2.17	0.48
19:8:11:ALA:HB1	19:8:87:SER:HA	1.94	0.48
21:A:817:CLA:H41	21:A:817:CLA:H62	1.51	0.48
21:A:819:CLA:H2	21:A:829:CLA:H92	47.34	0.48
21:A:819:CLA:H193	24:A:844:BCR:H372	1.95	0.48
2:B:687:LEU:HD11	10:L:39:ALA:HB1	1.95	0.48
16:1:619:GLY:HA3	16:1:629:HIS:HA	1.96	0.48
3:3:4:SER:HB3	3:3:6:LYS:HE2	1.95	0.48
21:A:813:CLA:H203	24:A:844:BCR:H351	12.52	0.48
21:A:819:CLA:H43	21:A:819:CLA:HMB2	9.37	0.48
1:A:8:ARG:HH11	21:A:810:CLA:HBA1	24.71	0.48
2:B:614:MET:O	2:B:618:ARG:HG2	5.21	0.48
21:B:825:CLA:HMB2	21:B:837:CLA:H3A	1.96	0.48
6:F:90:ILE:HD13	6:F:99:GLN:HB3	3.21	0.48
21:L:203:CLA:HHC	38:L:319:HOH:O	9.56	0.48
21:2:827:CLA:HMA1	24:2:847:BCR:H14C	1.94	0.48
2:B:87:ILE:HD13	2:B:113:VAL:HG21	1.95	0.48
2:B:115:ILE:O	21:B:809:CLA:HMD3	2.13	0.48
2:B:32:GLU:OE1	2:B:329:HIS:NE2	2.38	0.48
2:B:462:GLN:HG2	2:B:506:PHE:CD1	2.54	0.48
2:2:405:VAL:O	2:2:409:MET:HG2	2.13	0.48
1:A:486:VAL:CG1	21:A:835:CLA:HED1	2.44	0.48
1:A:58:PHE:CD2	21:A:804:CLA:HMC2	2.49	0.48
21:A:813:CLA:H3A	21:A:813:CLA:HBA1	2.18	0.48
2:B:213:LEU:O	26:K:105:LMG:H422	119.72	0.48
21:B:809:CLA:H142	21:B:809:CLA:H111	1.70	0.48
21:B:825:CLA:H3A	21:B:825:CLA:HBA2	1.59	0.48
2:B:580:MET:CG	21:B:825:CLA:HBC1	2.43	0.48
6:F:72:PHE:HB2	24:F:201:BCR:C32	2.44	0.48
1:A:86:TRP:HB2	24:J:1102:BCR:H391	3.15	0.48
21:L:205:CLA:H151	21:L:205:CLA:H111	3.63	0.48
16:1:304:PHE:HZ	21:1:819:CLA:H121	1.78	0.48
2:2:328:LEU:HD22	21:2:807:CLA:H203	1.95	0.48
21:2:810:CLA:O1A	21:2:829:CLA:HBD	2.14	0.48
2:2:85:ARG:NH2	2:2:117:TYR:OH	2.47	0.48
1:A:486:VAL:HG21	21:A:835:CLA:H12	1.96	0.48
1:A:168:MET:HG3	24:A:844:BCR:H322	2.09	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:ALA:HB1	21:B:827:CLA:HMA1	1.95	0.48
24:B:847:BCR:HC7	25:B:851:LHG:H223	1.96	0.48
10:L:27:SER:OG	10:L:30:THR:HG23	2.14	0.48
16:1:315:TRP:HZ3	21:1:812:CLA:HMA1	1.79	0.48
16:1:332:PHE:HB2	25:1:852:LHG:HC41	1.95	0.48
2:2:579:TRP:CZ2	21:2:803:CLA:HAB	2.47	0.48
21:2:808:CLA:H192	21:2:808:CLA:H93	1.96	0.48
1:A:739:THR:HG23	21:A:828:CLA:HBB2	18.64	0.48
21:A:828:CLA:H93	21:A:828:CLA:H61	4.44	0.48
1:A:356:LEU:HD21	21:A:830:CLA:CAB	26.41	0.48
22:A:841:PQN:H262	22:A:841:PQN:H302	3.76	0.48
16:1:114:ALA:HB3	16:1:139:ILE:HG21	1.95	0.48
16:1:419:ALA:HA	17:4:39:VAL:HG11	1.95	0.48
16:1:278:LYS:HA	16:1:502:LEU:HB2	1.96	0.48
21:1:820:CLA:H111	21:1:820:CLA:H91	1.62	0.48
16:1:352:LEU:HD21	21:1:830:CLA:C2B	2.44	0.48
1:A:595:LEU:HD21	21:A:830:CLA:HBC1	21.12	0.48
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.48	0.48
21:B:820:CLA:H151	24:B:843:BCR:H342	1.95	0.48
3:C:67:VAL:HG21	23:C:101:SF4:S2	2.64	0.48
2:B:542:LYS:NZ	6:F:139:PRO:HB2	2.51	0.48
21:L:205:CLA:H62	21:L:205:CLA:H41	1.46	0.48
21:2:806:CLA:H141	21:2:806:CLA:H162	1.61	0.47
21:2:834:CLA:HBB2	24:6:202:BCR:HC21	1.96	0.47
19:8:38:TYR:HE1	19:8:61:PHE:HE2	1.60	0.47
1:A:27:LYS:HA	1:A:30:LYS:HD2	1.96	0.47
1:A:362:LEU:HD21	21:A:819:CLA:H71	29.85	0.47
1:A:430:LEU:O	1:A:433:ARG:HD2	2.14	0.47
2:B:190:TRP:HD1	2:B:277:HIS:CD2	2.32	0.47
21:B:807:CLA:H162	21:B:828:CLA:HBB2	1.96	0.47
21:B:827:CLA:O1D	21:B:828:CLA:HMA1	2.14	0.47
6:F:82:VAL:HG21	21:F:202:CLA:OBD	2.27	0.47
21:F:202:CLA:HMA1	21:J:1103:CLA:H93	1.96	0.47
21:L:203:CLA:C2B	21:L:204:CLA:HED1	2.70	0.47
16:1:24:SER:O	21:1:811:CLA:HHB	2.14	0.47
21:1:806:CLA:H91	25:1:850:LHG:H351	1.96	0.47
21:1:855:CLA:HMA1	2:2:685:ALA:HB2	1.96	0.47
2:2:539:ARG:NH1	17:4:127:GLU:OE1	2.47	0.47
1:A:539:ALA:HB1	21:A:836:CLA:HMB3	1.96	0.47
2:B:273:ILE:O	2:B:277:HIS:ND1	2.39	0.47
21:J:1101:CLA:HBD	21:J:1101:CLA:HBA2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:5:ASN:N	20:0:5:ASN:OD1	2.46	0.47
16:1:462:ARG:NH1	2:2:634:PRO:HA	2.29	0.47
21:1:824:CLA:HBB1	24:1:847:BCR:H362	1.96	0.47
8:7:26:LEU:HD23	24:7:1102:BCR:HC7	1.96	0.47
1:A:282:ASN:HB3	1:A:285:THR:HG22	5.18	0.47
1:A:440:LEU:HG	1:A:547:LEU:HB2	2.05	0.47
21:A:808:CLA:HBB1	24:J:1102:BCR:C8	2.38	0.47
21:A:825:CLA:H2	21:A:835:CLA:HMA2	1.97	0.47
26:A:850:LMG:H342	26:A:850:LMG:H371	3.92	0.47
2:B:112:PRO:HG2	7:I:1:MET:HE1	1.96	0.47
2:B:429:PHE:CZ	24:F:201:BCR:H372	2.49	0.47
3:C:62:PHE:HE2	4:D:122:ILE:HG21	2.28	0.47
9:K:36:ILE:O	9:K:40:ALA:HB3	2.14	0.47
1:A:315:TRP:HB2	21:A:819:CLA:HED1	1.96	0.47
21:A:806:CLA:H61	21:A:830:CLA:HBC3	49.24	0.47
1:A:82:VAL:HG22	21:A:810:CLA:H161	1.96	0.47
21:B:813:CLA:H172	24:B:843:BCR:H271	1.95	0.47
21:I:101:CLA:H101	21:I:101:CLA:H62	1.63	0.47
7:I:37:GLU:HG2	10:L:105:GLN:OE1	4.32	0.47
11:M:22:ALA:HB2	30:M:7002:ECH:H37B	1.97	0.47
16:1:446:PHE:HE2	21:1:837:CLA:HBB1	1.80	0.47
2:2:291:TYR:HE1	21:2:821:CLA:HED1	1.79	0.47
2:2:29:HIS:ND1	21:2:808:CLA:O1A	2.33	0.47
10:L:151:ILE:HG23	21:2:812:CLA:HBA1	36.46	0.47
1:A:283:PRO:HD3	1:A:289:TRP:CZ2	2.50	0.47
1:A:704:HIS:NE2	21:A:839:CLA:HAC1	2.30	0.47
25:A:851:LHG:H371	25:A:851:LHG:H202	4.76	0.47
26:A:852:LMG:H361	26:A:852:LMG:H262	6.58	0.47
1:A:99:ASN:ND2	1:A:110:ILE:HD11	2.30	0.47
2:B:429:PHE:HZ	24:F:201:BCR:H372	1.79	0.47
16:1:203:GLY:HA3	21:1:813:CLA:HBB1	1.95	0.47
1:A:452:PHE:HE1	21:B:801:CLA:HMA1	1.80	0.47
21:A:805:CLA:HMB1	21:A:805:CLA:HBB1	2.02	0.47
21:A:840:CLA:H3A	21:A:840:CLA:HBA1	1.59	0.47
16:1:337:HIS:CE1	25:1:852:LHG:HC11	2.50	0.47
21:1:819:CLA:CAB	21:1:819:CLA:H62	2.44	0.47
1:A:167:VAL:HG22	24:A:848:BCR:H282	1.96	0.47
1:A:427:ASP:O	1:A:431:ARG:HG3	2.23	0.47
21:A:810:CLA:H92	21:A:810:CLA:H61	1.84	0.47
21:A:812:CLA:H3A	21:A:812:CLA:HBA1	1.72	0.47
21:A:817:CLA:HMC2	21:A:817:CLA:H93	4.84	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:825:CLA:H43	25:A:851:LHG:H381	1.96	0.47
21:B:819:CLA:OBD	21:B:822:CLA:HHD	2.15	0.47
21:I:101:CLA:HBA1	21:I:101:CLA:HMA2	1.97	0.47
16:1:238:LEU:HB2	16:1:241:GLU:HG3	1.96	0.47
2:2:177:HIS:CG	21:2:815:CLA:HMC2	2.50	0.47
2:2:704:LEU:HD11	26:2:850:LMG:H362	1.97	0.47
5:E:14:THR:N	38:E:106:HOH:O	2.47	0.47
21:A:834:CLA:H51	21:K:102:CLA:HAA1	1.95	0.47
16:1:484:GLN:HB3	26:1:853:LMG:HC5	1.97	0.47
16:1:557:ARG:HD2	16:1:566:ALA:HB2	1.97	0.47
21:1:834:CLA:H161	21:1:834:CLA:H141	1.68	0.47
2:2:104:PHE:HZ	2:2:642:VAL:HG23	1.79	0.47
2:2:309:LYS:O	21:2:842:CLA:HBC2	2.15	0.47
3:3:18:VAL:HG22	3:3:26:LEU:HB2	1.96	0.47
1:A:278:LYS:O	1:A:503:ALA:N	2.78	0.47
21:A:830:CLA:HAB	21:A:837:CLA:CBB	2.44	0.47
21:A:814:CLA:CHC	24:A:844:BCR:H14C	9.56	0.47
9:K:22:VAL:O	9:K:24:ILE:N	3.35	0.47
10:L:82:LEU:HD22	10:L:139:TYR:CD2	2.50	0.47
2:B:159:PRO:HB3	10:L:1:MET:SD	87.15	0.47
21:1:802:CLA:H111	21:1:802:CLA:H91	1.80	0.47
24:1:858:BCR:H271	21:7:1101:CLA:CBB	2.45	0.47
2:2:172:GLU:HG3	2:2:291:TYR:HB3	1.96	0.47
21:2:807:CLA:HMB3	21:2:808:CLA:HAA1	1.97	0.47
21:2:823:CLA:HBB1	21:2:823:CLA:H8	1.97	0.47
1:A:424:ASN:O	1:A:428:ARG:HG3	2.15	0.47
1:A:141:SER:HB2	21:A:829:CLA:HMA2	29.19	0.47
21:B:809:CLA:H143	21:B:809:CLA:H161	1.65	0.47
21:B:820:CLA:H3A	21:B:820:CLA:HBA2	1.54	0.47
24:L:207:BCR:HC32	31:L:208:SQD:H161	1.97	0.47
20:0:38:PRO:HG2	21:0:202:CLA:HED2	1.96	0.47
16:1:411:PHE:CD1	16:1:415:ASP:HB2	2.50	0.47
22:1:842:PQN:H162	24:6:202:BCR:H382	1.97	0.47
21:1:804:CLA:HMC1	25:1:850:LHG:H181	1.97	0.47
16:1:97:PHE:HE1	21:1:807:CLA:HED2	1.80	0.47
21:2:807:CLA:H91	21:2:807:CLA:H112	1.80	0.47
21:2:811:CLA:H112	21:2:811:CLA:H151	1.55	0.47
1:A:560:ARG:NH2	4:D:15:THR:O	2.88	0.47
21:A:802:CLA:H161	21:A:802:CLA:H141	1.65	0.47
21:A:824:CLA:H161	21:A:824:CLA:H141	1.66	0.47
21:A:807:CLA:HAB	24:J:1102:BCR:H382	10.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:809:CLA:HMA2	24:1:858:BCR:H12C	1.97	0.46
16:1:588:TRP:NE1	21:1:830:CLA:HMD1	2.30	0.46
2:2:705:VAL:HG13	2:2:709:HIS:CE1	2.50	0.46
1:A:99:ASN:HB3	1:A:134:PHE:CG	2.49	0.46
1:A:356:LEU:HD21	21:A:830:CLA:HAB	25.49	0.46
21:A:828:CLA:H62	21:A:828:CLA:H102	1.82	0.46
21:A:807:CLA:CAD	24:A:848:BCR:H14C	17.77	0.46
2:B:188:LEU:HG	21:B:815:CLA:CBB	2.45	0.46
2:B:299:HIS:NE2	21:B:822:CLA:OBD	2.48	0.46
2:B:475:LEU:HD13	21:B:833:CLA:HMD3	1.96	0.46
2:B:570:TRP:CD1	21:B:829:CLA:HMD1	2.50	0.46
4:D:31:THR:HA	4:D:55:ASN:O	2.15	0.46
1:A:315:TRP:HB3	9:K:64:PRO:CB	2.45	0.46
21:1:833:CLA:H162	21:0:202:CLA:HMB2	1.96	0.46
16:1:203:GLY:HA3	21:1:813:CLA:CBB	2.46	0.46
21:1:831:CLA:H3A	21:1:831:CLA:HBA1	1.58	0.46
21:1:827:CLA:HHB	21:1:834:CLA:H43	1.98	0.46
2:2:645:TRP:CE3	24:2:848:BCR:HC41	2.50	0.46
2:2:555:PRO:HB3	2:2:699:ILE:HD12	1.97	0.46
1:A:154:ASP:OD1	1:A:155:SER:N	2.48	0.46
1:A:31:PRO:HB2	1:A:51:LEU:HD11	1.97	0.46
1:A:12:ALA:HB1	21:A:812:CLA:HAA1	17.82	0.46
21:A:815:CLA:HMB1	21:A:815:CLA:HBB1	4.51	0.46
1:A:304:PHE:CZ	21:A:818:CLA:H121	2.47	0.46
21:A:836:CLA:H41	21:A:836:CLA:H61	3.70	0.46
21:B:839:CLA:HBA2	24:B:846:BCR:H352	1.96	0.46
6:F:75:ILE:HD11	21:J:1103:CLA:H111	4.25	0.46
20:0:99:TYR:CZ	20:0:103:THR:HG21	2.50	0.46
16:1:319:HIS:CG	16:1:324:ILE:HD11	2.51	0.46
2:2:513:ASP:HA	2:2:516:VAL:HG22	1.97	0.46
21:2:826:CLA:H71	21:2:828:CLA:H42	1.98	0.46
21:A:810:CLA:H12	21:A:812:CLA:C3D	21.89	0.46
21:A:813:CLA:HBA2	21:A:825:CLA:H43	41.63	0.46
21:A:818:CLA:H93	21:A:834:CLA:HAA2	19.07	0.46
1:A:395:TRP:CD1	21:A:827:CLA:HAB	2.50	0.46
21:A:834:CLA:H41	21:A:834:CLA:H61	1.66	0.46
21:A:835:CLA:H13	21:A:835:CLA:H171	2.75	0.46
21:A:854:CLA:H42	28:A:856:45D:H393	1.97	0.46
21:B:823:CLA:HBA1	24:B:847:BCR:H351	1.96	0.46
4:D:77:LYS:HB2	4:D:78:PRO:CD	2.55	0.46
2:2:339:LEU:HD12	2:2:342:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:843:PQN:H142	24:2:848:BCR:H271	1.97	0.46
1:A:189:TRP:CZ2	21:A:810:CLA:HMA1	22.76	0.46
26:A:852:LMG:HC72	26:A:852:LMG:HC2	4.13	0.46
21:B:801:CLA:H162	21:B:810:CLA:HMB2	1.97	0.46
21:B:832:CLA:HBB2	24:F:201:BCR:HC21	1.97	0.46
10:L:32:THR:HG22	31:L:208:SQD:H82	1.98	0.46
16:1:16:VAL:HG21	16:1:183:LYS:HD2	1.97	0.46
21:1:835:CLA:H41	21:1:835:CLA:H121	1.98	0.46
2:2:348:GLN:HG3	21:2:827:CLA:HED1	1.98	0.46
21:2:838:CLA:HMB2	21:2:839:CLA:C2D	2.46	0.46
1:A:197:MET:HG2	1:A:311:TYR:CE2	2.51	0.46
1:A:319:HIS:CG	1:A:324:ILE:HD11	2.58	0.46
1:A:414:ARG:HE	27:A:853:ACT:H3	1.81	0.46
26:A:850:LMG:H411	26:A:850:LMG:H382	3.35	0.46
21:B:809:CLA:H62	21:B:809:CLA:H101	1.61	0.46
2:B:185:VAL:HG11	24:B:843:BCR:H341	1.96	0.46
8:J:27:ILE:HD13	24:J:1107:BCR:H10C	1.97	0.46
16:1:597:TRP:HE1	21:2:805:CLA:C1D	2.28	0.46
21:2:806:CLA:H193	21:2:806:CLA:H161	1.85	0.46
28:2:854:45D:H401	28:2:854:45D:H421	1.56	0.46
3:3:2:SER:N	3:3:71:ALA:O	2.48	0.46
1:A:296:HIS:HB2	21:A:818:CLA:CHB	6.61	0.46
1:A:534:VAL:HG11	1:A:608:HIS:CG	3.18	0.46
1:A:638:SER:O	1:A:644:GLY:HA3	2.16	0.46
21:A:802:CLA:CGA	21:A:802:CLA:H3A	2.51	0.46
21:A:805:CLA:H41	21:A:805:CLA:H62	1.77	0.46
21:B:810:CLA:H71	24:B:846:BCR:H341	1.98	0.46
21:I:101:CLA:HMC1	21:I:101:CLA:HBC2	1.96	0.46
21:1:823:CLA:H61	21:1:823:CLA:H41	1.48	0.46
21:1:840:CLA:H41	21:1:840:CLA:H62	1.55	0.46
24:1:844:BCR:H363	24:8:1403:BCR:H343	1.97	0.46
21:6:201:CLA:H43	21:6:203:CLA:HBC3	1.97	0.46
16:1:269:GLY:N	19:8:13:PRO:HG3	2.31	0.46
21:A:827:CLA:O1D	21:A:828:CLA:HMA1	2.16	0.46
21:B:807:CLA:HBA1	21:B:829:CLA:HMB2	1.98	0.46
21:B:821:CLA:H162	21:B:821:CLA:H202	1.79	0.46
21:B:822:CLA:H143	21:B:822:CLA:H111	1.70	0.46
21:B:830:CLA:HBA2	25:B:849:LHG:H241	1.97	0.46
16:1:115:GLN:N	38:1:908:HOH:O	2.41	0.46
16:1:110:ILE:HG13	16:1:131:GLY:HA3	1.97	0.46
16:1:115:GLN:NE2	21:1:809:CLA:HMD1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:826:CLA:HAB	24:1:848:BCR:H311	1.98	0.46
21:2:809:CLA:H161	21:2:809:CLA:H202	1.72	0.46
2:2:426:PHE:CE2	21:2:838:CLA:HAB	2.51	0.46
25:2:851:LHG:H272	25:2:851:LHG:H121	1.98	0.46
2:B:441:VAL:HG13	2:B:446:THR:O	2.19	0.46
21:B:814:CLA:HMA1	30:B:844:ECH:H29A	1.97	0.46
21:B:817:CLA:H41	21:B:817:CLA:H62	1.70	0.46
21:B:819:CLA:H3A	21:B:819:CLA:HBA2	1.34	0.46
3:C:17:CYS:SG	3:C:18:VAL:N	4.36	0.46
6:F:77:GLY:HA3	6:F:118:TRP:CZ2	2.63	0.46
21:1:837:CLA:HAB	21:1:838:CLA:HHD	1.97	0.46
2:2:361:GLN:N	2:2:361:GLN:OE1	2.49	0.46
3:3:22:PRO:HG2	3:3:23:LEU:HD12	1.97	0.46
21:6:201:CLA:H42	8:7:15:ILE:HA	1.97	0.46
1:A:568:LEU:HD21	3:C:53:ARG:NH2	2.73	0.46
21:A:801:CLA:CGD	21:A:801:CLA:HAA2	2.57	0.46
21:A:821:CLA:HMA2	21:A:825:CLA:C1C	34.13	0.46
21:A:854:CLA:HAB	2:B:579:TRP:CZ2	2.51	0.46
2:B:643:TRP:CZ2	2:B:723:ILE:HG21	2.57	0.46
21:B:818:CLA:O1A	21:B:828:CLA:HMD1	2.16	0.46
21:B:836:CLA:CMA	21:B:837:CLA:HED2	2.45	0.46
30:B:844:ECH:H36	30:B:844:ECH:H20	1.52	0.46
9:K:48:LYS:HB3	9:K:48:LYS:HE2	1.61	0.46
16:1:189:TRP:CD1	21:1:812:CLA:HED2	2.51	0.46
6:6:75:ILE:HG23	21:6:203:CLA:HAA1	1.97	0.46
1:A:70:ARG:HD3	1:A:184:ALA:HB1	2.35	0.46
1:A:340:LEU:HD21	21:A:824:CLA:HBC3	8.55	0.46
21:A:813:CLA:HMA2	21:A:813:CLA:C2	8.02	0.46
21:A:820:CLA:H112	21:A:820:CLA:H142	3.35	0.46
2:B:203:ARG:HG2	2:B:250:ALA:HB1	2.14	0.46
2:B:342:ILE:HD13	21:B:824:CLA:H42	1.98	0.46
2:B:426:PHE:O	2:B:430:HIS:ND1	2.47	0.46
21:B:805:CLA:H141	21:B:805:CLA:H162	1.65	0.46
3:C:29:VAL:HG21	4:D:114:ALA:HB2	2.46	0.46
21:L:205:CLA:H203	21:L:205:CLA:H162	1.68	0.46
16:1:437:ILE:HG13	16:1:555:TYR:HE2	1.80	0.45
21:1:835:CLA:H41	21:1:835:CLA:H61	1.56	0.45
21:2:803:CLA:H41	21:2:803:CLA:H61	1.38	0.45
1:A:434:ASP:OD1	1:A:555:TYR:OH	2.80	0.45
2:B:44:GLN:OE1	2:B:162:ARG:NH2	2.69	0.45
21:B:808:CLA:HMA1	21:B:809:CLA:HHB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:828:CLA:H41	21:B:828:CLA:H61	1.65	0.45
1:A:31:PRO:HB3	21:J:1101:CLA:HAC1	2.52	0.45
10:L:112:ASP:HB3	10:L:115:GLN:HB2	1.98	0.45
10:L:144:ASN:O	10:L:147:VAL:HG12	2.16	0.45
21:L:205:CLA:H93	21:L:205:CLA:H111	1.73	0.45
21:1:813:CLA:H142	21:1:813:CLA:H111	1.76	0.45
24:1:845:BCR:H362	24:1:846:BCR:HC8	1.98	0.45
1:A:512:GLU:N	1:A:512:GLU:OE1	2.71	0.45
1:A:59:ASP:HB2	1:A:414:ARG:NH1	2.37	0.45
21:A:802:CLA:CMA	21:A:802:CLA:H2	2.59	0.45
1:A:86:TRP:HE1	21:A:807:CLA:HBA1	1.80	0.45
1:A:296:HIS:HB2	21:A:817:CLA:CHB	2.47	0.45
21:A:835:CLA:H121	25:A:851:LHG:H382	6.69	0.45
21:A:836:CLA:HBB1	21:A:836:CLA:HHC	2.14	0.45
1:A:309:HIS:NE2	24:A:843:BCR:H17C	4.90	0.45
2:B:633:ASN:HB3	2:B:635:TYR:H	1.80	0.45
21:B:814:CLA:H72	21:B:814:CLA:H112	1.41	0.45
2:B:3:THR:H	7:I:37:GLU:HA	1.81	0.45
21:J:1105:CLA:HED2	21:J:1105:CLA:H2A	1.97	0.45
9:K:54:GLN:CD	9:K:54:GLN:H	4.19	0.45
21:1:836:CLA:H62	21:1:836:CLA:H41	1.52	0.45
16:1:689:GLY:HA3	2:2:565:CYS:HB2	1.98	0.45
21:2:834:CLA:CBB	24:6:202:BCR:HC21	2.46	0.45
1:A:588:TRP:NE1	21:A:830:CLA:HMD1	28.52	0.45
1:A:657:VAL:HG21	1:A:742:PHE:HA	1.98	0.45
21:A:837:CLA:HHC	21:A:837:CLA:HBB1	1.98	0.45
21:A:823:CLA:H92	24:A:846:BCR:C14	2.47	0.45
2:B:235:ALA:HB3	2:B:253:ALA:HB2	2.46	0.45
21:B:808:CLA:HMA1	21:B:809:CLA:CHB	2.46	0.45
4:D:104:PHE:HB3	4:D:106:GLU:OE1	2.16	0.45
21:1:827:CLA:CED	21:1:834:CLA:HAB	2.46	0.45
16:1:482:PHE:HB3	21:1:836:CLA:H42	1.99	0.45
2:2:167:TRP:CZ2	21:2:813:CLA:HMA1	2.51	0.45
2:2:513:ASP:OD2	2:2:594:LYS:NZ	2.39	0.45
2:2:717:THR:HG23	21:2:804:CLA:O1D	2.16	0.45
2:2:368:ALA:HB1	21:2:829:CLA:HMA1	1.99	0.45
25:2:851:LHG:H372	25:2:851:LHG:H342	1.70	0.45
1:A:106:ASP:O	1:A:110:ILE:HG22	2.16	0.45
2:B:440:VAL:HG21	21:J:1103:CLA:HAC2	2.16	0.45
2:B:495:LEU:HA	2:B:498:ILE:HG22	1.98	0.45
21:B:805:CLA:C4D	25:I:103:LHG:H321	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:840:CLA:H201	31:F:205:SQD:H241	1.98	0.45
21:A:804:CLA:H193	24:J:1102:BCR:H23C	24.62	0.45
2:2:687:LEU:HD11	20:0:39:ALA:HB1	1.98	0.45
16:1:638:SER:O	16:1:644:GLY:HA3	2.17	0.45
2:2:299:HIS:CE1	21:2:824:CLA:HMD1	2.52	0.45
2:2:367:ALA:HB1	2:2:722:LEU:HD11	1.98	0.45
2:2:276:HIS:HB2	21:2:819:CLA:C1B	2.47	0.45
21:2:805:CLA:H151	24:2:848:BCR:H16C	1.97	0.45
1:A:309:HIS:NE2	24:A:843:BCR:H363	2.32	0.45
2:B:460:TRP:O	2:B:464:THR:HG23	2.25	0.45
21:A:804:CLA:H172	24:J:1102:BCR:H272	20.27	0.45
7:I:12:TRP:HH2	21:L:205:CLA:H43	30.83	0.45
21:1:818:CLA:H3A	21:1:818:CLA:CGA	2.47	0.45
21:1:805:CLA:HED2	21:1:830:CLA:HBB2	1.98	0.45
1:A:268:TRP:CZ2	21:A:817:CLA:HBB1	10.63	0.45
1:A:573:PRO:HG2	5:E:50:SER:HB3	2.30	0.45
21:A:806:CLA:H161	21:A:806:CLA:H143	1.75	0.45
21:A:827:CLA:H111	21:A:827:CLA:H152	3.75	0.45
21:A:833:CLA:H162	21:A:833:CLA:H193	1.63	0.45
21:B:828:CLA:H3A	21:B:828:CLA:HBA2	1.33	0.45
2:B:385:PHE:CE2	24:B:845:BCR:H373	2.51	0.45
2:B:158:GLN:HB3	31:B:852:SQD:H5	1.99	0.45
31:F:205:SQD:H152	31:F:205:SQD:H121	1.61	0.45
20:0:153:ARG:HB2	20:0:155:LEU:HD13	1.98	0.45
21:0:203:CLA:H161	21:0:203:CLA:H141	1.64	0.45
2:2:460:TRP:O	2:2:464:THR:HG23	2.16	0.45
2:2:452:LEU:HB3	2:2:511:PRO:HG3	1.99	0.45
25:2:801:LHG:H301	25:2:801:LHG:H331	1.46	0.45
2:2:183:PHE:CE2	21:2:815:CLA:H72	2.52	0.45
3:3:62:PHE:CD2	17:4:122:ILE:HG21	2.51	0.45
1:A:189:TRP:CE2	21:A:809:CLA:HMA1	2.52	0.45
1:A:203:GLY:HA3	21:A:813:CLA:CBB	11.92	0.45
1:A:313:THR:OG1	1:A:314:ASN:N	2.56	0.45
1:A:514:ILE:HG22	1:A:521:ALA:HB3	2.43	0.45
1:A:412:MET:O	1:A:557:ARG:HD3	2.17	0.45
21:A:804:CLA:H203	21:A:804:CLA:H161	1.71	0.45
21:A:823:CLA:H41	21:A:835:CLA:H201	1.99	0.45
21:A:807:CLA:H11	21:A:827:CLA:HMD1	1.98	0.45
2:B:460:TRP:CH2	25:B:855:LHG:H352	2.52	0.45
21:B:807:CLA:H72	21:B:807:CLA:H111	1.60	0.45
21:B:810:CLA:H102	21:B:827:CLA:H192	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:1101:CLA:H112	21:J:1101:CLA:H152	1.50	0.45
21:A:802:CLA:H193	21:J:1101:CLA:H18	3.13	0.45
20:0:67:LEU:HG	21:0:203:CLA:HMA1	1.98	0.45
16:1:452:PHE:CZ	16:1:456:ILE:HD11	2.52	0.45
16:1:714:GLN:HG2	16:1:716:ARG:NH1	2.32	0.45
16:1:189:TRP:CZ2	21:1:810:CLA:HMA1	2.52	0.45
2:2:526:THR:O	2:2:530:ILE:HG13	2.17	0.45
21:2:805:CLA:H61	21:2:805:CLA:H41	1.74	0.45
22:2:843:PQN:H2M1	22:2:843:PQN:H111	1.83	0.45
16:1:433:ARG:NH1	17:4:45:GLY:HA3	2.32	0.45
11:9:18:PRO:HB2	24:9:102:BCR:H351	1.99	0.45
1:A:376:TYR:CE2	21:A:829:CLA:HED2	35.06	0.45
1:A:424:ASN:N	1:A:424:ASN:OD1	2.86	0.45
21:A:822:CLA:HED2	21:A:822:CLA:H2A	4.85	0.45
25:A:849:LHG:H142	25:A:849:LHG:H111	1.56	0.45
2:B:100:ALA:O	2:B:104:PHE:HD2	2.24	0.45
21:B:825:CLA:C1B	24:B:845:BCR:H363	2.47	0.45
21:B:825:CLA:CMA	24:B:845:BCR:H14C	2.46	0.45
21:I:101:CLA:HED2	10:L:65:TRP:NE1	2.32	0.45
10:L:82:LEU:O	10:L:86:LEU:HG	2.19	0.45
16:1:331:PRO:HB3	20:0:5:ASN:O	2.17	0.45
21:1:829:CLA:H41	21:1:829:CLA:H61	1.52	0.45
1:A:356:LEU:HD21	21:A:829:CLA:HAB	1.98	0.45
21:A:810:CLA:H51	21:A:812:CLA:H91	21.25	0.45
21:A:822:CLA:H92	21:A:822:CLA:H62	2.57	0.45
21:A:824:CLA:HMB1	21:A:824:CLA:HBB1	1.99	0.45
21:A:833:CLA:H112	24:A:847:BCR:H362	2.50	0.45
2:B:543:LEU:O	2:B:561:ARG:NH2	2.85	0.45
8:J:12:PRO:HA	8:J:15:ILE:HG22	2.15	0.45
9:K:28:LEU:HD22	26:K:105:LMG:H273	1.98	0.45
10:L:7:VAL:HG23	25:L:210:LHG:HC2	1.98	0.45
20:0:57:HIS:HA	20:0:60:PHE:CD2	2.52	0.45
16:1:159:TYR:O	16:1:163:ILE:HG12	2.16	0.45
21:1:839:CLA:HBC1	22:1:842:PQN:H191	1.99	0.45
21:2:821:CLA:HMD3	21:2:823:CLA:HAB	1.99	0.45
21:7:1101:CLA:H112	21:7:1101:CLA:H152	1.63	0.45
21:A:819:CLA:HBA2	21:A:819:CLA:H3A	1.79	0.45
21:A:826:CLA:H62	21:A:826:CLA:H93	4.51	0.45
21:A:836:CLA:H71	21:A:836:CLA:H112	1.73	0.45
21:A:839:CLA:H112	21:A:839:CLA:H152	1.81	0.45
25:B:851:LHG:H361	25:B:851:LHG:H332	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:1103:CLA:H91	21:J:1103:CLA:H111	1.71	0.45
21:L:203:CLA:CBA	24:L:207:BCR:H363	2.47	0.45
16:1:692:TYR:OH	21:1:802:CLA:OBD	2.19	0.44
21:1:818:CLA:H161	21:1:818:CLA:H203	1.76	0.44
21:1:819:CLA:H111	21:1:819:CLA:H72	1.76	0.44
2:2:504:SER:HA	2:2:507:LEU:HD21	1.98	0.44
21:2:804:CLA:H152	21:2:804:CLA:H112	1.69	0.44
10:L:32:THR:HG21	25:9:101:LHG:H102	48.90	0.44
1:A:118:TRP:HE1	24:A:848:BCR:HC41	1.81	0.44
21:A:838:CLA:H202	21:F:202:CLA:HED3	11.58	0.44
2:B:301:ILE:HG21	21:B:824:CLA:HAC1	1.99	0.44
21:B:808:CLA:H61	21:B:808:CLA:H93	1.75	0.44
21:B:819:CLA:HBA1	21:B:824:CLA:HAB	1.99	0.44
4:D:85:ILE:HB	4:D:98:HIS:HB3	2.02	0.44
6:F:36:ARG:HG3	8:J:35:ASP:HB3	1.98	0.44
21:K:103:CLA:H18	21:K:103:CLA:H152	1.47	0.44
20:0:17:VAL:O	20:0:19:HIS:N	2.50	0.44
21:0:201:CLA:HBB2	24:0:205:BCR:H321	1.99	0.44
16:1:601:SER:O	16:1:605:VAL:HG23	2.17	0.44
21:1:818:CLA:H92	21:1:818:CLA:H61	1.81	0.44
21:1:821:CLA:HMA2	21:1:825:CLA:C1C	2.47	0.44
2:2:372:HIS:O	2:2:376:ILE:HG12	2.17	0.44
21:2:830:CLA:H202	24:2:845:BCR:H352	1.99	0.44
24:A:848:BCR:H351	24:A:848:BCR:H15C	1.74	0.44
2:B:682:THR:OG1	21:B:802:CLA:HMA1	2.17	0.44
5:E:9:VAL:HB	5:E:66:LEU:HB3	2.22	0.44
9:K:22:VAL:HB	21:K:103:CLA:H203	2.00	0.44
1:A:11:LYS:HB3	9:K:48:LYS:NZ	2.44	0.44
21:I:101:CLA:H151	24:0:205:BCR:H362	2.00	0.44
16:1:427:ASP:O	16:1:431:ARG:HG3	2.17	0.44
21:1:801:CLA:H102	21:1:801:CLA:H62	1.81	0.44
21:1:855:CLA:H62	21:1:855:CLA:H41	1.37	0.44
2:2:199:ILE:HG12	2:2:270:LEU:HB3	1.99	0.44
21:2:824:CLA:HBA2	21:2:824:CLA:HBD	1.98	0.44
5:5:3:LEU:HD11	5:5:63:GLU:HG2	2.00	0.44
1:A:571:ARG:HH21	25:A:849:LHG:HC31	3.36	0.44
1:A:384:ALA:HA	1:A:747:SER:HB2	1.98	0.44
2:B:289:HIS:CE1	24:B:842:BCR:H363	2.52	0.44
2:B:435:TYR:CZ	2:B:515:LEU:HB3	2.53	0.44
21:B:810:CLA:H161	21:B:810:CLA:H202	1.84	0.44
21:B:812:CLA:H11	21:B:812:CLA:H51	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:838:CLA:HBB2	22:B:841:PQN:H141	1.99	0.44
26:B:850:LMG:H182	26:B:850:LMG:H211	1.80	0.44
1:A:315:TRP:CD1	9:K:64:PRO:HG3	2.52	0.44
21:1:828:CLA:O1D	21:1:829:CLA:HMA1	2.18	0.44
16:1:446:PHE:CE2	21:1:837:CLA:HBB1	2.52	0.44
2:2:618:ARG:NH1	2:2:619:ASP:OD1	2.50	0.44
21:1:801:CLA:HAA1	21:2:804:CLA:CBB	2.48	0.44
21:2:808:CLA:H162	21:2:808:CLA:H143	1.75	0.44
3:3:12:ILE:HD11	3:3:59:PRO:HG2	2.00	0.44
17:4:120:ARG:NH1	17:4:141:VAL:O	2.44	0.44
1:A:344:LEU:HB3	21:A:825:CLA:HBC3	24.40	0.44
1:A:433:ARG:HG2	1:A:434:ASP:N	2.32	0.44
21:A:805:CLA:HBA1	21:A:805:CLA:H3A	4.14	0.44
21:A:807:CLA:CAB	24:J:1102:BCR:H382	10.08	0.44
21:A:831:CLA:HBA2	21:A:831:CLA:H3A	2.88	0.44
1:A:350:ALA:HB1	24:A:846:BCR:H312	2.00	0.44
2:B:43:TYR:CE1	2:B:328:LEU:HD21	2.66	0.44
2:B:513:ASP:O	2:B:517:HIS:ND1	2.49	0.44
2:B:577:MET:HG3	2:B:707:LEU:HD21	2.19	0.44
4:D:13:GLY:HA2	10:L:15:PRO:O	2.29	0.44
4:D:30:ILE:HG21	4:D:68:LEU:HD23	2.27	0.44
21:J:1105:CLA:H72	21:J:1105:CLA:H111	1.76	0.44
21:J:1106:CLA:H122	21:J:1106:CLA:H162	1.46	0.44
8:J:31:ARG:HD3	24:J:1107:BCR:C31	2.39	0.44
16:1:369:HIS:HB3	21:1:818:CLA:HED2	1.99	0.44
17:4:101:ASP:OD2	17:4:112:ARG:NE	2.40	0.44
24:6:202:BCR:H10C	21:6:203:CLA:C2B	2.47	0.44
21:A:813:CLA:H161	21:A:813:CLA:H121	4.30	0.44
21:A:813:CLA:CHA	21:A:815:CLA:HMB3	2.47	0.44
21:A:830:CLA:H91	25:A:851:LHG:H301	2.00	0.44
2:B:321:TYR:O	2:B:325:ASN:HB2	2.37	0.44
2:B:521:ALA:O	2:B:525:HIS:ND1	2.31	0.44
21:B:805:CLA:H161	21:B:805:CLA:H193	1.71	0.44
21:B:815:CLA:H41	21:B:815:CLA:H62	1.65	0.44
2:B:341:VAL:HG21	21:B:826:CLA:H51	1.98	0.44
3:C:28:MET:HE1	23:C:102:SF4:S1	2.58	0.44
21:J:1103:CLA:H161	21:J:1103:CLA:H143	1.77	0.44
9:K:22:VAL:HG23	9:K:23:GLY:H	1.83	0.44
10:L:95:ALA:HB1	24:L:206:BCR:C19	2.52	0.44
16:1:647:ARG:NE	16:1:648:ASP:OD1	2.48	0.44
16:1:279:GLY:HA2	21:1:818:CLA:O1A	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:810:CLA:H62	21:2:810:CLA:H102	1.39	0.44
21:2:827:CLA:HBA2	21:2:827:CLA:H3A	1.68	0.44
21:2:827:CLA:HAA2	21:2:828:CLA:OBD	2.17	0.44
21:2:833:CLA:H3A	21:2:833:CLA:HBA2	1.60	0.44
21:2:835:CLA:HMB1	21:2:835:CLA:HBB1	2.00	0.44
21:2:808:CLA:HMC2	24:2:845:BCR:H401	2.00	0.44
1:A:292:ASP:HB3	21:A:818:CLA:HMA1	7.31	0.44
1:A:67:ASP:O	1:A:71:LYS:HG3	2.18	0.44
21:A:806:CLA:H62	21:A:808:CLA:H72	2.00	0.44
21:A:824:CLA:H61	21:A:824:CLA:H41	4.44	0.44
21:A:825:CLA:H111	21:A:825:CLA:H142	1.85	0.44
2:B:589:PHE:CE2	21:B:803:CLA:H61	2.51	0.44
21:B:806:CLA:H3A	21:B:806:CLA:HBA1	1.61	0.44
2:B:422:TRP:HZ3	21:B:837:CLA:HBC2	1.82	0.44
30:B:844:ECH:H8	30:B:844:ECH:H11	1.78	0.44
5:E:12:LYS:HB3	5:E:12:LYS:HE2	2.38	0.44
10:L:66:THR:HG21	10:L:142:LEU:HD13	1.98	0.44
21:I:101:CLA:H191	26:0:206:LMG:H442	1.98	0.44
20:0:58:GLY:HA2	20:0:89:ILE:HD11	2.00	0.44
2:2:258:LEU:HD11	2:2:269:TRP:CE2	2.53	0.44
2:2:642:VAL:HG22	21:2:811:CLA:HHD	1.99	0.44
21:2:808:CLA:CHB	21:2:808:CLA:H152	2.48	0.44
21:2:808:CLA:HBA1	21:2:831:CLA:HMB2	1.99	0.44
21:2:811:CLA:H142	26:2:850:LMG:H212	2.00	0.44
21:A:804:CLA:H111	21:A:804:CLA:H142	2.89	0.44
21:A:813:CLA:H61	21:A:813:CLA:H41	3.32	0.44
21:A:833:CLA:H13	21:A:833:CLA:H102	2.51	0.44
2:B:580:MET:SD	2:B:584:LEU:HD12	2.58	0.44
21:A:854:CLA:HMA2	2:B:613:LEU:HD13	1.99	0.44
21:B:818:CLA:H41	21:B:818:CLA:H62	1.67	0.44
21:B:826:CLA:H193	21:B:837:CLA:HMB2	1.99	0.44
9:K:47:GLY:HA3	9:K:64:PRO:HG2	2.00	0.44
10:L:44:LEU:HG	10:L:48:LEU:HD23	2.00	0.44
20:0:96:LEU:HG	24:0:204:BCR:H24C	2.00	0.44
21:1:808:CLA:H141	21:1:808:CLA:H162	1.64	0.44
2:2:682:THR:HB	21:2:802:CLA:HMA1	1.99	0.44
21:2:830:CLA:H92	24:2:845:BCR:H21C	2.00	0.44
6:6:32:SER:HA	6:6:35:ILE:HG22	2.00	0.44
35:L:211:LMT:H62	24:9:102:BCR:H292	43.67	0.44
21:A:840:CLA:H112	21:A:840:CLA:H72	1.68	0.44
21:A:854:CLA:HED2	21:B:803:CLA:H71	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TRP:HA	21:A:806:CLA:CBB	2.46	0.44
21:B:810:CLA:H142	26:B:848:LMG:H222	1.99	0.44
21:B:840:CLA:H62	21:B:840:CLA:H102	1.55	0.44
26:K:101:LMG:H382	26:K:101:LMG:H351	1.64	0.44
26:K:101:LMG:H111	26:K:101:LMG:HC8	1.63	0.44
25:I:104:LHG:H351	21:0:203:CLA:C1D	2.48	0.44
20:0:23:PRO:HB3	31:0:207:SQD:H441	1.98	0.44
16:1:296:HIS:CE1	16:1:300:ILE:HG13	2.53	0.44
16:1:362:LEU:HD11	21:1:819:CLA:H93	1.99	0.44
21:1:828:CLA:H41	21:1:828:CLA:H62	1.89	0.44
2:2:437:HIS:CE1	2:2:451:ILE:HG13	2.53	0.44
22:2:843:PQN:H241	22:2:843:PQN:H261	1.74	0.44
21:A:826:CLA:HBD	21:A:835:CLA:HMB3	6.86	0.44
1:A:482:PHE:CE2	21:A:836:CLA:H42	2.53	0.44
21:A:837:CLA:H101	24:A:847:BCR:H373	2.00	0.44
21:A:838:CLA:H111	21:A:838:CLA:H152	3.47	0.44
21:A:840:CLA:H162	21:A:840:CLA:H141	1.67	0.44
21:B:809:CLA:H142	21:B:809:CLA:HMB2	2.00	0.44
21:F:202:CLA:H161	21:F:202:CLA:H141	1.61	0.44
10:L:132:MET:HB3	24:0:205:BCR:H393	2.00	0.44
10:L:133:GLY:C	24:L:207:BCR:H23C	2.38	0.44
16:1:304:PHE:HE1	21:1:821:CLA:HAB	1.83	0.43
16:1:523:MET:HE1	16:1:627:VAL:HG21	2.00	0.43
21:2:808:CLA:H151	21:2:808:CLA:H111	1.65	0.43
2:2:85:ARG:HH12	2:2:727:ALA:HA	1.82	0.43
21:6:201:CLA:H41	8:7:18:LEU:HD23	1.98	0.43
1:A:25:PHE:HB2	8:J:1:MET:HG2	2.00	0.43
1:A:733:LEU:HD22	21:A:840:CLA:HMA1	2.00	0.43
21:A:804:CLA:H112	21:A:804:CLA:H72	3.25	0.43
21:A:827:CLA:H41	21:A:827:CLA:H62	1.60	0.43
2:B:420:LEU:HG	21:B:837:CLA:CBB	2.47	0.43
21:B:836:CLA:H43	21:B:837:CLA:HMD2	1.99	0.43
11:M:20:PHE:CZ	11:M:24:ARG:HD2	2.53	0.43
20:0:54:GLY:O	20:0:131:GLY:HA2	2.18	0.43
16:1:189:TRP:CE2	21:1:810:CLA:HMA1	2.53	0.43
16:1:189:TRP:CZ2	21:1:813:CLA:HAC2	2.53	0.43
21:1:813:CLA:HMB1	21:1:813:CLA:HBB1	2.01	0.43
2:2:194:LEU:HA	2:2:198:ALA:HB3	2.00	0.43
21:1:832:CLA:HAA1	28:2:854:45D:C38	2.48	0.43
1:A:199:HIS:CG	21:A:813:CLA:HMC2	19.26	0.43
1:A:369:HIS:ND1	21:A:818:CLA:OBD	15.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ALA:HA	1:A:521:ALA:H	2.20	0.43
21:A:820:CLA:HMA2	21:A:824:CLA:C1C	2.48	0.43
21:A:826:CLA:O1A	21:A:835:CLA:HMA1	10.76	0.43
21:B:810:CLA:H112	21:B:810:CLA:H151	1.64	0.43
21:B:804:CLA:H192	24:B:846:BCR:H353	1.99	0.43
2:B:85:ARG:HA	2:B:85:ARG:HD3	1.63	0.43
21:F:202:CLA:H112	21:F:202:CLA:H151	1.75	0.43
9:K:44:THR:HG22	9:K:61:PHE:HB3	5.07	0.43
9:K:63:LEU:N	9:K:64:PRO:HD2	2.91	0.43
25:L:210:LHG:H131	25:L:210:LHG:H302	2.01	0.43
20:O:112:ASP:OD1	20:O:112:ASP:N	2.50	0.43
21:1:807:CLA:C4D	24:1:849:BCR:H14C	2.47	0.43
21:1:809:CLA:HMA1	8:7:27:ILE:HD13	1.99	0.43
21:1:813:CLA:H3A	21:1:813:CLA:HBA1	1.61	0.43
21:1:828:CLA:H161	21:1:828:CLA:H202	1.72	0.43
16:1:485:TRP:HB2	26:1:853:LMG:O7	2.18	0.43
21:2:810:CLA:H161	21:2:810:CLA:H143	1.76	0.43
16:1:702:TRP:CH2	21:2:833:CLA:HED1	2.53	0.43
21:2:824:CLA:C2B	21:2:842:CLA:HMC2	2.48	0.43
3:3:7:ILE:HG12	3:3:40:ALA:HB3	2.00	0.43
22:1:842:PQN:H201	21:7:1101:CLA:H12	2.00	0.43
21:A:806:CLA:H62	21:A:806:CLA:H41	2.97	0.43
21:A:808:CLA:H8	21:A:808:CLA:H51	3.98	0.43
21:A:811:CLA:H172	26:K:101:LMG:H191	2.00	0.43
21:A:812:CLA:H142	21:A:812:CLA:H111	4.66	0.43
21:A:822:CLA:HBA1	21:A:822:CLA:CHA	2.55	0.43
21:A:823:CLA:H102	21:A:823:CLA:HMC2	8.87	0.43
21:A:805:CLA:H162	24:A:845:BCR:H362	19.64	0.43
2:B:464:THR:O	2:B:476:LEU:HB2	2.19	0.43
2:B:539:ARG:NH2	6:F:143:ARG:O	2.51	0.43
9:K:17:GLY:C	9:K:18:TRP:HD1	5.76	0.43
21:L:203:CLA:H92	21:L:203:CLA:H62	4.48	0.43
25:M:7003:LHG:HC81	25:M:7003:LHG:HC5	1.70	0.43
21:1:837:CLA:H91	21:O:202:CLA:H201	2.01	0.43
16:1:462:ARG:NH1	38:1:910:HOH:O	2.45	0.43
21:1:813:CLA:H203	24:1:846:BCR:C11	2.48	0.43
2:2:570:TRP:CD1	21:2:831:CLA:HMD1	2.53	0.43
2:2:338:SER:HA	21:2:828:CLA:H41	2.01	0.43
19:8:59:LYS:HB2	19:8:59:LYS:HE2	1.78	0.43
1:A:141:SER:HB2	21:A:828:CLA:HMA2	1.99	0.43
1:A:168:MET:O	1:A:172:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:VAL:HG13	6:F:84:ARG:HG3	2.10	0.43
1:A:80:LEU:HD23	1:A:80:LEU:HA	2.05	0.43
21:A:837:CLA:H143	21:A:837:CLA:H112	1.74	0.43
2:B:376:ILE:O	2:B:380:LEU:HG	2.17	0.43
21:B:818:CLA:H122	21:B:818:CLA:H162	1.67	0.43
21:B:819:CLA:H101	21:B:819:CLA:H171	1.99	0.43
21:B:825:CLA:C2B	24:B:845:BCR:H363	2.48	0.43
6:F:48:GLU:HG2	6:F:50:TYR:H	2.40	0.43
1:A:267:ASN:OD1	9:K:13:PRO:HG2	2.35	0.43
21:0:201:CLA:H3A	21:0:201:CLA:HBA2	1.48	0.43
16:1:587:GLY:O	16:1:591:VAL:HG23	2.18	0.43
17:4:2:THR:OG1	17:4:3:GLU:N	2.51	0.43
5:5:13:ARG:HB3	5:5:16:SER:HB2	1.99	0.43
1:A:42:PRO:HB3	1:A:47:TRP:CE3	2.57	0.43
1:A:549:LEU:O	1:A:553:VAL:HG23	2.56	0.43
21:A:803:CLA:H203	21:A:808:CLA:H92	2.00	0.43
2:B:516:VAL:HG21	2:B:590:TYR:HB2	2.00	0.43
21:B:809:CLA:CGA	21:B:809:CLA:C1A	2.97	0.43
25:B:855:LHG:H211	21:F:203:CLA:C1B	2.48	0.43
9:K:14:THR:O	9:K:15:THR:OG1	4.65	0.43
16:1:733:LEU:HA	25:1:850:LHG:H383	2.00	0.43
21:A:804:CLA:HMB1	21:A:804:CLA:HBB1	2.00	0.43
21:A:817:CLA:H202	21:A:817:CLA:H161	3.74	0.43
21:A:820:CLA:H121	21:A:820:CLA:H162	4.24	0.43
21:A:830:CLA:H52	21:A:830:CLA:H11	1.81	0.43
25:A:851:LHG:H302	25:A:851:LHG:H272	2.53	0.43
2:B:688:VAL:HG13	10:L:99:TYR:CE1	2.60	0.43
2:B:287:ALA:HB2	21:B:819:CLA:HBC2	2.01	0.43
21:B:809:CLA:HBA1	21:B:827:CLA:OBD	2.18	0.43
9:K:15:THR:O	9:K:17:GLY:N	2.52	0.43
21:A:830:CLA:H102	21:L:204:CLA:H151	1.99	0.43
16:1:441:ASN:O	16:1:445:ILE:HG13	2.19	0.43
21:1:809:CLA:HBA1	21:1:809:CLA:HBD	2.00	0.43
21:1:804:CLA:HMA2	21:1:811:CLA:HMD2	2.01	0.43
25:2:801:LHG:H182	25:2:801:LHG:H151	1.86	0.43
21:2:803:CLA:H112	21:2:803:CLA:H93	1.81	0.43
21:2:830:CLA:H3A	21:2:830:CLA:HBA2	1.37	0.43
3:3:5:VAL:HG11	3:3:26:LEU:HD21	2.01	0.43
21:A:808:CLA:HBA2	21:A:808:CLA:H3A	3.80	0.43
21:A:811:CLA:H51	21:A:819:CLA:H41	2.00	0.43
21:A:826:CLA:HAB	24:A:847:BCR:H311	24.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:850:LMG:HC5	37:L:209:DGD:HA32	1.99	0.43
2:B:236:ASP:OD1	2:B:252:THR:OG1	2.35	0.43
2:B:694:PRO:HB3	21:B:838:CLA:C1C	2.49	0.43
21:B:807:CLA:H41	21:B:807:CLA:H61	1.38	0.43
21:B:814:CLA:H202	21:B:814:CLA:H161	1.78	0.43
16:1:350:ALA:HB1	24:1:847:BCR:H312	2.00	0.43
16:1:478:LEU:HB2	16:1:529:THR:HG23	1.99	0.43
21:1:821:CLA:H72	24:1:848:BCR:H14C	2.00	0.43
2:2:659:MET:HA	21:2:805:CLA:C2C	2.49	0.43
21:6:201:CLA:H91	21:6:201:CLA:H112	1.87	0.43
1:A:391:THR:HG21	1:A:743:PHE:CE2	2.54	0.43
21:A:807:CLA:HBB1	21:A:808:CLA:O1A	2.18	0.43
21:A:820:CLA:HBA1	21:A:824:CLA:CAB	2.49	0.43
21:A:826:CLA:CED	21:A:833:CLA:HAB	2.49	0.43
21:A:819:CLA:H141	24:A:844:BCR:H383	2.00	0.43
25:A:849:LHG:H382	25:A:849:LHG:H352	1.78	0.43
21:A:855:CLA:H41	21:A:855:CLA:H61	2.85	0.43
21:B:821:CLA:HMD2	24:B:842:BCR:H24C	2.00	0.43
21:A:838:CLA:HMA2	21:B:831:CLA:HMB3	2.01	0.43
2:B:672:ILE:HG12	24:B:846:BCR:H282	2.00	0.43
3:C:59:PRO:HD2	23:C:102:SF4:S4	2.59	0.43
21:I:101:CLA:HBA1	20:0:151:ILE:HG23	2.00	0.43
21:1:811:CLA:H62	21:1:811:CLA:H41	1.70	0.43
21:1:835:CLA:H161	21:1:835:CLA:H141	1.75	0.43
24:1:858:BCR:H15C	24:1:858:BCR:H351	1.85	0.43
21:2:807:CLA:H3A	21:2:807:CLA:HBA1	1.54	0.43
5:5:17:TYR:CE2	5:5:45:ASN:HA	2.53	0.43
6:6:10:CYS:HB3	6:6:16:TYR:CD2	2.54	0.43
1:A:344:LEU:HD23	1:A:344:LEU:HA	2.12	0.43
1:A:575:ASP:OD2	1:A:579:ARG:NH2	2.78	0.43
1:A:24:SER:O	21:A:811:CLA:HMA1	35.80	0.43
21:A:812:CLA:H3A	21:A:812:CLA:HBA2	3.15	0.43
21:A:813:CLA:HMB2	24:A:844:BCR:H10C	2.01	0.43
21:A:817:CLA:H3A	21:A:817:CLA:HBA2	1.70	0.43
1:A:588:TRP:NE1	21:A:829:CLA:HMD1	2.33	0.43
21:A:835:CLA:H41	21:A:835:CLA:H61	2.23	0.43
21:B:816:CLA:H143	21:B:816:CLA:H161	1.74	0.43
6:F:90:ILE:CG2	6:F:99:GLN:HB2	2.49	0.43
9:K:25:ILE:CD1	26:K:105:LMG:H221	2.49	0.43
16:1:342:GLU:OE1	16:1:342:GLU:N	2.43	0.43
16:1:439:HIS:CD2	21:1:831:CLA:HMB1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:80:LEU:HD23	16:1:80:LEU:HA	1.73	0.43
2:2:376:ILE:O	2:2:380:LEU:HG	2.19	0.43
21:2:809:CLA:HMA1	21:2:810:CLA:C2B	2.49	0.43
3:3:62:PHE:CE2	17:4:122:ILE:HG21	2.54	0.43
1:A:2:THR:HB	1:A:3:ILE:H	2.14	0.43
1:A:429:MET:HE2	1:A:436:ILE:HD11	2.01	0.43
21:A:808:CLA:H91	21:A:808:CLA:H111	1.72	0.43
21:B:835:CLA:H91	21:B:835:CLA:H111	1.74	0.43
25:B:851:LHG:H171	25:B:851:LHG:H142	1.87	0.43
3:C:52:LYS:HD2	3:C:55:GLU:OE1	2.19	0.43
3:C:55:GLU:HB3	3:C:63:LEU:HD13	2.01	0.43
4:D:77:LYS:HG3	4:D:78:PRO:HD2	4.85	0.43
21:F:203:CLA:H62	21:F:203:CLA:H93	4.51	0.43
38:B:936:HOH:O	31:F:205:SQD:H382	2.18	0.43
7:I:10:LEU:HD12	7:I:10:LEU:HA	1.86	0.43
7:I:14:LEU:HA	7:I:14:LEU:HD12	1.91	0.43
7:I:22:PHE:HA	25:I:103:LHG:H211	2.01	0.43
6:F:39:ARG:NH1	8:J:34:PRO:O	2.47	0.43
10:L:38:PRO:HG3	21:L:204:CLA:HED2	2.72	0.43
10:L:44:LEU:HD12	10:L:44:LEU:HA	2.25	0.43
16:1:364:ILE:HG23	16:1:394:MET:SD	2.59	0.42
16:1:433:ARG:HG3	16:1:555:TYR:CZ	2.54	0.42
21:1:808:CLA:HBB1	21:1:808:CLA:HMB1	2.01	0.42
21:1:839:CLA:HMB2	21:2:834:CLA:H52	2.01	0.42
21:2:822:CLA:H61	21:2:822:CLA:H41	1.40	0.42
3:3:28:MET:HE1	23:3:102:SF4:S1	2.59	0.42
25:B:857:LHG:H202	21:8:1401:CLA:HBA1	2.00	0.42
1:A:381:ILE:HD11	1:A:519:LYS:O	2.19	0.42
1:A:381:ILE:HG23	1:A:519:LYS:HD2	4.68	0.42
21:A:804:CLA:HMA2	21:A:811:CLA:HMD2	19.37	0.42
1:A:355:ASN:HB3	21:A:825:CLA:O1A	21.50	0.42
21:A:824:CLA:HAB	21:A:831:CLA:HMD2	32.91	0.42
21:A:826:CLA:H42	21:A:836:CLA:HBA1	16.44	0.42
21:A:839:CLA:H11	21:J:1101:CLA:HMA1	12.19	0.42
25:B:858:LHG:H172	25:B:858:LHG:H141	1.88	0.42
1:A:709:VAL:HG22	6:F:84:ARG:HE	2.07	0.42
8:J:18:LEU:O	8:J:18:LEU:HD12	2.18	0.42
10:L:150:GLY:HA2	10:L:155:LEU:HB2	2.17	0.42
7:I:21:LEU:HD21	21:L:203:CLA:H42	37.41	0.42
37:L:209:DGD:HAW1	37:L:209:DGD:HB52	2.01	0.42
16:1:561:LEU:HD23	16:1:561:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:821:CLA:H202	24:1:847:BCR:H332	2.01	0.42
21:1:837:CLA:HAB	21:1:838:CLA:CHD	2.48	0.42
2:2:656:THR:O	2:2:659:MET:HB3	2.20	0.42
1:A:13:LYS:HG3	1:A:314:ASN:HD21	2.62	0.42
1:A:280:GLY:N	1:A:503:ALA:HB3	2.77	0.42
21:A:831:CLA:HHC	21:A:837:CLA:CBB	21.73	0.42
21:A:839:CLA:H141	21:A:839:CLA:H162	3.85	0.42
1:A:551:LYS:HE3	2:B:667:TYR:CE1	2.54	0.42
21:B:831:CLA:CAB	21:B:832:CLA:H202	2.48	0.42
21:B:836:CLA:H162	21:B:836:CLA:H202	1.68	0.42
26:A:850:LMG:H422	25:L:210:LHG:H191	26.93	0.42
21:0:201:CLA:H202	21:0:201:CLA:H161	1.77	0.42
21:1:827:CLA:HED1	21:1:834:CLA:HAB	2.00	0.42
2:2:158:GLN:O	2:2:162:ARG:HG3	2.19	0.42
2:2:179:LEU:HD21	21:2:821:CLA:C3B	2.49	0.42
21:2:821:CLA:HMA2	21:2:826:CLA:C1C	2.49	0.42
21:2:829:CLA:O1D	21:2:830:CLA:HMA1	2.19	0.42
21:2:841:CLA:H202	21:2:841:CLA:H161	1.80	0.42
17:4:85:ILE:HB	17:4:98:HIS:HB3	2.01	0.42
21:8:1402:CLA:HMB1	21:8:1402:CLA:HBB1	2.00	0.42
1:A:17:ASP:OD2	1:A:70:ARG:NH2	2.38	0.42
1:A:313:THR:OG1	21:A:819:CLA:HED2	2.18	0.42
1:A:679:PHE:CD2	21:A:801:CLA:HMA1	2.53	0.42
21:A:813:CLA:H193	21:A:813:CLA:H162	1.85	0.42
21:A:817:CLA:H92	21:A:817:CLA:H62	3.14	0.42
21:A:827:CLA:HBB1	21:A:833:CLA:HMA2	27.04	0.42
24:A:843:BCR:H272	9:K:72:PHE:CE2	4.75	0.42
2:B:163:PRO:HB2	2:B:168:PHE:CE2	2.54	0.42
2:B:557:ASP:OD2	2:B:561:ARG:NH2	2.60	0.42
2:B:681:ARG:HD2	10:L:19:HIS:CD2	2.65	0.42
26:0:206:LMG:H232	26:0:206:LMG:H262	1.77	0.42
21:1:826:CLA:H93	21:1:826:CLA:H62	1.72	0.42
2:2:280:ILE:HA	2:2:280:ILE:HD13	1.81	0.42
2:2:420:LEU:HA	2:2:423:VAL:HG22	2.01	0.42
16:1:658:ILE:HB	2:2:618:ARG:HB3	2.01	0.42
21:2:808:CLA:H61	21:2:808:CLA:H41	1.66	0.42
21:2:809:CLA:HMA1	21:2:810:CLA:C1B	2.50	0.42
1:A:226:LEU:HD12	1:A:236:ILE:HG23	2.31	0.42
21:A:801:CLA:HAA2	21:A:801:CLA:O2D	2.43	0.42
21:A:829:CLA:H102	21:A:829:CLA:H62	2.96	0.42
1:A:666:SER:HB2	2:B:443:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:ILE:HD13	6:F:53:LEU:HB2	2.01	0.42
21:B:816:CLA:H2A	21:B:816:CLA:HED2	2.01	0.42
21:B:822:CLA:H141	21:B:822:CLA:H161	1.68	0.42
3:C:17:CYS:HB2	3:C:54:CYS:HB2	4.47	0.42
3:C:63:LEU:HG	3:C:63:LEU:H	1.50	0.42
31:F:205:SQD:H462	31:F:205:SQD:H242	4.12	0.42
16:1:114:ALA:HB1	38:1:908:HOH:O	2.18	0.42
16:1:278:LYS:HD2	16:1:289:TRP:CG	2.54	0.42
21:1:801:CLA:H203	21:1:803:CLA:C1B	2.50	0.42
2:2:544:MET:HE2	2:2:547:LYS:HA	2.00	0.42
2:2:701:GLN:HG3	26:2:850:LMG:H122	2.01	0.42
25:2:801:LHG:O10	25:2:801:LHG:H271	2.20	0.42
21:2:806:CLA:O1A	11:9:30:TYR:HB2	2.19	0.42
21:2:809:CLA:HHB	21:2:810:CLA:HHB	2.02	0.42
21:2:826:CLA:H161	21:2:826:CLA:H141	1.76	0.42
1:A:110:ILE:HG12	1:A:130:VAL:O	2.20	0.42
1:A:48:ILE:HD12	21:A:839:CLA:HMB3	2.02	0.42
1:A:677:PHE:HB2	21:A:855:CLA:O1A	41.10	0.42
28:A:856:45D:H401	28:A:856:45D:H421	1.94	0.42
2:B:120:VAL:HG13	2:B:124:PHE:CE2	2.65	0.42
2:B:655:ALA:O	2:B:658:PHE:HB2	2.27	0.42
21:B:811:CLA:HMD2	31:B:852:SQD:H131	2.01	0.42
2:B:276:HIS:HB2	21:B:817:CLA:CHB	2.49	0.42
21:B:820:CLA:H141	21:B:820:CLA:H161	1.83	0.42
21:B:839:CLA:H112	21:B:839:CLA:H91	1.64	0.42
21:1:817:CLA:CHD	21:1:818:CLA:HBB2	2.50	0.42
21:1:825:CLA:H51	21:1:825:CLA:HBD	2.01	0.42
16:1:588:TRP:CD1	21:1:830:CLA:HMD1	2.53	0.42
16:1:89:GLY:HA3	21:1:807:CLA:HBB1	2.01	0.42
2:2:163:PRO:HB2	2:2:168:PHE:CE2	2.55	0.42
21:2:839:CLA:H43	24:2:847:BCR:H12C	2.00	0.42
1:A:215:HIS:CD2	1:A:219:VAL:HB	3.42	0.42
1:A:429:MET:SD	21:A:830:CLA:HBC3	2.59	0.42
1:A:584:GLN:HG2	1:A:724:ARG:NH1	2.60	0.42
21:A:804:CLA:H111	24:A:845:BCR:H372	2.01	0.42
1:A:74:SER:HB3	21:A:810:CLA:HHH	2.01	0.42
21:A:834:CLA:O1A	21:K:102:CLA:H51	2.19	0.42
22:A:841:PQN:H2M1	22:A:841:PQN:H111	1.85	0.42
21:B:807:CLA:H162	21:B:807:CLA:H143	1.88	0.42
21:B:808:CLA:HED2	7:I:11:PRO:HB3	2.00	0.42
21:J:1101:CLA:H61	21:J:1101:CLA:H41	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:1101:CLA:H8	21:J:1101:CLA:H52	1.84	0.42
9:K:53:PRO:CG	24:K:104:BCR:H282	2.47	0.42
21:1:828:CLA:H143	21:1:828:CLA:H111	1.79	0.42
2:2:448:GLU:H	2:2:448:GLU:CD	2.23	0.42
1:A:185:PRO:HG2	1:A:190:PHE:CZ	2.55	0.42
1:A:687:PHE:HB2	21:A:802:CLA:HBC2	2.02	0.42
1:A:598:MET:CG	21:A:826:CLA:HBC1	20.96	0.42
21:A:833:CLA:H111	21:A:833:CLA:H91	2.09	0.42
21:A:838:CLA:H162	21:A:838:CLA:H141	1.84	0.42
2:B:387:HIS:HA	2:B:390:ILE:HD12	2.35	0.42
21:A:838:CLA:HED2	2:B:418:SER:O	2.20	0.42
2:B:491:LEU:HD12	2:B:491:LEU:HA	1.99	0.42
3:C:66:ARG:HD3	3:C:66:ARG:HA	2.03	0.42
16:1:668:TYR:OH	16:1:744:LEU:HD23	2.20	0.42
16:1:199:HIS:CG	21:1:813:CLA:HMC2	2.55	0.42
21:1:815:CLA:HBB1	21:1:815:CLA:HMB1	2.02	0.42
2:2:379:PHE:HZ	2:2:711:THR:HG21	1.83	0.42
2:2:654:TRP:CE3	21:2:804:CLA:HMA1	2.54	0.42
11:9:23:PHE:CE1	25:9:101:LHG:H112	2.53	0.42
1:A:249:MET:O	1:A:253:TYR:N	2.45	0.42
1:A:392:HIS:HB2	21:A:828:CLA:CHB	6.59	0.42
1:A:720:ILE:O	1:A:724:ARG:HG3	2.78	0.42
1:A:77:PHE:HE1	21:A:810:CLA:HBB1	17.75	0.42
21:A:814:CLA:H62	21:A:814:CLA:H102	1.43	0.42
21:A:838:CLA:H61	21:A:838:CLA:H41	3.63	0.42
2:B:484:SER:HA	2:B:491:LEU:HD21	2.01	0.42
21:B:807:CLA:HMC3	21:B:828:CLA:HAB	2.02	0.42
21:B:835:CLA:H18	25:B:849:LHG:H312	2.01	0.42
1:A:269:GLY:N	9:K:13:PRO:HG3	2.29	0.42
21:0:203:CLA:H41	21:0:203:CLA:H62	1.43	0.42
16:1:447:LEU:HB3	16:1:540:PHE:HB2	2.01	0.42
21:1:804:CLA:H61	21:1:804:CLA:H2	1.76	0.42
21:2:807:CLA:H111	21:2:807:CLA:H142	1.76	0.42
21:2:816:CLA:CBB	21:2:830:CLA:H121	2.50	0.42
17:4:27:LYS:HD3	17:4:58:TYR:HB3	2.02	0.42
1:A:125:ILE:HG21	2:B:444:PHE:HA	2.21	0.42
1:A:487:GLN:O	1:A:491:THR:HG23	5.43	0.42
1:A:497:THR:OG1	21:A:833:CLA:HMD1	2.20	0.42
21:A:809:CLA:H12	21:A:811:CLA:C3D	2.50	0.42
1:A:274:PHE:HE1	21:A:815:CLA:HAC2	18.26	0.42
21:A:819:CLA:CAB	21:A:819:CLA:H62	8.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:825:CLA:HAB	24:A:847:BCR:H311	2.01	0.42
21:A:834:CLA:HMB1	24:A:847:BCR:H292	3.57	0.42
21:A:855:CLA:HMA2	2:B:613:LEU:HD13	50.70	0.42
2:B:180:ALA:HB1	21:B:820:CLA:HAC2	2.01	0.42
5:E:61:PHE:HB2	5:E:66:LEU:HD21	2.01	0.42
6:F:118:TRP:CG	6:F:119:PRO:HD3	2.55	0.42
9:K:12:SER:HA	9:K:13:PRO:HD3	2.41	0.42
9:K:22:VAL:O	9:K:26:MET:N	2.53	0.42
31:O:207:SQD:H301	31:O:207:SQD:H331	1.74	0.42
16:1:219:VAL:HG13	16:1:239:PRO:HB3	2.02	0.42
16:1:325:LEU:O	16:1:337:HIS:HB2	2.19	0.42
16:1:429:MET:HA	16:1:432:HIS:CE1	2.55	0.42
16:1:561:LEU:O	17:4:61:ARG:NH2	2.52	0.42
2:2:269:TRP:O	2:2:273:ILE:HG13	2.19	0.42
2:2:420:LEU:HG	21:2:839:CLA:CBB	2.50	0.42
21:2:805:CLA:H192	24:2:848:BCR:H353	2.02	0.42
1:A:121:VAL:HB	21:J:1103:CLA:HMD1	2.02	0.42
21:A:801:CLA:HBA2	21:A:801:CLA:H3A	1.70	0.42
21:A:831:CLA:H93	21:A:831:CLA:H112	1.86	0.42
21:A:837:CLA:C12	24:A:846:BCR:H23C	2.46	0.42
2:B:225:PHE:HB2	2:B:233:TYR:CE2	2.55	0.42
2:B:609:ASN:O	2:B:615:GLY:HA3	2.20	0.42
21:B:821:CLA:HBB1	21:B:821:CLA:HMB1	2.02	0.42
21:B:835:CLA:H112	21:B:835:CLA:H142	1.71	0.42
21:A:811:CLA:H93	21:J:1101:CLA:CBB	37.55	0.42
9:K:58:LYS:H	9:K:58:LYS:HD2	1.83	0.42
24:A:843:BCR:C23	9:K:72:PHE:HB2	2.49	0.42
21:L:204:CLA:H91	21:L:204:CLA:H112	2.34	0.42
21:1:804:CLA:HBD	21:1:811:CLA:H2	2.01	0.41
21:1:829:CLA:H62	21:1:829:CLA:H102	1.72	0.41
2:2:583:THR:O	2:2:587:LEU:HD13	2.20	0.41
21:2:813:CLA:H41	21:2:813:CLA:H61	1.67	0.41
2:2:291:TYR:CE1	21:2:821:CLA:HED1	2.55	0.41
17:4:33:THR:HA	17:4:53:GLY:O	2.20	0.41
8:7:10:THR:O	8:7:14:MET:HG2	2.20	0.41
1:A:431:ARG:HD2	4:D:13:GLY:O	2.20	0.41
1:A:459:ASP:OD1	1:A:641:THR:HB	2.19	0.41
21:A:839:CLA:H112	21:A:839:CLA:H142	4.10	0.41
2:B:580:MET:HG3	21:B:825:CLA:HBC1	2.02	0.41
2:B:654:TRP:HZ3	21:B:801:CLA:HMD1	1.84	0.41
21:B:826:CLA:HBB1	21:B:833:CLA:HMA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:836:CLA:H41	21:B:836:CLA:H62	1.61	0.41
21:B:830:CLA:HBC2	24:B:847:BCR:H383	2.01	0.41
21:J:1103:CLA:HBA2	21:J:1103:CLA:H3A	1.91	0.41
6:F:36:ARG:NH1	8:J:35:ASP:OD2	2.53	0.41
10:L:38:PRO:HG2	21:L:204:CLA:HED2	2.02	0.41
21:B:805:CLA:O1A	11:M:30:TYR:HB2	2.19	0.41
20:O:118:ASP:OD2	38:O:1101:HOH:O	2.22	0.41
16:1:510:GLY:HA2	16:1:524:PRO:HG3	2.01	0.41
2:2:422:TRP:CD1	21:2:834:CLA:HED2	2.55	0.41
26:2:852:LMG:HC92	26:2:852:LMG:H321	2.01	0.41
3:3:62:PHE:HZ	3:3:66:ARG:HH21	1.68	0.41
17:4:31:THR:O	17:4:83:TYR:HA	2.21	0.41
21:7:1101:CLA:HBA2	21:7:1101:CLA:CBD	2.45	0.41
1:A:340:LEU:HD12	1:A:343:ILE:HD11	4.08	0.41
1:A:530:ALA:O	1:A:534:VAL:HG23	5.29	0.41
21:A:808:CLA:H112	21:A:808:CLA:H151	1.70	0.41
1:A:718:LEU:HD11	21:A:840:CLA:HMD3	2.02	0.41
2:B:474:VAL:HG12	2:B:475:LEU:HG	2.02	0.41
2:B:498:ILE:HG13	2:B:505:LEU:HG	2.35	0.41
2:B:589:PHE:HE2	21:B:803:CLA:H61	1.86	0.41
21:B:830:CLA:H3A	21:B:830:CLA:HBA1	1.70	0.41
1:A:708:ASN:O	6:F:88:ILE:HD11	2.20	0.41
7:I:28:GLY:O	7:I:32:ILE:HG13	2.38	0.41
9:K:52:LEU:HB3	9:K:53:PRO:HD2	3.31	0.41
10:L:99:TYR:CZ	10:L:103:THR:HG21	2.55	0.41
16:1:115:GLN:HE22	21:1:809:CLA:HMD1	1.86	0.41
16:1:74:SER:HB2	21:1:811:CLA:HHD	2.01	0.41
21:1:809:CLA:HMB2	24:7:1102:BCR:H10C	2.01	0.41
21:2:803:CLA:HMB3	21:2:804:CLA:H18	2.02	0.41
1:A:381:ILE:HG13	1:A:519:LYS:HB2	2.01	0.41
21:A:811:CLA:H93	21:A:811:CLA:H61	1.70	0.41
21:A:816:CLA:H51	21:A:816:CLA:H11	1.90	0.41
21:A:855:CLA:H62	21:A:855:CLA:H41	1.46	0.41
31:B:852:SQD:H341	31:B:852:SQD:H371	1.92	0.41
21:1:802:CLA:HBA1	2:2:425:LEU:HD12	2.02	0.41
21:1:832:CLA:H101	21:1:832:CLA:H62	1.76	0.41
21:2:810:CLA:H92	24:2:848:BCR:H342	2.01	0.41
5:5:33:ILE:HG22	5:5:35:TYR:H	1.86	0.41
21:A:801:CLA:CBB	21:B:803:CLA:HAA1	2.51	0.41
1:A:304:PHE:CE1	21:A:820:CLA:HAB	2.55	0.41
21:A:825:CLA:O1A	21:A:835:CLA:HMA1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:828:CLA:O1D	21:A:829:CLA:HBB	25.63	0.41
21:A:832:CLA:H141	21:A:832:CLA:H162	3.49	0.41
21:A:835:CLA:H202	21:A:837:CLA:H92	2.02	0.41
1:A:86:TRP:CD1	21:A:806:CLA:HBC1	12.94	0.41
2:B:397:ASP:OD1	2:B:399:VAL:HG22	2.21	0.41
21:B:813:CLA:H92	21:B:813:CLA:H61	1.75	0.41
21:B:816:CLA:H162	21:B:816:CLA:H203	1.73	0.41
21:B:835:CLA:H201	25:B:849:LHG:H281	2.03	0.41
2:B:591:TRP:CD1	21:B:835:CLA:HBC2	2.55	0.41
7:I:22:PHE:CE1	7:I:26:THR:HG21	2.55	0.41
10:L:45:SER:O	10:L:49:ARG:HG3	2.28	0.41
20:0:38:PRO:HG3	20:0:52:GLU:CD	2.41	0.41
20:0:82:LEU:O	20:0:86:LEU:HG	2.20	0.41
16:1:395:TRP:HZ3	16:1:599:TYR:HA	1.85	0.41
21:1:835:CLA:H102	21:1:835:CLA:H41	2.03	0.41
17:4:105:PRO:HA	17:4:112:ARG:HH12	1.85	0.41
2:B:290:MET:HA	21:B:821:CLA:HHD	2.02	0.41
2:B:580:MET:HE1	2:B:581:LEU:HD23	3.73	0.41
4:D:40:PHE:HB3	4:D:76:PHE:HZ	2.18	0.41
5:E:43:ARG:NH1	38:E:108:HOH:O	2.53	0.41
6:F:96:PRO:O	6:F:100:GLU:HG3	2.83	0.41
21:I:101:CLA:HBB1	21:I:101:CLA:HHC	2.01	0.41
25:I:104:LHG:H262	35:0:208:LMT:H42	2.01	0.41
11:M:20:PHE:CE2	11:M:24:ARG:HD2	2.55	0.41
11:M:3:LEU:HA	11:M:3:LEU:HD12	1.85	0.41
16:1:289:TRP:HB2	16:1:292:ASP:OD2	2.21	0.41
21:2:809:CLA:H161	21:2:809:CLA:H143	1.79	0.41
21:2:832:CLA:CBB	25:2:851:LHG:H311	2.51	0.41
19:8:58:LYS:HG2	19:8:58:LYS:H	1.50	0.41
1:A:203:GLY:O	1:A:207:LEU:HB2	2.24	0.41
1:A:332:PHE:CD1	10:L:7:VAL:HG11	2.54	0.41
1:A:742:PHE:CD2	21:A:801:CLA:HMD1	2.73	0.41
1:A:680:ALA:HB3	21:A:802:CLA:HBB2	2.03	0.41
21:A:806:CLA:H112	21:A:806:CLA:H151	1.58	0.41
21:A:816:CLA:H142	21:A:816:CLA:H112	1.79	0.41
21:A:821:CLA:H62	21:A:821:CLA:H41	2.56	0.41
21:A:835:CLA:H111	21:A:835:CLA:H142	3.31	0.41
25:A:851:LHG:H291	25:A:851:LHG:H322	3.28	0.41
2:B:174:ARG:HE	21:B:824:CLA:HMD1	1.86	0.41
21:J:1103:CLA:H2A	21:J:1103:CLA:HED2	2.01	0.41
9:K:47:GLY:HA3	9:K:64:PRO:HG3	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:134:GLY:HA2	10:L:137:VAL:HG12	2.14	0.41
21:L:204:CLA:HMB3	21:L:205:CLA:HBC2	2.12	0.41
16:1:540:PHE:O	16:1:544:VAL:HG23	2.21	0.41
16:1:718:LEU:HD11	21:1:840:CLA:HMD3	2.02	0.41
16:1:80:LEU:HD13	21:1:813:CLA:H52	2.01	0.41
2:2:642:VAL:HG21	21:2:811:CLA:HMD2	2.03	0.41
21:6:201:CLA:H111	21:6:201:CLA:H152	1.57	0.41
21:2:803:CLA:H191	24:7:1102:BCR:H362	2.02	0.41
19:8:63:LEU:N	19:8:64:PRO:HD2	2.36	0.41
1:A:310:MET:HB3	1:A:310:MET:HE3	1.94	0.41
21:A:804:CLA:H3A	21:A:804:CLA:HBA1	1.52	0.41
1:A:83:VAL:HG12	21:A:805:CLA:H92	17.39	0.41
21:A:814:CLA:H41	21:A:814:CLA:H61	1.53	0.41
21:A:818:CLA:H3A	21:A:818:CLA:HBA2	3.77	0.41
1:A:740:TRP:CD1	21:A:828:CLA:HMB2	11.44	0.41
21:A:827:CLA:CED	21:A:833:CLA:HAB	30.53	0.41
21:A:835:CLA:H203	21:A:835:CLA:H162	4.32	0.41
24:A:843:BCR:H383	24:A:843:BCR:H23C	2.47	0.41
2:B:346:VAL:O	2:B:350:MET:HG3	2.23	0.41
2:B:289:HIS:NE2	24:B:842:BCR:H363	2.35	0.41
4:D:30:ILE:HA	4:D:84:LYS:O	2.20	0.41
4:D:77:LYS:H	4:D:77:LYS:HG2	3.48	0.41
6:F:110:LYS:HB3	6:F:110:LYS:HE2	1.89	0.41
21:A:810:CLA:H93	21:J:1101:CLA:CBB	2.51	0.41
1:A:315:TRP:NE1	9:K:48:LYS:HB2	2.36	0.41
16:1:364:ILE:HG13	16:1:397:GLY:HA3	2.03	0.41
16:1:381:ILE:HG23	16:1:519:LYS:HE3	2.02	0.41
16:1:565:LYS:HE2	16:1:585:VAL:HG13	2.03	0.41
16:1:520:VAL:HG12	16:1:619:GLY:O	2.21	0.41
21:1:828:CLA:H62	21:1:828:CLA:H93	1.87	0.41
21:1:825:CLA:CBB	24:1:847:BCR:H341	2.51	0.41
2:2:316:GLY:O	2:2:405:VAL:HG22	2.21	0.41
21:1:802:CLA:H11	2:2:429:PHE:N	2.35	0.41
16:1:698:GLU:CD	2:2:542:LYS:HB2	2.41	0.41
2:2:613:LEU:HD12	21:2:803:CLA:H11	2.03	0.41
16:1:676:HIS:HB3	21:2:803:CLA:HBD	2.01	0.41
21:A:801:CLA:H102	21:A:801:CLA:H62	1.68	0.41
21:A:802:CLA:H62	21:A:840:CLA:HMC3	2.02	0.41
21:A:802:CLA:H91	21:A:802:CLA:H111	1.67	0.41
21:A:806:CLA:O1A	21:A:808:CLA:HBA2	2.20	0.41
21:A:827:CLA:H151	21:A:833:CLA:H121	47.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:835:CLA:H141	21:A:835:CLA:H161	1.81	0.41
21:B:816:CLA:CGA	21:B:816:CLA:C1A	2.99	0.41
21:B:819:CLA:HAA2	21:B:823:CLA:OBD	2.21	0.41
21:B:829:CLA:H161	21:B:829:CLA:H193	1.81	0.41
21:B:807:CLA:HMC2	24:B:843:BCR:H401	2.03	0.41
3:C:15:THR:HA	3:C:28:MET:CE	2.49	0.41
6:F:99:GLN:HA	6:F:102:VAL:O	2.21	0.41
7:I:31:PHE:HB2	24:L:206:BCR:H14C	2.36	0.41
9:K:25:ILE:HD13	26:K:105:LMG:H221	2.02	0.41
16:1:514:ILE:HG22	16:1:521:ALA:HB3	2.02	0.41
21:1:805:CLA:H3A	21:1:805:CLA:HBA1	1.42	0.41
21:1:813:CLA:HMA2	21:1:813:CLA:C2	2.51	0.41
21:1:821:CLA:HMB3	21:1:825:CLA:HED2	2.02	0.41
21:2:807:CLA:H2	21:2:807:CLA:H61	1.82	0.41
2:2:123:TRP:CZ2	21:2:815:CLA:H201	2.56	0.41
2:2:388:GLY:HA2	24:2:847:BCR:H393	2.03	0.41
1:A:56:HIS:CE1	21:A:805:CLA:HBB2	17.14	0.41
1:A:694:GLN:O	1:A:698:GLU:HG3	2.20	0.41
21:A:821:CLA:H161	21:A:821:CLA:H121	1.89	0.41
21:A:825:CLA:H71	21:A:825:CLA:CAD	14.62	0.41
21:A:836:CLA:H193	21:A:836:CLA:H162	1.63	0.41
21:A:839:CLA:H61	21:A:839:CLA:H93	4.45	0.41
21:A:801:CLA:HMB3	21:A:854:CLA:HMD1	2.03	0.41
1:A:88:SER:HB3	1:A:165:GLY:HA3	2.03	0.41
2:B:305:LEU:O	2:B:317:HIS:HB2	2.55	0.41
1:A:703:ALA:HB2	2:B:418:SER:OG	2.21	0.41
21:B:804:CLA:H143	24:B:846:BCR:H362	2.01	0.41
21:B:837:CLA:H12	24:B:845:BCR:C14	2.50	0.41
21:B:840:CLA:H101	21:B:840:CLA:HED3	2.02	0.41
21:B:826:CLA:H121	24:B:847:BCR:C20	2.51	0.41
6:F:13:ASN:O	6:F:17:LEU:HG	2.33	0.41
9:K:67:LEU:HD12	9:K:67:LEU:HA	1.93	0.41
21:L:205:CLA:H3A	21:L:205:CLA:HBA1	1.63	0.41
16:1:100:TYR:OH	16:1:152:PHE:O	2.31	0.41
16:1:418:PRO:HG3	17:4:41:GLU:HB2	2.02	0.41
2:2:375:TYR:HA	2:2:584:LEU:CD1	2.51	0.41
16:1:583:CYS:HB2	2:2:664:TRP:HB3	2.03	0.41
2:2:182:LEU:HD11	21:2:815:CLA:H43	2.03	0.41
21:2:823:CLA:H162	21:2:823:CLA:H141	1.81	0.41
21:2:823:CLA:H161	21:2:823:CLA:H193	1.93	0.41
1:A:428:ARG:NH2	38:A:901:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:847:BCR:H281	24:A:847:BCR:H393	4.21	0.41
2:B:265:THR:HB	2:B:357:ALA:HA	2.03	0.41
2:B:642:VAL:HG21	21:B:809:CLA:HAC1	2.03	0.41
21:B:812:CLA:HBA2	21:B:812:CLA:H3A	1.41	0.41
6:F:36:ARG:HD2	6:F:40:TYR:CE2	2.99	0.41
6:F:90:ILE:HG23	6:F:99:GLN:HB2	2.03	0.41
21:A:840:CLA:H171	21:J:1101:CLA:H203	2.03	0.41
21:K:102:CLA:H161	21:K:102:CLA:H203	1.84	0.41
11:M:4:SER:O	11:M:8:ILE:HG12	2.21	0.41
21:O:203:CLA:H92	21:O:203:CLA:H61	1.87	0.41
24:I:102:BCR:H343	26:O:206:LMG:H273	2.02	0.41
16:1:120:ILE:O	16:1:122:GLY:N	2.54	0.41
16:1:680:ALA:HB2	21:2:803:CLA:C3D	2.51	0.41
16:1:718:LEU:HD22	16:1:722:GLN:NE2	2.36	0.41
25:B:858:LHG:H242	21:1:841:CLA:HBC2	2.02	0.41
2:2:605:GLN:OE1	2:2:619:ASP:HB3	2.21	0.41
16:1:702:TRP:HH2	21:2:833:CLA:HED1	1.86	0.41
26:2:852:LMG:H322	26:2:852:LMG:H352	1.78	0.41
16:1:704:HIS:NE2	21:6:201:CLA:HAC1	2.36	0.41
19:8:87:SER:HB2	21:8:1401:CLA:H2A	2.02	0.41
1:A:129:ASP:OD1	1:A:129:ASP:N	4.42	0.41
1:A:721:ILE:HG22	25:A:849:LHG:HC41	3.40	0.41
21:A:807:CLA:H162	21:A:807:CLA:H141	1.74	0.41
21:A:821:CLA:H8	21:A:821:CLA:H52	4.32	0.41
21:A:835:CLA:H142	21:A:835:CLA:H112	1.92	0.41
21:A:824:CLA:H141	25:A:851:LHG:H172	30.12	0.41
2:B:195:VAL:HG21	21:B:815:CLA:HBC2	2.03	0.41
21:B:823:CLA:H61	21:B:823:CLA:H92	1.84	0.41
21:B:831:CLA:HAB	21:B:832:CLA:H202	2.03	0.41
21:F:203:CLA:H203	21:F:203:CLA:H162	3.66	0.41
7:I:38:GLY:N	38:I:202:HOH:O	2.54	0.41
8:J:21:PHE:CZ	8:J:25:ILE:HD11	2.71	0.41
16:1:311:TYR:HA	16:1:319:HIS:H	1.85	0.40
16:1:358:LEU:HD12	21:1:827:CLA:H62	2.02	0.40
22:1:842:PQN:H262	22:1:842:PQN:H302	1.89	0.40
21:1:815:CLA:C3B	24:1:844:BCR:H333	2.52	0.40
16:1:91:TYR:CE2	24:1:845:BCR:HC42	2.56	0.40
2:2:115:ILE:O	21:2:810:CLA:HMD3	2.21	0.40
2:2:257:PHE:CE2	21:2:819:CLA:HBB1	2.56	0.40
21:2:820:CLA:H13	21:2:826:CLA:H172	2.03	0.40
21:6:203:CLA:C3B	8:7:22:THR:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:312:ARG:NH1	19:8:43:LYS:HE2	2.35	0.40
1:A:244:LEU:O	1:A:246:PRO:HD3	2.20	0.40
1:A:345:THR:HG23	1:A:346:THR:HG23	2.60	0.40
21:A:837:CLA:C1C	25:A:851:LHG:H162	2.51	0.40
26:A:850:LMG:H322	26:A:850:LMG:H291	2.42	0.40
2:B:426:PHE:HD1	2:B:430:HIS:CE1	2.39	0.40
21:B:828:CLA:ND	24:B:843:BCR:H282	2.36	0.40
25:B:849:LHG:H321	25:B:849:LHG:H351	1.63	0.40
25:I:103:LHG:H152	25:I:103:LHG:H181	1.79	0.40
9:K:59:LYS:HE2	9:K:63:LEU:HB2	3.27	0.40
16:1:278:LYS:HA	16:1:502:LEU:HD12	2.03	0.40
21:1:855:CLA:H111	21:1:855:CLA:H91	1.83	0.40
2:2:408:ARG:HA	2:2:411:GLU:HB2	2.04	0.40
24:2:849:BCR:H20C	24:2:849:BCR:H23C	1.90	0.40
5:5:4:ASN:N	5:5:7:ASP:OD2	2.36	0.40
21:7:1101:CLA:H141	21:7:1101:CLA:H162	1.88	0.40
11:9:13:VAL:HG23	38:9:201:HOH:O	2.22	0.40
21:A:811:CLA:H62	21:A:811:CLA:H41	2.51	0.40
21:A:819:CLA:H112	26:K:101:LMG:H441	2.03	0.40
21:A:820:CLA:H93	21:A:820:CLA:H62	3.84	0.40
21:A:829:CLA:H142	21:A:829:CLA:H111	1.84	0.40
21:A:830:CLA:H41	21:A:830:CLA:H61	2.87	0.40
21:A:825:CLA:H52	21:A:833:CLA:HBB2	2.03	0.40
21:B:812:CLA:H71	21:B:820:CLA:O1A	2.21	0.40
3:C:10:THR:HG23	4:D:121:ARG:HG2	2.03	0.40
16:1:392:HIS:O	16:1:396:ILE:HG12	2.21	0.40
16:1:80:LEU:HD11	21:1:813:CLA:H2	2.03	0.40
21:1:830:CLA:H142	21:1:830:CLA:H111	1.75	0.40
16:1:674:ALA:HB1	24:1:856:BCR:H351	2.04	0.40
2:2:277:HIS:HE1	21:2:820:CLA:ND	2.19	0.40
2:2:452:LEU:O	6:6:53:LEU:N	2.38	0.40
21:2:832:CLA:HBB2	21:2:839:CLA:HMC2	2.03	0.40
21:2:818:CLA:HAA2	26:2:852:LMG:H332	2.02	0.40
1:A:59:ASP:HB2	1:A:414:ARG:HH11	1.97	0.40
1:A:482:PHE:O	1:A:486:VAL:HG23	2.21	0.40
1:A:171:LEU:HD11	21:A:815:CLA:H143	2.02	0.40
21:A:828:CLA:H142	21:A:828:CLA:H111	4.43	0.40
21:A:828:CLA:O1D	21:A:829:CLA:HMA1	27.96	0.40
21:A:829:CLA:H61	21:A:829:CLA:H41	1.49	0.40
21:A:831:CLA:HBB2	21:A:837:CLA:CMC	21.46	0.40
2:B:211:ASN:O	2:B:215:THR:HG22	4.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:HIS:HD2	2:B:277:HIS:CE1	2.39	0.40
2:B:398:PRO:O	31:F:205:SQD:H381	3.99	0.40
21:B:810:CLA:H111	24:I:102:BCR:H341	2.02	0.40
25:B:858:LHG:HC2	20:O:5:ASN:HB3	2.04	0.40
3:C:11:CYS:SG	23:C:102:SF4:S2	3.14	0.40
5:E:13:ARG:NH2	5:E:59:ASN:HD21	3.84	0.40
21:F:203:CLA:H111	21:F:203:CLA:H143	3.38	0.40
16:1:360:GLY:HA2	16:1:397:GLY:HA2	2.03	0.40
16:1:371:TYR:CD1	16:1:609:PHE:HE1	2.40	0.40
16:1:76:HIS:ND1	21:1:813:CLA:OBD	2.41	0.40
21:2:805:CLA:HMA1	21:2:805:CLA:H43	2.03	0.40
1:A:392:HIS:HB2	21:A:827:CLA:C1B	2.51	0.40
1:A:479:GLN:O	26:A:850:LMG:H321	6.05	0.40
1:A:592:PHE:CE1	1:A:728:VAL:HB	2.89	0.40
1:A:66:GLU:HB2	1:A:187:LEU:HB2	2.59	0.40
21:A:821:CLA:H52	21:A:821:CLA:H11	1.83	0.40
21:A:821:CLA:H202	24:A:846:BCR:HC41	40.83	0.40
2:B:199:ILE:HG12	2:B:270:LEU:HB3	2.34	0.40
2:B:381:MET:HB3	2:B:381:MET:HE2	3.07	0.40
1:A:686:LEU:HB3	2:B:662:ILE:HG12	2.03	0.40
21:B:836:CLA:H121	21:B:836:CLA:HMC2	2.02	0.40
21:B:804:CLA:H112	24:B:846:BCR:H362	2.04	0.40
21:B:827:CLA:C19	26:B:848:LMG:H251	2.52	0.40
3:C:59:PRO:CD	23:C:102:SF4:S4	3.09	0.40
2:B:542:LYS:HZ3	6:F:139:PRO:HB2	3.25	0.40
21:F:202:CLA:H3A	21:F:202:CLA:HBA1	2.06	0.40
1:A:706:LYS:HZ1	31:F:205:SQD:H1	1.86	0.40
16:1:387:LEU:O	16:1:391:THR:HG23	2.20	0.40
16:1:682:SER:HB3	16:1:730:HIS:HB2	2.03	0.40
21:1:805:CLA:H203	21:1:805:CLA:H161	1.69	0.40
21:1:823:CLA:CHA	21:1:823:CLA:HBA1	2.52	0.40
21:1:823:CLA:H92	21:1:823:CLA:H61	1.84	0.40
21:1:840:CLA:O1A	25:1:850:LHG:H171	2.21	0.40
2:2:323:THR:OG1	2:2:401:ASN:OD1	2.27	0.40
21:2:808:CLA:H72	21:2:808:CLA:H111	1.62	0.40
17:4:27:LYS:HG2	17:4:28:TYR:H	1.85	0.40
21:7:1101:CLA:H61	21:7:1101:CLA:H92	1.84	0.40
1:A:26:GLU:HG3	38:A:948:HOH:O	2.22	0.40
1:A:254:PRO:HD2	1:A:273:ASP:OD2	3.00	0.40
1:A:300:ILE:HA	1:A:300:ILE:HD13	1.96	0.40
1:A:352:LEU:HD21	21:A:830:CLA:C2B	28.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:THR:OG1	5:E:53:ALA:O	2.40	0.40
21:A:825:CLA:H61	21:A:825:CLA:H93	1.85	0.40
1:A:368:GLN:HG3	21:A:825:CLA:HED2	2.03	0.40
1:A:388:SER:CB	21:A:827:CLA:HMA1	2.47	0.40
1:A:722:GLN:NE2	25:A:849:LHG:HC81	2.36	0.40
2:B:192:GLY:O	2:B:196:HIS:HB2	2.43	0.40
2:B:420:LEU:HB3	2:B:529:LEU:HD13	2.04	0.40
5:E:3:LEU:HD13	5:E:37:VAL:HG11	2.03	0.40
6:F:70:ILE:HD11	21:F:203:CLA:H51	2.02	0.40
6:F:4:PHE:CE2	6:F:54:ILE:HD13	4.81	0.40
21:L:203:CLA:H62	21:L:203:CLA:H102	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	749/751 (100%)	719 (96%)	28 (4%)	2 (0%)	44 66
1	a	749/751 (100%)	712 (95%)	31 (4%)	6 (1%)	22 39
2	2	729/731 (100%)	694 (95%)	33 (4%)	2 (0%)	44 66
2	B	729/731 (100%)	697 (96%)	28 (4%)	4 (0%)	32 53
3	3	78/80 (98%)	72 (92%)	5 (6%)	1 (1%)	14 25
3	C	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	6 9
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100 100
4	d	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	25 43
5	5	67/69 (97%)	59 (88%)	6 (9%)	2 (3%)	5 7
5	E	67/69 (97%)	61 (91%)	6 (9%)	0	100 100
6	6	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	25 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	141/143 (99%)	135 (96%)	5 (4%)	1 (1%)	25	43
6	f	141/143 (99%)	134 (95%)	7 (5%)	0	100	100
7	I	38/40 (95%)	36 (95%)	1 (3%)	1 (3%)	6	9
7	i	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
8	7	38/40 (95%)	38 (100%)	0	0	100	100
8	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	K	79/80 (99%)	66 (84%)	6 (8%)	7 (9%)	1	1
10	L	155/157 (99%)	148 (96%)	7 (4%)	0	100	100
10	l	155/157 (99%)	150 (97%)	3 (2%)	2 (1%)	14	25
11	9	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	b	727/729 (100%)	701 (96%)	22 (3%)	4 (1%)	28	48
13	c	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	14	25
14	e	66/68 (97%)	62 (94%)	3 (4%)	1 (2%)	12	21
15	k	76/78 (97%)	60 (79%)	7 (9%)	9 (12%)	0	0
16	1	742/744 (100%)	706 (95%)	34 (5%)	2 (0%)	44	66
17	4	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
18	h	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	8
19	8	77/79 (98%)	64 (83%)	9 (12%)	4 (5%)	2	2
20	0	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	43
All	All	6706/6771 (99%)	6374 (95%)	277 (4%)	55 (1%)	22	39

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE
9	K	16	ALA
9	K	52	LEU
13	c	62	PHE
15	k	13	PRO
15	k	18	TRP
19	8	53	PRO

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Mol	Chain	Res	Type
1	A	6	PRO
2	B	228	GLY
9	K	22	VAL
1	a	6	PRO
1	a	182	VAL
12	b	235	ALA
15	k	23	GLY
10	l	18	GLY
2	2	556	CYS
3	3	62	PHE
5	5	14	THR
5	5	53	ALA
19	8	18	TRP
1	A	574	CYS
7	I	38	GLY
9	K	86	SER
15	k	15	THR
15	k	56	ALA
2	2	311	PRO
20	0	18	GLY
2	B	3	THR
1	a	115	GLN
12	b	221	GLY
12	b	556	CYS
15	k	54	GLN
18	h	37	GLU
19	8	86	SER
2	B	211	ASN
2	B	227	THR
4	d	77	LYS
15	k	55	LEU
6	F	65	PHE
9	K	13	PRO
9	K	57	SER
1	a	232	ALA
15	k	16	ALA
10	l	111	GLY
6	6	94	LYS
9	K	53	PRO
1	a	121	VAL
15	k	53	PRO
16	1	121	VAL

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Mol	Chain	Res	Type
16	1	623	PRO
19	8	13	PRO
12	b	228	GLY
3	C	59	PRO
14	e	36	PRO
1	a	334	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/603 (100%)	585 (97%)	18 (3%)	46	74
1	a	603/603 (100%)	588 (98%)	15 (2%)	53	79
2	2	583/583 (100%)	564 (97%)	19 (3%)	43	70
2	B	583/583 (100%)	563 (97%)	20 (3%)	42	69
3	3	68/68 (100%)	67 (98%)	1 (2%)	70	89
3	C	68/68 (100%)	64 (94%)	4 (6%)	23	42
4	D	116/116 (100%)	111 (96%)	5 (4%)	33	58
4	d	116/116 (100%)	109 (94%)	7 (6%)	22	41
5	5	58/58 (100%)	54 (93%)	4 (7%)	18	34
5	E	58/58 (100%)	51 (88%)	7 (12%)	6	11
6	6	119/119 (100%)	115 (97%)	4 (3%)	42	69
6	F	119/119 (100%)	117 (98%)	2 (2%)	66	87
6	f	119/119 (100%)	117 (98%)	2 (2%)	66	87
7	I	32/32 (100%)	30 (94%)	2 (6%)	21	38
7	i	32/32 (100%)	30 (94%)	2 (6%)	21	38
8	7	35/35 (100%)	34 (97%)	1 (3%)	48	75
8	J	35/35 (100%)	33 (94%)	2 (6%)	24	44
8	j	35/35 (100%)	34 (97%)	1 (3%)	48	75
9	K	60/60 (100%)	46 (77%)	14 (23%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	118/118 (100%)	110 (93%)	8 (7%)	18	34
10	l	118/118 (100%)	111 (94%)	7 (6%)	23	42
11	9	25/25 (100%)	23 (92%)	2 (8%)	14	27
11	M	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
12	b	582/582 (100%)	559 (96%)	23 (4%)	36	62
13	c	69/69 (100%)	67 (97%)	2 (3%)	48	75
14	e	57/57 (100%)	52 (91%)	5 (9%)	12	22
15	k	57/58 (98%)	46 (81%)	11 (19%)	1	3
16	1	596/596 (100%)	577 (97%)	19 (3%)	44	71
17	4	115/115 (100%)	112 (97%)	3 (3%)	51	78
18	h	31/31 (100%)	28 (90%)	3 (10%)	9	18
19	8	58/59 (98%)	51 (88%)	7 (12%)	6	11
20	0	116/116 (100%)	113 (97%)	3 (3%)	51	78
All	All	5434/5436 (100%)	5211 (96%)	223 (4%)	35	61

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	13	LYS
1	A	62	THR
1	A	110	ILE
1	A	171	LEU
1	A	210	LEU
1	A	234	LYS
1	A	277	PHE
1	A	303	LEU
1	A	345	THR
1	A	371	TYR
1	A	381	ILE
1	A	433	ARG
1	A	520	VAL
1	A	561	LEU
1	A	583	CYS
1	A	621	VAL
1	A	624	ASP

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Mol	Chain	Res	Type
2	B	50	HIS
2	B	85	ARG
2	B	113	VAL
2	B	120	VAL
2	B	143	LEU
2	B	257	PHE
2	B	258	LEU
2	B	299	HIS
2	B	313	THR
2	B	441	VAL
2	B	476	LEU
2	B	491	LEU
2	B	543	LEU
2	B	567	ILE
2	B	573	PHE
2	B	574	TYR
2	B	596	LEU
2	B	628	LEU
2	B	637	VAL
2	B	729	LYS
3	C	17	CYS
3	C	23	LEU
3	C	63	LEU
3	C	66	ARG
4	D	18	LEU
4	D	97	LEU
4	D	107	LYS
4	D	108	VAL
4	D	118	LYS
5	E	4	ASN
5	E	30	LYS
5	E	33	ILE
5	E	42	ASP
5	E	64	ASN
5	E	66	LEU
5	E	68	LEU
6	F	12	GLU
6	F	101	VAL
7	I	10	LEU
7	I	14	LEU
8	J	18	LEU
8	J	19	LEU

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Mol	Chain	Res	Type
9	K	18	TRP
9	K	20	LEU
9	K	22	VAL
9	K	28	LEU
9	K	34	PHE
9	K	36	ILE
9	K	49	ASP
9	K	50	LEU
9	K	52	LEU
9	K	55	LEU
9	K	58	LYS
9	K	67	LEU
9	K	82	LEU
9	K	86	SER
10	L	1	MET
10	L	42	LYS
10	L	47	ILE
10	L	49	ARG
10	L	60	PHE
10	L	62	ILE
10	L	101	LEU
10	L	155	LEU
1	a	7	GLU
1	a	11	LYS
1	a	74	SER
1	a	129	ASP
1	a	277	PHE
1	a	303	LEU
1	a	319	HIS
1	a	333	THR
1	a	340	LEU
1	a	371	TYR
1	a	481	ILE
1	a	513	THR
1	a	561	LEU
1	a	624	ASP
1	a	709	VAL
12	b	85	ARG
12	b	113	VAL
12	b	115	ILE
12	b	120	VAL
12	b	133	GLN

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Mol	Chain	Res	Type
12	b	143	LEU
12	b	145	LEU
12	b	160	LYS
12	b	195	VAL
12	b	215	THR
12	b	257	PHE
12	b	258	LEU
12	b	330	PHE
12	b	351	TYR
12	b	406	LEU
12	b	533	LYS
12	b	567	ILE
12	b	573	PHE
12	b	574	TYR
12	b	580	MET
12	b	584	LEU
12	b	596	LEU
12	b	730	PHE
13	c	73	THR
13	c	74	THR
4	d	2	THR
4	d	38	GLN
4	d	52	GLU
4	d	77	LYS
4	d	107	LYS
4	d	108	VAL
4	d	118	LYS
14	e	33	ILE
14	e	43	ARG
14	e	58	THR
14	e	66	LEU
14	e	68	LEU
6	f	94	LYS
6	f	101	VAL
7	i	10	LEU
7	i	14	LEU
8	j	26	LEU
15	k	10	GLN
15	k	18	TRP
15	k	34	PHE
15	k	36	ILE
15	k	46	LYS

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Mol	Chain	Res	Type
15	k	54	GLN
15	k	58	LYS
15	k	65	GLU
15	k	74	HIS
15	k	80	MET
15	k	84	LEU
10	l	19	HIS
10	l	42	LYS
10	l	44	LEU
10	l	101	LEU
10	l	136	PHE
10	l	143	GLU
10	l	155	LEU
16	1	11	LYS
16	1	73	PHE
16	1	153	THR
16	1	251	GLU
16	1	252	LEU
16	1	260	LEU
16	1	273	ASP
16	1	277	PHE
16	1	303	LEU
16	1	319	HIS
16	1	340	LEU
16	1	371	TYR
16	1	459	ASP
16	1	513	THR
16	1	561	LEU
16	1	583	CYS
16	1	585	VAL
16	1	709	VAL
16	1	714	GLN
2	2	34	HIS
2	2	47	PHE
2	2	65	LEU
2	2	115	ILE
2	2	137	SER
2	2	143	LEU
2	2	145	LEU
2	2	215	THR
2	2	226	PHE
2	2	257	PHE

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Mol	Chain	Res	Type
2	2	330	PHE
2	2	405	VAL
2	2	453	ILE
2	2	482	ILE
2	2	533	LYS
2	2	567	ILE
2	2	573	PHE
2	2	574	TYR
2	2	596	LEU
3	3	63	LEU
17	4	106	GLU
17	4	108	VAL
17	4	118	LYS
5	5	3	LEU
5	5	30	LYS
5	5	63	GLU
5	5	69	VAL
6	6	31	ASN
6	6	48	GLU
6	6	123	VAL
6	6	127	THR
18	h	10	LEU
18	h	26	THR
18	h	35	GLU
8	7	39	HIS
19	8	22	VAL
19	8	34	PHE
19	8	36	ILE
19	8	46	LYS
19	8	59	LYS
19	8	60	THR
19	8	82	LEU
20	0	19	HIS
20	0	101	LEU
20	0	155	LEU
11	9	6	THR
11	9	9	LEU

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

Mol	Chain	Res	Type
2	B	276	HIS

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Mol	Chain	Res	Type
2	2	277	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 443 ligands modelled in this entry, 11 are monoatomic - leaving 432 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	CLA	0	201	20	56,73,73	1.16	6 (10%)	65,113,113	1.17	5 (7%)
21	CLA	0	202	28	56,73,73	1.19	6 (10%)	65,113,113	1.24	6 (9%)
21	CLA	0	203	38	56,73,73	1.17	6 (10%)	65,113,113	1.14	4 (6%)
24	BCR	0	204	-	41,41,41	0.65	0	56,56,56	3.08	11 (19%)
24	BCR	0	205	-	41,41,41	0.69	0	56,56,56	3.24	13 (23%)
26	LMG	0	206	-	55,55,55	1.13	6 (10%)	63,63,63	1.31	7 (11%)
31	SQD	0	207	-	53,54,54	0.80	0	63,65,65	1.02	3 (4%)
35	LMT	0	208	-	36,36,36	1.14	4 (11%)	47,47,47	1.23	3 (6%)
21	CLA	1	801	-	56,73,73	1.17	7 (12%)	65,113,113	1.22	6 (9%)
21	CLA	1	802	-	56,73,73	1.18	7 (12%)	65,113,113	1.25	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	1	803	38	56,73,73	1.18	5 (8%)	65,113,113	1.24	7 (10%)
21	CLA	1	804	-	46,63,73	1.24	6 (13%)	53,101,113	1.43	9 (16%)
21	CLA	1	805	-	56,73,73	1.15	6 (10%)	65,113,113	1.17	3 (4%)
21	CLA	1	806	-	56,73,73	1.16	7 (12%)	65,113,113	1.17	5 (7%)
21	CLA	1	807	-	41,58,73	1.41	7 (17%)	47,95,113	1.28	4 (8%)
21	CLA	1	808	16	56,73,73	1.16	5 (8%)	65,113,113	1.23	5 (7%)
21	CLA	1	809	-	42,59,73	1.33	6 (14%)	48,96,113	1.40	6 (12%)
21	CLA	1	810	-	37,54,73	1.45	6 (16%)	43,90,113	1.29	3 (6%)
21	CLA	1	811	16	56,73,73	1.19	6 (10%)	65,113,113	1.19	6 (9%)
21	CLA	1	812	-	41,58,73	1.37	7 (17%)	47,95,113	1.28	4 (8%)
21	CLA	1	813	-	56,73,73	1.14	7 (12%)	65,113,113	1.16	8 (12%)
21	CLA	1	814	-	41,58,73	1.39	7 (17%)	47,95,113	1.36	6 (12%)
21	CLA	1	815	-	35,52,73	1.47	6 (17%)	39,87,113	1.45	4 (10%)
21	CLA	1	816	-	33,53,73	1.49	7 (21%)	37,89,113	1.35	4 (10%)
21	CLA	1	817	-	56,73,73	1.18	6 (10%)	65,113,113	1.12	6 (9%)
21	CLA	1	818	-	56,73,73	1.18	6 (10%)	65,113,113	1.20	5 (7%)
21	CLA	1	819	-	56,73,73	1.15	5 (8%)	65,113,113	1.15	5 (7%)
21	CLA	1	820	-	56,73,73	1.17	6 (10%)	65,113,113	1.18	7 (10%)
21	CLA	1	821	38	56,73,73	1.16	5 (8%)	65,113,113	1.28	5 (7%)
21	CLA	1	822	-	56,73,73	1.16	7 (12%)	65,113,113	1.22	5 (7%)
21	CLA	1	823	-	46,63,73	1.28	6 (13%)	53,101,113	1.29	6 (11%)
21	CLA	1	824	-	51,68,73	1.22	7 (13%)	59,107,113	1.19	3 (5%)
21	CLA	1	825	-	56,73,73	1.16	5 (8%)	65,113,113	1.25	6 (9%)
21	CLA	1	826	-	47,64,73	1.27	6 (12%)	54,102,113	1.29	6 (11%)
21	CLA	1	827	-	56,73,73	1.19	7 (12%)	65,113,113	1.22	5 (7%)
21	CLA	1	828	-	56,73,73	1.20	6 (10%)	65,113,113	1.23	5 (7%)
21	CLA	1	829	-	56,73,73	1.19	7 (12%)	65,113,113	1.10	5 (7%)
21	CLA	1	830	-	56,73,73	1.14	4 (7%)	65,113,113	1.28	7 (10%)
21	CLA	1	831	-	41,58,73	1.31	6 (14%)	47,95,113	1.46	7 (14%)
21	CLA	1	832	-	56,73,73	1.18	6 (10%)	65,113,113	1.11	4 (6%)
21	CLA	1	833	-	56,73,73	1.15	5 (8%)	65,113,113	1.23	6 (9%)
21	CLA	1	834	-	56,73,73	1.22	7 (12%)	65,113,113	1.17	4 (6%)
21	CLA	1	835	16	56,73,73	1.19	7 (12%)	65,113,113	1.17	4 (6%)
21	CLA	1	836	-	43,60,73	1.33	5 (11%)	49,97,113	1.33	7 (14%)
21	CLA	1	837	-	56,73,73	1.17	5 (8%)	65,113,113	1.21	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	1	838	-	42,59,73	1.34	6 (14%)	48,96,113	1.31	5 (10%)
21	CLA	1	839	-	51,68,73	1.22	7 (13%)	59,107,113	1.21	5 (8%)
21	CLA	1	840	-	56,73,73	1.15	6 (10%)	65,113,113	1.22	7 (10%)
21	CLA	1	841	25	47,64,73	1.26	7 (14%)	54,102,113	1.36	6 (11%)
22	PQN	1	842	-	34,34,34	0.41	0	43,45,45	1.03	2 (4%)
23	SF4	1	843	2,16	0,12,12	0.00	-	0,24,24	0.00	-
24	BCR	1	844	-	41,41,41	0.68	0	56,56,56	3.24	9 (16%)
24	BCR	1	845	-	41,41,41	0.63	0	56,56,56	3.23	12 (21%)
24	BCR	1	846	-	41,41,41	0.67	0	56,56,56	3.23	11 (19%)
24	BCR	1	847	-	41,41,41	0.62	0	56,56,56	3.24	10 (17%)
24	BCR	1	848	-	41,41,41	0.60	0	56,56,56	3.16	11 (19%)
24	BCR	1	849	-	41,41,41	0.65	0	56,56,56	3.32	8 (14%)
25	LHG	1	850	-	48,48,48	0.38	0	49,54,54	1.10	3 (6%)
26	LMG	1	851	-	50,50,55	1.02	4 (8%)	58,58,63	1.08	2 (3%)
25	LHG	1	852	21	48,48,48	0.39	0	49,54,54	1.14	3 (6%)
26	LMG	1	853	-	55,55,55	1.12	6 (10%)	63,63,63	1.06	2 (3%)
35	LMT	1	854	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	3 (6%)
21	CLA	1	855	38	56,73,73	1.14	6 (10%)	65,113,113	1.23	5 (7%)
24	BCR	1	856	-	41,41,41	0.66	0	56,56,56	2.92	9 (16%)
24	BCR	1	858	-	41,41,41	0.69	0	56,56,56	3.27	15 (26%)
25	LHG	2	801	-	48,48,48	0.40	0	49,54,54	1.07	3 (6%)
21	CLA	2	802	-	46,63,73	1.26	7 (15%)	53,101,113	1.25	6 (11%)
21	CLA	2	803	38	56,73,73	1.18	7 (12%)	65,113,113	1.22	8 (12%)
21	CLA	2	804	-	56,73,73	1.16	6 (10%)	65,113,113	1.22	5 (7%)
21	CLA	2	805	-	56,73,73	1.17	6 (10%)	65,113,113	1.28	6 (9%)
21	CLA	2	806	-	56,73,73	1.17	6 (10%)	65,113,113	1.27	6 (9%)
21	CLA	2	807	-	56,73,73	1.16	6 (10%)	65,113,113	1.23	6 (9%)
21	CLA	2	808	-	56,73,73	1.18	7 (12%)	65,113,113	1.15	5 (7%)
21	CLA	2	809	-	56,73,73	1.19	6 (10%)	65,113,113	1.26	5 (7%)
21	CLA	2	810	-	56,73,73	1.19	5 (8%)	65,113,113	1.25	5 (7%)
21	CLA	2	811	2	56,73,73	1.15	7 (12%)	65,113,113	1.26	6 (9%)
21	CLA	2	812	-	47,64,73	1.26	7 (14%)	54,102,113	1.27	7 (12%)
21	CLA	2	813	-	51,68,73	1.26	6 (11%)	59,107,113	1.19	5 (8%)
21	CLA	2	814	-	33,53,73	1.51	7 (21%)	37,89,113	1.44	5 (13%)
21	CLA	2	815	-	56,73,73	1.17	7 (12%)	65,113,113	1.17	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	816	-	41,58,73	1.37	7 (17%)	47,95,113	1.37	5 (10%)
21	CLA	2	817	-	32,49,73	1.55	7 (21%)	37,84,113	1.52	5 (13%)
21	CLA	2	818	-	41,58,73	1.38	6 (14%)	47,95,113	1.40	4 (8%)
21	CLA	2	819	-	50,67,73	1.18	7 (14%)	57,105,113	1.25	8 (14%)
21	CLA	2	820	-	51,68,73	1.20	7 (13%)	59,107,113	1.26	7 (11%)
21	CLA	2	821	-	41,58,73	1.37	5 (12%)	47,95,113	1.34	4 (8%)
21	CLA	2	822	-	43,60,73	1.34	6 (13%)	49,97,113	1.25	5 (10%)
21	CLA	2	823	-	56,73,73	1.16	7 (12%)	65,113,113	1.22	8 (12%)
21	CLA	2	824	-	44,61,73	1.32	6 (13%)	50,98,113	1.39	8 (16%)
21	CLA	2	825	-	33,53,73	1.50	7 (21%)	37,89,113	1.39	5 (13%)
21	CLA	2	826	-	56,73,73	1.16	6 (10%)	65,113,113	1.26	7 (10%)
21	CLA	2	827	-	41,58,73	1.37	4 (9%)	47,95,113	1.39	6 (12%)
21	CLA	2	828	-	46,63,73	1.31	7 (15%)	53,101,113	1.23	5 (9%)
21	CLA	2	829	-	46,63,73	1.25	6 (13%)	53,101,113	1.25	6 (11%)
21	CLA	2	830	-	56,73,73	1.17	6 (10%)	65,113,113	1.12	4 (6%)
21	CLA	2	831	-	46,63,73	1.28	7 (15%)	53,101,113	1.25	6 (11%)
21	CLA	2	832	-	33,53,73	1.50	7 (21%)	37,89,113	1.32	4 (10%)
21	CLA	2	833	-	33,53,73	1.47	7 (21%)	37,89,113	1.50	4 (10%)
21	CLA	2	834	-	56,73,73	1.19	6 (10%)	65,113,113	1.15	5 (7%)
21	CLA	2	835	38	37,54,73	1.41	6 (16%)	43,90,113	1.32	5 (11%)
21	CLA	2	836	-	33,53,73	1.52	7 (21%)	37,89,113	1.30	4 (10%)
21	CLA	2	837	-	41,58,73	1.38	6 (14%)	47,95,113	1.30	7 (14%)
21	CLA	2	838	-	44,61,73	1.32	7 (15%)	50,98,113	1.22	4 (8%)
21	CLA	2	839	-	41,58,73	1.37	6 (14%)	47,95,113	1.22	6 (12%)
21	CLA	2	840	38	56,73,73	1.16	6 (10%)	65,113,113	1.19	6 (9%)
21	CLA	2	841	-	56,73,73	1.20	6 (10%)	65,113,113	1.16	7 (10%)
21	CLA	2	842	-	32,49,73	1.55	7 (21%)	37,84,113	1.44	6 (16%)
22	PQN	2	843	-	34,34,34	0.37	0	43,45,45	1.21	3 (6%)
24	BCR	2	844	-	41,41,41	0.66	0	56,56,56	3.24	10 (17%)
24	BCR	2	845	-	41,41,41	0.71	0	56,56,56	3.30	10 (17%)
30	ECH	2	846	-	42,42,42	0.79	1 (2%)	55,58,58	2.53	16 (29%)
24	BCR	2	847	-	41,41,41	0.72	0	56,56,56	3.60	14 (25%)
24	BCR	2	848	-	41,41,41	0.64	0	56,56,56	3.20	11 (19%)
24	BCR	2	849	-	41,41,41	0.74	0	56,56,56	3.22	19 (33%)
26	LMG	2	850	-	55,55,55	1.12	6 (10%)	63,63,63	1.10	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	2	851	-	48,48,48	0.39	0	49,54,54	1.06	3 (6%)
26	LMG	2	852	-	55,55,55	1.12	6 (10%)	63,63,63	1.09	2 (3%)
28	45D	2	854	21	43,43,43	3.45	16 (37%)	54,60,60	3.40	25 (46%)
34	C7Z	2	855	-	43,43,43	0.83	2 (4%)	56,60,60	1.63	10 (17%)
23	SF4	3	101	-	0,12,12	0.00	-	0,24,24	0.00	-
23	SF4	3	102	-	0,12,12	0.00	-	0,24,24	0.00	-
21	CLA	6	201	-	56,73,73	1.19	6 (10%)	65,113,113	1.19	4 (6%)
24	BCR	6	202	-	41,41,41	0.71	0	56,56,56	3.31	13 (23%)
21	CLA	6	203	38	38,55,73	1.40	6 (15%)	44,91,113	1.45	6 (13%)
21	CLA	6	204	6	34,51,73	1.48	6 (17%)	39,86,113	1.71	8 (20%)
24	BCR	6	205	-	41,41,41	0.68	0	56,56,56	3.40	13 (23%)
25	LHG	6	206	-	11,11,48	0.46	0	11,14,54	0.51	0
21	CLA	7	1101	-	56,73,73	1.19	7 (12%)	65,113,113	1.26	6 (9%)
24	BCR	7	1102	-	41,41,41	0.66	0	56,56,56	3.20	9 (16%)
21	CLA	7	1103	-	38,55,73	1.45	7 (18%)	44,91,113	1.48	7 (15%)
21	CLA	7	1104	8	32,49,73	1.56	7 (21%)	37,84,113	1.40	5 (13%)
21	CLA	7	1105	-	32,49,73	1.52	5 (15%)	37,84,113	1.46	5 (13%)
21	CLA	8	1401	-	33,53,73	1.50	6 (18%)	37,89,113	1.45	5 (13%)
21	CLA	8	1402	-	37,54,73	1.45	7 (18%)	43,90,113	1.29	5 (11%)
24	BCR	8	1403	-	41,41,41	0.64	0	56,56,56	3.20	10 (17%)
25	LHG	9	101	-	48,48,48	0.38	0	49,54,54	1.13	3 (6%)
24	BCR	9	102	-	41,41,41	0.65	0	56,56,56	3.23	17 (30%)
21	CLA	A	801	-	56,73,73	1.20	6 (10%)	65,113,113	1.69	13 (20%)
21	CLA	A	802	-	56,73,73	1.15	7 (12%)	65,113,113	1.30	10 (15%)
21	CLA	A	803	21	56,73,73	1.14	6 (10%)	65,113,113	1.27	7 (10%)
21	CLA	A	804	-	56,73,73	1.14	6 (10%)	65,113,113	1.19	6 (9%)
21	CLA	A	805	-	56,73,73	1.17	7 (12%)	65,113,113	1.16	8 (12%)
21	CLA	A	806	-	56,73,73	1.18	6 (10%)	65,113,113	1.15	5 (7%)
21	CLA	A	807	1	56,73,73	1.13	6 (10%)	65,113,113	1.22	6 (9%)
21	CLA	A	808	1	56,73,73	1.20	6 (10%)	65,113,113	1.18	7 (10%)
21	CLA	A	809	-	44,61,73	1.34	7 (15%)	50,98,113	1.23	4 (8%)
21	CLA	A	810	21	56,73,73	1.17	5 (8%)	65,113,113	1.21	6 (9%)
21	CLA	A	811	-	56,73,73	1.17	6 (10%)	65,113,113	1.13	3 (4%)
21	CLA	A	812	-	56,73,73	1.17	7 (12%)	65,113,113	1.15	5 (7%)
21	CLA	A	813	-	56,73,73	1.19	7 (12%)	65,113,113	1.21	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	814	-	56,73,73	1.17	5 (8%)	65,113,113	1.25	7 (10%)
21	CLA	A	815	38	56,73,73	1.19	6 (10%)	65,113,113	1.12	5 (7%)
21	CLA	A	816	-	56,73,73	1.18	6 (10%)	65,113,113	1.10	5 (7%)
21	CLA	A	817	-	56,73,73	1.16	6 (10%)	65,113,113	1.18	5 (7%)
21	CLA	A	818	-	56,73,73	1.18	6 (10%)	65,113,113	1.23	5 (7%)
21	CLA	A	819	-	56,73,73	1.16	7 (12%)	65,113,113	1.15	5 (7%)
21	CLA	A	820	38	56,73,73	1.10	5 (8%)	65,113,113	1.16	4 (6%)
21	CLA	A	821	-	56,73,73	1.15	4 (7%)	65,113,113	1.26	9 (13%)
21	CLA	A	822	-	56,73,73	1.20	5 (8%)	65,113,113	1.18	4 (6%)
21	CLA	A	823	-	51,68,73	1.20	6 (11%)	59,107,113	1.24	7 (11%)
21	CLA	A	824	38	56,73,73	1.19	6 (10%)	65,113,113	1.22	5 (7%)
21	CLA	A	825	38	56,73,73	1.14	5 (8%)	65,113,113	1.31	7 (10%)
21	CLA	A	826	-	56,73,73	1.15	5 (8%)	65,113,113	1.25	8 (12%)
21	CLA	A	827	-	56,73,73	1.19	5 (8%)	65,113,113	1.14	4 (6%)
21	CLA	A	828	-	56,73,73	1.16	6 (10%)	65,113,113	1.13	6 (9%)
21	CLA	A	829	-	56,73,73	1.17	4 (7%)	65,113,113	1.33	8 (12%)
21	CLA	A	830	-	49,66,73	1.21	4 (8%)	56,104,113	1.31	7 (12%)
21	CLA	A	831	-	56,73,73	1.18	6 (10%)	65,113,113	1.11	3 (4%)
21	CLA	A	832	-	56,73,73	1.17	5 (8%)	65,113,113	1.14	6 (9%)
21	CLA	A	833	-	56,73,73	1.17	5 (8%)	65,113,113	1.16	3 (4%)
21	CLA	A	834	1	56,73,73	1.18	6 (10%)	65,113,113	1.19	6 (9%)
21	CLA	A	835	-	56,73,73	1.12	5 (8%)	65,113,113	1.22	6 (9%)
21	CLA	A	836	-	56,73,73	1.23	6 (10%)	65,113,113	1.16	6 (9%)
21	CLA	A	837	-	56,73,73	1.16	7 (12%)	65,113,113	1.11	5 (7%)
21	CLA	A	838	-	56,73,73	1.16	7 (12%)	65,113,113	1.16	6 (9%)
21	CLA	A	839	38	56,73,73	1.19	7 (12%)	65,113,113	1.16	3 (4%)
21	CLA	A	840	-	56,73,73	1.16	7 (12%)	65,113,113	1.17	5 (7%)
22	PQN	A	841	-	34,34,34	0.39	0	43,45,45	1.17	3 (6%)
23	SF4	A	842	1,2	0,12,12	0.00	-	0,24,24	0.00	-
24	BCR	A	843	-	41,41,41	0.66	0	56,56,56	3.04	12 (21%)
24	BCR	A	844	-	41,41,41	0.64	0	56,56,56	3.13	17 (30%)
24	BCR	A	845	-	41,41,41	0.67	0	56,56,56	3.14	13 (23%)
24	BCR	A	846	-	41,41,41	0.61	0	56,56,56	2.88	13 (23%)
24	BCR	A	847	-	41,41,41	0.63	0	56,56,56	2.89	9 (16%)
24	BCR	A	848	-	41,41,41	0.69	0	56,56,56	3.57	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	A	849	-	48,48,48	0.40	0	49,54,54	1.16	3 (6%)
26	LMG	A	850	-	50,50,55	1.05	5 (10%)	58,58,63	1.19	4 (6%)
25	LHG	A	851	21	48,48,48	0.39	0	49,54,54	1.06	4 (8%)
26	LMG	A	852	-	48,48,55	0.96	4 (8%)	56,56,63	1.11	3 (5%)
27	ACT	A	853	-	1,3,3	7.71	1 (100%)	0,3,3	0.00	-
21	CLA	A	854	38	56,73,73	1.13	6 (10%)	65,113,113	1.29	7 (10%)
21	CLA	A	855	38	56,73,73	1.15	4 (7%)	65,113,113	1.22	6 (9%)
28	45D	A	856	-	43,43,43	3.38	15 (34%)	54,60,60	2.23	18 (33%)
21	CLA	B	801	38	56,73,73	1.20	6 (10%)	65,113,113	1.14	5 (7%)
21	CLA	B	802	-	51,68,73	1.21	6 (11%)	59,107,113	1.37	10 (16%)
21	CLA	B	803	-	56,73,73	1.20	7 (12%)	65,113,113	1.20	5 (7%)
21	CLA	B	804	-	56,73,73	1.18	7 (12%)	65,113,113	1.21	5 (7%)
21	CLA	B	805	-	56,73,73	1.15	7 (12%)	65,113,113	1.14	4 (6%)
21	CLA	B	806	-	56,73,73	1.16	5 (8%)	65,113,113	1.25	5 (7%)
21	CLA	B	807	-	56,73,73	1.21	6 (10%)	65,113,113	1.08	4 (6%)
21	CLA	B	808	-	56,73,73	1.18	6 (10%)	65,113,113	1.22	5 (7%)
21	CLA	B	809	-	56,73,73	1.15	5 (8%)	65,113,113	1.21	4 (6%)
21	CLA	B	810	2	56,73,73	1.17	7 (12%)	65,113,113	1.24	7 (10%)
21	CLA	B	811	-	56,73,73	1.15	5 (8%)	65,113,113	1.21	5 (7%)
21	CLA	B	812	-	56,73,73	1.19	6 (10%)	65,113,113	1.25	7 (10%)
21	CLA	B	813	-	56,73,73	1.16	7 (12%)	65,113,113	1.23	7 (10%)
21	CLA	B	814	-	56,73,73	1.16	7 (12%)	65,113,113	1.17	5 (7%)
21	CLA	B	815	-	46,63,73	1.31	7 (15%)	53,101,113	1.25	6 (11%)
21	CLA	B	816	-	56,73,73	1.13	7 (12%)	65,113,113	1.29	7 (10%)
21	CLA	B	817	-	56,73,73	1.14	6 (10%)	65,113,113	1.13	5 (7%)
21	CLA	B	818	-	56,73,73	1.15	7 (12%)	65,113,113	1.24	5 (7%)
21	CLA	B	819	38	56,73,73	1.17	7 (12%)	65,113,113	1.13	5 (7%)
21	CLA	B	820	-	56,73,73	1.19	7 (12%)	65,113,113	1.24	6 (9%)
21	CLA	B	821	-	56,73,73	1.16	7 (12%)	65,113,113	1.20	7 (10%)
21	CLA	B	822	-	56,73,73	1.17	6 (10%)	65,113,113	1.20	5 (7%)
21	CLA	B	823	-	48,65,73	1.25	6 (12%)	54,103,113	1.29	5 (9%)
21	CLA	B	824	-	56,73,73	1.14	6 (10%)	65,113,113	1.19	6 (9%)
21	CLA	B	825	38	46,63,73	1.27	6 (13%)	53,101,113	1.33	7 (13%)
21	CLA	B	826	-	56,73,73	1.18	7 (12%)	65,113,113	1.16	5 (7%)
21	CLA	B	827	-	56,73,73	1.16	6 (10%)	65,113,113	1.15	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	828	-	56,73,73	1.22	6 (10%)	65,113,113	1.10	4 (6%)
21	CLA	B	829	-	56,73,73	1.14	5 (8%)	65,113,113	1.27	5 (7%)
21	CLA	B	830	-	46,63,73	1.28	6 (13%)	53,101,113	1.22	4 (7%)
21	CLA	B	831	-	56,73,73	1.14	6 (10%)	65,113,113	1.21	5 (7%)
21	CLA	B	832	-	56,73,73	1.21	6 (10%)	65,113,113	1.14	4 (6%)
21	CLA	B	833	38	56,73,73	1.15	7 (12%)	65,113,113	1.22	6 (9%)
21	CLA	B	834	-	41,58,73	1.41	7 (17%)	47,95,113	1.28	4 (8%)
21	CLA	B	835	-	56,73,73	1.18	5 (8%)	65,113,113	1.18	6 (9%)
21	CLA	B	836	-	56,73,73	1.18	5 (8%)	65,113,113	1.19	4 (6%)
21	CLA	B	837	-	41,58,73	1.38	6 (14%)	47,95,113	1.19	4 (8%)
21	CLA	B	838	38	56,73,73	1.19	6 (10%)	65,113,113	1.08	4 (6%)
21	CLA	B	839	-	56,73,73	1.20	7 (12%)	65,113,113	1.18	6 (9%)
21	CLA	B	840	-	56,73,73	1.18	7 (12%)	65,113,113	1.21	7 (10%)
22	PQN	B	841	-	34,34,34	0.87	2 (5%)	43,45,45	1.23	3 (6%)
24	BCR	B	842	-	41,41,41	0.66	0	56,56,56	3.17	12 (21%)
24	BCR	B	843	-	41,41,41	0.66	0	56,56,56	3.19	9 (16%)
30	ECH	B	844	-	42,42,42	0.89	2 (4%)	55,58,58	2.51	15 (27%)
24	BCR	B	845	-	41,41,41	0.63	0	56,56,56	3.16	11 (19%)
24	BCR	B	846	-	41,41,41	0.63	0	56,56,56	3.24	12 (21%)
24	BCR	B	847	-	41,41,41	0.70	0	56,56,56	3.43	14 (25%)
26	LMG	B	848	-	55,55,55	1.12	6 (10%)	63,63,63	1.08	4 (6%)
25	LHG	B	849	-	48,48,48	0.37	0	49,54,54	1.16	3 (6%)
26	LMG	B	850	-	55,55,55	1.11	6 (10%)	63,63,63	1.10	3 (4%)
25	LHG	B	851	-	48,48,48	0.39	0	49,54,54	1.10	3 (6%)
31	SQD	B	852	-	53,54,54	0.80	0	63,65,65	1.03	3 (4%)
25	LHG	B	855	-	48,48,48	0.37	0	49,54,54	1.00	2 (4%)
34	C7Z	B	856	-	43,43,43	0.79	2 (4%)	56,60,60	1.61	8 (14%)
25	LHG	B	857	-	48,48,48	0.39	0	49,54,54	1.07	3 (6%)
25	LHG	B	858	-	48,48,48	0.39	0	49,54,54	1.06	3 (6%)
23	SF4	C	101	3	0,12,12	0.00	-	0,24,24	0.00	-
23	SF4	C	102	3	0,12,12	0.00	-	0,24,24	0.00	-
27	ACT	D	201	-	1,3,3	6.78	1 (100%)	0,3,3	0.00	-
24	BCR	F	201	-	41,41,41	0.69	0	56,56,56	3.12	12 (21%)
21	CLA	F	202	38	56,73,73	1.16	6 (10%)	65,113,113	1.12	5 (7%)
21	CLA	F	203	6	56,73,73	1.18	7 (12%)	65,113,113	1.17	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	C7Z	F	204	-	43,43,43	0.80	1 (2%)	56,60,60	1.84	13 (23%)
31	SQD	F	205	-	53,54,54	0.80	0	63,65,65	1.06	3 (4%)
21	CLA	I	101	-	56,73,73	1.18	7 (12%)	65,113,113	1.33	8 (12%)
24	BCR	I	102	-	41,41,41	0.58	0	56,56,56	3.08	14 (25%)
25	LHG	I	103	-	48,48,48	0.38	0	49,54,54	1.09	2 (4%)
25	LHG	I	104	-	48,48,48	0.39	0	49,54,54	1.07	3 (6%)
21	CLA	J	1101	-	56,73,73	1.13	5 (8%)	65,113,113	1.31	7 (10%)
24	BCR	J	1102	-	41,41,41	0.69	0	56,56,56	3.09	10 (17%)
21	CLA	J	1103	-	56,73,73	1.18	6 (10%)	65,113,113	1.17	4 (6%)
35	LMT	J	1104	-	36,36,36	1.16	5 (13%)	47,47,47	1.03	2 (4%)
21	CLA	J	1105	8	56,73,73	1.20	7 (12%)	65,113,113	1.23	6 (9%)
21	CLA	J	1106	-	56,73,73	1.18	7 (12%)	65,113,113	1.18	6 (9%)
24	BCR	J	1107	-	41,41,41	0.67	0	56,56,56	3.20	12 (21%)
26	LMG	K	101	-	55,55,55	1.12	6 (10%)	63,63,63	1.06	2 (3%)
21	CLA	K	102	38	56,73,73	1.18	5 (8%)	65,113,113	1.33	9 (13%)
21	CLA	K	103	-	56,73,73	1.15	6 (10%)	65,113,113	1.20	4 (6%)
24	BCR	K	104	-	41,41,41	0.56	0	56,56,56	3.15	16 (28%)
26	LMG	K	105	-	55,55,55	1.15	7 (12%)	63,63,63	1.30	5 (7%)
36	EQ3	L	201	-	43,43,43	4.05	25 (58%)	55,60,60	2.21	21 (38%)
21	CLA	L	203	10	56,73,73	1.17	6 (10%)	65,113,113	1.15	6 (9%)
21	CLA	L	204	-	56,73,73	1.13	6 (10%)	65,113,113	1.21	4 (6%)
21	CLA	L	205	38	56,73,73	1.19	6 (10%)	65,113,113	1.19	7 (10%)
24	BCR	L	206	-	41,41,41	0.67	0	56,56,56	2.84	15 (26%)
24	BCR	L	207	-	41,41,41	0.59	0	56,56,56	3.04	10 (17%)
31	SQD	L	208	-	50,51,54	0.81	0	60,62,65	1.08	4 (6%)
37	DGD	L	209	-	67,67,67	1.05	6 (8%)	81,81,81	1.04	2 (2%)
25	LHG	L	210	-	48,48,48	0.39	0	49,54,54	0.99	2 (4%)
35	LMT	L	211	-	36,36,36	1.15	5 (13%)	47,47,47	1.23	4 (8%)
27	ACT	M	7001	-	1,3,3	6.45	1 (100%)	0,3,3	0.00	-
30	ECH	M	7002	-	42,42,42	0.63	0	55,58,58	1.68	11 (20%)
25	LHG	M	7003	-	48,48,48	0.41	0	49,54,54	1.16	3 (6%)
21	CLA	a	801	-	56,73,73	1.20	6 (10%)	65,113,113	1.24	8 (12%)
21	CLA	a	802	-	56,73,73	1.15	7 (12%)	65,113,113	1.23	7 (10%)
21	CLA	a	803	-	56,73,73	1.13	5 (8%)	65,113,113	1.24	7 (10%)
21	CLA	a	804	-	56,73,73	1.16	7 (12%)	65,113,113	1.25	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	a	805	-	56,73,73	1.13	5 (8%)	65,113,113	1.16	6 (9%)
21	CLA	a	806	-	56,73,73	1.19	6 (10%)	65,113,113	1.16	6 (9%)
21	CLA	a	807	-	49,66,73	1.25	5 (10%)	56,104,113	1.24	5 (8%)
21	CLA	a	808	-	56,73,73	1.17	6 (10%)	65,113,113	1.19	5 (7%)
21	CLA	a	809	1	41,58,73	1.36	6 (14%)	47,95,113	1.37	7 (14%)
21	CLA	a	810	-	48,65,73	1.30	7 (14%)	54,103,113	1.26	6 (11%)
21	CLA	a	811	-	56,73,73	1.16	6 (10%)	65,113,113	1.26	5 (7%)
21	CLA	a	812	-	50,67,73	1.23	7 (14%)	57,105,113	1.21	4 (7%)
21	CLA	a	813	-	56,73,73	1.17	7 (12%)	65,113,113	1.10	6 (9%)
21	CLA	a	814	-	56,73,73	1.18	7 (12%)	65,113,113	1.23	6 (9%)
21	CLA	a	815	-	41,58,73	1.38	7 (17%)	47,95,113	1.35	7 (14%)
21	CLA	a	816	-	43,60,73	1.33	7 (16%)	49,97,113	1.36	7 (14%)
21	CLA	a	817	-	56,73,73	1.19	6 (10%)	65,113,113	1.14	6 (9%)
21	CLA	a	818	-	51,68,73	1.22	7 (13%)	59,107,113	1.26	4 (6%)
21	CLA	a	819	-	56,73,73	1.16	7 (12%)	65,113,113	1.19	4 (6%)
21	CLA	a	820	-	56,73,73	1.16	5 (8%)	65,113,113	1.17	6 (9%)
21	CLA	a	821	-	56,73,73	1.14	6 (10%)	65,113,113	1.19	6 (9%)
21	CLA	a	822	-	46,63,73	1.28	6 (13%)	53,101,113	1.28	5 (9%)
21	CLA	a	823	-	56,73,73	1.15	7 (12%)	65,113,113	1.20	7 (10%)
21	CLA	a	824	-	56,73,73	1.17	7 (12%)	65,113,113	1.18	5 (7%)
21	CLA	a	825	1	56,73,73	1.15	7 (12%)	65,113,113	1.23	4 (6%)
21	CLA	a	826	-	46,63,73	1.28	7 (15%)	53,101,113	1.28	5 (9%)
21	CLA	a	827	-	56,73,73	1.18	7 (12%)	65,113,113	1.25	7 (10%)
21	CLA	a	828	-	56,73,73	1.19	6 (10%)	65,113,113	1.24	5 (7%)
21	CLA	a	829	-	56,73,73	1.17	7 (12%)	65,113,113	1.18	5 (7%)
21	CLA	a	830	-	56,73,73	1.15	6 (10%)	65,113,113	1.34	7 (10%)
21	CLA	a	831	-	43,60,73	1.30	6 (13%)	49,97,113	1.33	7 (14%)
21	CLA	a	832	-	56,73,73	1.20	7 (12%)	65,113,113	1.07	4 (6%)
21	CLA	a	833	-	56,73,73	1.17	6 (10%)	65,113,113	1.17	6 (9%)
21	CLA	a	834	1	40,57,73	1.36	7 (17%)	46,93,113	1.54	7 (15%)
21	CLA	a	835	-	56,73,73	1.16	6 (10%)	65,113,113	1.13	5 (7%)
21	CLA	a	836	-	56,73,73	1.19	7 (12%)	65,113,113	1.41	7 (10%)
21	CLA	a	837	-	41,58,73	1.37	7 (17%)	47,95,113	1.30	5 (10%)
21	CLA	a	838	38	56,73,73	1.16	7 (12%)	65,113,113	1.21	5 (7%)
21	CLA	a	839	-	56,73,73	1.18	6 (10%)	65,113,113	1.21	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	a	840	25	46,63,73	1.30	7 (15%)	53,101,113	1.24	5 (9%)
22	PQN	a	841	-	34,34,34	0.45	0	43,45,45	0.96	2 (4%)
23	SF4	a	842	1,12	0,12,12	0.00	-	0,24,24	0.00	-
24	BCR	a	843	-	41,41,41	0.68	0	56,56,56	3.41	14 (25%)
24	BCR	a	844	-	41,41,41	0.63	0	56,56,56	3.49	13 (23%)
24	BCR	a	845	-	41,41,41	0.71	0	56,56,56	3.29	11 (19%)
24	BCR	a	846	-	41,41,41	0.63	0	56,56,56	3.08	11 (19%)
24	BCR	a	847	-	41,41,41	0.63	0	56,56,56	3.25	12 (21%)
24	BCR	a	848	-	41,41,41	0.69	0	56,56,56	3.45	13 (23%)
25	LHG	a	849	-	48,48,48	0.40	0	49,54,54	1.15	3 (6%)
26	LMG	a	850	-	50,50,55	1.03	4 (8%)	58,58,63	1.10	2 (3%)
25	LHG	a	851	21	48,48,48	0.39	0	49,54,54	1.09	3 (6%)
26	LMG	a	852	-	55,55,55	1.13	7 (12%)	63,63,63	1.23	4 (6%)
25	LHG	a	853	-	48,48,48	0.38	0	49,54,54	1.15	3 (6%)
27	ACT	a	854	-	1,3,3	6.43	1 (100%)	0,3,3	0.00	-
21	CLA	a	855	38	56,73,73	1.13	7 (12%)	65,113,113	1.24	9 (13%)
21	CLA	a	856	38	56,73,73	1.14	6 (10%)	65,113,113	1.28	8 (12%)
30	ECH	a	857	-	42,42,42	0.81	1 (2%)	55,58,58	2.43	16 (29%)
24	BCR	a	859	-	41,41,41	0.72	0	56,56,56	3.23	13 (23%)
21	CLA	b	1801	25	56,73,73	1.14	6 (10%)	65,113,113	1.29	5 (7%)
25	LHG	b	1802	-	48,48,48	0.40	0	49,54,54	1.14	4 (8%)
25	LHG	b	1803	-	48,48,48	0.40	0	49,54,54	1.15	3 (6%)
21	CLA	b	1804	-	56,73,73	1.19	7 (12%)	65,113,113	1.10	4 (6%)
21	CLA	b	1805	-	56,73,73	1.20	7 (12%)	65,113,113	1.18	4 (6%)
21	CLA	b	1806	-	56,73,73	1.19	5 (8%)	65,113,113	1.17	5 (7%)
21	CLA	b	1807	-	56,73,73	1.20	6 (10%)	65,113,113	1.23	9 (13%)
21	CLA	b	1808	-	56,73,73	1.18	5 (8%)	65,113,113	1.26	6 (9%)
21	CLA	b	1809	-	56,73,73	1.18	7 (12%)	65,113,113	1.13	6 (9%)
21	CLA	b	1810	-	56,73,73	1.18	6 (10%)	65,113,113	1.18	5 (7%)
21	CLA	b	1811	-	56,73,73	1.13	6 (10%)	65,113,113	1.22	4 (6%)
21	CLA	b	1812	12	56,73,73	1.17	7 (12%)	65,113,113	1.22	7 (10%)
21	CLA	b	1813	-	56,73,73	1.17	7 (12%)	65,113,113	1.18	5 (7%)
21	CLA	b	1814	-	51,68,73	1.24	6 (11%)	59,107,113	1.14	5 (8%)
21	CLA	b	1815	-	56,73,73	1.17	6 (10%)	65,113,113	1.32	7 (10%)
21	CLA	b	1816	-	56,73,73	1.16	6 (10%)	65,113,113	1.18	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	b	1817	-	56,73,73	1.18	5 (8%)	65,113,113	1.12	3 (4%)
21	CLA	b	1818	-	56,73,73	1.17	7 (12%)	65,113,113	1.17	5 (7%)
21	CLA	b	1819	-	56,73,73	1.17	7 (12%)	65,113,113	1.24	6 (9%)
21	CLA	b	1820	-	56,73,73	1.16	6 (10%)	65,113,113	1.17	5 (7%)
21	CLA	b	1821	-	56,73,73	1.13	6 (10%)	65,113,113	1.24	6 (9%)
21	CLA	b	1822	38	56,73,73	1.16	7 (12%)	65,113,113	1.15	3 (4%)
21	CLA	b	1823	-	42,59,73	1.36	7 (16%)	48,96,113	1.31	5 (10%)
21	CLA	b	1824	-	56,73,73	1.15	5 (8%)	65,113,113	1.17	7 (10%)
21	CLA	b	1825	-	51,68,73	1.23	6 (11%)	59,107,113	1.24	5 (8%)
21	CLA	b	1826	-	56,73,73	1.18	7 (12%)	65,113,113	1.17	5 (7%)
21	CLA	b	1827	38	56,73,73	1.16	5 (8%)	65,113,113	1.34	7 (10%)
21	CLA	b	1828	38	56,73,73	1.14	5 (8%)	65,113,113	1.25	7 (10%)
21	CLA	b	1829	-	56,73,73	1.13	6 (10%)	65,113,113	1.21	6 (9%)
21	CLA	b	1830	-	56,73,73	1.15	6 (10%)	65,113,113	1.17	5 (7%)
21	CLA	b	1831	-	56,73,73	1.13	5 (8%)	65,113,113	1.10	6 (9%)
21	CLA	b	1832	-	56,73,73	1.16	6 (10%)	65,113,113	1.24	7 (10%)
21	CLA	b	1833	-	56,73,73	1.15	6 (10%)	65,113,113	1.17	5 (7%)
21	CLA	b	1834	-	56,73,73	1.18	7 (12%)	65,113,113	1.08	5 (7%)
21	CLA	b	1835	-	56,73,73	1.19	6 (10%)	65,113,113	1.18	6 (9%)
21	CLA	b	1836	38	56,73,73	1.18	7 (12%)	65,113,113	1.23	5 (7%)
21	CLA	b	1837	-	56,73,73	1.17	7 (12%)	65,113,113	1.15	5 (7%)
21	CLA	b	1838	-	44,61,73	1.31	5 (11%)	50,98,113	1.35	7 (14%)
21	CLA	b	1839	-	56,73,73	1.15	6 (10%)	65,113,113	1.18	4 (6%)
21	CLA	b	1840	-	56,73,73	1.20	6 (10%)	65,113,113	1.10	4 (6%)
21	CLA	b	1841	38	56,73,73	1.18	4 (7%)	65,113,113	1.22	6 (9%)
21	CLA	b	1842	-	56,73,73	1.21	6 (10%)	65,113,113	1.14	4 (6%)
21	CLA	b	1843	-	56,73,73	1.21	7 (12%)	65,113,113	1.18	4 (6%)
22	PQN	b	1844	-	34,34,34	0.76	2 (5%)	43,45,45	1.23	4 (9%)
24	BCR	b	1845	-	41,41,41	0.65	0	56,56,56	3.28	14 (25%)
24	BCR	b	1846	-	41,41,41	0.63	0	56,56,56	3.13	12 (21%)
30	ECH	b	1847	-	42,42,42	0.71	1 (2%)	55,58,58	2.25	15 (27%)
24	BCR	b	1848	-	41,41,41	0.62	0	56,56,56	3.05	7 (12%)
24	BCR	b	1849	-	41,41,41	0.61	0	56,56,56	3.26	10 (17%)
24	BCR	b	1850	-	41,41,41	0.68	0	56,56,56	3.30	8 (14%)
26	LMG	b	1851	-	55,55,55	1.12	6 (10%)	63,63,63	1.19	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	b	1852	-	48,48,48	0.38	0	49,54,54	1.11	3 (6%)
26	LMG	b	1853	-	55,55,55	1.12	6 (10%)	63,63,63	1.33	6 (9%)
31	SQD	b	1854	-	53,54,54	0.80	0	63,65,65	1.03	3 (4%)
26	LMG	b	1855	-	55,55,55	1.12	6 (10%)	63,63,63	1.16	3 (4%)
34	C7Z	b	1858	-	43,43,43	0.75	1 (2%)	56,60,60	1.89	12 (21%)
23	SF4	c	101	-	0,12,12	0.00	-	0,24,24	0.00	-
23	SF4	c	102	13	0,12,12	0.00	-	0,24,24	0.00	-
24	BCR	f	201	-	41,41,41	0.69	0	56,56,56	3.18	12 (21%)
21	CLA	f	202	38	41,58,73	1.38	5 (12%)	47,95,113	1.26	6 (12%)
21	CLA	f	203	-	56,73,73	1.19	7 (12%)	65,113,113	1.13	5 (7%)
24	BCR	f	204	-	41,41,41	0.71	0	56,56,56	3.26	12 (21%)
31	SQD	f	205	-	53,54,54	0.79	0	63,65,65	1.03	3 (4%)
24	BCR	h	101	-	41,41,41	0.68	0	56,56,56	3.30	11 (19%)
24	BCR	i	101	-	41,41,41	0.68	0	56,56,56	3.35	12 (21%)
21	CLA	j	1101	-	56,73,73	1.17	6 (10%)	65,113,113	1.31	8 (12%)
24	BCR	j	1102	-	41,41,41	0.67	0	56,56,56	3.10	14 (25%)
21	CLA	j	1103	-	56,73,73	1.21	7 (12%)	65,113,113	1.23	5 (7%)
21	CLA	j	1104	-	56,73,73	1.21	7 (12%)	65,113,113	1.22	5 (7%)
21	CLA	j	1105	-	46,63,73	1.31	7 (15%)	53,101,113	1.27	6 (11%)
21	CLA	k	1401	-	41,58,73	1.38	7 (17%)	47,95,113	1.32	6 (12%)
21	CLA	k	1402	-	40,57,73	1.41	7 (17%)	46,93,113	1.58	7 (15%)
24	BCR	k	1403	-	41,41,41	0.65	0	56,56,56	3.14	9 (16%)
21	CLA	l	201	-	56,73,73	1.16	6 (10%)	65,113,113	1.19	7 (10%)
30	ECH	l	202	-	42,42,42	0.80	1 (2%)	55,58,58	2.39	17 (30%)
21	CLA	l	203	10	56,73,73	1.15	6 (10%)	65,113,113	1.23	6 (9%)
21	CLA	l	204	-	56,73,73	1.14	6 (10%)	65,113,113	1.18	4 (6%)
21	CLA	l	205	-	56,73,73	1.16	5 (8%)	65,113,113	1.19	7 (10%)
24	BCR	l	206	-	41,41,41	0.62	0	56,56,56	2.87	12 (21%)
24	BCR	l	207	-	41,41,41	0.67	0	56,56,56	3.20	12 (21%)
25	LHG	l	208	-	48,48,48	0.39	0	49,54,54	1.14	3 (6%)
25	LHG	l	209	-	48,48,48	0.39	0	49,54,54	1.05	3 (6%)
25	LHG	l	210	-	48,48,48	0.39	0	49,54,54	1.08	3 (6%)
35	LMT	l	211	-	36,36,36	1.11	4 (11%)	47,47,47	1.25	4 (8%)
25	LHG	m	101	-	48,48,48	0.40	0	49,54,54	1.08	3 (6%)
31	SQD	m	102	-	53,54,54	0.80	0	63,65,65	1.01	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	m	103	-	56,73,73	1.18	7 (12%)	65,113,113	1.13	4 (6%)
30	ECH	m	104	-	42,42,42	0.63	0	55,58,58	1.69	11 (20%)

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
21	CLA	0	201	20	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	0	202	28	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	0	203	38	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	0	204	-	-	0/29/63/63	0/2/2/2
24	BCR	0	205	-	-	0/29/63/63	0/2/2/2
26	LMG	0	206	-	-	0/50/70/70	0/1/1/1
31	SQD	0	207	-	-	0/49/69/69	0/1/1/1
35	LMT	0	208	-	-	0/21/61/61	0/2/2/2
21	CLA	1	801	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	802	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	803	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	804	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	1	805	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	1	806	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	807	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	1	808	16	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	809	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	1	810	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	1	811	16	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	812	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	1	813	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	814	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	1	815	-	3/3/15/25	0/11/110/135	0/0/9/9
21	CLA	1	816	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	1	817	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	818	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	819	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	820	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	821	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	822	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	823	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	1	824	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	1	825	-	1/1/20/25	0/37/135/135	0/0/9/9
21	CLA	1	826	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	1	827	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	828	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	829	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	830	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	831	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	1	832	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	833	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	834	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	835	16	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	836	-	1/1/17/25	0/22/120/135	0/0/9/9
21	CLA	1	837	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	838	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	1	839	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	1	840	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	841	25	3/3/18/25	0/27/125/135	0/0/9/9
22	PQN	1	842	-	-	0/23/43/43	0/2/2/2
23	SF4	1	843	2,16	-	0/0/48/48	0/6/5/5
24	BCR	1	844	-	-	0/29/63/63	0/2/2/2
24	BCR	1	845	-	-	0/29/63/63	0/2/2/2
24	BCR	1	846	-	-	0/29/63/63	0/2/2/2
24	BCR	1	847	-	-	0/29/63/63	0/2/2/2
24	BCR	1	848	-	-	0/29/63/63	0/2/2/2
24	BCR	1	849	-	-	0/29/63/63	0/2/2/2
25	LHG	1	850	-	-	0/53/53/53	0/0/0/0
26	LMG	1	851	-	-	0/45/65/70	0/1/1/1
25	LHG	1	852	21	-	0/53/53/53	0/0/0/0
26	LMG	1	853	-	-	0/50/70/70	0/1/1/1
35	LMT	1	854	-	-	0/21/61/61	0/2/2/2
21	CLA	1	855	38	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	1	856	-	-	0/29/63/63	0/2/2/2
24	BCR	1	858	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	2	801	-	-	0/53/53/53	0/0/0/0
21	CLA	2	802	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	2	803	38	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	2	804	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	805	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	806	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	807	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	2	808	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	809	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	810	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	811	2	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	812	-	2/2/18/25	0/27/125/135	0/0/9/9
21	CLA	2	813	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	2	814	-	1/1/16/25	0/11/111/135	0/0/9/9
21	CLA	2	815	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	2	816	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	2	817	-	3/3/15/25	0/8/106/135	0/0/9/9
21	CLA	2	818	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	2	819	-	3/3/18/25	0/30/128/135	0/0/9/9
21	CLA	2	820	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	2	821	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	2	822	-	3/3/17/25	0/22/120/135	0/0/9/9
21	CLA	2	823	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	824	-	2/2/17/25	0/23/121/135	0/0/9/9
21	CLA	2	825	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	2	826	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	827	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	2	828	-	2/2/18/25	0/25/123/135	0/0/9/9
21	CLA	2	829	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	2	830	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	831	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	2	832	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	2	833	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	2	834	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	835	38	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	2	836	-	2/2/16/25	0/11/111/135	0/0/9/9
21	CLA	2	837	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	2	838	-	3/3/17/25	0/23/121/135	0/0/9/9
21	CLA	2	839	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	2	840	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	841	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	842	-	2/2/15/25	0/8/106/135	0/0/9/9
22	PQN	2	843	-	-	0/23/43/43	0/2/2/2
24	BCR	2	844	-	-	0/29/63/63	0/2/2/2
24	BCR	2	845	-	-	0/29/63/63	0/2/2/2
30	ECH	2	846	-	-	0/29/66/66	0/2/2/2
24	BCR	2	847	-	-	0/29/63/63	0/2/2/2
24	BCR	2	848	-	-	2/29/63/63	0/2/2/2
24	BCR	2	849	-	-	0/29/63/63	0/2/2/2
26	LMG	2	850	-	-	0/50/70/70	0/1/1/1
25	LHG	2	851	-	-	0/53/53/53	0/0/0/0
26	LMG	2	852	-	-	0/50/70/70	0/1/1/1
28	45D	2	854	21	-	0/29/69/69	0/2/2/2
34	C7Z	2	855	-	-	0/29/67/67	0/2/2/2
23	SF4	3	101	-	-	0/0/48/48	0/6/5/5
23	SF4	3	102	-	-	0/0/48/48	0/6/5/5
21	CLA	6	201	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	6	202	-	-	2/29/63/63	0/2/2/2
21	CLA	6	203	38	3/3/16/25	0/16/114/135	0/0/9/9
21	CLA	6	204	6	3/3/15/25	0/11/109/135	0/0/9/9
24	BCR	6	205	-	-	1/29/63/63	0/2/2/2
25	LHG	6	206	-	-	0/12/12/53	0/0/0/0
21	CLA	7	1101	-	1/1/20/25	0/37/135/135	0/0/9/9
24	BCR	7	1102	-	-	0/29/63/63	0/2/2/2
21	CLA	7	1103	-	3/3/16/25	0/16/114/135	0/0/9/9
21	CLA	7	1104	8	2/2/15/25	0/8/106/135	0/0/9/9
21	CLA	7	1105	-	3/3/15/25	0/8/106/135	0/0/9/9
21	CLA	8	1401	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	8	1402	-	3/3/16/25	0/15/113/135	0/0/9/9
24	BCR	8	1403	-	-	0/29/63/63	0/2/2/2
25	LHG	9	101	-	-	0/53/53/53	0/0/0/0
24	BCR	9	102	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	801	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	802	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	803	21	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	804	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	805	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	806	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	807	1	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	808	1	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	809	-	3/3/17/25	0/23/121/135	0/0/9/9
21	CLA	A	810	21	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	811	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	812	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	813	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	814	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	815	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	816	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	817	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	818	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	819	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	820	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	821	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	822	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	823	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	A	824	38	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	825	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	826	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	827	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	828	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	829	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	830	-	2/2/18/25	0/29/127/135	0/0/9/9
21	CLA	A	831	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	832	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	833	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	834	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
21	CLA	A	835	-	1/1/20/25	0/37/135/135	0/0/9/9
21	CLA	A	836	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	837	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	838	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	839	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	840	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PQN	A	841	-	-	0/23/43/43	0/2/2/2
23	SF4	A	842	1,2	-	0/0/48/48	0/6/5/5
24	BCR	A	843	-	-	0/29/63/63	0/2/2/2
24	BCR	A	844	-	-	0/29/63/63	0/2/2/2
24	BCR	A	845	-	-	0/29/63/63	0/2/2/2
24	BCR	A	846	-	-	0/29/63/63	0/2/2/2
24	BCR	A	847	-	-	0/29/63/63	0/2/2/2
24	BCR	A	848	-	-	0/29/63/63	0/2/2/2
25	LHG	A	849	-	-	0/53/53/53	0/0/0/0
26	LMG	A	850	-	-	0/45/65/70	0/1/1/1
25	LHG	A	851	21	-	0/53/53/53	0/0/0/0
26	LMG	A	852	-	-	0/43/63/70	0/1/1/1
27	ACT	A	853	-	-	0/0/0/0	0/0/0/0
21	CLA	A	854	38	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	855	38	3/3/20/25	0/37/135/135	0/0/9/9
28	45D	A	856	-	-	0/29/69/69	0/2/2/2
21	CLA	B	801	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	802	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	803	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	804	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	805	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	806	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	807	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	808	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	809	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	810	2	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	811	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	812	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	813	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	814	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	815	-	3/3/18/25	0/25/123/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	816	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	817	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	818	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	819	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	820	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	821	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	822	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	823	-	3/3/18/25	0/28/126/135	0/0/9/9
21	CLA	B	824	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	825	38	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	B	826	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	827	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	828	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	829	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	830	-	2/2/18/25	0/25/123/135	0/0/9/9
21	CLA	B	831	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	832	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	833	38	1/1/20/25	0/37/135/135	0/0/9/9
21	CLA	B	834	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	B	835	-	1/1/20/25	0/37/135/135	0/0/9/9
21	CLA	B	836	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	837	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	B	838	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	839	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	840	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PQN	B	841	-	-	0/23/43/43	0/2/2/2
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
24	BCR	B	843	-	-	0/29/63/63	0/2/2/2
30	ECH	B	844	-	-	0/29/66/66	0/2/2/2
24	BCR	B	845	-	-	0/29/63/63	0/2/2/2
24	BCR	B	846	-	-	0/29/63/63	0/2/2/2
24	BCR	B	847	-	-	0/29/63/63	0/2/2/2
26	LMG	B	848	-	-	0/50/70/70	0/1/1/1
25	LHG	B	849	-	-	0/53/53/53	0/0/0/0
26	LMG	B	850	-	-	0/50/70/70	0/1/1/1
25	LHG	B	851	-	-	1/53/53/53	0/0/0/0
31	SQD	B	852	-	-	0/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	B	855	-	-	0/53/53/53	0/0/0/0
34	C7Z	B	856	-	-	0/29/67/67	0/2/2/2
25	LHG	B	857	-	-	0/53/53/53	0/0/0/0
25	LHG	B	858	-	-	0/53/53/53	0/0/0/0
23	SF4	C	101	3	-	0/0/48/48	0/6/5/5
23	SF4	C	102	3	-	0/0/48/48	0/6/5/5
27	ACT	D	201	-	-	0/0/0/0	0/0/0/0
24	BCR	F	201	-	-	0/29/63/63	0/2/2/2
21	CLA	F	202	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	F	203	6	3/3/20/25	0/37/135/135	0/0/9/9
34	C7Z	F	204	-	-	0/29/67/67	0/2/2/2
31	SQD	F	205	-	-	0/49/69/69	0/1/1/1
21	CLA	I	101	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	I	102	-	-	0/29/63/63	0/2/2/2
25	LHG	I	103	-	-	0/53/53/53	0/0/0/0
25	LHG	I	104	-	-	0/53/53/53	0/0/0/0
21	CLA	J	1101	-	1/1/20/25	0/37/135/135	0/0/9/9
24	BCR	J	1102	-	-	0/29/63/63	0/2/2/2
21	CLA	J	1103	-	3/3/20/25	0/37/135/135	0/0/9/9
35	LMT	J	1104	-	-	0/21/61/61	0/2/2/2
21	CLA	J	1105	8	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	J	1106	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	J	1107	-	-	0/29/63/63	0/2/2/2
26	LMG	K	101	-	-	2/50/70/70	0/1/1/1
21	CLA	K	102	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	K	103	-	1/1/20/25	0/37/135/135	0/0/9/9
24	BCR	K	104	-	-	0/29/63/63	0/2/2/2
26	LMG	K	105	-	-	1/50/70/70	0/1/1/1
36	EQ3	L	201	-	-	0/29/68/68	0/2/2/2
21	CLA	L	203	10	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	L	204	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	L	205	38	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	L	206	-	-	0/29/63/63	0/2/2/2
24	BCR	L	207	-	-	0/29/63/63	0/2/2/2
31	SQD	L	208	-	-	0/46/66/69	0/1/1/1
37	DGD	L	209	-	-	0/55/95/95	0/2/2/2
25	LHG	L	210	-	-	0/53/53/53	0/0/0/0
35	LMT	L	211	-	-	0/21/61/61	0/2/2/2
27	ACT	M	7001	-	-	0/0/0/0	0/0/0/0
30	ECH	M	7002	-	-	0/29/66/66	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	M	7003	-	-	2/53/53/53	0/0/0/0
21	CLA	a	801	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	802	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	803	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	a	804	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	805	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	a	806	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	807	-	3/3/18/25	0/29/127/135	0/0/9/9
21	CLA	a	808	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	809	1	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	a	810	-	3/3/18/25	0/28/126/135	0/0/9/9
21	CLA	a	811	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	812	-	3/3/18/25	0/30/128/135	0/0/9/9
21	CLA	a	813	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	814	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	815	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	a	816	-	3/3/17/25	0/22/120/135	0/0/9/9
21	CLA	a	817	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	a	818	-	2/2/19/25	0/31/129/135	0/0/9/9
21	CLA	a	819	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	820	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	821	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	822	-	2/2/18/25	0/25/123/135	0/0/9/9
21	CLA	a	823	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	824	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	825	1	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	a	826	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	a	827	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	828	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	829	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	830	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	831	-	3/3/17/25	0/22/120/135	0/0/9/9
21	CLA	a	832	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	833	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	834	1	3/3/16/25	0/18/116/135	0/0/9/9
21	CLA	a	835	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	a	836	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	837	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	a	838	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	839	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	840	25	3/3/18/25	0/25/123/135	0/0/9/9
22	PQN	a	841	-	-	0/23/43/43	0/2/2/2
23	SF4	a	842	1,12	-	0/0/48/48	0/6/5/5
24	BCR	a	843	-	-	0/29/63/63	0/2/2/2
24	BCR	a	844	-	-	0/29/63/63	0/2/2/2
24	BCR	a	845	-	-	0/29/63/63	0/2/2/2
24	BCR	a	846	-	-	0/29/63/63	0/2/2/2
24	BCR	a	847	-	-	0/29/63/63	0/2/2/2
24	BCR	a	848	-	-	0/29/63/63	0/2/2/2
25	LHG	a	849	-	-	0/53/53/53	0/0/0/0
26	LMG	a	850	-	-	0/45/65/70	0/1/1/1
25	LHG	a	851	21	-	0/53/53/53	0/0/0/0
26	LMG	a	852	-	-	0/50/70/70	0/1/1/1
25	LHG	a	853	-	-	2/53/53/53	0/0/0/0
27	ACT	a	854	-	-	0/0/0/0	0/0/0/0
21	CLA	a	855	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	a	856	38	3/3/20/25	0/37/135/135	0/0/9/9
30	ECH	a	857	-	-	0/29/66/66	0/2/2/2
24	BCR	a	859	-	-	0/29/63/63	0/2/2/2
21	CLA	b	1801	25	3/3/20/25	0/37/135/135	0/0/9/9
25	LHG	b	1802	-	-	0/53/53/53	0/0/0/0
25	LHG	b	1803	-	-	2/53/53/53	0/0/0/0
21	CLA	b	1804	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1805	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1806	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1807	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1808	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1809	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1810	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1811	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1812	12	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	1813	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1814	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	b	1815	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1816	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1817	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1818	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1819	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1820	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1821	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1822	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1823	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	b	1824	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1825	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	b	1826	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1827	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1828	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1829	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1830	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1831	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1832	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1833	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1834	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1835	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1836	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1837	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1838	-	3/3/17/25	0/23/121/135	0/0/9/9
21	CLA	b	1839	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1840	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1841	38	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1842	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	b	1843	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PQN	b	1844	-	-	0/23/43/43	0/2/2/2
24	BCR	b	1845	-	-	0/29/63/63	0/2/2/2
24	BCR	b	1846	-	-	0/29/63/63	0/2/2/2
30	ECH	b	1847	-	-	0/29/66/66	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	1848	-	-	0/29/63/63	0/2/2/2
24	BCR	b	1849	-	-	2/29/63/63	0/2/2/2
24	BCR	b	1850	-	-	0/29/63/63	0/2/2/2
26	LMG	b	1851	-	-	0/50/70/70	0/1/1/1
25	LHG	b	1852	-	-	0/53/53/53	0/0/0/0
26	LMG	b	1853	-	-	0/50/70/70	0/1/1/1
31	SQD	b	1854	-	-	0/49/69/69	0/1/1/1
26	LMG	b	1855	-	-	0/50/70/70	0/1/1/1
34	C7Z	b	1858	-	-	0/29/67/67	0/2/2/2
23	SF4	c	101	-	-	0/0/48/48	0/6/5/5
23	SF4	c	102	13	-	0/0/48/48	0/6/5/5
24	BCR	f	201	-	-	0/29/63/63	0/2/2/2
21	CLA	f	202	38	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	f	203	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	f	204	-	-	1/29/63/63	0/2/2/2
31	SQD	f	205	-	-	0/49/69/69	0/1/1/1
24	BCR	h	101	-	-	2/29/63/63	0/2/2/2
24	BCR	i	101	-	-	2/29/63/63	0/2/2/2
21	CLA	j	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	j	1102	-	-	0/29/63/63	0/2/2/2
21	CLA	j	1103	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	j	1104	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	j	1105	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	k	1401	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	k	1402	-	3/3/16/25	0/18/116/135	0/0/9/9
24	BCR	k	1403	-	-	0/29/63/63	0/2/2/2
21	CLA	l	201	-	3/3/20/25	0/37/135/135	0/0/9/9
30	ECH	l	202	-	-	0/29/66/66	0/2/2/2
21	CLA	l	203	10	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	l	204	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	l	205	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	l	206	-	-	0/29/63/63	0/2/2/2
24	BCR	l	207	-	-	0/29/63/63	0/2/2/2
25	LHG	l	208	-	-	0/53/53/53	0/0/0/0
25	LHG	l	209	-	-	0/53/53/53	0/0/0/0
25	LHG	l	210	-	-	0/53/53/53	0/0/0/0
35	LMT	l	211	-	-	0/21/61/61	0/2/2/2
25	LHG	m	101	-	-	0/53/53/53	0/0/0/0
31	SQD	m	102	-	-	0/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	m	103	-	3/3/20/25	0/37/135/135	0/0/9/9
30	ECH	m	104	-	-	0/29/66/66	0/2/2/2

All (1964) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	201	EQ3	C2-C3	-6.06	1.43	1.52
36	L	201	EQ3	C1-C6	-4.74	1.47	1.53
36	L	201	EQ3	C4-C5	-4.45	1.43	1.51
36	L	201	EQ3	O3-C3	-3.29	1.33	1.43
26	K	105	LMG	C43-C42	-3.26	1.33	1.51
26	b	1851	LMG	C40-C39	-3.24	1.33	1.51
26	K	105	LMG	C37-C36	-3.24	1.33	1.51
26	B	848	LMG	C40-C39	-3.23	1.33	1.51
26	B	848	LMG	C25-C24	-3.22	1.33	1.51
26	b	1851	LMG	C43-C42	-3.22	1.33	1.51
26	b	1853	LMG	C40-C39	-3.22	1.33	1.51
26	K	105	LMG	C22-C21	-3.21	1.33	1.51
26	2	852	LMG	C37-C36	-3.21	1.33	1.51
26	B	848	LMG	C43-C42	-3.21	1.33	1.51
26	B	848	LMG	C19-C18	-3.21	1.33	1.51
26	2	850	LMG	C40-C39	-3.21	1.33	1.51
26	b	1853	LMG	C37-C36	-3.21	1.33	1.51
26	K	105	LMG	C40-C39	-3.20	1.33	1.51
26	b	1851	LMG	C37-C36	-3.20	1.33	1.51
26	B	848	LMG	C37-C36	-3.19	1.33	1.51
26	K	105	LMG	C19-C18	-3.19	1.33	1.51
26	2	852	LMG	C40-C39	-3.19	1.33	1.51
26	1	853	LMG	C19-C18	-3.19	1.33	1.51
26	2	852	LMG	C22-C21	-3.19	1.33	1.51
26	2	850	LMG	C37-C36	-3.19	1.33	1.51
26	2	850	LMG	C19-C18	-3.19	1.33	1.51
26	b	1855	LMG	C19-C18	-3.19	1.33	1.51
26	a	852	LMG	C40-C39	-3.19	1.33	1.51
26	0	206	LMG	C19-C18	-3.19	1.33	1.51
26	2	850	LMG	C43-C42	-3.18	1.33	1.51
26	1	853	LMG	C22-C21	-3.18	1.33	1.51
26	b	1851	LMG	C19-C18	-3.18	1.33	1.51
26	A	850	LMG	C37-C36	-3.18	1.33	1.51
26	B	850	LMG	C37-C36	-3.18	1.33	1.51
26	b	1853	LMG	C19-C18	-3.17	1.33	1.51
26	a	852	LMG	C43-C42	-3.17	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	L	209	DGD	CAB-C9B	-3.17	1.33	1.51
26	B	850	LMG	C40-C39	-3.17	1.33	1.51
26	K	101	LMG	C25-C24	-3.17	1.33	1.51
26	0	206	LMG	C22-C21	-3.17	1.33	1.51
26	1	853	LMG	C25-C24	-3.16	1.33	1.51
26	B	850	LMG	C22-C21	-3.16	1.33	1.51
26	0	206	LMG	C25-C24	-3.16	1.33	1.51
26	a	852	LMG	C25-C24	-3.16	1.33	1.51
26	a	850	LMG	C37-C36	-3.16	1.33	1.51
26	A	852	LMG	C25-C24	-3.16	1.33	1.51
26	A	850	LMG	C40-C39	-3.16	1.33	1.51
26	a	852	LMG	C37-C36	-3.16	1.33	1.51
26	2	852	LMG	C19-C18	-3.16	1.33	1.51
26	2	852	LMG	C25-C24	-3.16	1.33	1.51
26	B	850	LMG	C19-C18	-3.16	1.33	1.51
26	K	101	LMG	C40-C39	-3.15	1.33	1.51
26	B	850	LMG	C25-C24	-3.15	1.33	1.51
26	b	1855	LMG	C40-C39	-3.15	1.33	1.51
26	K	101	LMG	C22-C21	-3.15	1.33	1.51
26	1	851	LMG	C37-C36	-3.15	1.33	1.51
26	K	101	LMG	C19-C18	-3.15	1.33	1.51
26	1	851	LMG	C40-C39	-3.15	1.33	1.51
26	b	1853	LMG	C22-C21	-3.15	1.33	1.51
26	1	851	LMG	C19-C18	-3.15	1.33	1.51
26	K	101	LMG	C43-C42	-3.15	1.33	1.51
26	b	1851	LMG	C25-C24	-3.15	1.33	1.51
37	L	209	DGD	CDB-CCB	-3.15	1.33	1.51
26	0	206	LMG	C43-C42	-3.14	1.33	1.51
26	b	1855	LMG	C37-C36	-3.14	1.33	1.51
37	L	209	DGD	CDA-CCA	-3.14	1.33	1.51
26	2	850	LMG	C22-C21	-3.14	1.33	1.51
26	B	848	LMG	C22-C21	-3.14	1.33	1.51
26	a	852	LMG	C19-C18	-3.14	1.33	1.51
26	1	853	LMG	C40-C39	-3.14	1.33	1.51
26	1	853	LMG	C43-C42	-3.14	1.33	1.51
26	K	105	LMG	C25-C24	-3.14	1.33	1.51
26	b	1855	LMG	C43-C42	-3.14	1.33	1.51
26	a	850	LMG	C40-C39	-3.14	1.33	1.51
26	K	101	LMG	C37-C36	-3.13	1.33	1.51
26	b	1851	LMG	C22-C21	-3.13	1.33	1.51
26	b	1853	LMG	C25-C24	-3.13	1.33	1.51
26	1	851	LMG	C43-C42	-3.13	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	852	LMG	C22-C21	-3.13	1.33	1.51
26	b	1855	LMG	C22-C21	-3.13	1.33	1.51
21	2	831	CLA	C3B-C2B	-3.13	1.36	1.40
26	a	850	LMG	C19-C18	-3.13	1.33	1.51
26	b	1855	LMG	C25-C24	-3.13	1.33	1.51
26	a	850	LMG	C43-C42	-3.12	1.33	1.51
26	2	850	LMG	C25-C24	-3.12	1.33	1.51
26	a	852	LMG	C22-C21	-3.12	1.33	1.51
37	L	209	DGD	CGA-CFA	-3.12	1.33	1.51
37	L	209	DGD	CAA-C9A	-3.12	1.33	1.51
26	0	206	LMG	C37-C36	-3.12	1.33	1.51
26	2	852	LMG	C43-C42	-3.11	1.33	1.51
37	L	209	DGD	CGB-CFB	-3.11	1.33	1.51
26	A	850	LMG	C19-C18	-3.11	1.33	1.51
26	1	853	LMG	C37-C36	-3.11	1.33	1.51
26	0	206	LMG	C40-C39	-3.11	1.33	1.51
26	A	850	LMG	C43-C42	-3.10	1.33	1.51
26	b	1853	LMG	C43-C42	-3.10	1.33	1.51
26	A	852	LMG	C19-C18	-3.08	1.34	1.51
26	B	850	LMG	C43-C42	-3.08	1.34	1.51
21	a	835	CLA	C3B-C2B	-3.04	1.36	1.40
30	b	1847	ECH	C1-C6	-3.02	1.49	1.53
21	b	1818	CLA	C3B-C2B	-2.98	1.36	1.40
21	A	815	CLA	C3B-C2B	-2.96	1.36	1.40
21	B	828	CLA	C3B-C2B	-2.96	1.36	1.40
21	2	812	CLA	C3B-C2B	-2.95	1.36	1.40
21	B	832	CLA	C3B-C2B	-2.92	1.36	1.40
21	A	806	CLA	C3B-C2B	-2.91	1.36	1.40
21	2	841	CLA	C3B-C2B	-2.91	1.36	1.40
21	a	812	CLA	C3B-C2B	-2.90	1.36	1.40
21	2	834	CLA	C3B-C2B	-2.90	1.36	1.40
21	B	834	CLA	C3B-C2B	-2.88	1.36	1.40
21	b	1842	CLA	C3B-C2B	-2.88	1.36	1.40
21	b	1832	CLA	C3B-C2B	-2.88	1.36	1.40
21	A	811	CLA	C3B-C2B	-2.88	1.36	1.40
21	J	1101	CLA	C3B-C2B	-2.88	1.36	1.40
21	2	832	CLA	C3B-C2B	-2.87	1.36	1.40
21	b	1835	CLA	C3B-C2B	-2.87	1.36	1.40
21	B	826	CLA	C3B-C2B	-2.86	1.36	1.40
21	1	839	CLA	C3B-C2B	-2.85	1.36	1.40
21	B	822	CLA	C3B-C2B	-2.85	1.36	1.40
21	B	815	CLA	C3B-C2B	-2.85	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	833	CLA	C3B-C2B	-2.83	1.36	1.40
21	b	1813	CLA	C3B-C2B	-2.83	1.36	1.40
21	B	817	CLA	C3B-C2B	-2.82	1.36	1.40
21	1	834	CLA	C3B-C2B	-2.81	1.36	1.40
21	I	101	CLA	C3B-C2B	-2.80	1.36	1.40
21	a	837	CLA	C3B-C2B	-2.79	1.36	1.40
21	a	833	CLA	C3B-C2B	-2.79	1.36	1.40
21	b	1823	CLA	C3B-C2B	-2.77	1.36	1.40
21	a	829	CLA	C3B-C2B	-2.77	1.36	1.40
21	7	1101	CLA	C3B-C2B	-2.77	1.36	1.40
21	b	1834	CLA	C3B-C2B	-2.77	1.36	1.40
21	2	814	CLA	C3B-C2B	-2.76	1.36	1.40
35	0	208	LMT	O3'-C3'	-2.76	1.36	1.43
21	2	833	CLA	C3B-C2B	-2.75	1.36	1.40
21	B	837	CLA	C3B-C2B	-2.75	1.36	1.40
21	2	840	CLA	C3B-C2B	-2.75	1.36	1.40
21	A	837	CLA	C3B-C2B	-2.74	1.36	1.40
21	2	830	CLA	C3B-C2B	-2.74	1.36	1.40
21	F	203	CLA	C3B-C2B	-2.73	1.36	1.40
21	B	812	CLA	C3B-C2B	-2.73	1.36	1.40
35	J	1104	LMT	O3'-C3'	-2.73	1.36	1.43
21	b	1840	CLA	C3B-C2B	-2.73	1.36	1.40
21	2	828	CLA	C3B-C2B	-2.73	1.36	1.40
21	j	1103	CLA	C3B-C2B	-2.72	1.36	1.40
35	l	211	LMT	O3'-C3'	-2.72	1.36	1.43
21	a	832	CLA	C3B-C2B	-2.72	1.36	1.40
21	A	836	CLA	C3B-C2B	-2.71	1.36	1.40
21	1	829	CLA	C3B-C2B	-2.71	1.36	1.40
21	7	1104	CLA	C3B-C2B	-2.71	1.36	1.40
21	B	830	CLA	C3B-C2B	-2.70	1.36	1.40
21	b	1822	CLA	C3B-C2B	-2.70	1.36	1.40
21	b	1810	CLA	C3B-C2B	-2.70	1.36	1.40
21	A	831	CLA	C3B-C2B	-2.70	1.36	1.40
35	L	211	LMT	O3'-C3'	-2.70	1.36	1.43
21	b	1825	CLA	C3B-C2B	-2.69	1.36	1.40
30	B	844	ECH	C1-C6	-2.69	1.50	1.53
21	2	824	CLA	C3B-C2B	-2.68	1.36	1.40
21	2	822	CLA	C3B-C2B	-2.68	1.36	1.40
21	B	820	CLA	C3B-C2B	-2.68	1.36	1.40
21	a	818	CLA	C3B-C2B	-2.68	1.36	1.40
21	A	834	CLA	C3B-C2B	-2.68	1.36	1.40
21	1	832	CLA	C3B-C2B	-2.67	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	835	CLA	C3B-C2B	-2.67	1.36	1.40
21	B	819	CLA	C3B-C2B	-2.67	1.36	1.40
21	K	103	CLA	C3B-C2B	-2.66	1.36	1.40
21	1	837	CLA	C3B-C2B	-2.66	1.36	1.40
21	B	839	CLA	C3B-C2B	-2.66	1.36	1.40
21	1	812	CLA	C3B-C2B	-2.66	1.36	1.40
21	a	836	CLA	C3B-C2B	-2.65	1.36	1.40
21	a	807	CLA	C3B-C2B	-2.64	1.36	1.40
21	1	807	CLA	C3B-C2B	-2.64	1.36	1.40
21	2	813	CLA	C3B-C2B	-2.63	1.36	1.40
21	1	818	CLA	C3B-C2B	-2.62	1.36	1.40
21	a	838	CLA	C3B-C2B	-2.61	1.36	1.40
21	k	1402	CLA	C3B-C2B	-2.61	1.36	1.40
35	1	854	LMT	O3'-C3'	-2.59	1.37	1.43
21	1	838	CLA	C3B-C2B	-2.59	1.36	1.40
21	2	810	CLA	C3B-C2B	-2.58	1.36	1.40
21	A	840	CLA	C3B-C2B	-2.58	1.36	1.40
21	1	814	CLA	C3B-C2B	-2.57	1.37	1.40
21	a	834	CLA	C3B-C2B	-2.57	1.37	1.40
21	B	838	CLA	C3B-C2B	-2.54	1.37	1.40
26	A	852	LMG	C37-C36	-2.54	1.33	1.51
21	1	817	CLA	C3B-C2B	-2.54	1.37	1.40
21	J	1103	CLA	C3B-C2B	-2.53	1.37	1.40
21	a	817	CLA	C3B-C2B	-2.53	1.37	1.40
21	j	1101	CLA	C3B-C2B	-2.53	1.37	1.40
21	2	842	CLA	C3B-C2B	-2.53	1.37	1.40
21	A	817	CLA	C3B-C2B	-2.53	1.37	1.40
21	B	840	CLA	C3B-C2B	-2.53	1.37	1.40
28	A	856	45D	O02-C18	-2.52	1.17	1.23
30	l	202	ECH	C1-C6	-2.51	1.50	1.53
21	a	831	CLA	C3B-C2B	-2.51	1.37	1.40
21	b	1820	CLA	C3B-C2B	-2.50	1.37	1.40
21	2	839	CLA	C3B-C2B	-2.50	1.37	1.40
21	6	201	CLA	C3B-C2B	-2.49	1.37	1.40
21	f	203	CLA	C3B-C2B	-2.49	1.37	1.40
21	a	810	CLA	C3B-C2B	-2.48	1.37	1.40
22	B	841	PQN	C9-C10	-2.47	1.35	1.39
21	J	1105	CLA	C3B-C2B	-2.47	1.37	1.40
21	I	101	CLA	C1C-NC	-2.46	1.33	1.37
21	A	812	CLA	C3B-C2B	-2.46	1.37	1.40
21	2	826	CLA	C3B-C2B	-2.46	1.37	1.40
36	L	201	EQ3	C21-C22	-2.45	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	813	CLA	C3B-C2B	-2.44	1.37	1.40
21	B	807	CLA	C3B-C2B	-2.44	1.37	1.40
21	A	837	CLA	C1C-NC	-2.44	1.33	1.37
21	A	839	CLA	C3B-C2B	-2.44	1.37	1.40
21	7	1103	CLA	C3B-C2B	-2.43	1.37	1.40
21	j	1104	CLA	C3B-C2B	-2.43	1.37	1.40
21	B	824	CLA	C3B-C2B	-2.43	1.37	1.40
21	a	825	CLA	C3B-C2B	-2.42	1.37	1.40
21	b	1811	CLA	C3B-C2B	-2.42	1.37	1.40
21	2	836	CLA	C3B-C2B	-2.41	1.37	1.40
21	A	832	CLA	C3B-C2B	-2.41	1.37	1.40
35	0	208	LMT	O2B-C2B	-2.41	1.37	1.43
21	1	810	CLA	C3B-C2B	-2.40	1.37	1.40
21	j	1105	CLA	C3B-C2B	-2.40	1.37	1.40
21	a	816	CLA	C3B-C2B	-2.40	1.37	1.40
21	A	822	CLA	C3B-C2B	-2.38	1.37	1.40
21	1	840	CLA	C3B-C2B	-2.38	1.37	1.40
21	l	201	CLA	C3B-C2B	-2.38	1.37	1.40
21	2	815	CLA	C3B-C2B	-2.37	1.37	1.40
21	A	813	CLA	C3B-C2B	-2.37	1.37	1.40
35	0	208	LMT	O2'-C2'	-2.36	1.37	1.43
35	J	1104	LMT	O3B-C3B	-2.36	1.37	1.43
21	b	1805	CLA	C3B-C2B	-2.36	1.37	1.40
21	A	838	CLA	C3B-C2B	-2.36	1.37	1.40
35	J	1104	LMT	O2B-C2B	-2.35	1.37	1.43
21	1	811	CLA	C3B-C2B	-2.35	1.37	1.40
21	2	834	CLA	C1C-NC	-2.35	1.33	1.37
21	2	825	CLA	C3B-C2B	-2.34	1.37	1.40
21	0	203	CLA	C3B-C2B	-2.34	1.37	1.40
35	J	1104	LMT	O2'-C2'	-2.34	1.37	1.43
21	a	808	CLA	C3B-C2B	-2.34	1.37	1.40
21	2	808	CLA	C3B-C2B	-2.34	1.37	1.40
21	1	838	CLA	C1C-NC	-2.33	1.33	1.37
21	a	827	CLA	C3B-C2B	-2.33	1.37	1.40
21	2	809	CLA	C3B-C2B	-2.32	1.37	1.40
21	B	833	CLA	C3B-C2B	-2.32	1.37	1.40
21	b	1812	CLA	C3B-C2B	-2.32	1.37	1.40
21	1	855	CLA	C3B-C2B	-2.32	1.37	1.40
22	B	841	PQN	C10-C5	-2.31	1.36	1.40
21	B	813	CLA	C3B-C2B	-2.31	1.37	1.40
21	A	826	CLA	C1C-NC	-2.31	1.34	1.37
21	a	822	CLA	C3B-C2B	-2.30	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	816	CLA	C3B-C2B	-2.30	1.37	1.40
21	b	1839	CLA	C3B-C2B	-2.30	1.37	1.40
21	1	831	CLA	C3B-C2B	-2.30	1.37	1.40
21	2	815	CLA	C1C-NC	-2.30	1.34	1.37
21	b	1838	CLA	C1C-NC	-2.29	1.34	1.37
21	b	1809	CLA	C3B-C2B	-2.29	1.37	1.40
21	1	825	CLA	C3B-C2B	-2.29	1.37	1.40
21	b	1814	CLA	C3B-C2B	-2.29	1.37	1.40
21	J	1106	CLA	C3B-C2B	-2.29	1.37	1.40
28	2	854	45D	O02-C18	-2.28	1.18	1.23
21	b	1826	CLA	C1C-NC	-2.28	1.34	1.37
21	B	810	CLA	C3B-C2B	-2.28	1.37	1.40
21	2	809	CLA	C1C-NC	-2.28	1.34	1.37
21	J	1105	CLA	C1C-NC	-2.28	1.34	1.37
21	a	809	CLA	C1C-NC	-2.27	1.34	1.37
21	l	204	CLA	C3B-C2B	-2.27	1.37	1.40
21	a	827	CLA	C1C-NC	-2.27	1.34	1.37
34	2	855	C7Z	C1-C6	-2.26	1.50	1.53
21	2	841	CLA	C1C-NC	-2.26	1.34	1.37
21	1	805	CLA	C1C-NC	-2.26	1.34	1.37
21	2	819	CLA	C3B-C2B	-2.26	1.37	1.40
21	A	804	CLA	C1C-NC	-2.26	1.34	1.37
21	a	840	CLA	C3B-C2B	-2.26	1.37	1.40
21	a	855	CLA	C1C-NC	-2.26	1.34	1.37
21	b	1804	CLA	C3B-C2B	-2.26	1.37	1.40
21	2	838	CLA	C3B-C2B	-2.25	1.37	1.40
21	2	820	CLA	C3B-C2B	-2.25	1.37	1.40
35	L	211	LMT	O2'-C2'	-2.25	1.37	1.43
21	1	824	CLA	C1C-NC	-2.25	1.34	1.37
35	1	854	LMT	O2'-C2'	-2.25	1.37	1.43
21	a	813	CLA	C1C-NC	-2.25	1.34	1.37
35	l	211	LMT	O2B-C2B	-2.25	1.37	1.43
21	B	822	CLA	C1C-NC	-2.25	1.34	1.37
21	b	1818	CLA	C1C-NC	-2.25	1.34	1.37
21	m	103	CLA	C3B-C2B	-2.25	1.37	1.40
21	B	823	CLA	C1C-NC	-2.25	1.34	1.37
21	1	833	CLA	C3B-C2B	-2.25	1.37	1.40
35	1	854	LMT	O3B-C3B	-2.25	1.37	1.43
21	a	824	CLA	C3B-C2B	-2.24	1.37	1.40
21	b	1837	CLA	C3B-C2B	-2.24	1.37	1.40
21	1	820	CLA	C1C-NC	-2.24	1.34	1.37
34	F	204	C7Z	C24-C25	-2.24	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	823	CLA	C1C-NC	-2.24	1.34	1.37
22	b	1844	PQN	C10-C5	-2.24	1.36	1.40
21	B	830	CLA	C1C-NC	-2.24	1.34	1.37
21	B	834	CLA	C1C-NC	-2.24	1.34	1.37
35	0	208	LMT	O3B-C3B	-2.23	1.37	1.43
21	A	809	CLA	C3B-C2B	-2.23	1.37	1.40
21	b	1826	CLA	C3B-C2B	-2.23	1.37	1.40
21	a	805	CLA	C3B-C2B	-2.23	1.37	1.40
21	A	817	CLA	C1C-NC	-2.23	1.34	1.37
21	2	833	CLA	C1C-NC	-2.23	1.34	1.37
21	A	812	CLA	C1C-NC	-2.23	1.34	1.37
21	0	202	CLA	C1C-NC	-2.23	1.34	1.37
21	B	825	CLA	C1C-NC	-2.23	1.34	1.37
21	1	821	CLA	C1C-NC	-2.23	1.34	1.37
35	1	854	LMT	O2B-C2B	-2.23	1.37	1.43
21	A	816	CLA	C3B-C2B	-2.22	1.37	1.40
21	J	1103	CLA	C1C-NC	-2.22	1.34	1.37
34	b	1858	C7Z	C24-C25	-2.22	1.47	1.51
21	B	837	CLA	C1C-NC	-2.22	1.34	1.37
34	B	856	C7Z	C24-C25	-2.22	1.47	1.51
21	1	834	CLA	C1C-NC	-2.22	1.34	1.37
21	b	1840	CLA	C1C-NC	-2.22	1.34	1.37
21	a	814	CLA	C3B-C2B	-2.22	1.37	1.40
21	1	841	CLA	C3B-C2B	-2.22	1.37	1.40
21	a	826	CLA	C3B-C2B	-2.21	1.37	1.40
21	B	826	CLA	C1C-NC	-2.21	1.34	1.37
21	B	808	CLA	C3B-C2B	-2.21	1.37	1.40
21	A	838	CLA	C1C-NC	-2.21	1.34	1.37
21	0	203	CLA	C1C-NC	-2.21	1.34	1.37
21	B	821	CLA	C1C-NC	-2.21	1.34	1.37
21	b	1841	CLA	C1C-NC	-2.21	1.34	1.37
35	L	211	LMT	O2B-C2B	-2.21	1.37	1.43
21	b	1804	CLA	C1C-NC	-2.21	1.34	1.37
21	b	1807	CLA	C1C-NC	-2.21	1.34	1.37
21	7	1101	CLA	C1C-NC	-2.21	1.34	1.37
21	b	1819	CLA	C3B-C2B	-2.20	1.37	1.40
35	l	211	LMT	O2'-C2'	-2.20	1.37	1.43
21	b	1822	CLA	C1C-NC	-2.20	1.34	1.37
21	1	822	CLA	C3B-C2B	-2.20	1.37	1.40
21	2	812	CLA	C1C-NC	-2.20	1.34	1.37
21	a	839	CLA	C1C-NC	-2.20	1.34	1.37
21	L	203	CLA	C1C-NC	-2.20	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	0	201	CLA	C3B-C2B	-2.20	1.37	1.40
21	a	856	CLA	C1C-NC	-2.20	1.34	1.37
21	A	807	CLA	C1C-NC	-2.20	1.34	1.37
21	a	817	CLA	C1C-NC	-2.20	1.34	1.37
21	A	809	CLA	C1C-NC	-2.20	1.34	1.37
21	B	801	CLA	C3B-C2B	-2.19	1.37	1.40
21	b	1813	CLA	C1C-NC	-2.19	1.34	1.37
21	B	804	CLA	C3B-C2B	-2.19	1.37	1.40
21	a	837	CLA	C1C-NC	-2.19	1.34	1.37
21	a	814	CLA	C1C-NC	-2.19	1.34	1.37
21	A	824	CLA	C3B-C2B	-2.19	1.37	1.40
21	2	821	CLA	C3B-C2B	-2.19	1.37	1.40
21	2	825	CLA	C1C-NC	-2.19	1.34	1.37
21	7	1103	CLA	C1C-NC	-2.19	1.34	1.37
21	2	828	CLA	C1C-NC	-2.19	1.34	1.37
21	L	205	CLA	C3B-C2B	-2.19	1.37	1.40
21	1	829	CLA	C1C-NC	-2.19	1.34	1.37
21	A	818	CLA	C3B-C2B	-2.18	1.37	1.40
21	a	822	CLA	C1C-NC	-2.18	1.34	1.37
21	2	813	CLA	C1C-NC	-2.18	1.34	1.37
21	2	832	CLA	C1C-NC	-2.18	1.34	1.37
21	B	805	CLA	C3B-C2B	-2.18	1.37	1.40
21	A	822	CLA	C1C-NC	-2.18	1.34	1.37
21	B	808	CLA	C1C-NC	-2.18	1.34	1.37
21	a	828	CLA	C1C-NC	-2.18	1.34	1.37
21	b	1808	CLA	C1C-NC	-2.18	1.34	1.37
21	B	812	CLA	C1C-NC	-2.18	1.34	1.37
21	K	102	CLA	C1C-NC	-2.18	1.34	1.37
21	B	832	CLA	C1C-NC	-2.18	1.34	1.37
21	2	839	CLA	C1C-NC	-2.17	1.34	1.37
21	a	805	CLA	C1C-NC	-2.17	1.34	1.37
21	A	831	CLA	C1C-NC	-2.17	1.34	1.37
21	k	1401	CLA	C3B-C2B	-2.17	1.37	1.40
21	b	1806	CLA	C3B-C2B	-2.17	1.37	1.40
21	7	1105	CLA	C1C-NC	-2.17	1.34	1.37
21	a	829	CLA	C1C-NC	-2.17	1.34	1.37
21	A	839	CLA	C1C-NC	-2.17	1.34	1.37
34	2	855	C7Z	C24-C25	-2.17	1.47	1.51
35	l	211	LMT	O3B-C3B	-2.17	1.38	1.43
21	1	819	CLA	C1C-NC	-2.17	1.34	1.37
21	f	203	CLA	C1C-NC	-2.17	1.34	1.37
21	A	801	CLA	C1C-NC	-2.17	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1829	CLA	C1C-NC	-2.17	1.34	1.37
21	1	835	CLA	C1C-NC	-2.16	1.34	1.37
21	b	1833	CLA	C3B-C2B	-2.16	1.37	1.40
21	j	1104	CLA	C1C-NC	-2.16	1.34	1.37
21	b	1830	CLA	C1C-NC	-2.16	1.34	1.37
21	A	816	CLA	C1C-NC	-2.16	1.34	1.37
21	1	806	CLA	C3B-C2B	-2.16	1.37	1.40
21	A	808	CLA	C1C-NC	-2.16	1.34	1.37
21	1	817	CLA	C1C-NC	-2.16	1.34	1.37
21	6	203	CLA	C3B-C2B	-2.16	1.37	1.40
21	b	1828	CLA	C3B-C2B	-2.16	1.37	1.40
21	A	825	CLA	C1C-NC	-2.15	1.34	1.37
21	B	815	CLA	C1C-NC	-2.15	1.34	1.37
21	A	810	CLA	C1C-NC	-2.15	1.34	1.37
21	b	1816	CLA	C3B-C2B	-2.15	1.37	1.40
21	2	811	CLA	C1C-NC	-2.15	1.34	1.37
21	B	803	CLA	C3B-C2B	-2.15	1.37	1.40
21	B	804	CLA	C1C-NC	-2.15	1.34	1.37
21	A	806	CLA	C1C-NC	-2.15	1.34	1.37
21	1	810	CLA	C1C-NC	-2.15	1.34	1.37
21	a	820	CLA	C3B-C2B	-2.15	1.37	1.40
35	L	211	LMT	O4'-C4B	-2.15	1.38	1.43
21	2	824	CLA	C1C-NC	-2.15	1.34	1.37
21	a	804	CLA	C1C-NC	-2.15	1.34	1.37
21	B	829	CLA	C1C-NC	-2.15	1.34	1.37
21	B	827	CLA	C3B-C2B	-2.15	1.37	1.40
21	1	839	CLA	C1C-NC	-2.14	1.34	1.37
21	b	1815	CLA	C1C-NC	-2.14	1.34	1.37
21	2	835	CLA	C1C-NC	-2.14	1.34	1.37
21	a	824	CLA	C1C-NC	-2.14	1.34	1.37
21	1	803	CLA	C1C-NC	-2.14	1.34	1.37
21	a	836	CLA	C1C-NC	-2.14	1.34	1.37
21	2	807	CLA	C1C-NC	-2.14	1.34	1.37
21	a	840	CLA	C1C-NC	-2.14	1.34	1.37
21	a	819	CLA	C1C-NC	-2.14	1.34	1.37
21	2	814	CLA	C1C-NC	-2.14	1.34	1.37
21	a	830	CLA	C1C-NC	-2.14	1.34	1.37
21	B	821	CLA	C3B-C2B	-2.14	1.37	1.40
21	A	808	CLA	C3B-C2B	-2.14	1.37	1.40
21	A	819	CLA	C3B-C2B	-2.14	1.37	1.40
21	b	1835	CLA	C1C-NC	-2.14	1.34	1.37
21	B	817	CLA	C1C-NC	-2.14	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	822	CLA	C1C-NC	-2.14	1.34	1.37
21	2	805	CLA	C1C-NC	-2.14	1.34	1.37
21	B	816	CLA	C3B-C2B	-2.14	1.37	1.40
21	A	835	CLA	C3B-C2B	-2.13	1.37	1.40
21	1	840	CLA	C1C-NC	-2.13	1.34	1.37
21	a	803	CLA	C1C-NC	-2.13	1.34	1.37
21	b	1831	CLA	C1C-NC	-2.13	1.34	1.37
21	l	205	CLA	C1C-NC	-2.13	1.34	1.37
21	a	823	CLA	C3B-C2B	-2.13	1.37	1.40
21	2	804	CLA	C1C-NC	-2.13	1.34	1.37
21	a	831	CLA	C1C-NC	-2.13	1.34	1.37
21	a	802	CLA	C3B-C2B	-2.13	1.37	1.40
21	B	809	CLA	C1C-NC	-2.13	1.34	1.37
21	b	1817	CLA	C3B-C2B	-2.13	1.37	1.40
21	1	826	CLA	C3B-C2B	-2.13	1.37	1.40
21	1	813	CLA	C1C-NC	-2.12	1.34	1.37
21	2	830	CLA	C1C-NC	-2.12	1.34	1.37
21	8	1401	CLA	C1C-NC	-2.12	1.34	1.37
21	b	1810	CLA	C1C-NC	-2.12	1.34	1.37
21	2	818	CLA	C1C-NC	-2.12	1.34	1.37
21	0	202	CLA	C3B-C2B	-2.12	1.37	1.40
21	L	205	CLA	C1C-NC	-2.12	1.34	1.37
21	B	836	CLA	C1C-NC	-2.12	1.34	1.37
21	b	1842	CLA	C1C-NC	-2.12	1.34	1.37
21	a	821	CLA	C3B-C2B	-2.12	1.37	1.40
21	a	807	CLA	C1C-NC	-2.12	1.34	1.37
21	2	838	CLA	C1C-NC	-2.12	1.34	1.37
21	b	1836	CLA	C1C-NC	-2.12	1.34	1.37
21	a	815	CLA	C3B-C2B	-2.12	1.37	1.40
21	1	809	CLA	C3B-C2B	-2.12	1.37	1.40
21	A	801	CLA	C3B-C2B	-2.12	1.37	1.40
21	2	816	CLA	C3B-C2B	-2.12	1.37	1.40
21	b	1836	CLA	C3B-C2B	-2.12	1.37	1.40
21	A	811	CLA	C1C-NC	-2.12	1.34	1.37
21	B	819	CLA	C1C-NC	-2.11	1.34	1.37
21	a	812	CLA	C1C-NC	-2.11	1.34	1.37
21	1	805	CLA	C3B-C2B	-2.11	1.37	1.40
21	2	810	CLA	C1C-NC	-2.11	1.34	1.37
21	7	1104	CLA	C1C-NC	-2.11	1.34	1.37
21	1	812	CLA	C1C-NC	-2.11	1.34	1.37
21	2	817	CLA	C1C-NC	-2.11	1.34	1.37
21	A	804	CLA	C3B-C2B	-2.11	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	846	ECH	C1-C6	-2.11	1.50	1.53
22	b	1844	PQN	C9-C10	-2.11	1.36	1.39
21	B	810	CLA	C1C-NC	-2.11	1.34	1.37
21	1	827	CLA	C3B-C2B	-2.11	1.37	1.40
21	a	815	CLA	C1C-NC	-2.11	1.34	1.37
21	b	1834	CLA	C1C-NC	-2.11	1.34	1.37
21	B	820	CLA	C1C-NC	-2.11	1.34	1.37
21	a	839	CLA	C3B-C2B	-2.11	1.37	1.40
21	K	103	CLA	C1C-NC	-2.11	1.34	1.37
21	b	1815	CLA	C3B-C2B	-2.11	1.37	1.40
21	B	816	CLA	C1C-NC	-2.11	1.34	1.37
21	B	838	CLA	C1C-NC	-2.11	1.34	1.37
21	b	1830	CLA	C3B-C2B	-2.11	1.37	1.40
21	B	818	CLA	C1C-NC	-2.11	1.34	1.37
21	B	835	CLA	C1C-NC	-2.11	1.34	1.37
21	a	811	CLA	C1C-NC	-2.11	1.34	1.37
21	b	1812	CLA	C1C-NC	-2.11	1.34	1.37
21	B	805	CLA	C1C-NC	-2.11	1.34	1.37
21	m	103	CLA	C1C-NC	-2.11	1.34	1.37
28	A	856	45D	O01-C17	-2.11	1.18	1.23
21	2	816	CLA	C1C-NC	-2.10	1.34	1.37
21	1	836	CLA	C3B-C2B	-2.10	1.37	1.40
21	A	802	CLA	C3B-C2B	-2.10	1.37	1.40
35	L	211	LMT	O3B-C3B	-2.10	1.38	1.43
21	b	1843	CLA	C3B-C2B	-2.10	1.37	1.40
21	a	818	CLA	C1C-NC	-2.10	1.34	1.37
21	b	1819	CLA	C1C-NC	-2.10	1.34	1.37
21	B	839	CLA	C1C-NC	-2.10	1.34	1.37
30	a	857	ECH	C1-C6	-2.10	1.50	1.53
21	2	837	CLA	C1C-NC	-2.10	1.34	1.37
21	B	827	CLA	C1C-NC	-2.10	1.34	1.37
21	B	811	CLA	C1C-NC	-2.10	1.34	1.37
21	1	824	CLA	C3B-C2B	-2.09	1.37	1.40
21	B	828	CLA	C1C-NC	-2.09	1.34	1.37
21	A	855	CLA	C1C-NC	-2.09	1.34	1.37
21	2	802	CLA	C1C-NC	-2.09	1.34	1.37
21	1	823	CLA	C3B-C2B	-2.09	1.37	1.40
21	a	834	CLA	C1C-NC	-2.09	1.34	1.37
21	F	202	CLA	C1C-NC	-2.09	1.34	1.37
21	2	829	CLA	C3B-C2B	-2.09	1.37	1.40
21	2	823	CLA	C3B-C2B	-2.09	1.37	1.40
21	2	808	CLA	C1C-NC	-2.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	1402	CLA	C1C-NC	-2.09	1.34	1.37
21	2	829	CLA	C1C-NC	-2.09	1.34	1.37
21	F	203	CLA	C1C-NC	-2.09	1.34	1.37
21	1	802	CLA	C3B-C2B	-2.09	1.37	1.40
21	1	806	CLA	C1C-NC	-2.09	1.34	1.37
21	1	813	CLA	C3B-C2B	-2.09	1.37	1.40
35	J	1104	LMT	O4'-C4B	-2.09	1.38	1.43
21	A	819	CLA	C1C-NC	-2.08	1.34	1.37
21	b	1821	CLA	C1C-NC	-2.08	1.34	1.37
21	b	1827	CLA	C1C-NC	-2.08	1.34	1.37
21	a	809	CLA	C3B-C2B	-2.08	1.37	1.40
21	l	203	CLA	C1C-NC	-2.08	1.34	1.37
21	b	1825	CLA	C1C-NC	-2.08	1.34	1.37
21	L	204	CLA	C3B-C2B	-2.08	1.37	1.40
21	B	809	CLA	C3B-C2B	-2.08	1.37	1.40
21	2	811	CLA	C3B-C2B	-2.08	1.37	1.40
30	B	844	ECH	C25-C26	-2.08	1.32	1.35
21	b	1814	CLA	C1C-NC	-2.08	1.34	1.37
21	2	803	CLA	C1C-NC	-2.08	1.34	1.37
21	B	813	CLA	C1C-NC	-2.08	1.34	1.37
21	a	832	CLA	C1C-NC	-2.08	1.34	1.37
21	A	840	CLA	C1C-NC	-2.08	1.34	1.37
21	b	1805	CLA	C1C-NC	-2.08	1.34	1.37
21	b	1843	CLA	C1C-NC	-2.08	1.34	1.37
21	B	829	CLA	C3B-C2B	-2.08	1.37	1.40
21	1	814	CLA	C1C-NC	-2.08	1.34	1.37
21	B	831	CLA	C1C-NC	-2.08	1.34	1.37
21	1	802	CLA	C1C-NC	-2.07	1.34	1.37
21	1	828	CLA	C1C-NC	-2.07	1.34	1.37
21	a	823	CLA	C1C-NC	-2.07	1.34	1.37
21	1	807	CLA	C1C-NC	-2.07	1.34	1.37
21	1	855	CLA	C1C-NC	-2.07	1.34	1.37
21	A	827	CLA	C1C-NC	-2.07	1.34	1.37
21	a	821	CLA	C1C-NC	-2.07	1.34	1.37
21	a	830	CLA	C3B-C2B	-2.07	1.37	1.40
21	8	1402	CLA	C3B-C2B	-2.07	1.37	1.40
21	B	840	CLA	C1C-NC	-2.07	1.34	1.37
21	1	831	CLA	C1C-NC	-2.07	1.34	1.37
21	B	814	CLA	C1C-NC	-2.07	1.34	1.37
21	A	815	CLA	C1C-NC	-2.07	1.34	1.37
21	1	801	CLA	C3B-C2B	-2.07	1.37	1.40
21	a	833	CLA	C1C-NC	-2.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	801	CLA	C1C-NC	-2.06	1.34	1.37
21	A	807	CLA	C3B-C2B	-2.06	1.37	1.40
21	1	830	CLA	C3B-C2B	-2.06	1.37	1.40
21	6	203	CLA	C1C-NC	-2.06	1.34	1.37
21	A	820	CLA	C1C-NC	-2.06	1.34	1.37
21	B	806	CLA	C1C-NC	-2.06	1.34	1.37
21	A	813	CLA	C1C-NC	-2.06	1.34	1.37
21	j	1103	CLA	C1C-NC	-2.06	1.34	1.37
21	1	827	CLA	C1C-NC	-2.06	1.34	1.37
21	1	804	CLA	C1C-NC	-2.06	1.34	1.37
21	2	802	CLA	C3B-C2B	-2.06	1.37	1.40
21	B	833	CLA	C1C-NC	-2.06	1.34	1.37
21	k	1401	CLA	C1C-NC	-2.05	1.34	1.37
21	A	818	CLA	C1C-NC	-2.05	1.34	1.37
21	A	854	CLA	C3B-C2B	-2.05	1.37	1.40
21	B	802	CLA	C1C-NC	-2.05	1.34	1.37
21	f	202	CLA	C1C-NC	-2.05	1.34	1.37
21	2	840	CLA	C1C-NC	-2.05	1.34	1.37
21	2	803	CLA	C3B-C2B	-2.05	1.37	1.40
21	1	809	CLA	C1C-NC	-2.05	1.34	1.37
21	1	815	CLA	C1C-NC	-2.05	1.34	1.37
21	1	801	CLA	C1C-NC	-2.05	1.34	1.37
21	a	804	CLA	C3B-C2B	-2.05	1.37	1.40
21	a	835	CLA	C1C-NC	-2.04	1.34	1.37
21	A	828	CLA	C1C-NC	-2.04	1.34	1.37
21	L	204	CLA	C1C-NC	-2.04	1.34	1.37
21	0	201	CLA	C1C-NC	-2.04	1.34	1.37
21	B	803	CLA	C1C-NC	-2.04	1.34	1.37
21	k	1402	CLA	C1C-NC	-2.04	1.34	1.37
21	a	855	CLA	C3B-C2B	-2.04	1.37	1.40
21	b	1811	CLA	C1C-NC	-2.04	1.34	1.37
21	1	818	CLA	C1C-NC	-2.04	1.34	1.37
21	A	803	CLA	C1C-NC	-2.04	1.34	1.37
21	2	819	CLA	C1C-NC	-2.04	1.34	1.37
21	j	1105	CLA	C1C-NC	-2.04	1.34	1.37
21	A	802	CLA	C1C-NC	-2.03	1.34	1.37
21	B	818	CLA	C3B-C2B	-2.03	1.37	1.40
21	A	824	CLA	C1C-NC	-2.03	1.34	1.37
21	b	1801	CLA	C1C-NC	-2.03	1.34	1.37
21	2	836	CLA	C1C-NC	-2.03	1.34	1.37
21	a	819	CLA	C3B-C2B	-2.03	1.37	1.40
21	2	806	CLA	C1C-NC	-2.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	826	CLA	C1C-NC	-2.03	1.34	1.37
21	2	842	CLA	C1C-NC	-2.03	1.34	1.37
21	a	806	CLA	C1C-NC	-2.03	1.34	1.37
21	B	814	CLA	C3B-C2B	-2.03	1.37	1.40
21	a	816	CLA	C1C-NC	-2.03	1.34	1.37
21	l	203	CLA	C3B-C2B	-2.03	1.37	1.40
35	1	854	LMT	O4'-C4B	-2.03	1.38	1.43
21	a	856	CLA	C3B-C2B	-2.03	1.37	1.40
21	2	817	CLA	C3B-C2B	-2.02	1.37	1.40
21	2	820	CLA	C1C-NC	-2.02	1.34	1.37
21	a	838	CLA	C1C-NC	-2.02	1.34	1.37
21	a	802	CLA	C1C-NC	-2.02	1.34	1.37
21	1	816	CLA	C1C-NC	-2.02	1.34	1.37
21	A	835	CLA	C1C-NC	-2.02	1.34	1.37
21	1	841	CLA	C1C-NC	-2.02	1.34	1.37
21	J	1106	CLA	C1C-NC	-2.02	1.34	1.37
21	a	825	CLA	C1C-NC	-2.02	1.34	1.37
21	b	1837	CLA	C1C-NC	-2.02	1.34	1.37
21	a	810	CLA	C1C-NC	-2.02	1.34	1.37
21	1	808	CLA	C1C-NC	-2.01	1.34	1.37
21	A	829	CLA	C1C-NC	-2.01	1.34	1.37
21	2	831	CLA	C1C-NC	-2.01	1.34	1.37
21	b	1839	CLA	C1C-NC	-2.01	1.34	1.37
21	1	832	CLA	C1C-NC	-2.01	1.34	1.37
21	b	1809	CLA	C1C-NC	-2.01	1.34	1.37
21	A	805	CLA	C3B-C2B	-2.01	1.37	1.40
28	2	854	45D	O01-C17	-2.01	1.18	1.23
21	1	823	CLA	C1C-NC	-2.01	1.34	1.37
21	A	805	CLA	C1C-NC	-2.01	1.34	1.37
21	A	814	CLA	C1C-NC	-2.01	1.34	1.37
21	b	1823	CLA	C1C-NC	-2.01	1.34	1.37
34	B	856	C7Z	C1-C6	-2.01	1.51	1.53
21	2	823	CLA	C1C-NC	-2.01	1.34	1.37
21	l	201	CLA	C1C-NC	-2.01	1.34	1.37
21	b	1833	CLA	C1C-NC	-2.00	1.34	1.37
21	b	1821	CLA	C3B-C2B	-2.00	1.37	1.40
21	b	1832	CLA	C1C-NC	-2.00	1.34	1.37
21	B	801	CLA	C1C-NC	-2.00	1.34	1.37
21	b	1820	CLA	C1C-NC	-2.00	1.34	1.37
21	6	204	CLA	C1C-NC	-2.00	1.34	1.37
21	l	204	CLA	C1C-NC	-2.00	1.34	1.37
21	b	1811	CLA	CHC-C1C	2.00	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1809	CLA	C1A-CHA	2.00	1.51	1.43
21	A	840	CLA	C1A-CHA	2.00	1.51	1.43
21	2	819	CLA	C1A-CHA	2.00	1.51	1.43
21	B	825	CLA	CHC-C1C	2.00	1.41	1.35
21	a	856	CLA	CHC-C1C	2.00	1.41	1.35
21	2	831	CLA	C1A-CHA	2.00	1.51	1.43
21	1	813	CLA	CHC-C1C	2.00	1.41	1.35
21	2	815	CLA	C1A-CHA	2.01	1.51	1.43
21	b	1812	CLA	CHC-C1C	2.01	1.41	1.35
26	K	105	LMG	O1-C1	2.01	1.43	1.40
21	B	824	CLA	C1A-CHA	2.01	1.51	1.43
21	1	807	CLA	C1A-CHA	2.01	1.51	1.43
21	A	819	CLA	C1A-CHA	2.01	1.51	1.43
21	b	1829	CLA	C1A-CHA	2.01	1.51	1.43
21	1	816	CLA	C1A-CHA	2.01	1.51	1.43
21	a	802	CLA	C1A-CHA	2.01	1.51	1.43
21	2	823	CLA	C1A-CHA	2.01	1.51	1.43
21	B	834	CLA	CHC-C1C	2.01	1.41	1.35
21	a	832	CLA	C1A-CHA	2.01	1.51	1.43
21	1	805	CLA	C1A-CHA	2.01	1.51	1.43
21	B	833	CLA	C1A-CHA	2.02	1.51	1.43
21	b	1842	CLA	CHC-C1C	2.02	1.41	1.35
21	1	826	CLA	C1A-CHA	2.02	1.51	1.43
21	2	842	CLA	C1A-CHA	2.02	1.51	1.43
21	b	1840	CLA	CHC-C1C	2.02	1.41	1.35
21	a	815	CLA	C1A-CHA	2.02	1.51	1.43
21	B	802	CLA	C1A-CHA	2.02	1.51	1.43
21	A	828	CLA	C1A-CHA	2.02	1.51	1.43
21	j	1105	CLA	C1A-CHA	2.02	1.51	1.43
21	1	835	CLA	C1A-CHA	2.02	1.51	1.43
21	2	812	CLA	CHC-C1C	2.02	1.41	1.35
21	B	813	CLA	CHC-C1C	2.02	1.41	1.35
21	b	1809	CLA	CHC-C1C	2.02	1.41	1.35
21	1	824	CLA	CHC-C1C	2.02	1.41	1.35
21	K	103	CLA	C1A-CHA	2.02	1.51	1.43
21	2	816	CLA	C1A-CHA	2.02	1.51	1.43
21	B	807	CLA	CHC-C1C	2.02	1.41	1.35
21	1	804	CLA	CHC-C1C	2.03	1.41	1.35
21	b	1837	CLA	C1A-CHA	2.03	1.51	1.43
21	B	815	CLA	C1A-CHA	2.03	1.51	1.43
21	B	821	CLA	CHC-C1C	2.03	1.41	1.35
21	b	1822	CLA	C1A-CHA	2.03	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	825	CLA	CHC-C1C	2.03	1.41	1.35
21	f	203	CLA	C1A-CHA	2.03	1.51	1.43
21	A	805	CLA	C1A-CHA	2.03	1.51	1.43
21	8	1401	CLA	C1A-CHA	2.03	1.51	1.43
21	a	828	CLA	C1A-CHA	2.03	1.51	1.43
21	a	829	CLA	C1A-CHA	2.03	1.51	1.43
21	a	808	CLA	C1A-CHA	2.03	1.51	1.43
21	B	825	CLA	C1A-CHA	2.03	1.51	1.43
21	b	1801	CLA	C1A-CHA	2.03	1.51	1.43
21	A	836	CLA	C1A-CHA	2.03	1.51	1.43
21	1	836	CLA	CHC-C1C	2.03	1.41	1.35
21	b	1836	CLA	C1A-CHA	2.03	1.51	1.43
21	A	809	CLA	C1A-CHA	2.03	1.51	1.43
21	b	1810	CLA	CHC-C1C	2.03	1.41	1.35
21	F	203	CLA	CHC-C1C	2.03	1.41	1.35
21	2	811	CLA	CHC-C1C	2.03	1.41	1.35
21	1	828	CLA	C1A-CHA	2.03	1.51	1.43
21	B	805	CLA	C1A-CHA	2.03	1.51	1.43
21	b	1827	CLA	C1A-CHA	2.03	1.51	1.43
21	2	802	CLA	C1A-CHA	2.04	1.51	1.43
21	2	804	CLA	C1A-CHA	2.04	1.51	1.43
21	A	812	CLA	C1A-CHA	2.04	1.51	1.43
21	a	816	CLA	C1A-CHA	2.04	1.51	1.43
21	A	839	CLA	C1A-CHA	2.04	1.51	1.43
21	b	1818	CLA	C1A-CHA	2.04	1.51	1.43
21	1	814	CLA	CHC-C1C	2.04	1.41	1.35
21	B	840	CLA	C1A-CHA	2.04	1.51	1.43
21	2	837	CLA	C1A-CHA	2.04	1.51	1.43
21	B	831	CLA	C1A-CHA	2.04	1.51	1.43
21	A	823	CLA	C1A-CHA	2.04	1.51	1.43
21	7	1103	CLA	C1A-CHA	2.04	1.51	1.43
21	2	808	CLA	C1A-CHA	2.04	1.51	1.43
21	2	838	CLA	C1A-CHA	2.04	1.51	1.43
21	a	824	CLA	CHC-C1C	2.04	1.41	1.35
21	B	827	CLA	CHC-C1C	2.04	1.41	1.35
21	a	819	CLA	C1A-CHA	2.04	1.51	1.43
21	a	837	CLA	C1A-CHA	2.04	1.51	1.43
21	1	806	CLA	C1A-CHA	2.04	1.51	1.43
21	A	804	CLA	CHC-C1C	2.04	1.41	1.35
21	m	103	CLA	C1A-CHA	2.04	1.51	1.43
21	7	1101	CLA	CHC-C1C	2.04	1.41	1.35
21	A	802	CLA	C1A-CHA	2.04	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	803	CLA	C1A-CHA	2.04	1.51	1.43
21	a	806	CLA	C1A-CHA	2.04	1.51	1.43
21	B	821	CLA	C1A-CHA	2.05	1.51	1.43
21	7	1103	CLA	CHC-C1C	2.05	1.41	1.35
21	b	1830	CLA	C1A-CHA	2.05	1.51	1.43
21	F	202	CLA	C1A-CHA	2.05	1.51	1.43
21	1	841	CLA	C1A-CHA	2.05	1.51	1.43
21	F	203	CLA	C1A-CHA	2.05	1.51	1.43
21	1	826	CLA	CHC-C1C	2.05	1.41	1.35
21	8	1402	CLA	C1A-CHA	2.05	1.51	1.43
21	a	838	CLA	C1A-CHA	2.05	1.51	1.43
21	B	807	CLA	C1A-CHA	2.05	1.51	1.43
21	1	820	CLA	C1A-CHA	2.05	1.51	1.43
21	B	826	CLA	C1A-CHA	2.05	1.51	1.43
21	b	1819	CLA	C1A-CHA	2.05	1.51	1.43
21	2	824	CLA	CHC-C1C	2.05	1.41	1.35
21	B	803	CLA	C1A-CHA	2.05	1.51	1.43
21	l	203	CLA	C1A-CHA	2.05	1.51	1.43
21	2	822	CLA	CHC-C1C	2.05	1.41	1.35
21	b	1831	CLA	CHC-C1C	2.05	1.41	1.35
21	1	834	CLA	C1A-CHA	2.05	1.51	1.43
21	a	826	CLA	CHC-C1C	2.05	1.41	1.35
21	2	826	CLA	CHC-C1C	2.05	1.41	1.35
21	b	1834	CLA	CHC-C1C	2.06	1.41	1.35
21	f	203	CLA	CHC-C1C	2.06	1.41	1.35
21	2	835	CLA	C1A-CHA	2.06	1.51	1.43
21	B	818	CLA	C1A-CHA	2.06	1.51	1.43
21	j	1101	CLA	C1A-CHA	2.06	1.51	1.43
21	F	202	CLA	CHC-C1C	2.06	1.41	1.35
21	1	820	CLA	CHC-C1C	2.06	1.41	1.35
21	b	1804	CLA	C1A-CHA	2.06	1.51	1.43
21	7	1101	CLA	C1A-CHA	2.06	1.51	1.43
21	A	813	CLA	CHC-C1C	2.06	1.41	1.35
21	B	818	CLA	CHC-C1C	2.06	1.41	1.35
21	L	204	CLA	CHC-C1C	2.06	1.41	1.35
21	B	834	CLA	C1A-CHA	2.06	1.51	1.43
21	K	102	CLA	CHC-C1C	2.06	1.41	1.35
21	A	826	CLA	CHC-C1C	2.06	1.41	1.35
21	2	829	CLA	CHC-C1C	2.06	1.41	1.35
21	a	840	CLA	CHC-C1C	2.07	1.41	1.35
21	a	855	CLA	CHC-C1C	2.07	1.41	1.35
21	2	814	CLA	CHC-C1C	2.07	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	828	CLA	CHC-C1C	2.07	1.41	1.35
21	A	834	CLA	C1A-CHA	2.07	1.51	1.43
21	1	829	CLA	C1A-CHA	2.07	1.51	1.43
21	B	822	CLA	CHC-C1C	2.07	1.41	1.35
21	L	203	CLA	CHC-C1C	2.07	1.41	1.35
21	6	201	CLA	C1A-CHA	2.07	1.51	1.43
21	1	806	CLA	CHC-C1C	2.07	1.41	1.35
21	b	1843	CLA	CHC-C1C	2.07	1.41	1.35
21	A	837	CLA	C1A-CHA	2.07	1.51	1.43
21	2	820	CLA	C1A-CHA	2.07	1.51	1.43
21	b	1829	CLA	CHC-C1C	2.07	1.41	1.35
21	2	826	CLA	C1A-CHA	2.07	1.51	1.43
21	2	828	CLA	C1A-CHA	2.07	1.51	1.43
21	6	203	CLA	CHC-C1C	2.07	1.41	1.35
21	b	1816	CLA	C1A-CHA	2.07	1.51	1.43
21	a	813	CLA	C1A-CHA	2.07	1.51	1.43
21	A	807	CLA	CHC-C1C	2.07	1.41	1.35
21	a	835	CLA	CHC-C1C	2.08	1.41	1.35
21	2	822	CLA	C1A-CHA	2.08	1.51	1.43
21	2	818	CLA	C1A-CHA	2.08	1.51	1.43
21	2	831	CLA	CHC-C1C	2.08	1.41	1.35
21	B	823	CLA	C1A-CHA	2.08	1.51	1.43
21	a	814	CLA	CHC-C1C	2.08	1.41	1.35
21	j	1103	CLA	C1A-CHA	2.08	1.51	1.43
21	1	811	CLA	C1A-CHA	2.08	1.51	1.43
21	B	804	CLA	C1A-CHA	2.08	1.51	1.43
21	2	804	CLA	CHC-C1C	2.08	1.41	1.35
21	j	1104	CLA	CHC-C1C	2.08	1.41	1.35
21	a	812	CLA	C1A-CHA	2.08	1.51	1.43
21	b	1833	CLA	CHC-C1C	2.08	1.41	1.35
21	b	1815	CLA	CHC-C1C	2.08	1.41	1.35
21	k	1402	CLA	C1A-CHA	2.08	1.51	1.43
21	B	811	CLA	CHC-C1C	2.08	1.41	1.35
21	b	1823	CLA	CHC-C1C	2.08	1.41	1.35
21	0	203	CLA	CHC-C1C	2.08	1.41	1.35
21	2	825	CLA	CHC-C1C	2.08	1.41	1.35
21	a	813	CLA	CHC-C1C	2.08	1.41	1.35
21	B	824	CLA	CHC-C1C	2.08	1.41	1.35
21	1	823	CLA	C1A-CHA	2.08	1.51	1.43
21	1	825	CLA	C1A-CHA	2.08	1.51	1.43
21	A	834	CLA	CHC-C1C	2.08	1.41	1.35
21	a	806	CLA	CHC-C1C	2.08	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	1106	CLA	C1A-CHA	2.08	1.51	1.43
21	a	822	CLA	C1A-CHA	2.08	1.51	1.43
21	1	827	CLA	C1A-CHA	2.08	1.51	1.43
21	a	809	CLA	CHC-C1C	2.09	1.41	1.35
21	a	811	CLA	CHC-C1C	2.09	1.41	1.35
21	a	823	CLA	C1A-CHA	2.09	1.51	1.43
21	2	833	CLA	CHC-C1C	2.09	1.41	1.35
21	A	838	CLA	C1A-CHA	2.09	1.51	1.43
21	L	205	CLA	CHC-C1C	2.09	1.41	1.35
21	b	1813	CLA	C1A-CHA	2.09	1.51	1.43
21	a	804	CLA	CHC-C1C	2.09	1.41	1.35
21	A	806	CLA	CHC-C1C	2.09	1.41	1.35
21	2	807	CLA	C1A-CHA	2.09	1.51	1.43
21	B	819	CLA	C1A-CHA	2.09	1.51	1.43
21	1	824	CLA	C1A-CHA	2.09	1.51	1.43
21	B	839	CLA	CHC-C1C	2.09	1.41	1.35
21	a	826	CLA	C1A-CHA	2.09	1.51	1.43
21	a	818	CLA	C1A-CHA	2.09	1.51	1.43
21	A	808	CLA	CHC-C1C	2.09	1.41	1.35
21	B	820	CLA	CHC-C1C	2.09	1.41	1.35
21	b	1834	CLA	C1A-CHA	2.09	1.51	1.43
21	2	835	CLA	CHC-C1C	2.09	1.41	1.35
21	1	810	CLA	CHC-C1C	2.09	1.41	1.35
21	a	808	CLA	CHC-C1C	2.09	1.41	1.35
21	B	817	CLA	C1A-CHA	2.10	1.51	1.43
21	a	817	CLA	CHC-C1C	2.10	1.41	1.35
21	2	802	CLA	CHC-C1C	2.10	1.41	1.35
21	6	201	CLA	CHC-C1C	2.10	1.41	1.35
21	A	823	CLA	CHC-C1C	2.10	1.41	1.35
21	1	812	CLA	CHC-C1C	2.10	1.41	1.35
21	1	819	CLA	CHC-C1C	2.10	1.41	1.35
21	1	834	CLA	CHC-C1C	2.10	1.41	1.35
21	2	825	CLA	C1A-CHA	2.10	1.51	1.43
21	2	832	CLA	C1A-CHA	2.10	1.51	1.43
21	B	812	CLA	C1A-CHA	2.10	1.51	1.43
21	1	811	CLA	CHC-C1C	2.10	1.41	1.35
21	b	1812	CLA	C1A-CHA	2.10	1.51	1.43
21	a	836	CLA	CHC-C1C	2.10	1.41	1.35
21	2	841	CLA	C1A-CHA	2.10	1.51	1.43
21	b	1804	CLA	CHC-C1C	2.10	1.41	1.35
21	a	827	CLA	C1A-CHA	2.10	1.51	1.43
21	b	1813	CLA	CHC-C1C	2.10	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	816	CLA	CHC-C1C	2.10	1.41	1.35
21	b	1823	CLA	C1A-CHA	2.11	1.52	1.43
21	B	813	CLA	C1A-CHA	2.11	1.52	1.43
21	B	836	CLA	CHC-C1C	2.11	1.41	1.35
26	a	852	LMG	O1-C1	2.11	1.43	1.40
21	A	815	CLA	CHC-C1C	2.11	1.41	1.35
21	1	808	CLA	CHC-C1C	2.11	1.41	1.35
21	a	824	CLA	C1A-CHA	2.11	1.52	1.43
21	a	834	CLA	C1A-CHA	2.11	1.52	1.43
21	1	815	CLA	C1A-CHA	2.11	1.52	1.43
21	8	1401	CLA	CHC-C1C	2.11	1.41	1.35
21	1	816	CLA	CHC-C1C	2.11	1.41	1.35
21	2	836	CLA	CHC-C1C	2.11	1.41	1.35
21	a	837	CLA	CHC-C1C	2.11	1.41	1.35
21	B	814	CLA	C1A-CHA	2.11	1.52	1.43
21	1	839	CLA	C1A-CHA	2.11	1.52	1.43
21	B	816	CLA	CHC-C1C	2.11	1.41	1.35
21	a	840	CLA	C1A-CHA	2.11	1.52	1.43
21	a	855	CLA	C1A-CHA	2.11	1.52	1.43
21	b	1824	CLA	C1A-CHA	2.11	1.52	1.43
21	B	805	CLA	CHC-C1C	2.11	1.41	1.35
21	a	830	CLA	CHC-C1C	2.11	1.41	1.35
21	1	855	CLA	CHC-C1C	2.11	1.41	1.35
21	A	839	CLA	CHC-C1C	2.11	1.41	1.35
21	2	833	CLA	C1A-CHA	2.11	1.52	1.43
21	B	808	CLA	CHC-C1C	2.11	1.41	1.35
21	A	816	CLA	CHC-C1C	2.11	1.41	1.35
21	1	812	CLA	C1A-CHA	2.11	1.52	1.43
21	1	815	CLA	CHC-C1C	2.11	1.41	1.35
21	b	1826	CLA	CHC-C1C	2.11	1.41	1.35
21	a	810	CLA	C1A-CHA	2.11	1.52	1.43
21	a	811	CLA	C1A-CHA	2.11	1.52	1.43
21	J	1106	CLA	CHC-C1C	2.11	1.41	1.35
21	a	839	CLA	CHC-C1C	2.11	1.41	1.35
21	1	817	CLA	CHC-C1C	2.12	1.41	1.35
21	B	826	CLA	CHC-C1C	2.12	1.41	1.35
21	1	821	CLA	CHC-C1C	2.12	1.41	1.35
21	B	833	CLA	CHC-C1C	2.12	1.41	1.35
21	1	813	CLA	C1A-CHA	2.12	1.52	1.43
21	A	831	CLA	CHC-C1C	2.12	1.41	1.35
21	7	1104	CLA	C1A-CHA	2.12	1.52	1.43
21	A	854	CLA	CHC-C1C	2.12	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	809	CLA	CHC-C1C	2.12	1.41	1.35
21	a	804	CLA	C1A-CHA	2.12	1.52	1.43
21	B	810	CLA	C1A-CHA	2.12	1.52	1.43
21	b	1805	CLA	CHC-C1C	2.12	1.41	1.35
21	a	815	CLA	CHC-C1C	2.12	1.41	1.35
21	B	806	CLA	CHC-C1C	2.12	1.41	1.35
21	j	1104	CLA	C1A-CHA	2.12	1.52	1.43
21	b	1814	CLA	CHC-C1C	2.12	1.41	1.35
21	a	821	CLA	CHC-C1C	2.12	1.41	1.35
21	1	822	CLA	CHC-C1C	2.12	1.41	1.35
21	A	812	CLA	CHC-C1C	2.12	1.41	1.35
21	j	1103	CLA	CHC-C1C	2.12	1.41	1.35
21	b	1819	CLA	CHC-C1C	2.13	1.41	1.35
21	1	803	CLA	CHC-C1C	2.13	1.41	1.35
21	A	803	CLA	CHC-C1C	2.13	1.41	1.35
21	l	201	CLA	CHC-C1C	2.13	1.41	1.35
21	2	819	CLA	CHC-C1C	2.13	1.41	1.35
21	b	1824	CLA	CHC-C1C	2.13	1.41	1.35
21	B	803	CLA	CHC-C1C	2.13	1.41	1.35
21	2	817	CLA	C1A-CHA	2.13	1.52	1.43
21	A	854	CLA	C1A-CHA	2.13	1.52	1.43
21	A	817	CLA	CHC-C1C	2.13	1.41	1.35
21	a	833	CLA	CHC-C1C	2.13	1.41	1.35
21	a	814	CLA	C1A-CHA	2.13	1.52	1.43
21	b	1838	CLA	CHC-C1C	2.13	1.41	1.35
21	b	1843	CLA	C1A-CHA	2.13	1.52	1.43
21	L	203	CLA	C1A-CHA	2.13	1.52	1.43
21	2	807	CLA	CHC-C1C	2.13	1.41	1.35
21	B	839	CLA	C1A-CHA	2.13	1.52	1.43
21	1	840	CLA	CHC-C1C	2.13	1.41	1.35
21	2	838	CLA	CHC-C1C	2.13	1.41	1.35
21	a	816	CLA	CHC-C1C	2.13	1.41	1.35
21	2	839	CLA	CHC-C1C	2.13	1.41	1.35
21	B	832	CLA	CHC-C1C	2.13	1.41	1.35
21	j	1105	CLA	CHC-C1C	2.13	1.41	1.35
21	7	1105	CLA	C1A-CHA	2.13	1.52	1.43
21	2	812	CLA	C1A-CHA	2.14	1.52	1.43
21	2	803	CLA	C1A-CHA	2.14	1.52	1.43
21	B	810	CLA	CHC-C1C	2.14	1.41	1.35
21	a	838	CLA	CHC-C1C	2.14	1.41	1.35
21	2	832	CLA	CHC-C1C	2.14	1.41	1.35
21	2	811	CLA	C1A-CHA	2.14	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	k	1402	CLA	CHC-C1C	2.14	1.41	1.35
21	a	829	CLA	CHC-C1C	2.14	1.41	1.35
21	1	804	CLA	C1A-CHA	2.14	1.52	1.43
21	1	829	CLA	CHC-C1C	2.14	1.41	1.35
21	2	830	CLA	CHC-C1C	2.14	1.41	1.35
21	k	1401	CLA	C1A-CHA	2.14	1.52	1.43
21	7	1104	CLA	CHC-C1C	2.14	1.41	1.35
21	a	823	CLA	CHC-C1C	2.14	1.41	1.35
21	a	819	CLA	CHC-C1C	2.14	1.41	1.35
21	b	1821	CLA	CHC-C1C	2.14	1.41	1.35
21	1	814	CLA	C1A-CHA	2.14	1.52	1.43
21	2	806	CLA	C1A-CHA	2.15	1.52	1.43
21	a	818	CLA	CHC-C1C	2.15	1.41	1.35
21	b	1816	CLA	CHC-C1C	2.15	1.41	1.35
21	A	810	CLA	CHC-C1C	2.15	1.41	1.35
21	A	820	CLA	CHC-C1C	2.15	1.41	1.35
21	B	835	CLA	CHC-C1C	2.15	1.41	1.35
21	f	202	CLA	CHC-C1C	2.15	1.41	1.35
21	2	814	CLA	C1A-CHA	2.15	1.52	1.43
21	B	820	CLA	C1A-CHA	2.15	1.52	1.43
21	2	820	CLA	CHC-C1C	2.15	1.41	1.35
21	B	816	CLA	C1A-CHA	2.15	1.52	1.43
21	a	801	CLA	C1A-CHA	2.15	1.52	1.43
21	2	834	CLA	CHC-C1C	2.15	1.41	1.35
21	I	101	CLA	CHC-C1C	2.15	1.41	1.35
21	1	838	CLA	CHC-C1C	2.15	1.41	1.35
21	a	827	CLA	CHC-C1C	2.16	1.41	1.35
21	B	840	CLA	CHC-C1C	2.16	1.41	1.35
21	a	803	CLA	CHC-C1C	2.16	1.41	1.35
21	b	1825	CLA	CHC-C1C	2.16	1.41	1.35
21	2	842	CLA	CHC-C1C	2.16	1.41	1.35
21	b	1805	CLA	C1A-CHA	2.16	1.52	1.43
21	A	830	CLA	CHC-C1C	2.16	1.41	1.35
21	1	822	CLA	C1A-CHA	2.16	1.52	1.43
21	A	837	CLA	CHC-C1C	2.16	1.41	1.35
21	8	1402	CLA	CHC-C1C	2.16	1.41	1.35
21	A	825	CLA	CHC-C1C	2.16	1.41	1.35
21	1	818	CLA	CHC-C1C	2.16	1.41	1.35
21	B	830	CLA	CHC-C1C	2.16	1.41	1.35
21	b	1826	CLA	C1A-CHA	2.16	1.52	1.43
21	b	1822	CLA	CHC-C1C	2.17	1.41	1.35
21	B	837	CLA	CHC-C1C	2.17	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	831	CLA	CHC-C1C	2.17	1.41	1.35
21	a	825	CLA	C1A-CHA	2.17	1.52	1.43
21	2	836	CLA	C1A-CHA	2.17	1.52	1.43
21	1	801	CLA	C1A-CHA	2.17	1.52	1.43
21	A	818	CLA	CHC-C1C	2.17	1.41	1.35
21	2	815	CLA	CHC-C1C	2.17	1.41	1.35
21	2	818	CLA	CHC-C1C	2.17	1.41	1.35
21	2	808	CLA	CHC-C1C	2.17	1.41	1.35
21	b	1807	CLA	C1A-CHA	2.17	1.52	1.43
21	b	1808	CLA	CHC-C1C	2.17	1.41	1.35
21	1	835	CLA	CHC-C1C	2.17	1.41	1.35
21	1	809	CLA	CHC-C1C	2.17	1.41	1.35
21	1	839	CLA	CHC-C1C	2.17	1.41	1.35
26	A	850	LMG	O1-C1	2.17	1.44	1.40
21	J	1105	CLA	CHC-C1C	2.17	1.41	1.35
21	J	1105	CLA	C1A-CHA	2.17	1.52	1.43
21	a	810	CLA	CHC-C1C	2.17	1.41	1.35
21	B	815	CLA	CHC-C1C	2.17	1.41	1.35
21	a	812	CLA	CHC-C1C	2.18	1.41	1.35
21	b	1820	CLA	CHC-C1C	2.18	1.41	1.35
21	j	1101	CLA	CHC-C1C	2.18	1.41	1.35
21	B	802	CLA	CHC-C1C	2.18	1.41	1.35
21	A	832	CLA	CHC-C1C	2.18	1.41	1.35
21	A	813	CLA	C1A-CHA	2.18	1.52	1.43
21	0	201	CLA	CHC-C1C	2.18	1.41	1.35
21	A	833	CLA	CHC-C1C	2.18	1.41	1.35
21	1	832	CLA	CHC-C1C	2.18	1.41	1.35
21	2	840	CLA	CHC-C1C	2.18	1.41	1.35
21	b	1806	CLA	CHC-C1C	2.18	1.41	1.35
21	2	813	CLA	CHC-C1C	2.18	1.41	1.35
21	k	1401	CLA	CHC-C1C	2.18	1.41	1.35
21	2	837	CLA	CHC-C1C	2.18	1.41	1.35
21	A	821	CLA	CHC-C1C	2.18	1.41	1.35
21	1	801	CLA	CHC-C1C	2.19	1.41	1.35
21	b	1836	CLA	CHC-C1C	2.19	1.41	1.35
21	2	805	CLA	C1A-CHA	2.19	1.52	1.43
21	B	823	CLA	CHC-C1C	2.19	1.41	1.35
21	B	819	CLA	CHC-C1C	2.19	1.41	1.35
21	A	819	CLA	CHC-C1C	2.19	1.41	1.35
21	1	833	CLA	CHC-C1C	2.19	1.41	1.35
21	2	817	CLA	CHC-C1C	2.19	1.41	1.35
21	B	814	CLA	CHC-C1C	2.19	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1837	CLA	CHC-C1C	2.19	1.41	1.35
21	m	103	CLA	CHC-C1C	2.20	1.41	1.35
21	A	811	CLA	CHC-C1C	2.20	1.41	1.35
21	B	831	CLA	CHC-C1C	2.20	1.41	1.35
21	a	834	CLA	CHC-C1C	2.20	1.41	1.35
21	2	806	CLA	CHC-C1C	2.20	1.41	1.35
21	b	1839	CLA	CHC-C1C	2.20	1.41	1.35
21	l	205	CLA	CHC-C1C	2.20	1.41	1.35
21	2	805	CLA	CHC-C1C	2.20	1.41	1.35
21	2	823	CLA	CHC-C1C	2.20	1.41	1.35
21	J	1103	CLA	CHC-C1C	2.21	1.41	1.35
21	2	803	CLA	CHC-C1C	2.21	1.41	1.35
21	A	805	CLA	CHC-C1C	2.21	1.41	1.35
21	1	807	CLA	CHC-C1C	2.21	1.41	1.35
21	A	828	CLA	CHC-C1C	2.21	1.41	1.35
21	a	802	CLA	CHC-C1C	2.21	1.41	1.35
21	a	836	CLA	C1A-CHA	2.21	1.52	1.43
21	1	827	CLA	CHC-C1C	2.21	1.41	1.35
21	0	202	CLA	CHC-C1C	2.21	1.41	1.35
21	1	802	CLA	CHC-C1C	2.22	1.41	1.35
21	B	828	CLA	CHC-C1C	2.22	1.41	1.35
21	a	832	CLA	CHC-C1C	2.22	1.41	1.35
21	b	1817	CLA	CHC-C1C	2.22	1.41	1.35
21	a	820	CLA	CHC-C1C	2.22	1.41	1.35
21	B	801	CLA	CHC-C1C	2.22	1.41	1.35
21	b	1801	CLA	CHC-C1C	2.23	1.41	1.35
21	b	1818	CLA	CHC-C1C	2.23	1.41	1.35
21	A	824	CLA	C1A-CHA	2.23	1.52	1.43
21	l	204	CLA	CHC-C1C	2.23	1.41	1.35
21	b	1835	CLA	CHC-C1C	2.23	1.41	1.35
21	A	809	CLA	CHC-C1C	2.23	1.41	1.35
21	b	1828	CLA	CHC-C1C	2.23	1.41	1.35
21	a	828	CLA	CHC-C1C	2.24	1.41	1.35
21	a	831	CLA	CHC-C1C	2.24	1.41	1.35
21	B	829	CLA	C1C-C2C	2.24	1.48	1.44
21	A	838	CLA	CHC-C1C	2.24	1.41	1.35
21	2	821	CLA	CHC-C1C	2.24	1.41	1.35
21	B	825	CLA	C1C-C2C	2.25	1.48	1.44
21	b	1832	CLA	CHC-C1C	2.26	1.41	1.35
21	A	827	CLA	CHC-C1C	2.26	1.41	1.35
21	1	828	CLA	CHC-C1C	2.26	1.41	1.35
21	a	801	CLA	CHC-C1C	2.26	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	827	CLA	CHC-C1C	2.26	1.41	1.35
21	B	838	CLA	CHC-C1C	2.26	1.41	1.35
21	6	204	CLA	CHC-C1C	2.27	1.41	1.35
21	6	204	CLA	C1A-CHA	2.27	1.52	1.43
21	A	840	CLA	CHC-C1C	2.27	1.41	1.35
36	L	201	EQ3	C27-C26	2.27	1.52	1.47
21	1	802	CLA	C1A-CHA	2.27	1.52	1.43
21	I	101	CLA	C1A-CHA	2.27	1.52	1.43
21	A	814	CLA	CHC-C1C	2.28	1.41	1.35
21	A	801	CLA	CHC-C1C	2.29	1.41	1.35
21	b	1807	CLA	CHC-C1C	2.31	1.42	1.35
21	B	809	CLA	C1C-C2C	2.31	1.49	1.44
21	1	837	CLA	CHC-C1C	2.32	1.42	1.35
36	L	201	EQ3	C17-C18	2.34	1.38	1.35
21	1	841	CLA	CHC-C1C	2.34	1.42	1.35
21	A	804	CLA	C1C-C2C	2.34	1.49	1.44
21	b	1827	CLA	C1C-C2C	2.34	1.49	1.44
21	B	804	CLA	CHC-C1C	2.35	1.42	1.35
28	2	854	45D	C18-C16	2.36	1.52	1.47
28	A	856	45D	C17-C15	2.37	1.52	1.47
21	A	836	CLA	CHC-C1C	2.37	1.42	1.35
21	1	830	CLA	C1C-C2C	2.39	1.49	1.44
21	1	805	CLA	C1C-C2C	2.39	1.49	1.44
21	A	802	CLA	CHC-C1C	2.40	1.42	1.35
21	B	805	CLA	C1C-C2C	2.41	1.49	1.44
21	2	810	CLA	C1C-C2C	2.41	1.49	1.44
21	J	1101	CLA	CHC-C1C	2.42	1.42	1.35
21	a	805	CLA	C1C-C2C	2.42	1.49	1.44
36	L	201	EQ3	C40-C30	2.43	1.58	1.53
21	A	855	CLA	C1C-C2C	2.43	1.49	1.44
21	A	824	CLA	C1C-C2C	2.45	1.49	1.44
21	A	829	CLA	C1C-C2C	2.45	1.49	1.44
21	b	1812	CLA	C1C-C2C	2.46	1.49	1.44
36	L	201	EQ3	C28-C27	2.47	1.54	1.50
21	a	811	CLA	C1C-C2C	2.47	1.49	1.44
21	A	835	CLA	C1C-C2C	2.49	1.49	1.44
21	a	856	CLA	C1C-C2C	2.50	1.49	1.44
21	b	1841	CLA	C1C-C2C	2.50	1.49	1.44
21	A	822	CLA	C1C-C2C	2.51	1.49	1.44
21	1	804	CLA	C1C-C2C	2.51	1.49	1.44
21	2	841	CLA	C1C-C2C	2.51	1.49	1.44
21	2	831	CLA	C1C-C2C	2.51	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	807	CLA	C1C-C2C	2.52	1.49	1.44
28	2	854	45D	C17-C15	2.52	1.53	1.47
21	A	823	CLA	C1C-C2C	2.52	1.49	1.44
21	A	825	CLA	C1C-C2C	2.54	1.49	1.44
21	b	1811	CLA	C1C-C2C	2.54	1.49	1.44
21	A	838	CLA	C1C-C2C	2.54	1.49	1.44
21	b	1840	CLA	C1C-C2C	2.54	1.49	1.44
21	1	825	CLA	C1C-C2C	2.55	1.49	1.44
21	1	819	CLA	C1C-C2C	2.55	1.49	1.44
21	7	1105	CLA	C1C-C2C	2.55	1.49	1.44
21	A	810	CLA	C1C-C2C	2.56	1.49	1.44
21	A	816	CLA	C1C-C2C	2.56	1.49	1.44
21	a	804	CLA	C1C-C2C	2.56	1.49	1.44
21	1	824	CLA	C1C-C2C	2.56	1.49	1.44
21	a	826	CLA	C1C-C2C	2.56	1.49	1.44
21	m	103	CLA	C1C-C2C	2.57	1.49	1.44
21	b	1810	CLA	C1C-C2C	2.57	1.49	1.44
21	K	103	CLA	C1C-C2C	2.57	1.49	1.44
21	l	203	CLA	C1C-C2C	2.57	1.49	1.44
21	B	813	CLA	C1C-C2C	2.57	1.49	1.44
21	L	204	CLA	C1C-C2C	2.57	1.49	1.44
21	b	1828	CLA	C1C-C2C	2.58	1.49	1.44
21	B	817	CLA	C1C-C2C	2.58	1.49	1.44
21	1	821	CLA	C1C-C2C	2.58	1.49	1.44
21	B	821	CLA	C1C-C2C	2.58	1.49	1.44
21	2	819	CLA	C1C-C2C	2.58	1.49	1.44
21	a	824	CLA	C1C-C2C	2.58	1.49	1.44
21	2	829	CLA	C1C-C2C	2.59	1.49	1.44
21	a	809	CLA	C1C-C2C	2.59	1.49	1.44
21	A	837	CLA	C1C-C2C	2.59	1.49	1.44
21	2	840	CLA	C1C-C2C	2.59	1.49	1.44
21	A	839	CLA	C1C-C2C	2.59	1.49	1.44
21	2	804	CLA	C1C-C2C	2.60	1.49	1.44
21	1	835	CLA	C1C-C2C	2.60	1.49	1.44
21	b	1832	CLA	C1C-C2C	2.60	1.49	1.44
21	a	830	CLA	C1C-C2C	2.60	1.49	1.44
21	b	1833	CLA	C1C-C2C	2.61	1.49	1.44
21	1	806	CLA	C1C-C2C	2.61	1.49	1.44
21	a	822	CLA	C1C-C2C	2.61	1.49	1.44
21	F	203	CLA	C1C-C2C	2.61	1.49	1.44
21	A	813	CLA	C1C-C2C	2.61	1.49	1.44
21	a	807	CLA	C1C-C2C	2.61	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	834	CLA	C1C-C2C	2.61	1.49	1.44
21	B	810	CLA	C1C-C2C	2.61	1.49	1.44
21	A	854	CLA	C1C-C2C	2.61	1.49	1.44
21	0	203	CLA	C1C-C2C	2.61	1.49	1.44
21	2	802	CLA	C1C-C2C	2.62	1.49	1.44
21	a	840	CLA	C1C-C2C	2.62	1.49	1.44
21	B	802	CLA	C1C-C2C	2.62	1.49	1.44
21	1	813	CLA	C1C-C2C	2.62	1.49	1.44
21	1	823	CLA	C1C-C2C	2.62	1.49	1.44
21	1	817	CLA	C1C-C2C	2.62	1.49	1.44
21	1	855	CLA	C1C-C2C	2.62	1.49	1.44
21	b	1831	CLA	C1C-C2C	2.62	1.49	1.44
21	b	1816	CLA	C1C-C2C	2.63	1.49	1.44
21	a	816	CLA	C1C-C2C	2.63	1.49	1.44
21	b	1819	CLA	C1C-C2C	2.63	1.49	1.44
21	2	826	CLA	C1C-C2C	2.63	1.49	1.44
21	b	1809	CLA	C1C-C2C	2.63	1.49	1.44
21	1	826	CLA	C1C-C2C	2.63	1.49	1.44
21	K	102	CLA	C1C-C2C	2.63	1.49	1.44
21	F	202	CLA	C1C-C2C	2.64	1.49	1.44
21	b	1814	CLA	C1C-C2C	2.64	1.49	1.44
21	B	833	CLA	C1C-C2C	2.64	1.49	1.44
21	A	812	CLA	C1C-C2C	2.64	1.49	1.44
21	A	820	CLA	C1C-C2C	2.64	1.49	1.44
21	6	203	CLA	C1C-C2C	2.64	1.49	1.44
21	B	824	CLA	C1C-C2C	2.64	1.49	1.44
21	2	824	CLA	C1C-C2C	2.64	1.49	1.44
21	A	831	CLA	C1C-C2C	2.64	1.49	1.44
21	B	834	CLA	C1C-C2C	2.65	1.49	1.44
21	1	814	CLA	C1C-C2C	2.65	1.49	1.44
21	b	1829	CLA	C1C-C2C	2.65	1.49	1.44
21	A	815	CLA	C1C-C2C	2.65	1.49	1.44
21	A	808	CLA	C1C-C2C	2.65	1.49	1.44
21	A	802	CLA	C1C-C2C	2.65	1.49	1.44
21	a	808	CLA	C1C-C2C	2.65	1.49	1.44
21	j	1103	CLA	C1C-C2C	2.66	1.49	1.44
21	a	833	CLA	C1C-C2C	2.66	1.49	1.44
21	A	834	CLA	C1C-C2C	2.66	1.49	1.44
21	2	835	CLA	C1C-C2C	2.66	1.49	1.44
21	l	201	CLA	C1C-C2C	2.66	1.49	1.44
21	2	830	CLA	C1C-C2C	2.66	1.49	1.44
21	a	813	CLA	C1C-C2C	2.67	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1815	CLA	C1C-C2C	2.67	1.49	1.44
21	B	808	CLA	C1C-C2C	2.67	1.49	1.44
21	f	203	CLA	C1C-C2C	2.67	1.49	1.44
21	b	1830	CLA	C1C-C2C	2.67	1.49	1.44
21	b	1839	CLA	C1C-C2C	2.67	1.49	1.44
21	2	811	CLA	C1C-C2C	2.67	1.49	1.44
21	2	836	CLA	C1C-C2C	2.67	1.49	1.44
36	L	201	EQ3	C20-C21	2.67	1.51	1.43
21	j	1104	CLA	C1C-C2C	2.67	1.49	1.44
21	a	837	CLA	C1C-C2C	2.67	1.49	1.44
21	1	820	CLA	C1C-C2C	2.67	1.49	1.44
21	b	1801	CLA	C1C-C2C	2.67	1.49	1.44
21	2	817	CLA	C1C-C2C	2.68	1.49	1.44
21	L	203	CLA	C1C-C2C	2.68	1.49	1.44
21	2	814	CLA	C1C-C2C	2.68	1.49	1.44
21	8	1401	CLA	C1C-C2C	2.68	1.49	1.44
21	1	836	CLA	C1C-C2C	2.68	1.49	1.44
21	b	1817	CLA	C1C-C2C	2.68	1.49	1.44
21	A	830	CLA	C1C-C2C	2.68	1.49	1.44
21	b	1822	CLA	C1C-C2C	2.68	1.49	1.44
21	a	835	CLA	C1C-C2C	2.68	1.49	1.44
21	L	205	CLA	C1C-C2C	2.68	1.49	1.44
21	A	833	CLA	C1C-C2C	2.68	1.49	1.44
21	b	1834	CLA	C1C-C2C	2.68	1.49	1.44
21	1	816	CLA	C1C-C2C	2.68	1.49	1.44
21	A	807	CLA	C1C-C2C	2.68	1.49	1.44
21	a	825	CLA	C1C-C2C	2.68	1.49	1.44
21	1	840	CLA	C1C-C2C	2.68	1.49	1.44
21	6	201	CLA	C1C-C2C	2.68	1.49	1.44
21	B	812	CLA	C1C-C2C	2.69	1.49	1.44
21	a	814	CLA	C1C-C2C	2.69	1.49	1.44
21	a	806	CLA	C1C-C2C	2.69	1.49	1.44
21	B	803	CLA	C1C-C2C	2.69	1.49	1.44
21	B	827	CLA	C1C-C2C	2.69	1.49	1.44
21	b	1836	CLA	C1C-C2C	2.69	1.49	1.44
21	2	832	CLA	C1C-C2C	2.69	1.49	1.44
21	b	1826	CLA	C1C-C2C	2.69	1.49	1.44
21	A	826	CLA	C1C-C2C	2.69	1.49	1.44
21	a	817	CLA	C1C-C2C	2.69	1.49	1.44
21	B	820	CLA	C1C-C2C	2.69	1.49	1.44
21	1	808	CLA	C1C-C2C	2.69	1.49	1.44
21	k	1401	CLA	C1C-C2C	2.70	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	827	CLA	C1C-C2C	2.70	1.49	1.44
21	2	809	CLA	C1C-C2C	2.70	1.49	1.44
21	2	833	CLA	C1C-C2C	2.70	1.49	1.44
21	8	1402	CLA	C1C-C2C	2.70	1.49	1.44
21	2	823	CLA	C1C-C2C	2.70	1.49	1.44
21	A	840	CLA	C1C-C2C	2.71	1.49	1.44
21	2	815	CLA	C1C-C2C	2.71	1.49	1.44
21	1	838	CLA	C1C-C2C	2.71	1.49	1.44
21	b	1842	CLA	C1C-C2C	2.71	1.49	1.44
21	2	818	CLA	C1C-C2C	2.71	1.49	1.44
21	a	819	CLA	C1C-C2C	2.71	1.49	1.44
21	2	822	CLA	C1C-C2C	2.71	1.49	1.44
21	a	839	CLA	C1C-C2C	2.71	1.49	1.44
36	L	201	EQ3	C24-C25	2.71	1.55	1.45
21	2	812	CLA	C1C-C2C	2.72	1.49	1.44
21	a	836	CLA	C1C-C2C	2.72	1.49	1.44
21	0	201	CLA	C1C-C2C	2.72	1.49	1.44
21	A	801	CLA	C1C-C2C	2.72	1.49	1.44
21	B	811	CLA	C1C-C2C	2.72	1.49	1.44
21	1	811	CLA	C1C-C2C	2.72	1.49	1.44
21	a	821	CLA	C1C-C2C	2.72	1.49	1.44
21	b	1821	CLA	C1C-C2C	2.72	1.49	1.44
21	B	822	CLA	C1C-C2C	2.73	1.49	1.44
21	A	806	CLA	C1C-C2C	2.73	1.49	1.44
21	a	827	CLA	C1C-C2C	2.73	1.49	1.44
21	2	816	CLA	C1C-C2C	2.73	1.49	1.44
21	a	823	CLA	C1C-C2C	2.73	1.49	1.44
21	B	818	CLA	C1C-C2C	2.73	1.49	1.44
21	b	1823	CLA	C1C-C2C	2.73	1.49	1.44
21	2	825	CLA	C1C-C2C	2.73	1.49	1.44
21	b	1805	CLA	C1C-C2C	2.73	1.49	1.44
21	B	840	CLA	C1C-C2C	2.73	1.49	1.44
21	B	816	CLA	C1C-C2C	2.73	1.49	1.44
21	1	822	CLA	C1C-C2C	2.74	1.49	1.44
21	2	828	CLA	C1C-C2C	2.74	1.49	1.44
21	2	806	CLA	C1C-C2C	2.74	1.49	1.44
21	k	1402	CLA	C1C-C2C	2.74	1.49	1.44
36	L	201	EQ3	C33-C5	2.74	1.55	1.51
21	b	1813	CLA	C1C-C2C	2.74	1.49	1.44
21	a	832	CLA	C1C-C2C	2.75	1.49	1.44
21	1	812	CLA	C1C-C2C	2.75	1.49	1.44
21	J	1103	CLA	C1C-C2C	2.75	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	1103	CLA	C1C-C2C	2.75	1.49	1.44
21	b	1807	CLA	C1C-C2C	2.75	1.49	1.44
21	a	815	CLA	C1C-C2C	2.75	1.49	1.44
21	7	1104	CLA	C1C-C2C	2.75	1.49	1.44
21	b	1837	CLA	C1C-C2C	2.75	1.49	1.44
21	2	807	CLA	C1C-C2C	2.75	1.49	1.44
21	A	817	CLA	C1C-C2C	2.76	1.49	1.44
21	J	1106	CLA	C1C-C2C	2.76	1.49	1.44
21	b	1804	CLA	C1C-C2C	2.76	1.49	1.44
21	J	1105	CLA	C1C-C2C	2.76	1.49	1.44
21	7	1101	CLA	C1C-C2C	2.76	1.49	1.44
21	I	101	CLA	C1C-C2C	2.76	1.49	1.44
21	1	810	CLA	C1C-C2C	2.76	1.49	1.44
21	1	815	CLA	C1C-C2C	2.76	1.49	1.44
28	A	856	45D	C19-C07	2.76	1.55	1.45
21	a	802	CLA	C1C-C2C	2.77	1.49	1.44
21	a	834	CLA	C1C-C2C	2.77	1.49	1.44
21	B	826	CLA	C1C-C2C	2.77	1.49	1.44
21	b	1825	CLA	C1C-C2C	2.77	1.49	1.44
21	a	838	CLA	C1C-C2C	2.77	1.49	1.44
21	a	812	CLA	C1C-C2C	2.77	1.49	1.44
21	l	205	CLA	C1C-C2C	2.77	1.49	1.44
21	1	809	CLA	C1C-C2C	2.77	1.49	1.44
21	1	831	CLA	C1C-C2C	2.77	1.49	1.44
21	2	808	CLA	C1C-C2C	2.78	1.49	1.44
21	1	818	CLA	C1C-C2C	2.78	1.49	1.44
21	A	811	CLA	C1C-C2C	2.78	1.49	1.44
21	B	823	CLA	C1C-C2C	2.79	1.49	1.44
21	a	831	CLA	C1C-C2C	2.79	1.49	1.44
21	a	810	CLA	C1C-C2C	2.79	1.49	1.44
21	b	1808	CLA	C1C-C2C	2.79	1.49	1.44
21	b	1818	CLA	C1C-C2C	2.79	1.49	1.44
21	A	814	CLA	C1C-C2C	2.79	1.49	1.44
21	6	204	CLA	C1C-C2C	2.79	1.49	1.44
21	B	831	CLA	C1C-C2C	2.79	1.49	1.44
21	B	814	CLA	C1C-C2C	2.80	1.49	1.44
21	b	1824	CLA	C1C-C2C	2.80	1.49	1.44
21	A	805	CLA	C1C-C2C	2.80	1.49	1.44
21	A	819	CLA	C1C-C2C	2.80	1.49	1.44
21	l	204	CLA	C1C-C2C	2.80	1.49	1.44
21	a	803	CLA	C1C-C2C	2.80	1.49	1.44
21	2	838	CLA	C1C-C2C	2.80	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	818	CLA	C1C-C2C	2.80	1.49	1.44
21	A	809	CLA	C1C-C2C	2.80	1.50	1.44
21	a	855	CLA	C1C-C2C	2.80	1.50	1.44
21	1	839	CLA	C1C-C2C	2.81	1.50	1.44
21	2	805	CLA	C1C-C2C	2.81	1.50	1.44
21	b	1843	CLA	C1C-C2C	2.81	1.50	1.44
21	B	838	CLA	C1C-C2C	2.81	1.50	1.44
21	1	833	CLA	C1C-C2C	2.81	1.50	1.44
21	2	820	CLA	C1C-C2C	2.82	1.50	1.44
21	1	802	CLA	C1C-C2C	2.82	1.50	1.44
21	B	839	CLA	C1C-C2C	2.82	1.50	1.44
21	2	813	CLA	C1C-C2C	2.83	1.50	1.44
21	1	807	CLA	C1C-C2C	2.83	1.50	1.44
21	j	1101	CLA	C1C-C2C	2.83	1.50	1.44
21	B	836	CLA	C1C-C2C	2.83	1.50	1.44
21	A	821	CLA	C1C-C2C	2.83	1.50	1.44
21	B	837	CLA	C1C-C2C	2.83	1.50	1.44
21	a	829	CLA	C1C-C2C	2.83	1.50	1.44
21	B	835	CLA	C1C-C2C	2.83	1.50	1.44
21	2	803	CLA	C1C-C2C	2.83	1.50	1.44
28	2	854	45D	C19-C07	2.83	1.55	1.45
21	j	1105	CLA	C1C-C2C	2.84	1.50	1.44
21	2	821	CLA	C1C-C2C	2.84	1.50	1.44
21	b	1835	CLA	C1C-C2C	2.84	1.50	1.44
21	a	828	CLA	C1C-C2C	2.84	1.50	1.44
21	A	803	CLA	C1C-C2C	2.84	1.50	1.44
21	A	827	CLA	C1C-C2C	2.84	1.50	1.44
21	2	834	CLA	C1C-C2C	2.85	1.50	1.44
21	1	832	CLA	C1C-C2C	2.85	1.50	1.44
36	L	201	EQ3	C16-C17	2.85	1.52	1.43
21	b	1806	CLA	C1C-C2C	2.85	1.50	1.44
21	A	818	CLA	C1C-C2C	2.85	1.50	1.44
21	2	839	CLA	C1C-C2C	2.85	1.50	1.44
21	a	801	CLA	C1C-C2C	2.86	1.50	1.44
21	b	1820	CLA	C1C-C2C	2.86	1.50	1.44
21	b	1838	CLA	C1C-C2C	2.87	1.50	1.44
21	2	842	CLA	C1C-C2C	2.87	1.50	1.44
21	1	803	CLA	C1C-C2C	2.87	1.50	1.44
21	A	832	CLA	C1C-C2C	2.87	1.50	1.44
21	1	801	CLA	C1C-C2C	2.87	1.50	1.44
21	B	815	CLA	C1C-C2C	2.87	1.50	1.44
21	a	820	CLA	C1C-C2C	2.88	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	0	202	CLA	C1C-C2C	2.88	1.50	1.44
21	B	806	CLA	C1C-C2C	2.88	1.50	1.44
21	1	829	CLA	C1C-C2C	2.88	1.50	1.44
21	B	830	CLA	C1C-C2C	2.89	1.50	1.44
21	f	202	CLA	C1C-C2C	2.89	1.50	1.44
21	2	837	CLA	C1C-C2C	2.90	1.50	1.44
21	B	832	CLA	C1C-C2C	2.90	1.50	1.44
21	1	841	CLA	C1C-C2C	2.90	1.50	1.44
21	B	819	CLA	C1C-C2C	2.91	1.50	1.44
21	1	837	CLA	C1C-C2C	2.91	1.50	1.44
21	B	828	CLA	C1C-C2C	2.91	1.50	1.44
21	1	828	CLA	C1C-C2C	2.93	1.50	1.44
21	A	828	CLA	C1C-C2C	2.93	1.50	1.44
21	A	836	CLA	C1C-C2C	2.95	1.50	1.44
21	B	804	CLA	C1C-C2C	2.95	1.50	1.44
21	1	827	CLA	C1C-C2C	2.96	1.50	1.44
28	2	854	45D	C32-C30	2.97	1.52	1.43
36	L	201	EQ3	C2-C1	2.98	1.64	1.54
28	A	856	45D	C20-C08	3.00	1.56	1.45
21	J	1101	CLA	C1C-C2C	3.01	1.50	1.44
21	B	801	CLA	C1C-C2C	3.02	1.50	1.44
28	2	854	45D	C20-C08	3.03	1.56	1.45
21	1	855	CLA	CBB-CAB	3.09	1.50	1.28
21	A	855	CLA	CBB-CAB	3.10	1.50	1.28
21	J	1101	CLA	CBB-CAB	3.10	1.50	1.28
21	2	831	CLA	CBB-CAB	3.12	1.50	1.28
21	b	1820	CLA	CBB-CAB	3.13	1.50	1.28
21	b	1818	CLA	CBB-CAB	3.13	1.50	1.28
21	1	839	CLA	CBB-CAB	3.14	1.51	1.28
21	b	1841	CLA	CBB-CAB	3.14	1.51	1.28
21	1	837	CLA	CBB-CAB	3.14	1.51	1.28
36	L	201	EQ3	C38-C26	3.14	1.57	1.50
21	A	817	CLA	CBB-CAB	3.14	1.51	1.28
21	b	1839	CLA	CBB-CAB	3.14	1.51	1.28
21	A	833	CLA	CBB-CAB	3.15	1.51	1.28
21	B	815	CLA	CBB-CAB	3.15	1.51	1.28
21	2	834	CLA	CBB-CAB	3.15	1.51	1.28
21	B	809	CLA	CBB-CAB	3.15	1.51	1.28
21	B	840	CLA	CBB-CAB	3.15	1.51	1.28
21	2	825	CLA	CBB-CAB	3.16	1.51	1.28
21	b	1831	CLA	CBB-CAB	3.16	1.51	1.28
21	b	1823	CLA	CBB-CAB	3.16	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	813	CLA	CBB-CAB	3.16	1.51	1.28
21	B	817	CLA	CBB-CAB	3.16	1.51	1.28
21	2	812	CLA	CBB-CAB	3.16	1.51	1.28
21	b	1835	CLA	CBB-CAB	3.16	1.51	1.28
21	b	1815	CLA	CBB-CAB	3.16	1.51	1.28
21	2	810	CLA	CBB-CAB	3.16	1.51	1.28
21	1	818	CLA	CBB-CAB	3.17	1.51	1.28
21	a	837	CLA	CBB-CAB	3.17	1.51	1.28
21	a	812	CLA	CBB-CAB	3.17	1.51	1.28
21	A	836	CLA	CBB-CAB	3.17	1.51	1.28
21	2	833	CLA	CBB-CAB	3.17	1.51	1.28
21	B	830	CLA	CBB-CAB	3.17	1.51	1.28
21	B	828	CLA	CBB-CAB	3.17	1.51	1.28
21	1	814	CLA	CBB-CAB	3.17	1.51	1.28
21	F	203	CLA	CBB-CAB	3.17	1.51	1.28
21	1	823	CLA	CBB-CAB	3.18	1.51	1.28
21	A	840	CLA	CBB-CAB	3.18	1.51	1.28
21	B	832	CLA	CBB-CAB	3.18	1.51	1.28
21	2	832	CLA	CBB-CAB	3.18	1.51	1.28
21	B	822	CLA	CBB-CAB	3.18	1.51	1.28
21	1	829	CLA	CBB-CAB	3.18	1.51	1.28
21	1	832	CLA	CBB-CAB	3.18	1.51	1.28
21	A	808	CLA	CBB-CAB	3.18	1.51	1.28
21	a	856	CLA	CBB-CAB	3.18	1.51	1.28
21	b	1826	CLA	CBB-CAB	3.18	1.51	1.28
21	b	1832	CLA	CBB-CAB	3.18	1.51	1.28
21	0	201	CLA	CBB-CAB	3.18	1.51	1.28
21	2	819	CLA	CBB-CAB	3.18	1.51	1.28
21	A	811	CLA	CBB-CAB	3.18	1.51	1.28
21	a	835	CLA	CBB-CAB	3.18	1.51	1.28
21	1	838	CLA	CBB-CAB	3.18	1.51	1.28
21	A	830	CLA	CBB-CAB	3.18	1.51	1.28
21	a	818	CLA	CBB-CAB	3.19	1.51	1.28
21	1	813	CLA	CBB-CAB	3.19	1.51	1.28
21	B	801	CLA	CBB-CAB	3.19	1.51	1.28
21	1	812	CLA	CBB-CAB	3.19	1.51	1.28
21	a	831	CLA	CBB-CAB	3.19	1.51	1.28
21	A	822	CLA	CBB-CAB	3.19	1.51	1.28
21	L	204	CLA	CBB-CAB	3.19	1.51	1.28
21	1	831	CLA	CBB-CAB	3.19	1.51	1.28
21	b	1837	CLA	CBB-CAB	3.19	1.51	1.28
21	A	801	CLA	CBB-CAB	3.19	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	808	CLA	CBB-CAB	3.19	1.51	1.28
21	I	101	CLA	CBB-CAB	3.19	1.51	1.28
21	2	830	CLA	CBB-CAB	3.19	1.51	1.28
21	A	815	CLA	CBB-CAB	3.19	1.51	1.28
21	2	804	CLA	CBB-CAB	3.19	1.51	1.28
21	j	1101	CLA	CBB-CAB	3.19	1.51	1.28
21	A	827	CLA	CBB-CAB	3.19	1.51	1.28
21	A	816	CLA	CBB-CAB	3.19	1.51	1.28
21	a	813	CLA	CBB-CAB	3.19	1.51	1.28
21	B	839	CLA	CBB-CAB	3.19	1.51	1.28
36	L	201	EQ3	C35-C13	3.19	1.57	1.50
21	A	839	CLA	CBB-CAB	3.20	1.51	1.28
21	1	834	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1814	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1819	CLA	CBB-CAB	3.20	1.51	1.28
21	B	808	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1816	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1810	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1822	CLA	CBB-CAB	3.20	1.51	1.28
21	1	807	CLA	CBB-CAB	3.20	1.51	1.28
21	a	821	CLA	CBB-CAB	3.20	1.51	1.28
21	a	829	CLA	CBB-CAB	3.20	1.51	1.28
21	B	826	CLA	CBB-CAB	3.20	1.51	1.28
21	a	833	CLA	CBB-CAB	3.20	1.51	1.28
21	a	801	CLA	CBB-CAB	3.20	1.51	1.28
21	2	828	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1834	CLA	CBB-CAB	3.20	1.51	1.28
21	a	805	CLA	CBB-CAB	3.20	1.51	1.28
21	a	838	CLA	CBB-CAB	3.20	1.51	1.28
21	2	840	CLA	CBB-CAB	3.20	1.51	1.28
21	0	202	CLA	CBB-CAB	3.20	1.51	1.28
21	B	811	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1825	CLA	CBB-CAB	3.20	1.51	1.28
21	B	805	CLA	CBB-CAB	3.20	1.51	1.28
21	B	836	CLA	CBB-CAB	3.20	1.51	1.28
21	B	818	CLA	CBB-CAB	3.20	1.51	1.28
21	a	809	CLA	CBB-CAB	3.20	1.51	1.28
21	A	837	CLA	CBB-CAB	3.20	1.51	1.28
21	A	821	CLA	CBB-CAB	3.20	1.51	1.28
21	7	1104	CLA	CBB-CAB	3.20	1.51	1.28
21	a	839	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1805	CLA	CBB-CAB	3.20	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	807	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1809	CLA	CBB-CAB	3.20	1.51	1.28
21	1	826	CLA	CBB-CAB	3.20	1.51	1.28
21	A	823	CLA	CBB-CAB	3.20	1.51	1.28
21	A	835	CLA	CBB-CAB	3.20	1.51	1.28
21	A	825	CLA	CBB-CAB	3.20	1.51	1.28
21	B	834	CLA	CBB-CAB	3.20	1.51	1.28
21	2	842	CLA	CBB-CAB	3.20	1.51	1.28
21	1	828	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1811	CLA	CBB-CAB	3.20	1.51	1.28
21	b	1833	CLA	CBB-CAB	3.20	1.51	1.28
21	a	832	CLA	CBB-CAB	3.20	1.51	1.28
21	2	823	CLA	CBB-CAB	3.21	1.51	1.28
21	A	819	CLA	CBB-CAB	3.21	1.51	1.28
21	1	840	CLA	CBB-CAB	3.21	1.51	1.28
21	f	203	CLA	CBB-CAB	3.21	1.51	1.28
21	b	1807	CLA	CBB-CAB	3.21	1.51	1.28
21	1	810	CLA	CBB-CAB	3.21	1.51	1.28
21	2	816	CLA	CBB-CAB	3.21	1.51	1.28
21	f	202	CLA	CBB-CAB	3.21	1.51	1.28
21	a	817	CLA	CBB-CAB	3.21	1.51	1.28
21	a	824	CLA	CBB-CAB	3.21	1.51	1.28
21	2	820	CLA	CBB-CAB	3.21	1.51	1.28
21	A	806	CLA	CBB-CAB	3.21	1.51	1.28
21	B	807	CLA	CBB-CAB	3.21	1.51	1.28
21	2	813	CLA	CBB-CAB	3.21	1.51	1.28
21	1	803	CLA	CBB-CAB	3.21	1.51	1.28
21	2	824	CLA	CBB-CAB	3.21	1.51	1.28
21	6	201	CLA	CBB-CAB	3.21	1.51	1.28
21	b	1842	CLA	CBB-CAB	3.21	1.51	1.28
21	0	203	CLA	CBB-CAB	3.21	1.51	1.28
21	1	801	CLA	CBB-CAB	3.21	1.51	1.28
21	b	1801	CLA	CBB-CAB	3.21	1.51	1.28
21	B	819	CLA	CBB-CAB	3.21	1.51	1.28
21	1	809	CLA	CBB-CAB	3.21	1.51	1.28
21	B	803	CLA	CBB-CAB	3.21	1.51	1.28
21	A	809	CLA	CBB-CAB	3.21	1.51	1.28
21	a	834	CLA	CBB-CAB	3.21	1.51	1.28
21	a	836	CLA	CBB-CAB	3.21	1.51	1.28
21	2	835	CLA	CBB-CAB	3.21	1.51	1.28
21	B	824	CLA	CBB-CAB	3.21	1.51	1.28
21	2	826	CLA	CBB-CAB	3.21	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	836	CLA	CBB-CAB	3.21	1.51	1.28
21	b	1829	CLA	CBB-CAB	3.21	1.51	1.28
21	B	812	CLA	CBB-CAB	3.21	1.51	1.28
21	A	829	CLA	CBB-CAB	3.21	1.51	1.28
21	B	838	CLA	CBB-CAB	3.21	1.51	1.28
21	2	806	CLA	CBB-CAB	3.21	1.51	1.28
21	A	814	CLA	CBB-CAB	3.21	1.51	1.28
21	J	1106	CLA	CBB-CAB	3.21	1.51	1.28
21	b	1824	CLA	CBB-CAB	3.21	1.51	1.28
21	b	1817	CLA	CBB-CAB	3.21	1.51	1.28
21	1	825	CLA	CBB-CAB	3.21	1.51	1.28
21	2	822	CLA	CBB-CAB	3.21	1.51	1.28
21	A	854	CLA	CBB-CAB	3.21	1.51	1.28
21	a	814	CLA	CBB-CAB	3.21	1.51	1.28
21	b	1813	CLA	CBB-CAB	3.21	1.51	1.28
21	2	803	CLA	CBB-CAB	3.21	1.51	1.28
21	A	826	CLA	CBB-CAB	3.21	1.51	1.28
21	1	817	CLA	CBB-CAB	3.21	1.51	1.28
21	a	810	CLA	CBB-CAB	3.21	1.51	1.28
21	b	1806	CLA	CBB-CAB	3.22	1.51	1.28
21	B	833	CLA	CBB-CAB	3.22	1.51	1.28
21	B	820	CLA	CBB-CAB	3.22	1.51	1.28
21	l	204	CLA	CBB-CAB	3.22	1.51	1.28
21	b	1827	CLA	CBB-CAB	3.22	1.51	1.28
21	a	803	CLA	CBB-CAB	3.22	1.51	1.28
21	a	822	CLA	CBB-CAB	3.22	1.51	1.28
21	J	1103	CLA	CBB-CAB	3.22	1.51	1.28
21	k	1402	CLA	CBB-CAB	3.22	1.51	1.28
21	B	829	CLA	CBB-CAB	3.22	1.51	1.28
21	a	827	CLA	CBB-CAB	3.22	1.51	1.28
21	a	826	CLA	CBB-CAB	3.22	1.51	1.28
21	b	1804	CLA	CBB-CAB	3.22	1.51	1.28
21	B	814	CLA	CBB-CAB	3.22	1.51	1.28
21	B	821	CLA	CBB-CAB	3.22	1.51	1.28
21	F	202	CLA	CBB-CAB	3.22	1.51	1.28
21	2	818	CLA	CBB-CAB	3.22	1.51	1.28
21	a	811	CLA	CBB-CAB	3.22	1.51	1.28
21	2	808	CLA	CBB-CAB	3.22	1.51	1.28
21	b	1812	CLA	CBB-CAB	3.22	1.51	1.28
21	A	807	CLA	CBB-CAB	3.22	1.51	1.28
21	2	802	CLA	CBB-CAB	3.22	1.51	1.28
21	2	838	CLA	CBB-CAB	3.22	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	804	CLA	CBB-CAB	3.22	1.51	1.28
21	A	812	CLA	CBB-CAB	3.22	1.51	1.28
21	a	825	CLA	CBB-CAB	3.22	1.51	1.28
21	1	819	CLA	CBB-CAB	3.22	1.51	1.28
21	m	103	CLA	CBB-CAB	3.22	1.51	1.28
21	a	802	CLA	CBB-CAB	3.22	1.51	1.28
21	1	806	CLA	CBB-CAB	3.22	1.51	1.28
21	j	1103	CLA	CBB-CAB	3.22	1.51	1.28
21	A	834	CLA	CBB-CAB	3.22	1.51	1.28
21	2	841	CLA	CBB-CAB	3.22	1.51	1.28
21	J	1105	CLA	CBB-CAB	3.22	1.51	1.28
21	2	807	CLA	CBB-CAB	3.22	1.51	1.28
21	L	205	CLA	CBB-CAB	3.22	1.51	1.28
21	1	802	CLA	CBB-CAB	3.22	1.51	1.28
21	7	1105	CLA	CBB-CAB	3.22	1.51	1.28
21	A	832	CLA	CBB-CAB	3.22	1.51	1.28
21	A	804	CLA	CBB-CAB	3.22	1.51	1.28
21	a	816	CLA	CBB-CAB	3.22	1.51	1.28
21	1	824	CLA	CBB-CAB	3.22	1.51	1.28
21	a	855	CLA	CBB-CAB	3.22	1.51	1.28
21	2	829	CLA	CBB-CAB	3.22	1.51	1.28
21	2	815	CLA	CBB-CAB	3.22	1.51	1.28
21	j	1105	CLA	CBB-CAB	3.22	1.51	1.28
21	1	841	CLA	CBB-CAB	3.22	1.51	1.28
21	B	825	CLA	CBB-CAB	3.22	1.51	1.28
21	1	830	CLA	CBB-CAB	3.22	1.51	1.28
21	1	822	CLA	CBB-CAB	3.22	1.51	1.28
21	1	811	CLA	CBB-CAB	3.22	1.51	1.28
21	1	808	CLA	CBB-CAB	3.23	1.51	1.28
21	b	1840	CLA	CBB-CAB	3.23	1.51	1.28
21	b	1843	CLA	CBB-CAB	3.23	1.51	1.28
21	2	827	CLA	CBB-CAB	3.23	1.51	1.28
21	B	823	CLA	CBB-CAB	3.23	1.51	1.28
21	2	839	CLA	CBB-CAB	3.23	1.51	1.28
21	2	809	CLA	CBB-CAB	3.23	1.51	1.28
21	B	837	CLA	CBB-CAB	3.23	1.51	1.28
21	K	103	CLA	CBB-CAB	3.23	1.51	1.28
21	B	813	CLA	CBB-CAB	3.23	1.51	1.28
21	1	821	CLA	CBB-CAB	3.23	1.51	1.28
21	l	201	CLA	CBB-CAB	3.23	1.51	1.28
21	7	1101	CLA	CBB-CAB	3.23	1.51	1.28
21	2	836	CLA	CBB-CAB	3.23	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	805	CLA	CBB-CAB	3.23	1.51	1.28
21	b	1821	CLA	CBB-CAB	3.23	1.51	1.28
21	b	1836	CLA	CBB-CAB	3.23	1.51	1.28
21	8	1401	CLA	CBB-CAB	3.23	1.51	1.28
21	B	804	CLA	CBB-CAB	3.23	1.51	1.28
21	1	816	CLA	CBB-CAB	3.23	1.51	1.28
21	2	811	CLA	CBB-CAB	3.23	1.51	1.28
21	1	820	CLA	CBB-CAB	3.23	1.51	1.28
21	1	815	CLA	CBB-CAB	3.23	1.51	1.28
21	2	821	CLA	CBB-CAB	3.23	1.51	1.28
21	2	814	CLA	CBB-CAB	3.23	1.51	1.28
21	1	827	CLA	CBB-CAB	3.23	1.51	1.28
21	B	802	CLA	CBB-CAB	3.23	1.51	1.28
21	1	835	CLA	CBB-CAB	3.23	1.51	1.28
21	b	1830	CLA	CBB-CAB	3.23	1.51	1.28
21	A	820	CLA	CBB-CAB	3.23	1.51	1.28
21	a	804	CLA	CBB-CAB	3.23	1.51	1.28
21	a	828	CLA	CBB-CAB	3.23	1.51	1.28
21	a	806	CLA	CBB-CAB	3.23	1.51	1.28
21	a	820	CLA	CBB-CAB	3.23	1.51	1.28
21	A	838	CLA	CBB-CAB	3.23	1.51	1.28
21	1	805	CLA	CBB-CAB	3.23	1.51	1.28
21	B	827	CLA	CBB-CAB	3.23	1.51	1.28
21	A	803	CLA	CBB-CAB	3.23	1.51	1.28
21	K	102	CLA	CBB-CAB	3.23	1.51	1.28
21	k	1401	CLA	CBB-CAB	3.23	1.51	1.28
21	a	823	CLA	CBB-CAB	3.23	1.51	1.28
21	a	840	CLA	CBB-CAB	3.23	1.51	1.28
21	a	830	CLA	CBB-CAB	3.23	1.51	1.28
21	A	831	CLA	CBB-CAB	3.23	1.51	1.28
21	2	817	CLA	CBB-CAB	3.23	1.51	1.28
21	8	1402	CLA	CBB-CAB	3.23	1.51	1.28
21	b	1828	CLA	CBB-CAB	3.23	1.51	1.28
21	B	810	CLA	CBB-CAB	3.24	1.51	1.28
21	A	810	CLA	CBB-CAB	3.24	1.51	1.28
21	2	805	CLA	CBB-CAB	3.24	1.51	1.28
21	l	205	CLA	CBB-CAB	3.24	1.51	1.28
21	7	1103	CLA	CBB-CAB	3.24	1.51	1.28
21	L	203	CLA	CBB-CAB	3.24	1.51	1.28
21	6	203	CLA	CBB-CAB	3.24	1.51	1.28
21	B	831	CLA	CBB-CAB	3.24	1.51	1.28
21	b	1838	CLA	CBB-CAB	3.24	1.51	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	824	CLA	CBB-CAB	3.24	1.51	1.28
21	B	835	CLA	CBB-CAB	3.24	1.51	1.28
21	l	203	CLA	CBB-CAB	3.24	1.51	1.28
21	B	816	CLA	CBB-CAB	3.24	1.51	1.28
21	a	819	CLA	CBB-CAB	3.24	1.51	1.28
21	a	815	CLA	CBB-CAB	3.24	1.51	1.28
21	6	204	CLA	CBB-CAB	3.24	1.51	1.28
21	1	833	CLA	CBB-CAB	3.25	1.51	1.28
21	A	802	CLA	CBB-CAB	3.25	1.51	1.28
21	A	828	CLA	CBB-CAB	3.25	1.51	1.28
21	2	837	CLA	CBB-CAB	3.25	1.51	1.28
21	j	1104	CLA	CBB-CAB	3.25	1.51	1.28
21	b	1808	CLA	CBB-CAB	3.27	1.51	1.28
21	A	818	CLA	CBB-CAB	3.27	1.51	1.28
21	B	806	CLA	CBB-CAB	3.27	1.51	1.28
28	2	854	45D	C31-C29	3.40	1.54	1.43
28	2	854	45D	C41-C37	3.46	1.54	1.43
28	A	856	45D	C31-C29	3.48	1.54	1.43
28	A	856	45D	C32-C30	3.57	1.54	1.43
28	2	854	45D	C42-C38	3.65	1.54	1.43
28	A	856	45D	C41-C37	3.68	1.54	1.43
36	L	201	EQ3	C19-C18	3.70	1.53	1.45
36	L	201	EQ3	C7-C6	3.70	1.58	1.45
28	A	856	45D	C42-C38	3.72	1.55	1.43
36	L	201	EQ3	C12-C13	3.74	1.54	1.45
36	L	201	EQ3	C23-C22	3.92	1.54	1.45
28	2	854	45D	C34-C36	4.03	1.54	1.45
28	2	854	45D	C24-C26	4.05	1.54	1.45
28	A	856	45D	C34-C36	4.21	1.55	1.45
28	2	854	45D	C33-C35	4.21	1.55	1.45
28	A	856	45D	C33-C35	4.34	1.55	1.45
28	A	856	45D	C24-C26	4.46	1.55	1.45
36	L	201	EQ3	C15-C14	4.51	1.57	1.43
36	L	201	EQ3	C11-C10	4.53	1.57	1.43
28	2	854	45D	C23-C25	4.63	1.56	1.45
28	A	856	45D	C23-C25	4.74	1.56	1.45
21	J	1101	CLA	CHB-C4A	5.08	1.40	1.33
21	1	831	CLA	CHB-C4A	5.32	1.40	1.33
21	2	833	CLA	CHB-C4A	5.34	1.40	1.33
21	A	820	CLA	CHB-C4A	5.35	1.40	1.33
21	A	835	CLA	CHB-C4A	5.39	1.40	1.33
21	2	812	CLA	CHB-C4A	5.39	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	831	CLA	CHB-C4A	5.40	1.40	1.33
21	A	837	CLA	CHB-C4A	5.40	1.40	1.33
21	a	855	CLA	CHB-C4A	5.41	1.40	1.33
21	B	816	CLA	CHB-C4A	5.44	1.40	1.33
21	B	830	CLA	CHB-C4A	5.44	1.40	1.33
21	2	819	CLA	CHB-C4A	5.46	1.40	1.33
21	b	1811	CLA	CHB-C4A	5.47	1.40	1.33
21	B	817	CLA	CHB-C4A	5.48	1.40	1.33
21	a	835	CLA	CHB-C4A	5.49	1.40	1.33
21	b	1821	CLA	CHB-C4A	5.49	1.40	1.33
21	b	1818	CLA	CHB-C4A	5.49	1.40	1.33
21	I	101	CLA	CHB-C4A	5.51	1.40	1.33
21	a	812	CLA	CHB-C4A	5.51	1.40	1.33
21	1	839	CLA	CHB-C4A	5.51	1.40	1.33
21	b	1832	CLA	CHB-C4A	5.51	1.40	1.33
21	A	807	CLA	CHB-C4A	5.52	1.40	1.33
21	2	832	CLA	CHB-C4A	5.53	1.40	1.33
21	l	204	CLA	CHB-C4A	5.55	1.40	1.33
21	a	803	CLA	CHB-C4A	5.56	1.40	1.33
21	a	829	CLA	CHB-C4A	5.56	1.40	1.33
21	b	1822	CLA	CHB-C4A	5.57	1.40	1.33
21	A	811	CLA	CHB-C4A	5.57	1.40	1.33
21	1	833	CLA	CHB-C4A	5.58	1.40	1.33
21	b	1813	CLA	CHB-C4A	5.58	1.40	1.33
21	2	831	CLA	CHB-C4A	5.58	1.40	1.33
21	2	829	CLA	CHB-C4A	5.58	1.40	1.33
21	A	802	CLA	CHB-C4A	5.59	1.40	1.33
21	1	838	CLA	CHB-C4A	5.61	1.40	1.33
21	a	834	CLA	CHB-C4A	5.61	1.40	1.33
21	B	822	CLA	CHB-C4A	5.61	1.40	1.33
21	b	1829	CLA	CHB-C4A	5.62	1.40	1.33
21	2	820	CLA	CHB-C4A	5.62	1.40	1.33
21	1	840	CLA	CHB-C4A	5.63	1.40	1.33
21	B	819	CLA	CHB-C4A	5.63	1.40	1.33
21	A	838	CLA	CHB-C4A	5.63	1.40	1.33
21	1	841	CLA	CHB-C4A	5.63	1.40	1.33
21	b	1828	CLA	CHB-C4A	5.64	1.40	1.33
21	A	804	CLA	CHB-C4A	5.64	1.40	1.33
21	A	854	CLA	CHB-C4A	5.65	1.40	1.33
21	A	817	CLA	CHB-C4A	5.65	1.40	1.33
21	K	103	CLA	CHB-C4A	5.65	1.40	1.33
21	a	818	CLA	CHB-C4A	5.65	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1830	CLA	CHB-C4A	5.66	1.40	1.33
21	2	814	CLA	CHB-C4A	5.66	1.40	1.33
21	L	204	CLA	CHB-C4A	5.66	1.40	1.33
21	a	805	CLA	CHB-C4A	5.66	1.40	1.33
21	a	825	CLA	CHB-C4A	5.66	1.40	1.33
21	B	831	CLA	CHB-C4A	5.66	1.40	1.33
21	B	833	CLA	CHB-C4A	5.66	1.40	1.33
21	B	837	CLA	CHB-C4A	5.67	1.40	1.33
21	A	825	CLA	CHB-C4A	5.67	1.40	1.33
21	B	824	CLA	CHB-C4A	5.68	1.40	1.33
21	1	813	CLA	CHB-C4A	5.68	1.40	1.33
21	A	833	CLA	CHB-C4A	5.68	1.40	1.33
21	b	1801	CLA	CHB-C4A	5.68	1.40	1.33
21	1	809	CLA	CHB-C4A	5.68	1.40	1.33
21	a	802	CLA	CHB-C4A	5.68	1.40	1.33
21	2	840	CLA	CHB-C4A	5.69	1.40	1.33
21	B	804	CLA	CHB-C4A	5.69	1.40	1.33
21	a	838	CLA	CHB-C4A	5.69	1.40	1.33
21	A	840	CLA	CHB-C4A	5.70	1.40	1.33
21	A	806	CLA	CHB-C4A	5.70	1.40	1.33
21	A	832	CLA	CHB-C4A	5.70	1.40	1.33
21	A	803	CLA	CHB-C4A	5.71	1.40	1.33
21	a	833	CLA	CHB-C4A	5.71	1.40	1.33
21	A	826	CLA	CHB-C4A	5.71	1.40	1.33
21	A	828	CLA	CHB-C4A	5.72	1.40	1.33
21	a	837	CLA	CHB-C4A	5.72	1.40	1.33
21	1	804	CLA	CHB-C4A	5.72	1.40	1.33
21	2	839	CLA	CHB-C4A	5.72	1.40	1.33
21	b	1839	CLA	CHB-C4A	5.72	1.40	1.33
21	B	826	CLA	CHB-C4A	5.73	1.40	1.33
21	b	1820	CLA	CHB-C4A	5.73	1.40	1.33
21	B	806	CLA	CHB-C4A	5.74	1.40	1.33
21	1	855	CLA	CHB-C4A	5.74	1.40	1.33
21	a	823	CLA	CHB-C4A	5.74	1.40	1.33
21	2	802	CLA	CHB-C4A	5.74	1.40	1.33
21	B	815	CLA	CHB-C4A	5.74	1.40	1.33
21	A	830	CLA	CHB-C4A	5.74	1.40	1.33
21	a	821	CLA	CHB-C4A	5.75	1.40	1.33
21	2	830	CLA	CHB-C4A	5.75	1.40	1.33
21	1	837	CLA	CHB-C4A	5.75	1.40	1.33
21	2	811	CLA	CHB-C4A	5.75	1.40	1.33
21	B	818	CLA	CHB-C4A	5.75	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1825	CLA	CHB-C4A	5.75	1.40	1.33
21	a	830	CLA	CHB-C4A	5.75	1.40	1.33
21	A	821	CLA	CHB-C4A	5.76	1.40	1.33
21	1	812	CLA	CHB-C4A	5.76	1.40	1.33
21	b	1831	CLA	CHB-C4A	5.76	1.40	1.33
21	A	819	CLA	CHB-C4A	5.77	1.40	1.33
21	l	203	CLA	CHB-C4A	5.77	1.40	1.33
21	b	1838	CLA	CHB-C4A	5.77	1.40	1.33
21	a	819	CLA	CHB-C4A	5.77	1.40	1.33
21	a	856	CLA	CHB-C4A	5.77	1.40	1.33
21	1	822	CLA	CHB-C4A	5.77	1.40	1.33
21	2	815	CLA	CHB-C4A	5.77	1.40	1.33
21	1	832	CLA	CHB-C4A	5.78	1.40	1.33
21	2	838	CLA	CHB-C4A	5.78	1.40	1.33
21	1	816	CLA	CHB-C4A	5.78	1.40	1.33
21	1	819	CLA	CHB-C4A	5.78	1.40	1.33
21	b	1823	CLA	CHB-C4A	5.79	1.40	1.33
21	a	813	CLA	CHB-C4A	5.80	1.40	1.33
21	J	1103	CLA	CHB-C4A	5.80	1.40	1.33
21	2	834	CLA	CHB-C4A	5.80	1.40	1.33
21	2	825	CLA	CHB-C4A	5.80	1.40	1.33
21	2	835	CLA	CHB-C4A	5.80	1.40	1.33
21	B	814	CLA	CHB-C4A	5.81	1.40	1.33
21	a	807	CLA	CHB-C4A	5.81	1.40	1.33
21	B	823	CLA	CHB-C4A	5.81	1.40	1.33
21	B	821	CLA	CHB-C4A	5.82	1.40	1.33
21	b	1835	CLA	CHB-C4A	5.82	1.40	1.33
21	B	805	CLA	CHB-C4A	5.82	1.40	1.33
21	2	826	CLA	CHB-C4A	5.82	1.40	1.33
21	B	829	CLA	CHB-C4A	5.82	1.40	1.33
21	a	809	CLA	CHB-C4A	5.82	1.40	1.33
21	B	809	CLA	CHB-C4A	5.82	1.40	1.33
21	2	823	CLA	CHB-C4A	5.83	1.40	1.33
21	A	812	CLA	CHB-C4A	5.83	1.40	1.33
21	b	1824	CLA	CHB-C4A	5.83	1.40	1.33
21	b	1815	CLA	CHB-C4A	5.83	1.40	1.33
21	1	805	CLA	CHB-C4A	5.83	1.40	1.33
21	7	1101	CLA	CHB-C4A	5.83	1.40	1.33
21	a	827	CLA	CHB-C4A	5.83	1.40	1.33
21	l	205	CLA	CHB-C4A	5.83	1.40	1.33
21	1	830	CLA	CHB-C4A	5.84	1.40	1.33
21	B	802	CLA	CHB-C4A	5.84	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	822	CLA	CHB-C4A	5.84	1.40	1.33
21	a	822	CLA	CHB-C4A	5.84	1.41	1.33
21	2	807	CLA	CHB-C4A	5.84	1.41	1.33
21	B	812	CLA	CHB-C4A	5.84	1.41	1.33
21	a	820	CLA	CHB-C4A	5.84	1.41	1.33
21	2	824	CLA	CHB-C4A	5.85	1.41	1.33
21	b	1834	CLA	CHB-C4A	5.85	1.41	1.33
21	2	805	CLA	CHB-C4A	5.85	1.41	1.33
21	A	805	CLA	CHB-C4A	5.85	1.41	1.33
21	2	828	CLA	CHB-C4A	5.85	1.41	1.33
21	b	1810	CLA	CHB-C4A	5.86	1.41	1.33
21	0	201	CLA	CHB-C4A	5.86	1.41	1.33
21	B	810	CLA	CHB-C4A	5.86	1.41	1.33
21	A	818	CLA	CHB-C4A	5.87	1.41	1.33
21	a	816	CLA	CHB-C4A	5.87	1.41	1.33
21	1	817	CLA	CHB-C4A	5.87	1.41	1.33
21	B	838	CLA	CHB-C4A	5.87	1.41	1.33
21	j	1101	CLA	CHB-C4A	5.88	1.41	1.33
21	B	827	CLA	CHB-C4A	5.88	1.41	1.33
21	1	829	CLA	CHB-C4A	5.88	1.41	1.33
21	A	831	CLA	CHB-C4A	5.88	1.41	1.33
21	1	824	CLA	CHB-C4A	5.88	1.41	1.33
21	1	806	CLA	CHB-C4A	5.88	1.41	1.33
21	1	836	CLA	CHB-C4A	5.88	1.41	1.33
21	B	811	CLA	CHB-C4A	5.89	1.41	1.33
21	b	1816	CLA	CHB-C4A	5.89	1.41	1.33
21	l	201	CLA	CHB-C4A	5.89	1.41	1.33
21	b	1837	CLA	CHB-C4A	5.89	1.41	1.33
21	A	815	CLA	CHB-C4A	5.89	1.41	1.33
21	1	802	CLA	CHB-C4A	5.89	1.41	1.33
21	b	1833	CLA	CHB-C4A	5.90	1.41	1.33
21	a	826	CLA	CHB-C4A	5.90	1.41	1.33
21	b	1826	CLA	CHB-C4A	5.90	1.41	1.33
21	B	820	CLA	CHB-C4A	5.90	1.41	1.33
21	L	203	CLA	CHB-C4A	5.91	1.41	1.33
21	6	203	CLA	CHB-C4A	5.91	1.41	1.33
21	1	801	CLA	CHB-C4A	5.92	1.41	1.33
21	B	813	CLA	CHB-C4A	5.92	1.41	1.33
21	a	808	CLA	CHB-C4A	5.92	1.41	1.33
21	B	828	CLA	CHB-C4A	5.92	1.41	1.33
21	1	825	CLA	CHB-C4A	5.92	1.41	1.33
21	2	842	CLA	CHB-C4A	5.92	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	823	CLA	CHB-C4A	5.92	1.41	1.33
21	1	818	CLA	CHB-C4A	5.92	1.41	1.33
21	A	834	CLA	CHB-C4A	5.93	1.41	1.33
21	1	821	CLA	CHB-C4A	5.93	1.41	1.33
21	F	203	CLA	CHB-C4A	5.93	1.41	1.33
21	0	203	CLA	CHB-C4A	5.93	1.41	1.33
21	B	839	CLA	CHB-C4A	5.94	1.41	1.33
21	1	826	CLA	CHB-C4A	5.94	1.41	1.33
21	A	814	CLA	CHB-C4A	5.94	1.41	1.33
21	2	836	CLA	CHB-C4A	5.94	1.41	1.33
21	2	808	CLA	CHB-C4A	5.94	1.41	1.33
21	a	814	CLA	CHB-C4A	5.94	1.41	1.33
21	2	821	CLA	CHB-C4A	5.95	1.41	1.33
21	6	204	CLA	CHB-C4A	5.95	1.41	1.33
21	2	837	CLA	CHB-C4A	5.95	1.41	1.33
21	b	1819	CLA	CHB-C4A	5.95	1.41	1.33
21	0	202	CLA	CHB-C4A	5.95	1.41	1.33
21	1	835	CLA	CHB-C4A	5.95	1.41	1.33
21	8	1401	CLA	CHB-C4A	5.96	1.41	1.33
21	m	103	CLA	CHB-C4A	5.96	1.41	1.33
21	B	840	CLA	CHB-C4A	5.96	1.41	1.33
21	a	824	CLA	CHB-C4A	5.96	1.41	1.33
21	F	202	CLA	CHB-C4A	5.96	1.41	1.33
21	2	809	CLA	CHB-C4A	5.96	1.41	1.33
21	2	804	CLA	CHB-C4A	5.97	1.41	1.33
21	j	1105	CLA	CHB-C4A	5.97	1.41	1.33
21	2	841	CLA	CHB-C4A	5.97	1.41	1.33
21	2	803	CLA	CHB-C4A	5.97	1.41	1.33
21	A	809	CLA	CHB-C4A	5.97	1.41	1.33
21	a	804	CLA	CHB-C4A	5.97	1.41	1.33
21	B	825	CLA	CHB-C4A	5.97	1.41	1.33
21	1	815	CLA	CHB-C4A	5.98	1.41	1.33
21	A	810	CLA	CHB-C4A	5.98	1.41	1.33
21	1	803	CLA	CHB-C4A	5.98	1.41	1.33
21	7	1104	CLA	CHB-C4A	5.98	1.41	1.33
21	2	816	CLA	CHB-C4A	5.98	1.41	1.33
21	a	836	CLA	CHB-C4A	5.98	1.41	1.33
21	B	834	CLA	CHB-C4A	5.98	1.41	1.33
21	b	1812	CLA	CHB-C4A	5.98	1.41	1.33
21	J	1106	CLA	CHB-C4A	5.98	1.41	1.33
21	B	832	CLA	CHB-C4A	5.99	1.41	1.33
21	K	102	CLA	CHB-C4A	5.99	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	815	CLA	CHB-C4A	5.99	1.41	1.33
21	J	1105	CLA	CHB-C4A	5.99	1.41	1.33
21	7	1105	CLA	CHB-C4A	6.01	1.41	1.33
21	2	827	CLA	CHB-C4A	6.01	1.41	1.33
21	b	1817	CLA	CHB-C4A	6.01	1.41	1.33
21	2	813	CLA	CHB-C4A	6.01	1.41	1.33
21	a	817	CLA	CHB-C4A	6.02	1.41	1.33
21	B	836	CLA	CHB-C4A	6.02	1.41	1.33
21	f	202	CLA	CHB-C4A	6.02	1.41	1.33
21	B	801	CLA	CHB-C4A	6.02	1.41	1.33
21	f	203	CLA	CHB-C4A	6.03	1.41	1.33
21	A	801	CLA	CHB-C4A	6.03	1.41	1.33
21	1	814	CLA	CHB-C4A	6.03	1.41	1.33
21	1	827	CLA	CHB-C4A	6.03	1.41	1.33
21	2	806	CLA	CHB-C4A	6.03	1.41	1.33
21	a	832	CLA	CHB-C4A	6.04	1.41	1.33
21	a	839	CLA	CHB-C4A	6.04	1.41	1.33
21	1	823	CLA	CHB-C4A	6.04	1.41	1.33
21	b	1836	CLA	CHB-C4A	6.04	1.41	1.33
21	A	829	CLA	CHB-C4A	6.04	1.41	1.33
21	a	840	CLA	CHB-C4A	6.04	1.41	1.33
21	k	1401	CLA	CHB-C4A	6.04	1.41	1.33
21	B	808	CLA	CHB-C4A	6.05	1.41	1.33
21	A	855	CLA	CHB-C4A	6.06	1.41	1.33
21	1	808	CLA	CHB-C4A	6.06	1.41	1.33
21	2	818	CLA	CHB-C4A	6.06	1.41	1.33
21	1	810	CLA	CHB-C4A	6.06	1.41	1.33
21	b	1840	CLA	CHB-C4A	6.06	1.41	1.33
21	B	835	CLA	CHB-C4A	6.07	1.41	1.33
21	k	1402	CLA	CHB-C4A	6.07	1.41	1.33
21	b	1808	CLA	CHB-C4A	6.07	1.41	1.33
21	1	820	CLA	CHB-C4A	6.07	1.41	1.33
21	A	839	CLA	CHB-C4A	6.07	1.41	1.33
21	1	807	CLA	CHB-C4A	6.08	1.41	1.33
21	A	816	CLA	CHB-C4A	6.08	1.41	1.33
21	b	1806	CLA	CHB-C4A	6.09	1.41	1.33
21	b	1804	CLA	CHB-C4A	6.09	1.41	1.33
21	2	817	CLA	CHB-C4A	6.10	1.41	1.33
21	b	1827	CLA	CHB-C4A	6.10	1.41	1.33
21	A	824	CLA	CHB-C4A	6.11	1.41	1.33
21	b	1809	CLA	CHB-C4A	6.12	1.41	1.33
21	b	1842	CLA	CHB-C4A	6.12	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1814	CLA	CHB-C4A	6.13	1.41	1.33
21	8	1402	CLA	CHB-C4A	6.13	1.41	1.33
21	L	205	CLA	CHB-C4A	6.14	1.41	1.33
21	a	828	CLA	CHB-C4A	6.14	1.41	1.33
21	j	1103	CLA	CHB-C4A	6.14	1.41	1.33
21	A	827	CLA	CHB-C4A	6.14	1.41	1.33
21	1	834	CLA	CHB-C4A	6.14	1.41	1.33
21	a	811	CLA	CHB-C4A	6.15	1.41	1.33
21	A	813	CLA	CHB-C4A	6.15	1.41	1.33
21	7	1103	CLA	CHB-C4A	6.15	1.41	1.33
21	a	806	CLA	CHB-C4A	6.16	1.41	1.33
21	b	1805	CLA	CHB-C4A	6.17	1.41	1.33
21	2	810	CLA	CHB-C4A	6.17	1.41	1.33
21	1	811	CLA	CHB-C4A	6.17	1.41	1.33
21	a	801	CLA	CHB-C4A	6.17	1.41	1.33
21	j	1104	CLA	CHB-C4A	6.17	1.41	1.33
21	6	201	CLA	CHB-C4A	6.17	1.41	1.33
21	b	1841	CLA	CHB-C4A	6.19	1.41	1.33
21	a	810	CLA	CHB-C4A	6.21	1.41	1.33
21	A	808	CLA	CHB-C4A	6.23	1.41	1.33
21	b	1807	CLA	CHB-C4A	6.23	1.41	1.33
21	1	828	CLA	CHB-C4A	6.25	1.41	1.33
21	A	836	CLA	CHB-C4A	6.28	1.41	1.33
21	b	1843	CLA	CHB-C4A	6.29	1.41	1.33
21	B	803	CLA	CHB-C4A	6.29	1.41	1.33
21	A	822	CLA	CHB-C4A	6.36	1.41	1.33
27	a	854	ACT	CH3-C	6.43	1.57	1.48
21	B	807	CLA	CHB-C4A	6.44	1.41	1.33
27	M	7001	ACT	CH3-C	6.45	1.57	1.48
27	D	201	ACT	CH3-C	6.78	1.57	1.48
27	A	853	ACT	CH3-C	7.71	1.58	1.48
36	L	201	EQ3	C5-C6	10.91	1.53	1.34
36	L	201	EQ3	C4-C3	11.12	1.71	1.52
28	A	856	45D	C07-C15	11.70	1.52	1.35
28	2	854	45D	C07-C15	12.43	1.53	1.35
28	A	856	45D	C08-C16	12.70	1.53	1.35
36	L	201	EQ3	C25-C26	13.14	1.54	1.35
28	2	854	45D	C08-C16	13.22	1.54	1.35

All (2697) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	854	45D	C42-C38-C36	-10.25	112.69	127.31
30	2	846	ECH	C16-C17-C18	-9.92	113.15	127.31
30	1	202	ECH	C15-C14-C13	-9.84	113.26	127.31
28	2	854	45D	C24-C26-C30	-9.77	103.94	118.94
30	B	844	ECH	C16-C17-C18	-9.19	114.20	127.31
30	a	857	ECH	C15-C14-C13	-8.81	114.74	127.31
30	b	1847	ECH	C20-C21-C22	-8.67	114.94	127.31
28	2	854	45D	C32-C34-C36	-8.28	103.16	126.42
30	2	846	ECH	C24-C23-C22	-7.46	115.01	126.21
34	F	204	C7Z	C21-C26-C25	-7.32	112.30	122.59
30	B	844	ECH	C24-C23-C22	-6.62	116.26	126.21
28	2	854	45D	C24-C20-C08	-6.52	109.00	127.25
28	A	856	45D	C20-C24-C26	-6.27	116.79	126.21
30	l	202	ECH	C7-C8-C9	-6.12	117.01	126.21
30	a	857	ECH	C20-C21-C22	-6.03	118.70	127.31
28	A	856	45D	C41-C37-C35	-5.87	118.94	127.31
21	A	801	CLA	C3D-CAD-CBD	-5.75	99.47	107.60
36	L	201	EQ3	C11-C10-C9	-5.48	119.48	127.31
30	B	844	ECH	C11-C10-C9	-5.47	119.50	127.31
28	A	856	45D	C31-C29-C25	-5.44	119.54	127.31
30	B	844	ECH	C16-C15-C14	-5.42	111.89	123.46
31	F	205	SQD	O7-S-C6	-5.28	102.31	106.83
36	L	201	EQ3	C33-C5-C6	-5.27	118.60	124.51
21	A	829	CLA	CMB-C2B-C1B	-5.24	120.41	128.46
34	b	1858	C7Z	C7-C8-C9	-5.24	118.34	126.21
34	b	1858	C7Z	C21-C26-C25	-5.16	115.34	122.59
31	b	1854	SQD	O7-S-C6	-4.91	102.63	106.83
34	F	204	C7Z	C27-C26-C25	-4.90	109.86	121.54
31	L	208	SQD	O7-S-C6	-4.88	102.65	106.83
34	2	855	C7Z	C7-C8-C9	-4.79	119.02	126.21
31	f	205	SQD	O7-S-C6	-4.78	102.74	106.83
30	a	857	ECH	C7-C8-C9	-4.75	119.08	126.21
30	b	1847	ECH	C33-C5-C6	-4.72	119.22	124.51
21	a	830	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
30	b	1847	ECH	C7-C8-C9	-4.70	119.15	126.21
30	2	846	ECH	C16-C15-C14	-4.70	113.44	123.46
30	b	1847	ECH	C24-C23-C22	-4.64	119.23	126.21
30	B	844	ECH	C33-C5-C6	-4.64	119.31	124.51
34	B	856	C7Z	C7-C8-C9	-4.60	119.31	126.21
22	B	841	PQN	C11-C12-C13	-4.57	119.06	126.71
24	6	205	BCR	C35-C13-C14	-4.56	116.54	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	1858	C7Z	C27-C26-C25	-4.53	110.73	121.54
31	0	207	SQD	O7-S-C6	-4.50	102.98	106.83
21	B	829	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
36	L	201	EQ3	C16-C17-C18	-4.47	120.93	127.31
30	B	844	ECH	C20-C21-C22	-4.42	121.00	127.31
21	K	102	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
31	m	102	SQD	O7-S-C6	-4.41	103.06	106.83
30	2	846	ECH	C33-C5-C6	-4.38	119.60	124.51
30	2	846	ECH	C7-C8-C9	-4.38	119.63	126.21
30	b	1847	ECH	C15-C14-C13	-4.33	121.14	127.31
31	B	852	SQD	O7-S-C6	-4.32	103.13	106.83
30	l	202	ECH	C15-C16-C17	-4.32	114.25	123.46
30	m	104	ECH	C20-C21-C22	-4.31	121.17	127.31
28	2	854	45D	C41-C37-C35	-4.30	121.18	127.31
30	a	857	ECH	C28-C27-C26	-4.27	114.99	118.80
24	f	204	BCR	C35-C13-C14	-4.25	116.97	122.92
21	1	831	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
34	B	856	C7Z	C21-C26-C25	-4.14	116.78	122.59
21	A	835	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
21	1	803	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
30	a	857	ECH	C24-C23-C22	-4.10	120.05	126.21
21	1	830	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
21	6	204	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
21	2	811	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
30	m	104	ECH	C7-C8-C9	-4.06	120.12	126.21
21	B	806	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
22	2	843	PQN	C11-C12-C13	-4.00	120.03	126.71
34	2	855	C7Z	C27-C26-C25	-3.99	112.01	121.54
34	b	1858	C7Z	C31-C32-C33	-3.99	115.21	126.42
21	2	827	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
30	l	202	ECH	C10-C11-C12	-3.98	111.01	123.23
21	A	854	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
30	M	7002	ECH	C24-C23-C22	-3.96	120.26	126.21
30	M	7002	ECH	C33-C5-C6	-3.95	120.09	124.51
28	A	856	45D	C42-C38-C36	-3.94	121.69	127.31
30	M	7002	ECH	C7-C8-C9	-3.93	120.31	126.21
34	2	855	C7Z	C21-C26-C25	-3.93	117.07	122.59
34	b	1858	C7Z	C31-C30-C29	-3.89	121.76	127.31
30	M	7002	ECH	C20-C21-C22	-3.89	121.76	127.31
24	6	205	BCR	C40-C30-C25	-3.87	104.03	110.31
35	0	208	LMT	C3'-C4'-C5'	-3.80	102.80	110.88
21	B	831	CLA	CMB-C2B-C1B	-3.80	122.62	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	m	104	ECH	C33-C5-C6	-3.80	120.26	124.51
34	B	856	C7Z	C27-C26-C25	-3.79	112.50	121.54
30	B	844	ECH	C28-C27-C26	-3.76	115.45	118.80
24	9	102	BCR	C30-C25-C26	-3.76	117.31	122.59
24	A	847	BCR	C39-C30-C25	-3.76	104.22	110.31
24	a	845	BCR	C30-C25-C26	-3.75	117.31	122.59
21	b	1841	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
36	L	201	EQ3	C15-C14-C13	-3.74	121.98	127.31
21	1	808	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
30	m	104	ECH	C15-C14-C13	-3.73	121.99	127.31
30	a	857	ECH	C33-C5-C6	-3.73	120.34	124.51
24	b	1845	BCR	C39-C30-C25	-3.72	104.27	110.31
34	F	204	C7Z	C28-C27-C26	-3.71	116.86	127.25
30	2	846	ECH	C28-C27-C26	-3.71	115.50	118.80
36	L	201	EQ3	C7-C8-C9	-3.70	120.65	126.21
28	2	854	45D	C23-C19-C07	-3.70	116.90	127.25
28	2	854	45D	C40-C36-C38	-3.69	117.75	122.92
24	1	858	BCR	C38-C26-C25	-3.68	120.39	124.51
36	L	201	EQ3	C23-C24-C25	-3.67	116.97	127.25
21	b	1812	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
24	0	205	BCR	C36-C18-C19	-3.66	112.27	118.10
21	1	809	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
21	0	202	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
36	L	201	EQ3	C8-C7-C6	-3.62	117.11	127.25
30	a	857	ECH	C10-C11-C12	-3.61	112.17	123.23
21	b	1801	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
21	J	1101	CLA	CAA-C2A-C3A	-3.60	102.93	112.81
21	b	1832	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
30	B	844	ECH	C20-C19-C18	-3.60	116.32	126.42
21	a	828	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
24	2	849	BCR	C38-C26-C25	-3.58	120.50	124.51
24	B	843	BCR	C38-C26-C25	-3.57	120.51	124.51
24	a	848	BCR	C15-C14-C13	-3.56	122.23	127.31
30	l	202	ECH	C33-C5-C6	-3.56	120.53	124.51
21	1	815	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
24	a	859	BCR	C38-C26-C25	-3.55	120.53	124.51
21	j	1101	CLA	CAA-C2A-C3A	-3.53	103.12	112.81
21	a	819	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
24	J	1107	BCR	C38-C26-C25	-3.51	120.58	124.51
21	1	828	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
34	F	204	C7Z	C7-C8-C9	-3.50	120.96	126.21
21	A	814	CLA	CMB-C2B-C1B	-3.49	123.10	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	810	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
28	A	856	45D	C23-C19-C07	-3.46	117.56	127.25
21	A	823	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
21	a	811	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
24	9	102	BCR	C35-C13-C14	-3.45	118.09	122.92
24	2	845	BCR	C40-C30-C25	-3.44	104.72	110.31
24	8	1403	BCR	C40-C30-C25	-3.44	104.73	110.31
34	b	1858	C7Z	C39-C29-C30	-3.44	118.11	122.92
24	A	845	BCR	C1-C6-C5	-3.43	117.77	122.59
21	2	825	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
30	a	857	ECH	C35-C13-C12	-3.42	112.64	118.10
21	1	821	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
21	b	1829	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
21	7	1101	CLA	CAA-C2A-C3A	-3.40	103.50	112.81
21	A	807	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
24	L	206	BCR	C40-C30-C25	-3.38	104.82	110.31
25	9	101	LHG	C5-O7-C7	-3.38	109.89	117.88
30	l	202	ECH	C20-C21-C22	-3.37	122.50	127.31
35	l	211	LMT	C3'-C4'-C5'	-3.36	103.75	110.88
24	a	848	BCR	C40-C30-C25	-3.36	104.86	110.31
24	2	844	BCR	C40-C30-C25	-3.36	104.87	110.31
30	M	7002	ECH	C16-C17-C18	-3.35	122.52	127.31
30	B	844	ECH	C11-C12-C13	-3.35	117.00	126.42
30	a	857	ECH	C15-C16-C17	-3.35	116.31	123.46
24	a	844	BCR	C40-C30-C25	-3.35	104.88	110.31
24	a	846	BCR	C40-C30-C25	-3.34	104.89	110.31
30	M	7002	ECH	C15-C14-C13	-3.34	122.55	127.31
30	B	844	ECH	C7-C8-C9	-3.32	121.22	126.21
30	b	1847	ECH	C28-C27-C26	-3.32	115.84	118.80
30	a	857	ECH	C20-C19-C18	-3.32	117.10	126.42
24	b	1849	BCR	C39-C30-C25	-3.28	104.99	110.31
24	b	1846	BCR	C40-C30-C25	-3.27	105.00	110.31
22	A	841	PQN	C11-C12-C13	-3.27	121.24	126.71
21	2	805	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
30	2	846	ECH	C21-C20-C19	-3.27	113.21	123.23
24	j	1102	BCR	C39-C30-C25	-3.27	105.01	110.31
24	1	845	BCR	C38-C26-C25	-3.26	120.86	124.51
24	f	204	BCR	C40-C30-C25	-3.25	105.03	110.31
24	h	101	BCR	C40-C30-C25	-3.24	105.05	110.31
30	b	1847	ECH	C19-C18-C17	-3.23	113.98	118.94
24	A	844	BCR	C40-C30-C25	-3.23	105.07	110.31
21	B	811	CLA	CMB-C2B-C1B	-3.23	123.50	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	l	202	ECH	C23-C24-C25	-3.22	118.24	127.25
21	2	820	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
24	B	843	BCR	C40-C30-C25	-3.21	105.10	110.31
24	l	206	BCR	C34-C9-C10	-3.21	118.42	122.92
24	a	843	BCR	C30-C25-C26	-3.20	118.09	122.59
34	2	855	C7Z	C31-C32-C33	-3.19	117.44	126.42
30	m	104	ECH	C16-C17-C18	-3.19	122.75	127.31
30	m	104	ECH	C24-C23-C22	-3.19	121.42	126.21
34	B	856	C7Z	C31-C32-C33	-3.18	117.50	126.42
25	A	849	LHG	C5-O7-C7	-3.18	110.37	117.88
21	B	818	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
34	B	856	C7Z	C39-C29-C30	-3.17	118.48	122.92
24	1	845	BCR	C40-C30-C25	-3.17	105.17	110.31
21	A	830	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
21	b	1821	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
24	b	1846	BCR	C38-C26-C25	-3.16	120.97	124.51
21	B	835	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
21	7	1105	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
21	2	817	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
24	h	101	BCR	C39-C30-C25	-3.13	105.23	110.31
21	A	818	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
21	A	803	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
21	B	833	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
24	1	856	BCR	C39-C30-C25	-3.12	105.25	110.31
21	B	813	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
21	A	810	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
21	B	823	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
24	0	205	BCR	C40-C30-C25	-3.10	105.29	110.31
25	1	852	LHG	C5-O7-C7	-3.09	110.57	117.88
28	2	854	45D	C31-C29-C25	-3.09	122.90	127.31
35	J	1104	LMT	C3'-C4'-C5'	-3.09	104.31	110.88
21	1	841	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
21	A	820	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
21	A	801	CLA	CHA-C1A-NA	-3.07	119.04	126.18
24	1	848	BCR	C40-C30-C25	-3.07	105.33	110.31
24	A	843	BCR	C34-C9-C10	-3.07	118.62	122.92
21	A	801	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
21	1	822	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
21	b	1815	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
36	L	201	EQ3	C24-C23-C22	-3.04	121.64	126.21
24	A	845	BCR	C40-C30-C25	-3.04	105.37	110.31
36	L	201	EQ3	C21-C20-C19	-3.04	113.91	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	858	BCR	C34-C9-C10	-3.02	118.70	122.92
34	B	856	C7Z	C37-C21-C26	-3.02	105.42	110.31
24	L	206	BCR	C39-C30-C25	-3.00	105.44	110.31
30	2	846	ECH	C23-C22-C21	-2.99	114.35	118.94
21	a	814	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
21	b	1838	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
25	a	849	LHG	C5-O7-C7	-2.97	110.86	117.88
24	B	842	BCR	C38-C26-C25	-2.96	121.20	124.51
21	A	825	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
21	a	803	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
24	9	102	BCR	C40-C30-C25	-2.95	105.53	110.31
24	a	859	BCR	C34-C9-C10	-2.95	118.80	122.92
34	2	855	C7Z	C17-C1-C6	-2.95	105.53	110.31
30	a	857	ECH	C23-C24-C25	-2.95	119.00	127.25
21	1	825	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
24	l	207	BCR	C40-C30-C25	-2.94	105.54	110.31
21	2	835	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
31	L	208	SQD	O8-S-C6	-2.94	102.42	106.01
21	b	1806	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
24	a	847	BCR	C38-C26-C25	-2.93	121.23	124.51
21	b	1808	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
35	1	854	LMT	C1'-O5'-C5'	-2.92	108.21	113.72
31	0	207	SQD	O8-S-C6	-2.92	102.45	106.01
21	2	804	CLA	CMB-C2B-C1B	-2.91	123.98	128.46
24	K	104	BCR	C40-C30-C25	-2.91	105.59	110.31
21	a	801	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
36	L	201	EQ3	C16-C15-C14	-2.91	117.26	123.46
28	2	854	45D	C19-C23-C25	-2.90	121.85	126.21
21	a	801	CLA	C3D-CAD-CBD	-2.90	103.50	107.60
24	F	201	BCR	C39-C30-C25	-2.90	105.61	110.31
36	L	201	EQ3	C20-C21-C22	-2.89	123.18	127.31
24	1	858	BCR	C40-C30-C25	-2.89	105.62	110.31
31	m	102	SQD	O8-S-C6	-2.89	102.48	106.01
28	A	856	45D	C31-C33-C35	-2.89	118.30	126.42
21	b	1827	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
21	2	808	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
24	0	204	BCR	C40-C30-C25	-2.88	105.64	110.31
24	B	847	BCR	C15-C14-C13	-2.87	123.22	127.31
24	1	846	BCR	C1-C6-C5	-2.86	118.57	122.59
31	b	1854	SQD	O8-S-C6	-2.86	102.52	106.01
21	1	819	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
36	L	201	EQ3	C10-C11-C12	-2.86	114.46	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	1401	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
22	b	1844	PQN	C17-C16-C15	-2.86	105.17	113.11
24	I	102	BCR	C40-C30-C25	-2.86	105.68	110.31
28	A	856	45D	O02-C18-C16	-2.85	118.40	120.93
21	2	817	CLA	CAA-C2A-C3A	-2.85	110.61	116.38
24	f	201	BCR	C39-C30-C25	-2.85	105.68	110.31
24	a	859	BCR	C39-C30-C25	-2.85	105.69	110.31
24	0	204	BCR	C34-C9-C10	-2.85	118.93	122.92
25	b	1802	LHG	C5-O7-C7	-2.85	111.15	117.88
31	B	852	SQD	O8-S-C6	-2.84	102.54	106.01
24	J	1102	BCR	C38-C26-C25	-2.84	121.33	124.51
30	m	104	ECH	C28-C27-C26	-2.84	116.27	118.80
21	B	803	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
24	i	101	BCR	C40-C30-C25	-2.84	105.71	110.31
21	b	1836	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
21	b	1826	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
28	2	854	45D	C21-C15-C07	-2.83	120.11	123.92
24	a	844	BCR	C34-C9-C10	-2.82	118.97	122.92
24	0	204	BCR	C38-C26-C25	-2.81	121.36	124.51
24	2	847	BCR	C34-C9-C10	-2.81	118.99	122.92
24	a	845	BCR	C27-C26-C25	-2.81	118.62	122.74
30	l	202	ECH	C28-C27-C26	-2.81	116.30	118.80
34	2	855	C7Z	C39-C29-C30	-2.80	119.00	122.92
21	B	815	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
21	f	202	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
21	7	1104	CLA	CAA-C2A-C3A	-2.79	110.74	116.38
24	J	1107	BCR	C39-C30-C25	-2.79	105.79	110.31
24	A	844	BCR	C34-C9-C10	-2.78	119.02	122.92
35	L	211	LMT	C3B-C4B-C5B	-2.78	105.31	110.22
28	2	854	45D	C31-C33-C35	-2.78	118.60	126.42
36	L	201	EQ3	C38-C26-C25	-2.77	120.19	123.92
21	A	826	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
25	l	208	LHG	C5-O7-C7	-2.77	111.32	117.88
21	A	813	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
24	2	849	BCR	C36-C18-C19	-2.77	113.68	118.10
34	2	855	C7Z	C37-C21-C26	-2.77	105.82	110.31
24	B	842	BCR	C40-C30-C25	-2.77	105.82	110.31
21	A	819	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
21	a	839	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
21	a	816	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
24	1	847	BCR	C40-C30-C25	-2.76	105.83	110.31
24	1	845	BCR	C34-C9-C10	-2.75	119.07	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	856	45D	C28-C26-C30	-2.75	119.07	122.92
24	I	102	BCR	C39-C30-C25	-2.75	105.86	110.31
24	2	845	BCR	C38-C26-C25	-2.75	121.44	124.51
24	a	847	BCR	C39-C30-C25	-2.74	105.86	110.31
24	J	1102	BCR	C39-C30-C25	-2.74	105.86	110.31
21	A	821	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
21	1	840	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
24	6	202	BCR	C40-C30-C25	-2.73	105.88	110.31
21	1	820	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
34	F	204	C7Z	C1-C6-C5	-2.73	118.75	122.59
21	A	801	CLA	O1D-CGD-CBD	-2.73	119.70	124.60
21	B	840	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
31	F	205	SQD	O8-S-C6	-2.72	102.69	106.01
24	B	847	BCR	C38-C26-C25	-2.72	121.46	124.51
24	K	104	BCR	C23-C24-C25	-2.71	119.66	127.25
28	A	856	45D	C21-C15-C07	-2.71	120.27	123.92
24	A	845	BCR	C36-C18-C19	-2.71	113.78	118.10
21	a	801	CLA	CHA-C1A-NA	-2.71	119.89	126.18
24	f	204	BCR	C32-C1-C6	-2.70	105.93	110.31
21	2	837	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
24	b	1846	BCR	C39-C30-C25	-2.70	105.93	110.31
21	1	818	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
26	b	1853	LMG	O1-C7-C8	-2.70	104.57	110.99
21	2	806	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
21	B	801	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
24	1	847	BCR	C38-C26-C25	-2.70	121.49	124.51
24	8	1403	BCR	C34-C9-C10	-2.69	119.15	122.92
21	1	838	CLA	CAA-CBA-CGA	-2.69	105.24	113.35
24	F	201	BCR	C36-C18-C19	-2.69	113.81	118.10
21	a	821	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
24	A	848	BCR	C34-C9-C10	-2.69	119.16	122.92
24	l	206	BCR	C40-C30-C25	-2.69	105.95	110.31
24	b	1845	BCR	C38-C26-C25	-2.68	121.50	124.51
21	2	816	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
28	A	856	45D	C19-C23-C25	-2.68	122.18	126.21
30	m	104	ECH	C37-C22-C23	-2.68	113.83	118.10
26	b	1851	LMG	C7-O1-C1	-2.68	108.26	113.76
24	a	846	BCR	C38-C26-C25	-2.68	121.51	124.51
21	2	815	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
21	A	801	CLA	CED-O2D-CGD	-2.68	109.69	115.97
24	I	102	BCR	C12-C13-C14	-2.68	114.83	118.94
31	f	205	SQD	O8-S-C6	-2.67	102.74	106.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	1849	BCR	C38-C26-C25	-2.67	121.52	124.51
21	J	1103	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
24	b	1850	BCR	C38-C26-C25	-2.66	121.53	124.51
24	i	101	BCR	C39-C30-C25	-2.66	105.99	110.31
24	7	1102	BCR	C39-C30-C25	-2.66	105.99	110.31
24	b	1849	BCR	C34-C9-C10	-2.66	119.19	122.92
34	B	856	C7Z	C31-C30-C29	-2.66	123.51	127.31
24	f	201	BCR	C36-C18-C19	-2.66	113.86	118.10
24	A	846	BCR	C40-C30-C25	-2.66	106.00	110.31
24	B	847	BCR	C39-C30-C25	-2.65	106.00	110.31
25	A	851	LHG	C5-O7-C7	-2.65	111.61	117.88
24	k	1403	BCR	C40-C30-C25	-2.65	106.01	110.31
34	b	1858	C7Z	C28-C27-C26	-2.65	119.83	127.25
24	1	846	BCR	C39-C30-C25	-2.65	106.01	110.31
21	A	830	CLA	O2D-CGD-O1D	-2.65	118.49	123.82
21	F	202	CLA	CMB-C2B-C1B	-2.65	124.40	128.46
24	b	1848	BCR	C40-C30-C25	-2.65	106.02	110.31
24	6	202	BCR	C39-C30-C25	-2.64	106.02	110.31
24	2	849	BCR	C34-C9-C10	-2.64	119.22	122.92
30	B	844	ECH	C8-C7-C6	-2.64	119.86	127.25
24	A	848	BCR	C35-C13-C14	-2.64	119.22	122.92
21	a	827	CLA	OBD-CAD-C3D	-2.64	123.17	128.03
24	0	205	BCR	C34-C9-C10	-2.63	119.24	122.92
21	a	831	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
25	B	849	LHG	C5-O7-C7	-2.63	111.67	117.88
21	1	809	CLA	CAA-C2A-C3A	-2.62	105.62	112.81
24	B	846	BCR	C38-C26-C25	-2.62	121.57	124.51
21	1	801	CLA	CHA-C1A-NA	-2.62	120.09	126.18
24	A	843	BCR	C40-C30-C25	-2.62	106.06	110.31
25	a	851	LHG	C5-O7-C7	-2.62	111.69	117.88
24	9	102	BCR	C34-C9-C10	-2.62	119.26	122.92
24	i	101	BCR	C38-C26-C25	-2.61	121.58	124.51
21	A	802	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
24	J	1107	BCR	C40-C30-C25	-2.60	106.09	110.31
36	L	201	EQ3	C7-C6-C5	-2.60	115.33	121.54
24	a	847	BCR	C40-C30-C25	-2.60	106.09	110.31
21	1	804	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
21	J	1101	CLA	CHA-C1A-NA	-2.60	120.14	126.18
30	M	7002	ECH	C28-C27-C26	-2.60	116.48	118.80
21	a	824	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
24	1	847	BCR	C39-C30-C25	-2.59	106.11	110.31
24	b	1845	BCR	C30-C25-C26	-2.59	118.96	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	849	BCR	C40-C30-C25	-2.58	106.12	110.31
21	0	201	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
24	b	1845	BCR	C34-C9-C10	-2.58	119.31	122.92
24	B	846	BCR	C36-C18-C19	-2.58	113.99	118.10
34	2	855	C7Z	C31-C30-C29	-2.58	123.63	127.31
24	A	846	BCR	C34-C9-C10	-2.58	119.31	122.92
36	L	201	EQ3	C15-C16-C17	-2.57	117.97	123.46
30	2	846	ECH	C8-C7-C6	-2.57	120.05	127.25
22	a	841	PQN	C12-C11-C3	-2.57	104.63	111.85
24	A	848	BCR	C15-C14-C13	-2.57	123.65	127.31
21	7	1103	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
24	B	846	BCR	C40-C30-C25	-2.56	106.15	110.31
24	a	845	BCR	C39-C30-C25	-2.56	106.16	110.31
24	j	1102	BCR	C34-C9-C10	-2.56	119.34	122.92
34	B	856	C7Z	C40-C33-C34	-2.56	119.34	122.92
25	2	801	LHG	C5-O7-C7	-2.56	111.84	117.88
21	B	805	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
21	j	1101	CLA	CHA-C1A-NA	-2.55	120.25	126.18
21	2	842	CLA	CAA-C2A-C3A	-2.55	111.23	116.38
21	2	826	CLA	CMB-C2B-C1B	-2.55	124.55	128.46
28	A	856	45D	C30-C32-C34	-2.55	115.42	123.23
24	L	207	BCR	C39-C30-C25	-2.54	106.18	110.31
31	f	205	SQD	O3-C3-C2	-2.54	104.82	110.36
24	6	205	BCR	C30-C25-C26	-2.54	119.02	122.59
25	B	851	LHG	C5-O7-C7	-2.54	111.87	117.88
24	7	1102	BCR	C40-C30-C25	-2.54	106.19	110.31
24	1	844	BCR	C40-C30-C25	-2.54	106.19	110.31
24	A	845	BCR	C39-C30-C25	-2.54	106.19	110.31
21	7	1105	CLA	CAA-C2A-C3A	-2.54	111.25	116.38
24	F	201	BCR	C40-C30-C25	-2.54	106.20	110.31
24	f	201	BCR	C40-C30-C25	-2.53	106.20	110.31
24	2	847	BCR	C39-C30-C25	-2.53	106.21	110.31
24	A	848	BCR	C30-C25-C26	-2.52	119.04	122.59
30	2	846	ECH	C11-C10-C9	-2.52	123.71	127.31
21	A	838	CLA	CMB-C2B-C1B	-2.52	124.58	128.46
24	a	843	BCR	C40-C30-C25	-2.52	106.22	110.31
21	K	102	CLA	CAA-CBA-CGA	-2.52	105.75	113.35
21	B	814	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
25	b	1852	LHG	C5-O7-C7	-2.51	111.94	117.88
24	B	845	BCR	C39-C30-C25	-2.51	106.23	110.31
25	2	851	LHG	C5-O7-C7	-2.50	111.96	117.88
21	1	831	CLA	O2D-CGD-O1D	-2.50	118.78	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	820	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
24	A	844	BCR	C38-C26-C25	-2.50	121.71	124.51
21	1	806	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
21	b	1809	CLA	O2D-CGD-O1D	-2.50	118.79	123.82
21	b	1831	CLA	CMB-C2B-C1B	-2.50	124.63	128.46
30	l	202	ECH	C24-C23-C22	-2.50	122.46	126.21
21	a	834	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
30	l	202	ECH	C7-C6-C5	-2.49	115.61	121.54
21	7	1101	CLA	CHA-C1A-NA	-2.49	120.41	126.18
31	B	852	SQD	O3-C3-C2	-2.48	104.96	110.36
24	2	847	BCR	C38-C26-C25	-2.48	121.73	124.51
21	A	828	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
34	b	1858	C7Z	C19-C9-C10	-2.48	119.45	122.92
30	l	202	ECH	C29-C30-C25	-2.48	106.60	110.48
24	L	206	BCR	C34-C9-C10	-2.47	119.46	122.92
21	2	824	CLA	CHA-C1A-NA	-2.47	120.44	126.18
24	0	205	BCR	C38-C26-C25	-2.47	121.75	124.51
25	b	1803	LHG	O7-C7-O9	-2.47	117.53	123.68
35	L	211	LMT	C3'-C4'-C5'	-2.46	105.65	110.88
24	a	844	BCR	C38-C26-C25	-2.46	121.75	124.51
24	F	201	BCR	C34-C9-C10	-2.46	119.48	122.92
34	F	204	C7Z	C11-C12-C13	-2.46	119.52	126.42
24	1	846	BCR	C40-C30-C25	-2.45	106.33	110.31
21	2	833	CLA	O1D-CGD-CBD	-2.45	120.20	124.60
21	1	801	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
25	I	104	LHG	C5-O7-C7	-2.45	112.09	117.88
21	A	854	CLA	CHA-C1A-NA	-2.44	120.51	126.18
21	B	825	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
30	l	202	ECH	C8-C9-C10	-2.44	115.20	118.94
30	M	7002	ECH	C23-C24-C25	-2.43	120.44	127.25
21	K	102	CLA	CAA-C2A-C1A	-2.43	104.00	111.97
24	l	206	BCR	C38-C26-C25	-2.43	121.79	124.51
24	k	1403	BCR	C38-C26-C25	-2.43	121.79	124.51
24	J	1107	BCR	C34-C9-C10	-2.43	119.52	122.92
30	2	846	ECH	C36-C18-C19	-2.42	114.24	118.10
24	a	848	BCR	C35-C13-C14	-2.42	119.53	122.92
24	a	845	BCR	C40-C30-C25	-2.42	106.38	110.31
25	l	210	LHG	C5-O7-C7	-2.42	112.15	117.88
24	2	844	BCR	C38-C26-C25	-2.42	121.80	124.51
24	A	843	BCR	C30-C25-C26	-2.42	119.19	122.59
24	B	845	BCR	C34-C9-C10	-2.42	119.54	122.92
31	0	207	SQD	O3-C3-C2	-2.41	105.11	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	848	BCR	C38-C26-C25	-2.41	121.81	124.51
21	1	836	CLA	CMB-C2B-C1B	-2.41	124.77	128.46
21	2	826	CLA	O1D-CGD-CBD	-2.41	120.28	124.60
24	2	848	BCR	C40-C30-C25	-2.40	106.41	110.31
21	j	1103	CLA	CMB-C2B-C1B	-2.40	124.77	128.46
21	6	204	CLA	CHA-C1A-NA	-2.40	120.60	126.18
26	b	1853	LMG	O6-C1-O1	-2.40	104.32	110.02
25	M	7003	LHG	O7-C7-O9	-2.40	117.69	123.68
21	A	801	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
24	b	1845	BCR	C24-C25-C26	-2.40	115.83	121.54
21	b	1833	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
21	f	203	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
21	A	802	CLA	C2C-C1C-NC	-2.39	108.58	110.22
24	a	846	BCR	C34-C9-C10	-2.38	119.58	122.92
24	a	848	BCR	C30-C25-C26	-2.38	119.24	122.59
21	a	836	CLA	O1D-CGD-CBD	-2.38	120.32	124.60
24	j	1102	BCR	C30-C25-C26	-2.38	119.25	122.59
21	1	802	CLA	CMB-C2B-C1B	-2.37	124.82	128.46
21	2	824	CLA	CAA-C2A-C3A	-2.37	106.31	112.81
34	2	855	C7Z	C40-C33-C34	-2.37	119.61	122.92
21	a	855	CLA	O2D-CGD-O1D	-2.37	119.06	123.82
21	a	808	CLA	CMB-C2B-C1B	-2.37	124.83	128.46
36	L	201	EQ3	C12-C13-C14	-2.37	115.31	118.94
24	J	1102	BCR	C34-C9-C10	-2.37	119.61	122.92
24	I	102	BCR	C32-C1-C6	-2.36	106.47	110.31
24	0	204	BCR	C32-C1-C6	-2.36	106.48	110.31
21	A	826	CLA	OBD-CAD-C3D	-2.36	123.67	128.03
30	M	7002	ECH	C8-C7-C6	-2.36	120.64	127.25
21	2	803	CLA	CHA-C1A-NA	-2.36	120.70	126.18
30	m	104	ECH	C23-C24-C25	-2.36	120.65	127.25
24	b	1849	BCR	C40-C30-C25	-2.36	106.48	110.31
24	B	843	BCR	C34-C9-C10	-2.36	119.62	122.92
24	2	849	BCR	C40-C30-C25	-2.36	106.49	110.31
21	a	823	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
31	F	205	SQD	O3-C3-C2	-2.35	105.25	110.36
24	a	847	BCR	C32-C1-C6	-2.35	106.50	110.31
31	L	208	SQD	O3-C3-C2	-2.35	105.25	110.36
24	a	843	BCR	C27-C26-C25	-2.34	119.30	122.74
24	6	202	BCR	C36-C18-C19	-2.34	114.36	118.10
21	2	802	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
21	1	813	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
24	A	847	BCR	C32-C1-C6	-2.34	106.51	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	841	CLA	CAA-CBA-CGA	-2.34	106.30	113.35
24	B	843	BCR	C39-C30-C25	-2.34	106.52	110.31
21	a	836	CLA	O2D-CGD-O1D	-2.33	119.12	123.82
21	b	1818	CLA	CHA-C1A-NA	-2.33	120.76	126.18
24	a	843	BCR	C39-C30-C25	-2.33	106.53	110.31
21	b	1824	CLA	CMB-C2B-C1B	-2.33	124.88	128.46
24	K	104	BCR	C34-C9-C10	-2.33	119.66	122.92
30	m	104	ECH	C8-C7-C6	-2.33	120.73	127.25
21	2	839	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
24	B	847	BCR	C34-C9-C10	-2.33	119.66	122.92
21	l	203	CLA	CMB-C2B-C1B	-2.32	124.89	128.46
25	l	209	LHG	C5-O7-C7	-2.32	112.39	117.88
22	B	841	PQN	O4-C4-C5	-2.32	117.73	121.55
24	2	847	BCR	C36-C18-C19	-2.32	114.40	118.10
24	2	848	BCR	C39-C30-C25	-2.32	106.55	110.31
34	b	1858	C7Z	C11-C12-C13	-2.32	119.90	126.42
30	l	202	ECH	C35-C13-C12	-2.32	114.41	118.10
22	b	1844	PQN	O1-C1-C10	-2.32	117.74	121.55
24	L	207	BCR	C12-C13-C14	-2.31	115.39	118.94
24	a	848	BCR	C34-C9-C10	-2.31	119.68	122.92
21	b	1827	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
24	B	846	BCR	C39-C30-C25	-2.31	106.57	110.31
25	1	850	LHG	C6-C5-C4	-2.31	106.65	111.86
24	A	848	BCR	C40-C30-C25	-2.31	106.57	110.31
21	a	809	CLA	CMB-C2B-C1B	-2.31	124.92	128.46
24	B	846	BCR	C34-C9-C10	-2.30	119.70	122.92
21	6	204	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
21	a	856	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
21	B	812	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
34	F	204	C7Z	C40-C33-C34	-2.29	119.72	122.92
31	b	1854	SQD	O3-C3-C2	-2.29	105.38	110.36
21	b	1820	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
21	1	804	CLA	CAA-CBA-CGA	-2.29	106.46	113.35
24	l	206	BCR	C39-C30-C25	-2.28	106.61	110.31
24	2	845	BCR	C39-C30-C25	-2.28	106.61	110.31
30	B	844	ECH	C23-C24-C25	-2.28	120.88	127.25
24	6	202	BCR	C34-C9-C10	-2.28	119.73	122.92
21	a	855	CLA	CMB-C2B-C1B	-2.28	124.97	128.46
21	b	1818	CLA	O2D-CGD-O1D	-2.27	119.25	123.82
21	2	803	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
24	9	102	BCR	C27-C26-C25	-2.27	119.41	122.74
21	A	805	CLA	CAA-C2A-C3A	-2.27	106.58	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	1102	BCR	C40-C30-C25	-2.27	106.63	110.31
21	2	819	CLA	OBD-CAD-C3D	-2.27	123.85	128.03
21	a	805	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
30	b	1847	ECH	C23-C24-C25	-2.26	120.92	127.25
24	j	1102	BCR	C27-C26-C25	-2.26	119.42	122.74
21	B	812	CLA	O1D-CGD-CBD	-2.26	120.54	124.60
21	1	855	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
21	2	821	CLA	CHA-C1A-NA	-2.25	120.94	126.18
24	1	845	BCR	C31-C1-C6	-2.25	106.65	110.31
24	B	842	BCR	C34-C9-C10	-2.25	119.77	122.92
21	a	826	CLA	CAA-CBA-CGA	-2.25	106.56	113.35
22	2	843	PQN	C2M-C2-C3	-2.25	119.64	124.20
24	J	1102	BCR	C40-C30-C25	-2.25	106.67	110.31
24	f	201	BCR	C34-C9-C10	-2.24	119.78	122.92
21	1	823	CLA	CHA-C1A-NA	-2.24	120.97	126.18
30	2	846	ECH	C12-C13-C14	-2.24	115.50	118.94
24	B	846	BCR	C32-C1-C6	-2.24	106.67	110.31
21	B	802	CLA	CAA-C2A-C3A	-2.24	106.67	112.81
24	0	204	BCR	C39-C30-C25	-2.24	106.68	110.31
24	a	845	BCR	C35-C13-C14	-2.24	119.79	122.92
24	A	845	BCR	C34-C9-C10	-2.24	119.79	122.92
30	b	1847	ECH	C8-C7-C6	-2.24	120.99	127.25
24	1	844	BCR	C15-C14-C13	-2.24	124.12	127.31
21	2	819	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
30	a	857	ECH	C7-C6-C5	-2.24	116.21	121.54
30	b	1847	ECH	C37-C22-C23	-2.24	114.54	118.10
21	b	1819	CLA	CAA-C2A-C3A	-2.24	106.68	112.81
25	a	853	LHG	O7-C7-O9	-2.24	118.10	123.68
21	B	825	CLA	CBC-CAC-C3C	-2.23	106.07	112.41
21	j	1105	CLA	OBD-CAD-C3D	-2.23	123.91	128.03
30	b	1847	ECH	C15-C16-C17	-2.23	118.70	123.46
24	2	849	BCR	C10-C11-C12	-2.23	116.39	123.23
21	A	834	CLA	CHA-C1A-NA	-2.23	121.00	126.18
21	2	819	CLA	CHA-C1A-NA	-2.23	121.00	126.18
21	B	813	CLA	CHA-C1A-NA	-2.23	121.00	126.18
21	1	813	CLA	CHA-C1A-NA	-2.23	121.00	126.18
21	A	826	CLA	O2D-CGD-O1D	-2.23	119.33	123.82
24	A	844	BCR	C12-C13-C14	-2.23	115.52	118.94
21	b	1807	CLA	C2C-C1C-NC	-2.23	108.69	110.22
21	b	1827	CLA	C6-C7-C8	-2.23	108.42	115.73
21	A	805	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
21	B	816	CLA	CHA-C1A-NA	-2.23	121.01	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	m	102	SQD	O3-C3-C2	-2.22	105.52	110.36
24	a	859	BCR	C24-C25-C26	-2.22	116.24	121.54
21	l	205	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
21	A	808	CLA	CAA-C2A-C3A	-2.22	106.72	112.81
24	b	1846	BCR	C24-C25-C26	-2.22	116.25	121.54
28	2	854	45D	C22-C16-C08	-2.22	120.94	123.92
24	a	847	BCR	C34-C9-C10	-2.22	119.82	122.92
21	B	825	CLA	O2D-CGD-O1D	-2.21	119.37	123.82
26	B	848	LMG	C7-O1-C1	-2.21	109.22	113.76
24	b	1848	BCR	C39-C30-C25	-2.21	106.72	110.31
34	2	855	C7Z	C11-C12-C13	-2.21	120.21	126.42
21	B	824	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
24	2	847	BCR	C40-C30-C25	-2.21	106.73	110.31
26	b	1851	LMG	O7-C10-O9	-2.21	118.17	123.68
24	1	844	BCR	C30-C25-C26	-2.21	119.49	122.59
24	B	842	BCR	C36-C18-C19	-2.20	114.59	118.10
21	A	817	CLA	O1D-CGD-CBD	-2.20	120.65	124.60
21	a	855	CLA	CHA-C1A-NA	-2.20	121.07	126.18
21	a	823	CLA	CHA-C1A-NA	-2.20	121.07	126.18
21	2	814	CLA	OBD-CAD-C3D	-2.20	123.98	128.03
21	A	829	CLA	O2D-CGD-O1D	-2.20	119.40	123.82
24	2	848	BCR	C30-C25-C26	-2.20	119.50	122.59
21	b	1828	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
24	a	844	BCR	C31-C1-C6	-2.19	106.75	110.31
21	A	834	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
24	B	847	BCR	C40-C30-C25	-2.19	106.76	110.31
24	B	845	BCR	C40-C30-C25	-2.19	106.76	110.31
21	A	805	CLA	CHA-C1A-NA	-2.19	121.10	126.18
21	A	804	CLA	CAA-CBA-CGA	-2.19	106.76	113.35
24	K	104	BCR	C10-C11-C12	-2.18	116.53	123.23
21	L	203	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
21	2	829	CLA	CHA-C1A-NA	-2.18	121.11	126.18
21	B	802	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
21	A	810	CLA	O2D-CGD-O1D	-2.18	119.44	123.82
24	i	101	BCR	C34-C9-C10	-2.18	119.87	122.92
35	1	854	LMT	C3'-C4'-C5'	-2.18	106.26	110.88
21	2	812	CLA	CHA-C1A-NA	-2.17	121.13	126.18
21	J	1106	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
21	a	817	CLA	OBD-CAD-C3D	-2.17	124.03	128.03
21	b	1806	CLA	CHA-C1A-NA	-2.17	121.14	126.18
24	h	101	BCR	C32-C1-C6	-2.17	106.80	110.31
21	2	805	CLA	CHA-C1A-NA	-2.16	121.15	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	825	CLA	CHA-C1A-NA	-2.16	121.16	126.18
24	K	104	BCR	C39-C30-C25	-2.16	106.81	110.31
21	1	811	CLA	CMD-C2D-C3D	-2.16	120.89	124.89
24	l	207	BCR	C34-C9-C10	-2.16	119.90	122.92
24	1	848	BCR	C39-C30-C25	-2.16	106.81	110.31
21	k	1401	CLA	CHA-C1A-NA	-2.16	121.17	126.18
34	F	204	C7Z	C31-C32-C33	-2.16	120.36	126.42
21	b	1807	CLA	CHA-C1A-NA	-2.16	121.17	126.18
21	b	1811	CLA	O2D-CGD-O1D	-2.15	119.48	123.82
21	b	1835	CLA	C6-C7-C8	-2.15	108.66	115.73
21	a	809	CLA	CAA-C2A-C3A	-2.15	106.91	112.81
21	b	1838	CLA	O2D-CGD-O1D	-2.15	119.49	123.82
24	h	101	BCR	C30-C25-C26	-2.15	119.57	122.59
24	k	1403	BCR	C34-C9-C10	-2.15	119.91	122.92
21	2	807	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
21	B	822	CLA	CHA-C1A-NA	-2.15	121.19	126.18
24	2	844	BCR	C39-C30-C25	-2.15	106.83	110.31
24	L	206	BCR	C32-C1-C6	-2.15	106.83	110.31
26	K	105	LMG	O7-C10-O9	-2.15	118.32	123.68
21	1	831	CLA	CHA-C1A-NA	-2.15	121.20	126.18
30	l	202	ECH	C28-C29-C30	-2.14	109.14	113.11
21	2	840	CLA	CHA-C1A-NA	-2.14	121.20	126.18
24	8	1403	BCR	C38-C26-C25	-2.14	122.11	124.51
24	a	845	BCR	C34-C9-C10	-2.14	119.92	122.92
21	a	810	CLA	CHA-C1A-NA	-2.14	121.20	126.18
24	A	844	BCR	C39-C30-C25	-2.14	106.84	110.31
21	b	1809	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
24	a	843	BCR	C32-C1-C6	-2.13	106.85	110.31
21	j	1104	CLA	O1D-CGD-CBD	-2.13	120.77	124.60
21	2	831	CLA	CHA-C1A-NA	-2.13	121.23	126.18
21	a	822	CLA	CHA-C1A-NA	-2.13	121.23	126.18
30	b	1847	ECH	C11-C10-C9	-2.13	124.27	127.31
24	1	849	BCR	C39-C30-C25	-2.13	106.85	110.31
24	b	1845	BCR	C36-C18-C19	-2.13	114.70	118.10
24	1	846	BCR	C34-C9-C10	-2.13	119.94	122.92
24	L	206	BCR	C38-C26-C25	-2.13	122.12	124.51
21	a	816	CLA	CHA-C1A-NA	-2.13	121.23	126.18
21	l	201	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
21	a	820	CLA	CHA-C1A-NA	-2.13	121.23	126.18
28	2	854	45D	C42-C41-C37	-2.13	118.92	123.46
21	2	823	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
21	1	802	CLA	CHA-C1A-NA	-2.12	121.24	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	807	CLA	CAA-C2A-C1A	-2.12	105.01	111.97
24	l	206	BCR	C32-C1-C6	-2.12	106.86	110.31
21	2	832	CLA	CHA-C1A-NA	-2.12	121.26	126.18
21	1	803	CLA	CHA-C1A-NA	-2.12	121.26	126.18
21	I	101	CLA	CHA-C1A-NA	-2.12	121.26	126.18
24	a	846	BCR	C30-C25-C26	-2.11	119.62	122.59
21	2	815	CLA	CHA-C1A-NA	-2.11	121.27	126.18
21	A	813	CLA	CHA-C1A-NA	-2.11	121.27	126.18
24	B	847	BCR	C11-C12-C13	-2.11	120.48	126.42
24	6	205	BCR	C27-C26-C25	-2.11	119.64	122.74
21	A	814	CLA	O2D-CGD-O1D	-2.11	119.58	123.82
21	L	205	CLA	C6-C7-C8	-2.11	108.81	115.73
21	B	817	CLA	CHA-C1A-NA	-2.11	121.29	126.18
24	l	207	BCR	C32-C1-C6	-2.11	106.89	110.31
28	A	856	45D	C41-C42-C38	-2.10	118.97	123.46
21	A	837	CLA	CAA-CBA-CGA	-2.10	107.01	113.35
21	1	803	CLA	OBD-CAD-C3D	-2.10	124.15	128.03
21	1	814	CLA	CHA-C1A-NA	-2.10	121.30	126.18
30	M	7002	ECH	C7-C6-C5	-2.10	116.53	121.54
21	a	802	CLA	C2C-C1C-NC	-2.10	108.78	110.22
21	2	839	CLA	CHA-C1A-NA	-2.10	121.30	126.18
24	I	102	BCR	C38-C26-C25	-2.10	122.16	124.51
21	2	814	CLA	CHA-C1A-NA	-2.10	121.31	126.18
21	b	1804	CLA	CAA-C2A-C3A	-2.10	107.06	112.81
21	A	812	CLA	O2D-CGD-O1D	-2.10	119.60	123.82
21	2	807	CLA	O2D-CGD-O1D	-2.10	119.60	123.82
21	2	842	CLA	CHA-C1A-NA	-2.10	121.31	126.18
21	a	838	CLA	CHA-C1A-NA	-2.09	121.31	126.18
21	1	816	CLA	CHA-C1A-NA	-2.09	121.31	126.18
24	K	104	BCR	C12-C13-C14	-2.09	115.73	118.94
21	b	1830	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
24	A	844	BCR	C31-C1-C6	-2.09	106.91	110.31
24	A	846	BCR	C38-C26-C25	-2.09	122.17	124.51
21	1	822	CLA	CHA-C1A-NA	-2.09	121.32	126.18
21	a	830	CLA	O2D-CGD-O1D	-2.09	119.61	123.82
35	J	1104	LMT	C1'-O5'-C5'	-2.09	109.77	113.72
21	2	833	CLA	CHA-C1A-NA	-2.09	121.32	126.18
21	a	802	CLA	O2D-CGD-O1D	-2.09	119.61	123.82
21	8	1402	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
21	B	824	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
21	B	804	CLA	CHA-C1A-NA	-2.09	121.33	126.18
21	b	1832	CLA	CHA-C1A-NA	-2.09	121.33	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	858	LHG	C5-O7-C7	-2.09	112.94	117.88
24	A	846	BCR	C39-C30-C25	-2.09	106.92	110.31
22	b	1844	PQN	C11-C12-C13	-2.09	123.22	126.71
21	2	825	CLA	CHA-C1A-NA	-2.09	121.33	126.18
21	a	815	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
24	B	847	BCR	C35-C13-C14	-2.08	120.00	122.92
21	B	802	CLA	O2D-CGD-O1D	-2.08	119.63	123.82
25	m	101	LHG	C5-O7-C7	-2.08	112.96	117.88
21	2	810	CLA	O1D-CGD-CBD	-2.08	120.86	124.60
21	A	815	CLA	CHA-C1A-NA	-2.08	121.35	126.18
21	2	804	CLA	CHA-C1A-NA	-2.08	121.35	126.18
21	A	803	CLA	CAA-CBA-CGA	-2.08	107.08	113.35
21	8	1402	CLA	CHA-C1A-NA	-2.08	121.35	126.18
21	a	840	CLA	CHA-C1A-NA	-2.08	121.35	126.18
21	A	836	CLA	OBD-CAD-C3D	-2.08	124.20	128.03
25	B	857	LHG	O7-C7-O9	-2.08	118.49	123.68
21	2	831	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
21	8	1401	CLA	CHA-C1A-NA	-2.08	121.36	126.18
21	B	821	CLA	CHA-C1A-NA	-2.07	121.36	126.18
25	A	851	LHG	O8-C23-O10	-2.07	118.40	123.55
34	b	1858	C7Z	C40-C33-C34	-2.07	120.02	122.92
24	1	858	BCR	C36-C18-C19	-2.07	114.80	118.10
21	a	806	CLA	CHA-C1A-NA	-2.07	121.37	126.18
21	B	803	CLA	CHA-C1A-NA	-2.07	121.37	126.18
21	a	833	CLA	CHA-C1A-NA	-2.07	121.37	126.18
26	b	1851	LMG	C30-C29-C28	-2.07	106.03	113.58
24	1	207	BCR	C36-C18-C19	-2.07	114.80	118.10
21	J	1106	CLA	CHA-C1A-NA	-2.07	121.37	126.18
21	a	834	CLA	CHA-C1A-NA	-2.07	121.37	126.18
21	f	202	CLA	CHA-C1A-NA	-2.07	121.37	126.18
21	2	803	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
21	a	837	CLA	CHA-C1A-NA	-2.07	121.38	126.18
21	F	203	CLA	CHA-C1A-NA	-2.07	121.38	126.18
21	A	835	CLA	CHA-C1A-NA	-2.07	121.38	126.18
21	a	804	CLA	CHA-C1A-NA	-2.07	121.38	126.18
26	B	848	LMG	C30-C29-C28	-2.07	106.04	113.58
24	a	859	BCR	C40-C30-C25	-2.07	106.96	110.31
21	1	820	CLA	CHA-C1A-NA	-2.06	121.38	126.18
31	L	208	SQD	O5-C1-O6	-2.06	105.12	110.02
34	F	204	C7Z	C20-C13-C14	-2.06	120.03	122.92
21	1	201	CLA	OBD-CAD-C3D	-2.06	124.22	128.03
24	B	845	BCR	C38-C26-C25	-2.06	122.20	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	830	CLA	CHA-C1A-NA	-2.06	121.39	126.18
30	2	846	ECH	C29-C30-C25	-2.06	107.25	110.48
21	A	819	CLA	CHA-C1A-NA	-2.06	121.39	126.18
21	1	840	CLA	CHA-C1A-NA	-2.06	121.39	126.18
24	9	102	BCR	C39-C30-C25	-2.06	106.97	110.31
21	A	802	CLA	O2D-CGD-O1D	-2.06	119.67	123.82
21	J	1105	CLA	CHA-C1A-NA	-2.06	121.40	126.18
21	k	1402	CLA	CHA-C1A-NA	-2.06	121.40	126.18
30	M	7002	ECH	C11-C10-C9	-2.06	124.37	127.31
21	a	831	CLA	CHA-C1A-NA	-2.06	121.40	126.18
21	2	824	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
21	B	840	CLA	CHA-C1A-NA	-2.05	121.41	126.18
21	A	823	CLA	CHA-C1A-NA	-2.05	121.41	126.18
34	b	1858	C7Z	C17-C1-C6	-2.05	106.98	110.31
26	a	852	LMG	O7-C10-O9	-2.05	118.56	123.68
21	I	101	CLA	CAC-C3C-C4C	-2.05	121.94	124.83
21	A	821	CLA	OBD-CAD-C3D	-2.05	124.25	128.03
21	B	839	CLA	O2D-CGD-O1D	-2.05	119.69	123.82
24	I	102	BCR	C10-C11-C12	-2.05	116.94	123.23
21	a	827	CLA	CHA-C1A-NA	-2.05	121.41	126.18
21	B	826	CLA	CHA-C1A-NA	-2.05	121.42	126.18
21	b	1841	CLA	CHA-C1A-NA	-2.05	121.42	126.18
21	b	1816	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
21	J	1101	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
21	2	822	CLA	CHA-C1A-NA	-2.05	121.42	126.18
24	2	848	BCR	C34-C9-C10	-2.05	120.06	122.92
24	h	101	BCR	C38-C26-C25	-2.04	122.22	124.51
24	j	1102	BCR	C32-C1-C6	-2.04	107.00	110.31
21	2	828	CLA	CHA-C1A-NA	-2.04	121.44	126.18
21	a	814	CLA	CHA-C1A-NA	-2.04	121.44	126.18
24	2	845	BCR	C34-C9-C10	-2.04	120.06	122.92
21	2	835	CLA	CHA-C1A-NA	-2.04	121.44	126.18
21	B	840	CLA	O1D-CGD-CBD	-2.04	120.94	124.60
21	2	806	CLA	CHA-C1A-NA	-2.04	121.44	126.18
21	A	832	CLA	CHA-C1A-NA	-2.04	121.44	126.18
21	a	803	CLA	CHA-C1A-NA	-2.04	121.44	126.18
21	1	804	CLA	CHA-C1A-NA	-2.04	121.44	126.18
21	B	810	CLA	CHA-C1A-NA	-2.04	121.44	126.18
21	2	811	CLA	CHA-C1A-NA	-2.04	121.44	126.18
28	2	854	45D	C29-C31-C33	-2.04	116.98	123.23
21	b	1815	CLA	CHA-C1A-NA	-2.04	121.44	126.18
24	1	858	BCR	C39-C30-C25	-2.04	107.00	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	l	201	CLA	CHA-C1A-NA	-2.04	121.45	126.18
21	A	814	CLA	CHA-C1A-NA	-2.04	121.45	126.18
21	j	1105	CLA	CHA-C1A-NA	-2.04	121.45	126.18
21	A	806	CLA	CHA-C1A-NA	-2.04	121.45	126.18
21	2	841	CLA	O2D-CGD-O1D	-2.03	119.72	123.82
21	1	817	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
21	1	826	CLA	CHA-C1A-NA	-2.03	121.46	126.18
24	a	844	BCR	C10-C11-C12	-2.03	117.00	123.23
21	a	813	CLA	CHA-C1A-NA	-2.03	121.46	126.18
21	a	815	CLA	CHA-C1A-NA	-2.03	121.46	126.18
21	1	839	CLA	CHA-C1A-NA	-2.03	121.47	126.18
21	K	102	CLA	CHA-C1A-NA	-2.03	121.47	126.18
21	b	1829	CLA	CHA-C1A-NA	-2.03	121.47	126.18
21	A	802	CLA	CHA-C1A-NA	-2.03	121.47	126.18
24	2	849	BCR	C30-C25-C26	-2.03	119.74	122.59
21	b	1828	CLA	CBC-CAC-C3C	-2.03	106.66	112.41
30	m	104	ECH	C7-C6-C5	-2.03	116.71	121.54
21	2	826	CLA	CHA-C1A-NA	-2.02	121.48	126.18
21	B	815	CLA	CHA-C1A-NA	-2.02	121.48	126.18
21	L	205	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
24	1	847	BCR	C31-C1-C6	-2.02	107.03	110.31
21	A	829	CLA	OBD-CAD-CBD	-2.02	122.88	125.94
21	b	1824	CLA	CHA-C1A-NA	-2.02	121.48	126.18
26	B	850	LMG	O7-C10-O9	-2.02	118.63	123.68
24	2	847	BCR	C1-C6-C5	-2.02	119.75	122.59
21	2	823	CLA	CHA-C1A-NA	-2.02	121.48	126.18
21	6	204	CLA	O2D-CGD-O1D	-2.02	119.75	123.82
21	2	820	CLA	CHA-C1A-NA	-2.02	121.48	126.18
24	K	104	BCR	C38-C26-C25	-2.02	122.25	124.51
24	A	844	BCR	C30-C25-C26	-2.02	119.75	122.59
21	1	811	CLA	CHA-C1A-NA	-2.02	121.49	126.18
21	A	808	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
21	b	1834	CLA	CHA-C1A-NA	-2.02	121.49	126.18
24	K	104	BCR	C27-C26-C25	-2.02	119.78	122.74
26	A	850	LMG	O7-C10-O9	-2.02	118.64	123.68
21	2	836	CLA	CHA-C1A-NA	-2.02	121.50	126.18
24	J	1107	BCR	C35-C13-C14	-2.02	120.10	122.92
22	1	842	PQN	C12-C11-C3	-2.02	106.19	111.85
21	b	1828	CLA	O2D-CGD-O1D	-2.01	119.77	123.82
21	a	835	CLA	CHA-C1A-NA	-2.01	121.51	126.18
25	b	1802	LHG	O7-C7-O9	-2.01	118.66	123.68
21	2	827	CLA	CAA-CBA-CGA	-2.01	107.29	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	807	CLA	CHA-C1A-NA	-2.01	121.51	126.18
21	A	821	CLA	C2C-C1C-NC	-2.01	108.84	110.22
21	a	856	CLA	CHA-C1A-NA	-2.01	121.51	126.18
21	b	1812	CLA	CHA-C1A-NA	-2.01	121.51	126.18
24	A	848	BCR	C1-C6-C5	-2.01	119.77	122.59
22	A	841	PQN	C17-C16-C15	-2.01	107.53	113.11
26	b	1853	LMG	O8-C28-O10	-2.01	118.57	123.55
21	7	1104	CLA	CHA-C1A-NA	-2.01	121.52	126.18
21	2	813	CLA	CHA-C1A-NA	-2.01	121.52	126.18
24	a	843	BCR	C34-C9-C10	-2.01	120.11	122.92
30	a	857	ECH	C8-C7-C6	-2.01	121.64	127.25
21	B	835	CLA	CHA-C1A-NA	-2.00	121.52	126.18
28	2	854	45D	C23-C25-C29	-2.00	115.87	118.94
21	1	829	CLA	CHA-C1A-NA	-2.00	121.53	126.18
21	a	839	CLA	CHA-C1A-NA	-2.00	121.53	126.18
21	7	1103	CLA	O1D-CGD-CBD	-2.00	121.01	124.60
21	0	202	CLA	O1D-CGD-CBD	-2.00	121.01	124.60
21	1	836	CLA	CHA-C1A-NA	-2.00	121.53	126.18
24	B	847	BCR	C37-C22-C23	2.00	121.29	118.10
21	b	1817	CLA	O2A-CGA-CBA	2.00	117.73	111.90
21	2	819	CLA	CMB-C2B-C3B	2.00	128.61	124.89
24	1	845	BCR	C30-C25-C24	2.00	121.36	115.73
21	a	813	CLA	CAC-C3C-C4C	2.01	127.66	124.83
24	2	848	BCR	C8-C9-C10	2.01	122.02	118.94
21	F	203	CLA	C1-O2A-CGA	2.01	121.59	116.77
24	B	842	BCR	C37-C22-C23	2.01	121.30	118.10
21	A	824	CLA	CMA-C3A-C2A	2.01	121.92	113.77
21	b	1830	CLA	CMA-C3A-C4A	2.01	117.17	111.77
21	B	802	CLA	C6-C5-C3	2.01	117.21	112.66
35	l	211	LMT	O1B-C1B-C2B	2.01	112.64	108.11
21	A	832	CLA	CMA-C3A-C4A	2.01	117.18	111.77
24	K	104	BCR	C35-C13-C12	2.02	121.31	118.10
21	B	819	CLA	C1-O2A-CGA	2.02	121.61	116.77
24	J	1107	BCR	C8-C9-C10	2.02	122.03	118.94
24	2	844	BCR	C37-C22-C23	2.02	121.31	118.10
21	2	842	CLA	CMA-C3A-C2A	2.02	120.46	116.38
24	A	846	BCR	C2-C1-C6	2.02	113.63	110.48
21	a	856	CLA	CMB-C2B-C3B	2.02	128.64	124.89
24	a	848	BCR	C19-C18-C17	2.02	122.04	118.94
21	b	1814	CLA	O2A-CGA-CBA	2.02	117.78	111.90
21	1	827	CLA	CMB-C2B-C3B	2.02	128.64	124.89
21	B	815	CLA	O2A-CGA-CBA	2.02	117.78	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	803	CLA	CMA-C3A-C4A	2.02	117.20	111.77
24	a	848	BCR	C38-C26-C27	2.02	117.29	113.45
21	a	830	CLA	C1-O2A-CGA	2.02	121.63	116.77
24	9	102	BCR	C23-C24-C25	2.02	132.92	127.25
34	F	204	C7Z	C31-C30-C29	2.03	130.20	127.31
24	1	856	BCR	C37-C22-C23	2.03	121.33	118.10
21	a	831	CLA	CMA-C3A-C4A	2.03	117.22	111.77
24	1	849	BCR	C37-C22-C23	2.03	121.33	118.10
30	2	846	ECH	C15-C16-C17	2.03	127.80	123.46
21	A	838	CLA	O2A-CGA-CBA	2.03	117.81	111.90
21	B	821	CLA	CMB-C2B-C3B	2.03	128.66	124.89
21	A	805	CLA	CMA-C3A-C4A	2.03	117.23	111.77
21	2	802	CLA	O2A-CGA-CBA	2.03	117.81	111.90
24	b	1845	BCR	C35-C13-C12	2.03	121.34	118.10
21	a	833	CLA	C1-O2A-CGA	2.03	121.65	116.77
21	1	802	CLA	C2A-C1A-CHA	2.03	127.53	123.92
21	a	801	CLA	C1-O2A-CGA	2.03	121.65	116.77
24	2	845	BCR	C37-C22-C23	2.04	121.34	118.10
21	1	833	CLA	C1-O2A-CGA	2.04	121.66	116.77
21	a	855	CLA	C2A-C1A-CHA	2.04	127.53	123.92
21	1	811	CLA	O2A-CGA-CBA	2.04	117.83	111.90
21	1	832	CLA	CMA-C3A-C4A	2.04	117.25	111.77
21	a	802	CLA	C1-O2A-CGA	2.04	121.66	116.77
21	2	835	CLA	CMA-C3A-C4A	2.04	117.26	111.77
24	1	848	BCR	C38-C26-C27	2.04	117.33	113.45
21	B	829	CLA	CMA-C3A-C4A	2.04	117.27	111.77
21	a	804	CLA	CMB-C2B-C3B	2.04	128.69	124.89
30	1	202	ECH	C33-C5-C4	2.05	117.33	113.45
21	A	832	CLA	C1-O2A-CGA	2.05	121.69	116.77
21	2	837	CLA	C1-O2A-CGA	2.05	121.69	116.77
21	A	829	CLA	CMA-C3A-C4A	2.06	117.30	111.77
21	1	837	CLA	C1-O2A-CGA	2.06	121.71	116.77
24	A	843	BCR	C29-C28-C27	2.06	116.25	111.34
21	B	807	CLA	CMA-C3A-C4A	2.06	117.31	111.77
24	1	846	BCR	C37-C22-C23	2.06	121.38	118.10
21	2	812	CLA	CMA-C3A-C2A	2.06	122.14	113.77
21	B	837	CLA	CMA-C3A-C4A	2.06	117.31	111.77
21	b	1807	CLA	C2A-C1A-CHA	2.06	127.57	123.92
21	L	205	CLA	C1-O2A-CGA	2.06	121.72	116.77
24	L	206	BCR	C35-C13-C12	2.06	121.39	118.10
21	1	817	CLA	O2A-CGA-CBA	2.06	117.90	111.90
21	b	1837	CLA	CMB-C2B-C3B	2.06	128.72	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	846	BCR	C1-C6-C7	2.06	121.53	115.73
21	A	854	CLA	CMA-C3A-C4A	2.06	117.32	111.77
24	l	207	BCR	C35-C13-C12	2.07	121.39	118.10
24	l	207	BCR	C37-C22-C23	2.07	121.39	118.10
24	l	206	BCR	C37-C22-C23	2.07	121.39	118.10
24	A	843	BCR	C37-C22-C23	2.07	121.39	118.10
24	8	1403	BCR	C37-C22-C23	2.07	121.39	118.10
21	6	203	CLA	CMB-C2B-C3B	2.07	128.73	124.89
24	1	844	BCR	C29-C28-C27	2.07	116.28	111.34
24	0	204	BCR	C8-C9-C10	2.07	122.12	118.94
21	B	812	CLA	C1-O2A-CGA	2.07	121.74	116.77
21	L	203	CLA	O2A-CGA-CBA	2.07	117.93	111.90
24	2	844	BCR	C38-C26-C27	2.07	117.39	113.45
21	A	824	CLA	C1-O2A-CGA	2.07	121.75	116.77
24	1	845	BCR	C29-C28-C27	2.08	116.29	111.34
21	b	1801	CLA	C1-O2A-CGA	2.08	121.75	116.77
21	A	804	CLA	C1C-NC-C4C	2.08	108.25	107.06
21	J	1103	CLA	O2A-CGA-CBA	2.08	117.94	111.90
24	1	858	BCR	C37-C22-C23	2.08	121.41	118.10
24	L	206	BCR	C38-C26-C27	2.08	117.39	113.45
24	a	844	BCR	C37-C22-C23	2.08	121.41	118.10
21	b	1808	CLA	CMA-C3A-C4A	2.08	117.36	111.77
21	2	841	CLA	C1-O2A-CGA	2.08	121.76	116.77
24	9	102	BCR	C8-C7-C6	2.08	133.08	127.25
21	a	839	CLA	O2A-CGA-CBA	2.09	117.97	111.90
24	A	847	BCR	C38-C26-C27	2.09	117.41	113.45
21	A	837	CLA	CMA-C3A-C4A	2.09	117.38	111.77
26	0	206	LMG	O6-C5-C6	2.09	111.41	106.41
21	2	829	CLA	CMB-C2B-C3B	2.09	128.77	124.89
21	1	803	CLA	C1-O2A-CGA	2.09	121.78	116.77
21	A	830	CLA	CMA-C3A-C4A	2.09	117.39	111.77
26	0	206	LMG	C9-O8-C28	2.09	123.42	117.13
24	1	856	BCR	C38-C26-C27	2.09	117.42	113.45
21	2	812	CLA	C1-O2A-CGA	2.09	121.79	116.77
24	0	205	BCR	C15-C14-C13	2.09	130.29	127.31
24	L	207	BCR	C37-C22-C23	2.09	121.43	118.10
21	1	819	CLA	O2A-CGA-CBA	2.09	117.99	111.90
36	L	201	EQ3	C36-C18-C19	2.09	121.44	118.10
30	B	844	ECH	C37-C22-C21	2.10	125.86	122.92
34	F	204	C7Z	C39-C29-C28	2.10	121.44	118.10
21	1	833	CLA	CMA-C3A-C4A	2.10	117.41	111.77
30	a	857	ECH	O27-C27-C26	2.10	122.79	120.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	823	CLA	C1-O2A-CGA	2.10	121.81	116.77
24	h	101	BCR	C38-C26-C27	2.10	117.44	113.45
24	A	845	BCR	C35-C13-C12	2.10	121.45	118.10
21	a	829	CLA	O2A-CGA-CBA	2.10	118.02	111.90
21	b	1823	CLA	C1-O2A-CGA	2.10	121.82	116.77
21	B	801	CLA	CMA-C3A-C4A	2.11	117.44	111.77
21	A	855	CLA	CMB-C2B-C3B	2.11	128.80	124.89
21	a	817	CLA	O2A-CGA-CBA	2.11	118.03	111.90
21	a	802	CLA	CMB-C2B-C3B	2.11	128.81	124.89
24	2	848	BCR	C35-C13-C12	2.11	121.47	118.10
21	A	804	CLA	O2A-CGA-CBA	2.11	118.05	111.90
24	6	202	BCR	C37-C22-C23	2.11	121.47	118.10
21	1	820	CLA	CMB-C2B-C3B	2.12	128.82	124.89
24	L	206	BCR	C23-C24-C25	2.12	133.18	127.25
30	l	202	ECH	C34-C9-C10	2.12	125.89	122.92
24	l	206	BCR	C35-C13-C12	2.12	121.47	118.10
21	2	823	CLA	C1-O2A-CGA	2.12	121.85	116.77
24	a	859	BCR	C19-C18-C17	2.12	122.19	118.94
21	l	203	CLA	CMB-C2B-C3B	2.12	128.82	124.89
21	2	837	CLA	CMB-C2B-C3B	2.12	128.82	124.89
24	A	846	BCR	C35-C13-C12	2.12	121.48	118.10
21	A	833	CLA	O2A-CGA-CBA	2.12	118.08	111.90
26	b	1853	LMG	C1-C2-C3	2.12	113.93	109.98
30	a	857	ECH	C19-C18-C17	2.12	122.20	118.94
28	A	856	45D	C10-C18-C16	2.12	120.70	118.80
21	0	201	CLA	O2A-CGA-CBA	2.13	118.08	111.90
24	j	1102	BCR	C37-C22-C23	2.13	121.49	118.10
35	l	211	LMT	C1B-O5B-C5B	2.13	117.73	113.72
21	j	1104	CLA	O2A-CGA-CBA	2.13	118.10	111.90
24	A	848	BCR	C37-C22-C23	2.13	121.50	118.10
21	1	808	CLA	O2A-CGA-CBA	2.13	118.10	111.90
24	B	842	BCR	C29-C28-C27	2.13	116.43	111.34
21	a	806	CLA	CMB-C2B-C3B	2.14	128.85	124.89
21	b	1809	CLA	O2A-CGA-CBA	2.14	118.11	111.90
21	A	801	CLA	C1C-NC-C4C	2.14	108.28	107.06
21	A	803	CLA	CMB-C2B-C3B	2.14	128.86	124.89
21	b	1828	CLA	CMA-C3A-C4A	2.14	117.53	111.77
21	1	805	CLA	O2A-CGA-CBA	2.14	118.13	111.90
21	a	813	CLA	O2A-CGA-CBA	2.14	118.14	111.90
21	A	840	CLA	C1-O2A-CGA	2.14	121.92	116.77
35	1	854	LMT	O5B-C5B-C6B	2.14	111.55	106.41
21	A	808	CLA	C1-O2A-CGA	2.14	121.92	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	845	BCR	C37-C22-C23	2.15	121.52	118.10
21	a	829	CLA	C1-O2A-CGA	2.15	121.92	116.77
24	i	101	BCR	C15-C14-C13	2.15	130.37	127.31
21	B	827	CLA	CMA-C3A-C4A	2.15	117.56	111.77
24	A	846	BCR	C15-C14-C13	2.15	130.38	127.31
21	A	823	CLA	CMB-C2B-C3B	2.16	128.89	124.89
30	B	844	ECH	C19-C18-C17	2.16	122.25	118.94
21	a	840	CLA	O2A-CGA-CBA	2.16	118.17	111.90
24	f	204	BCR	C29-C28-C27	2.16	116.48	111.34
21	B	820	CLA	C1-C2-C3	2.16	129.93	125.96
21	1	812	CLA	O2A-CGA-CBA	2.16	118.17	111.90
21	1	840	CLA	O2A-CGA-CBA	2.16	118.18	111.90
21	b	1807	CLA	CMA-C3A-C4A	2.16	117.59	111.77
24	b	1846	BCR	C30-C25-C24	2.16	121.81	115.73
21	A	812	CLA	C1-O2A-CGA	2.16	121.97	116.77
21	2	834	CLA	O2A-CGA-CBA	2.16	118.20	111.90
21	A	809	CLA	O2A-CGA-CBA	2.16	118.20	111.90
34	F	204	C7Z	C27-C28-C29	2.17	129.47	126.21
24	a	843	BCR	C23-C24-C25	2.17	133.32	127.25
24	i	101	BCR	C2-C1-C6	2.17	113.87	110.48
21	a	811	CLA	O2A-CGA-CBA	2.17	118.21	111.90
26	A	850	LMG	O1-C1-C2	2.17	111.77	108.23
24	B	845	BCR	C35-C13-C12	2.17	121.56	118.10
21	a	837	CLA	CMA-C3A-C4A	2.17	117.61	111.77
21	A	836	CLA	C1-O2A-CGA	2.17	121.99	116.77
24	a	848	BCR	C37-C22-C23	2.17	121.56	118.10
21	b	1821	CLA	CMA-C3A-C4A	2.18	117.62	111.77
21	B	833	CLA	CMA-C3A-C4A	2.18	117.63	111.77
24	a	843	BCR	C2-C1-C6	2.18	113.88	110.48
21	A	832	CLA	O2A-CGA-CBA	2.18	118.24	111.90
21	B	821	CLA	C1-O2A-CGA	2.18	122.00	116.77
21	a	831	CLA	O2A-CGA-CBA	2.18	118.24	111.90
24	b	1846	BCR	C35-C13-C12	2.18	121.57	118.10
21	A	801	CLA	C2A-C3A-C4A	2.18	105.39	101.87
24	f	201	BCR	C8-C9-C10	2.18	122.29	118.94
24	a	847	BCR	C37-C22-C23	2.18	121.58	118.10
21	1	840	CLA	C1-O2A-CGA	2.18	122.01	116.77
21	B	835	CLA	O2A-CGA-CBA	2.19	118.26	111.90
21	B	802	CLA	CMA-C3A-C4A	2.19	117.65	111.77
24	6	205	BCR	C38-C26-C27	2.19	117.60	113.45
24	1	858	BCR	C30-C25-C24	2.19	121.88	115.73
21	B	812	CLA	O2A-CGA-CBA	2.19	118.27	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	808	CLA	O2A-CGA-CBA	2.19	118.28	111.90
21	2	803	CLA	C2A-C1A-CHA	2.19	127.80	123.92
21	1	813	CLA	CMB-C2B-C3B	2.19	128.96	124.89
21	a	810	CLA	O2A-CGA-CBA	2.19	118.28	111.90
21	1	836	CLA	CMB-C2B-C3B	2.19	128.96	124.89
24	B	845	BCR	C37-C22-C23	2.20	121.60	118.10
21	A	802	CLA	O2A-CGA-CBA	2.20	118.29	111.90
24	6	205	BCR	C15-C14-C13	2.20	130.45	127.31
21	F	203	CLA	O2A-CGA-CBA	2.20	118.30	111.90
24	1	847	BCR	C37-C22-C23	2.20	121.60	118.10
24	7	1102	BCR	C8-C9-C10	2.20	122.32	118.94
21	l	201	CLA	CMA-C3A-C4A	2.20	117.69	111.77
24	k	1403	BCR	C37-C22-C23	2.20	121.61	118.10
21	b	1812	CLA	O2A-CGA-CBA	2.20	118.31	111.90
24	2	849	BCR	C35-C13-C12	2.20	121.61	118.10
21	l	201	CLA	O2A-CGA-CBA	2.20	118.31	111.90
24	2	849	BCR	C15-C14-C13	2.20	130.46	127.31
21	b	1819	CLA	CMA-C3A-C4A	2.20	117.70	111.77
24	a	843	BCR	C37-C22-C23	2.20	121.61	118.10
21	1	823	CLA	CMB-C2B-C3B	2.20	128.98	124.89
21	B	820	CLA	O2A-CGA-CBA	2.21	118.32	111.90
21	A	826	CLA	O2A-CGA-CBA	2.21	118.32	111.90
24	J	1102	BCR	C37-C22-C23	2.21	121.62	118.10
28	A	856	45D	C06-C04-C08	2.21	113.93	110.48
21	2	803	CLA	CMA-C3A-C4A	2.21	117.71	111.77
21	2	824	CLA	CBA-CAA-C2A	2.21	120.41	113.80
21	a	808	CLA	O2A-CGA-CBA	2.21	118.33	111.90
21	B	814	CLA	O2A-CGA-CBA	2.21	118.34	111.90
24	1	858	BCR	C19-C18-C17	2.21	122.34	118.94
21	B	807	CLA	O2A-CGA-CBA	2.21	118.34	111.90
21	a	821	CLA	CMB-C2B-C3B	2.21	129.00	124.89
21	b	1807	CLA	CMB-C2B-C3B	2.21	129.00	124.89
21	b	1833	CLA	O2A-CGA-CBA	2.21	118.34	111.90
21	2	805	CLA	C2A-C1A-CHA	2.22	127.85	123.92
21	a	801	CLA	O2D-CGD-CBD	2.22	115.26	111.30
24	b	1850	BCR	C37-C22-C23	2.22	121.64	118.10
21	a	812	CLA	O2A-CGA-CBA	2.22	118.36	111.90
21	A	827	CLA	CMA-C3A-C4A	2.22	117.74	111.77
21	B	824	CLA	O2A-CGA-CBA	2.22	118.36	111.90
21	b	1838	CLA	CMB-C2B-C3B	2.22	129.01	124.89
21	2	834	CLA	C1-O2A-CGA	2.22	122.11	116.77
21	b	1810	CLA	O2A-CGA-CBA	2.22	118.37	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	844	BCR	C29-C28-C27	2.22	116.64	111.34
21	b	1809	CLA	CMA-C3A-C4A	2.22	117.75	111.77
24	b	1849	BCR	C15-C14-C13	2.23	130.49	127.31
21	A	840	CLA	O2A-CGA-CBA	2.23	118.38	111.90
24	l	207	BCR	C19-C18-C17	2.23	122.36	118.94
24	1	848	BCR	C29-C28-C27	2.23	116.66	111.34
24	K	104	BCR	C37-C22-C23	2.23	121.65	118.10
24	a	846	BCR	C38-C26-C27	2.23	117.69	113.45
24	j	1102	BCR	C38-C26-C27	2.23	117.69	113.45
24	B	847	BCR	C12-C13-C14	2.24	122.37	118.94
21	B	825	CLA	CMA-C3A-C4A	2.24	117.78	111.77
24	b	1850	BCR	C29-C28-C27	2.24	116.68	111.34
21	A	826	CLA	C1-O2A-CGA	2.24	122.14	116.77
24	A	846	BCR	C37-C22-C23	2.24	121.67	118.10
24	J	1107	BCR	C37-C22-C23	2.24	121.67	118.10
21	j	1101	CLA	CBA-CAA-C2A	2.24	120.50	113.80
21	B	832	CLA	CMA-C3A-C4A	2.24	117.80	111.77
21	a	810	CLA	C1-O2A-CGA	2.24	122.15	116.77
21	a	803	CLA	CMB-C2B-C3B	2.24	129.06	124.89
21	a	856	CLA	CMA-C3A-C4A	2.24	117.80	111.77
21	a	809	CLA	O2A-CGA-CBA	2.24	118.43	111.90
21	2	840	CLA	O2A-CGA-CBA	2.25	118.43	111.90
28	2	854	45D	C27-C25-C23	2.25	121.68	118.10
21	B	825	CLA	O2A-CGA-CBA	2.25	118.44	111.90
21	a	822	CLA	C1-O2A-CGA	2.25	122.17	116.77
21	2	840	CLA	C1-O2A-CGA	2.25	122.17	116.77
21	K	102	CLA	O2A-CGA-CBA	2.25	118.45	111.90
21	B	816	CLA	C1-O2A-CGA	2.25	122.18	116.77
24	a	847	BCR	C35-C13-C12	2.25	121.69	118.10
21	2	823	CLA	CMB-C2B-C3B	2.26	129.08	124.89
21	I	101	CLA	O2D-CGD-CBD	2.26	115.33	111.30
21	a	805	CLA	O2A-CGA-CBA	2.26	118.47	111.90
21	j	1105	CLA	O2A-CGA-CBA	2.26	118.47	111.90
21	2	820	CLA	O2A-CGA-CBA	2.26	118.47	111.90
24	1	858	BCR	C29-C28-C27	2.26	116.73	111.34
21	a	805	CLA	CMB-C2B-C3B	2.26	129.09	124.89
21	f	202	CLA	O2A-CGA-CBA	2.26	118.47	111.90
21	1	804	CLA	CMA-C3A-C4A	2.26	117.85	111.77
21	1	831	CLA	CMA-C3A-C4A	2.26	117.85	111.77
21	B	830	CLA	O2A-CGA-CBA	2.26	118.48	111.90
24	a	859	BCR	C37-C22-C23	2.26	121.70	118.10
24	6	205	BCR	C37-C22-C23	2.27	121.71	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	816	CLA	CBA-CAA-C2A	2.27	120.58	113.80
21	1	825	CLA	O2A-CGA-CBA	2.27	118.51	111.90
24	7	1102	BCR	C37-C22-C23	2.27	121.72	118.10
21	2	838	CLA	O2A-CGA-CBA	2.27	118.51	111.90
21	1	813	CLA	CAC-C3C-C4C	2.28	128.04	124.83
21	1	814	CLA	C1-O2A-CGA	2.28	122.23	116.77
21	L	203	CLA	CMB-C2B-C3B	2.28	129.12	124.89
24	2	849	BCR	C37-C22-C23	2.28	121.73	118.10
21	A	821	CLA	O2A-CGA-CBA	2.28	118.54	111.90
21	A	835	CLA	O2A-CGA-CBA	2.28	118.54	111.90
21	a	832	CLA	CMA-C3A-C4A	2.28	117.91	111.77
34	F	204	C7Z	C38-C25-C24	2.28	118.50	114.33
21	A	831	CLA	O2A-CGA-CBA	2.29	118.55	111.90
21	A	830	CLA	CMB-C2B-C3B	2.29	129.13	124.89
21	a	823	CLA	CMB-C2B-C3B	2.29	129.13	124.89
21	B	833	CLA	O2A-CGA-CBA	2.29	118.55	111.90
21	b	1831	CLA	CMB-C2B-C3B	2.29	129.13	124.89
21	b	1819	CLA	CBA-CAA-C2A	2.29	120.64	113.80
21	A	827	CLA	O2A-CGA-CBA	2.29	118.56	111.90
21	A	825	CLA	O2A-CGA-CBA	2.29	118.56	111.90
21	1	802	CLA	O2A-CGA-CBA	2.29	118.57	111.90
21	b	1828	CLA	O2A-CGA-CBA	2.29	118.57	111.90
24	a	846	BCR	C35-C13-C12	2.29	121.75	118.10
21	b	1838	CLA	O2A-CGA-CBA	2.29	118.57	111.90
21	A	815	CLA	O2A-CGA-CBA	2.30	118.58	111.90
24	A	844	BCR	C38-C26-C27	2.30	117.81	113.45
24	B	842	BCR	C19-C18-C17	2.30	122.47	118.94
21	1	823	CLA	O2A-CGA-CBA	2.30	118.59	111.90
24	8	1403	BCR	C29-C28-C27	2.30	116.84	111.34
21	A	854	CLA	C2A-C1A-CHA	2.31	128.01	123.92
21	a	815	CLA	CMB-C2B-C3B	2.31	129.17	124.89
21	0	202	CLA	O2A-CGA-CBA	2.31	118.61	111.90
21	B	831	CLA	CMA-C3A-C4A	2.31	117.97	111.77
21	a	832	CLA	O2A-CGA-CBA	2.31	118.61	111.90
21	j	1103	CLA	O2A-CGA-CBA	2.31	118.61	111.90
21	2	826	CLA	O2A-CGA-CBA	2.31	118.62	111.90
21	A	816	CLA	O2A-CGA-CBA	2.31	118.62	111.90
21	A	804	CLA	CMB-C2B-C3B	2.31	129.18	124.89
21	B	818	CLA	O2A-CGA-CBA	2.31	118.62	111.90
21	A	835	CLA	O2D-CGD-CBD	2.31	115.43	111.30
24	b	1845	BCR	C19-C18-C17	2.31	122.49	118.94
21	A	816	CLA	C1-O2A-CGA	2.31	122.33	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	102	BCR	C38-C26-C27	2.31	117.84	113.45
21	6	203	CLA	O2A-CGA-CBA	2.32	118.64	111.90
21	A	812	CLA	CMA-C3A-C4A	2.32	118.00	111.77
21	2	826	CLA	CMA-C3A-C4A	2.32	118.00	111.77
21	F	202	CLA	O2A-CGA-CBA	2.32	118.64	111.90
21	A	801	CLA	O2A-CGA-CBA	2.32	118.66	111.90
21	b	1832	CLA	C1-O2A-CGA	2.32	122.34	116.77
21	k	1401	CLA	C1-O2A-CGA	2.32	122.34	116.77
21	a	835	CLA	O2A-CGA-CBA	2.32	118.66	111.90
21	A	855	CLA	C1-O2A-CGA	2.32	122.35	116.77
21	b	1832	CLA	O2A-CGA-CBA	2.33	118.67	111.90
24	6	202	BCR	C8-C9-C10	2.33	122.51	118.94
21	2	829	CLA	CMA-C3A-C4A	2.33	118.03	111.77
21	2	830	CLA	O2A-CGA-CBA	2.33	118.67	111.90
21	2	821	CLA	CMA-C3A-C4A	2.33	118.03	111.77
21	2	822	CLA	O2A-CGA-CBA	2.33	118.68	111.90
21	B	813	CLA	CAC-C3C-C4C	2.33	128.12	124.83
21	1	806	CLA	CMA-C3A-C4A	2.33	118.04	111.77
28	A	856	45D	C09-C05-C03	2.33	117.42	113.11
21	A	805	CLA	CMB-C2B-C3B	2.33	129.22	124.89
21	A	807	CLA	CMA-C3A-C4A	2.33	118.04	111.77
21	1	802	CLA	CMA-C3A-C4A	2.33	118.04	111.77
36	L	201	EQ3	C37-C22-C23	2.33	121.82	118.10
21	1	833	CLA	CMB-C2B-C3B	2.33	129.22	124.89
28	2	854	45D	C10-C18-C16	2.33	120.88	118.80
21	j	1101	CLA	C1-O2A-CGA	2.34	122.38	116.77
21	a	839	CLA	C1-O2A-CGA	2.34	122.38	116.77
21	A	810	CLA	CMA-C3A-C4A	2.34	118.05	111.77
21	A	836	CLA	O2A-CGA-CBA	2.34	118.70	111.90
21	2	819	CLA	O2A-CGA-CBA	2.34	118.71	111.90
21	b	1835	CLA	O2A-CGA-CBA	2.34	118.72	111.90
21	A	825	CLA	C1-O2A-CGA	2.34	122.39	116.77
21	1	834	CLA	CMA-C3A-C4A	2.34	118.07	111.77
21	b	1807	CLA	C1C-NC-C4C	2.35	108.40	107.06
21	a	809	CLA	C1-O2A-CGA	2.35	122.40	116.77
21	b	1834	CLA	O2A-CGA-CBA	2.35	118.72	111.90
21	b	1810	CLA	CMA-C3A-C4A	2.35	118.08	111.77
21	l	204	CLA	O2A-CGA-CBA	2.35	118.73	111.90
24	2	849	BCR	C8-C9-C10	2.35	122.54	118.94
21	2	802	CLA	CMA-C3A-C4A	2.35	118.08	111.77
21	B	803	CLA	O2A-CGA-CBA	2.35	118.74	111.90
21	0	203	CLA	CMA-C3A-C4A	2.35	118.09	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1842	CLA	CMA-C3A-C4A	2.35	118.09	111.77
21	B	821	CLA	O2A-CGA-CBA	2.35	118.74	111.90
21	1	802	CLA	CMB-C2B-C3B	2.35	129.26	124.89
21	a	825	CLA	O2A-CGA-CBA	2.35	118.75	111.90
21	b	1835	CLA	C1-O2A-CGA	2.35	122.42	116.77
21	a	817	CLA	C1-O2A-CGA	2.36	122.42	116.77
21	a	803	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	B	809	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	A	826	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	a	813	CLA	CMA-C3A-C4A	2.36	118.11	111.77
24	0	205	BCR	C8-C9-C10	2.36	122.56	118.94
21	1	832	CLA	O2A-CGA-CBA	2.36	118.77	111.90
21	B	819	CLA	O2A-CGA-CBA	2.36	118.78	111.90
21	2	808	CLA	CMA-C3A-C4A	2.36	118.13	111.77
21	1	833	CLA	O2A-CGA-CBA	2.36	118.78	111.90
24	F	201	BCR	C8-C9-C10	2.37	122.58	118.94
35	0	208	LMT	C1'-C2'-C3'	2.37	114.39	109.98
21	K	102	CLA	C1-O2A-CGA	2.37	122.47	116.77
21	A	817	CLA	O2A-CGA-CBA	2.37	118.81	111.90
21	1	806	CLA	O2A-CGA-CBA	2.38	118.82	111.90
21	b	1833	CLA	CMA-C3A-C4A	2.38	118.17	111.77
24	K	104	BCR	C38-C26-C27	2.38	117.97	113.45
21	b	1836	CLA	O2A-CGA-CBA	2.38	118.83	111.90
21	2	813	CLA	O2A-CGA-CBA	2.38	118.84	111.90
21	2	816	CLA	O2A-CGA-CBA	2.38	118.84	111.90
21	1	836	CLA	O2A-CGA-CBA	2.39	118.84	111.90
21	1	839	CLA	O2A-CGA-CBA	2.39	118.84	111.90
24	A	844	BCR	C37-C22-C23	2.39	121.90	118.10
21	a	828	CLA	O2A-CGA-CBA	2.39	118.85	111.90
35	0	208	LMT	O1B-C4'-C3'	2.39	112.94	107.19
21	1	820	CLA	O2A-CGA-CBA	2.39	118.85	111.90
21	B	829	CLA	O2A-CGA-CBA	2.39	118.86	111.90
21	1	813	CLA	C1-O2A-CGA	2.39	122.51	116.77
28	2	854	45D	C03-C07-C19	2.39	122.45	115.73
24	1	848	BCR	C37-C22-C23	2.39	121.91	118.10
21	f	203	CLA	O2A-CGA-CBA	2.40	118.87	111.90
28	A	856	45D	C24-C26-C30	2.40	122.62	118.94
21	a	824	CLA	C1-O2A-CGA	2.40	122.53	116.77
21	B	810	CLA	CMA-C3A-C4A	2.40	118.22	111.77
21	A	805	CLA	O2A-CGA-CBA	2.40	118.88	111.90
21	b	1827	CLA	O2A-CGA-CBA	2.40	118.89	111.90
21	m	103	CLA	CMA-C3A-C4A	2.40	118.23	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	801	CLA	O2A-CGA-CBA	2.41	118.90	111.90
21	a	802	CLA	O2A-CGA-CBA	2.41	118.90	111.90
24	A	845	BCR	C1-C6-C7	2.41	122.50	115.73
21	A	838	CLA	O2D-CGD-CBD	2.41	115.60	111.30
21	1	831	CLA	O2A-CGA-CBA	2.41	118.92	111.90
21	B	836	CLA	O2A-CGA-CBA	2.41	118.92	111.90
24	2	847	BCR	C19-C18-C17	2.42	122.65	118.94
30	B	844	ECH	C12-C13-C14	2.42	122.65	118.94
21	I	101	CLA	C1-O2A-CGA	2.42	122.57	116.77
21	A	821	CLA	CMB-C2B-C3B	2.42	129.38	124.89
21	b	1839	CLA	O2A-CGA-CBA	2.42	118.94	111.90
21	a	821	CLA	O2A-CGA-CBA	2.42	118.94	111.90
21	a	805	CLA	CMA-C3A-C4A	2.42	118.28	111.77
24	L	207	BCR	C35-C13-C12	2.42	121.96	118.10
21	1	826	CLA	C1-O2A-CGA	2.42	122.58	116.77
21	a	823	CLA	O2A-CGA-CBA	2.42	118.95	111.90
24	L	207	BCR	C15-C14-C13	2.43	130.78	127.31
24	i	101	BCR	C37-C22-C23	2.43	121.97	118.10
24	6	202	BCR	C19-C18-C17	2.43	122.67	118.94
21	J	1105	CLA	O2A-CGA-CBA	2.43	118.97	111.90
21	j	1101	CLA	O2A-CGA-CBA	2.43	118.97	111.90
21	1	821	CLA	CMA-C3A-C4A	2.43	118.31	111.77
21	a	806	CLA	O2A-CGA-CBA	2.43	118.98	111.90
21	2	809	CLA	CMA-C3A-C4A	2.44	118.32	111.77
21	b	1839	CLA	CMA-C3A-C4A	2.44	118.32	111.77
21	L	204	CLA	O2A-CGA-CBA	2.44	118.99	111.90
21	B	840	CLA	O2A-CGA-CBA	2.44	119.00	111.90
21	6	204	CLA	C2A-C1A-CHA	2.44	128.25	123.92
21	k	1402	CLA	C1-O2A-CGA	2.44	122.63	116.77
21	1	821	CLA	O2A-CGA-CBA	2.44	119.01	111.90
21	b	1834	CLA	CMA-C3A-C4A	2.44	118.34	111.77
21	A	822	CLA	O2A-CGA-CBA	2.45	119.01	111.90
21	6	201	CLA	C1-O2A-CGA	2.45	122.64	116.77
21	A	821	CLA	C1-O2A-CGA	2.45	122.64	116.77
21	b	1826	CLA	CMA-C3A-C4A	2.45	118.35	111.77
21	7	1103	CLA	O2A-CGA-CBA	2.45	119.03	111.90
21	1	820	CLA	CMA-C3A-C4A	2.45	118.36	111.77
21	B	837	CLA	O2A-CGA-CBA	2.45	119.03	111.90
24	k	1403	BCR	C40-C30-C29	2.45	118.47	108.80
21	A	819	CLA	O2A-CGA-CBA	2.45	119.04	111.90
24	A	847	BCR	C40-C30-C29	2.45	118.48	108.80
21	b	1825	CLA	C1-O2A-CGA	2.46	122.66	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	0	205	BCR	C29-C28-C27	2.47	117.22	111.34
21	l	205	CLA	C1-O2A-CGA	2.47	122.69	116.77
21	a	855	CLA	CMA-C3A-C4A	2.47	118.41	111.77
26	K	105	LMG	O6-C1-C2	2.47	115.06	110.30
21	b	1814	CLA	CMA-C3A-C4A	2.47	118.41	111.77
24	2	844	BCR	C40-C30-C29	2.47	118.56	108.80
21	1	804	CLA	C1-O2A-CGA	2.47	122.71	116.77
21	k	1401	CLA	O2A-CGA-CBA	2.47	119.10	111.90
21	2	803	CLA	O2A-CGA-CBA	2.48	119.10	111.90
21	a	833	CLA	CMA-C3A-C4A	2.48	118.43	111.77
21	B	816	CLA	CMB-C2B-C3B	2.48	129.49	124.89
21	b	1807	CLA	O2A-CGA-CBA	2.48	119.11	111.90
21	1	841	CLA	C1-O2A-CGA	2.48	122.72	116.77
24	F	201	BCR	C40-C30-C29	2.48	118.58	108.80
21	A	808	CLA	O2A-CGA-CBA	2.48	119.11	111.90
24	b	1848	BCR	C40-C30-C29	2.48	118.58	108.80
21	b	1819	CLA	C1-O2A-CGA	2.48	122.72	116.77
21	b	1818	CLA	C1-O2A-CGA	2.48	122.72	116.77
24	B	845	BCR	C40-C30-C29	2.48	118.58	108.80
21	l	205	CLA	CMB-C2B-C3B	2.48	129.49	124.89
21	B	831	CLA	O2A-CGA-CBA	2.48	119.12	111.90
21	L	205	CLA	CMA-C3A-C4A	2.48	118.44	111.77
21	B	808	CLA	CMA-C3A-C4A	2.48	118.44	111.77
21	a	834	CLA	O2A-CGA-CBA	2.48	119.12	111.90
21	1	835	CLA	O2A-CGA-CBA	2.48	119.12	111.90
21	2	839	CLA	O2D-CGD-CBD	2.48	115.74	111.30
21	F	202	CLA	CMA-C3A-C4A	2.48	118.45	111.77
24	j	1102	BCR	C40-C30-C29	2.49	118.61	108.80
21	a	808	CLA	CMA-C3A-C4A	2.49	118.46	111.77
24	1	844	BCR	C40-C30-C29	2.49	118.61	108.80
24	A	848	BCR	C40-C30-C29	2.49	118.61	108.80
21	A	855	CLA	CMA-C3A-C4A	2.49	118.46	111.77
24	0	204	BCR	C40-C30-C29	2.49	118.62	108.80
24	L	206	BCR	C40-C30-C29	2.49	118.62	108.80
21	B	822	CLA	O2A-CGA-CBA	2.49	119.15	111.90
21	B	839	CLA	C1-O2A-CGA	2.49	122.75	116.77
21	2	804	CLA	O2A-CGA-CBA	2.49	119.16	111.90
21	1	203	CLA	CMA-C3A-C4A	2.49	118.48	111.77
24	1	848	BCR	C40-C30-C29	2.49	118.64	108.80
21	2	832	CLA	CMA-C3A-C4A	2.49	118.48	111.77
24	1	849	BCR	C40-C30-C29	2.50	118.65	108.80
24	A	843	BCR	C8-C9-C10	2.50	122.77	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	827	CLA	O2A-CGA-CBA	2.50	119.17	111.90
21	A	837	CLA	O2A-CGA-CBA	2.50	119.17	111.90
21	b	1812	CLA	CMA-C3A-C4A	2.50	118.49	111.77
24	l	207	BCR	C40-C30-C29	2.50	118.66	108.80
24	l	845	BCR	C40-C30-C29	2.50	118.67	108.80
21	m	103	CLA	O2A-CGA-CBA	2.50	119.18	111.90
21	b	1806	CLA	O2A-CGA-CBA	2.50	119.18	111.90
24	2	847	BCR	C40-C30-C29	2.50	118.67	108.80
24	f	204	BCR	C40-C30-C29	2.50	118.67	108.80
24	1	858	BCR	C40-C30-C29	2.50	118.68	108.80
26	1	851	LMG	O8-C28-C29	2.50	119.18	111.90
24	1	856	BCR	C40-C30-C29	2.50	118.68	108.80
36	L	201	EQ3	C38-C26-C27	2.50	119.31	115.48
21	l	203	CLA	O2A-CGA-CBA	2.50	119.19	111.90
24	B	842	BCR	C40-C30-C29	2.50	118.68	108.80
24	A	844	BCR	C40-C30-C29	2.50	118.68	108.80
21	1	834	CLA	O2A-CGA-CBA	2.51	119.19	111.90
21	1	809	CLA	O2A-CGA-CBA	2.51	119.19	111.90
24	a	845	BCR	C40-C30-C29	2.51	118.69	108.80
24	K	104	BCR	C40-C30-C29	2.51	118.69	108.80
24	B	847	BCR	C40-C30-C29	2.51	118.69	108.80
24	B	846	BCR	C40-C30-C29	2.51	118.69	108.80
24	2	849	BCR	C40-C30-C29	2.51	118.69	108.80
21	b	1821	CLA	O2A-CGA-CBA	2.51	119.19	111.90
24	8	1403	BCR	C40-C30-C29	2.51	118.69	108.80
24	L	207	BCR	C40-C30-C29	2.51	118.69	108.80
21	A	817	CLA	CMA-C3A-C4A	2.51	118.51	111.77
24	1	846	BCR	C40-C30-C29	2.51	118.70	108.80
24	a	846	BCR	C40-C30-C29	2.51	118.70	108.80
24	b	1846	BCR	C40-C30-C29	2.51	118.71	108.80
24	A	846	BCR	C40-C30-C29	2.51	118.71	108.80
21	a	815	CLA	O2A-CGA-CBA	2.51	119.21	111.90
24	0	205	BCR	C40-C30-C29	2.51	118.71	108.80
21	2	815	CLA	CMA-C3A-C4A	2.51	118.53	111.77
24	A	843	BCR	C40-C30-C29	2.51	118.72	108.80
24	l	206	BCR	C40-C30-C29	2.51	118.72	108.80
24	J	1107	BCR	C40-C30-C29	2.51	118.72	108.80
24	6	205	BCR	C40-C30-C29	2.51	118.72	108.80
24	B	843	BCR	C40-C30-C29	2.52	118.72	108.80
24	a	844	BCR	C40-C30-C29	2.52	118.73	108.80
24	b	1849	BCR	C40-C30-C29	2.52	118.73	108.80
21	A	801	CLA	OBD-CAD-CBD	2.52	129.74	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	f	201	BCR	C40-C30-C29	2.52	118.73	108.80
21	l	205	CLA	CMA-C3A-C4A	2.52	118.54	111.77
21	A	813	CLA	CMA-C3A-C4A	2.52	118.54	111.77
24	9	102	BCR	C40-C30-C29	2.52	118.73	108.80
21	A	828	CLA	CMB-C2B-C3B	2.52	129.56	124.89
24	2	845	BCR	C40-C30-C29	2.52	118.74	108.80
24	a	848	BCR	C40-C30-C29	2.52	118.74	108.80
21	a	806	CLA	CMA-C3A-C4A	2.52	118.55	111.77
21	1	813	CLA	CMA-C3A-C4A	2.52	118.55	111.77
21	1	817	CLA	C1-O2A-CGA	2.52	122.82	116.77
24	2	848	BCR	C40-C30-C29	2.52	118.75	108.80
24	I	102	BCR	C40-C30-C29	2.52	118.75	108.80
24	6	202	BCR	C40-C30-C29	2.52	118.75	108.80
21	B	811	CLA	O2A-CGA-CBA	2.52	119.24	111.90
24	b	1845	BCR	C40-C30-C29	2.52	118.75	108.80
21	1	807	CLA	O2A-CGA-CBA	2.52	119.24	111.90
24	i	101	BCR	C40-C30-C29	2.52	118.75	108.80
24	A	845	BCR	C40-C30-C29	2.52	118.75	108.80
21	2	831	CLA	O2A-CGA-CBA	2.52	119.24	111.90
24	a	859	BCR	C40-C30-C29	2.52	118.76	108.80
21	A	828	CLA	CMA-C3A-C4A	2.52	118.56	111.77
24	1	847	BCR	C40-C30-C29	2.53	118.77	108.80
24	a	843	BCR	C40-C30-C29	2.53	118.78	108.80
21	B	832	CLA	O2A-CGA-CBA	2.53	119.27	111.90
21	2	812	CLA	CMA-C3A-C4A	2.53	118.58	111.77
21	L	205	CLA	O2A-CGA-CBA	2.53	119.27	111.90
24	b	1850	BCR	C40-C30-C29	2.53	118.80	108.80
24	A	844	BCR	C35-C13-C12	2.53	122.14	118.10
21	B	813	CLA	O2A-CGA-CBA	2.53	119.28	111.90
21	2	837	CLA	O2A-CGA-CBA	2.54	119.28	111.90
36	L	201	EQ3	C29-C30-C25	2.54	114.44	110.48
21	a	801	CLA	O2A-CGA-CBA	2.54	119.28	111.90
21	b	1840	CLA	CMA-C3A-C4A	2.54	118.59	111.77
24	h	101	BCR	C40-C30-C29	2.54	118.82	108.80
21	B	839	CLA	CMA-C3A-C4A	2.54	118.60	111.77
21	A	834	CLA	CMA-C3A-C4A	2.54	118.60	111.77
21	b	1831	CLA	O2A-CGA-CBA	2.54	119.29	111.90
21	2	819	CLA	CMA-C3A-C4A	2.54	118.61	111.77
24	J	1102	BCR	C40-C30-C29	2.54	118.84	108.80
24	9	102	BCR	C8-C9-C10	2.55	122.85	118.94
21	b	1815	CLA	O2A-CGA-CBA	2.55	119.31	111.90
21	A	830	CLA	O2A-CGA-CBA	2.55	119.32	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1829	CLA	O2A-CGA-CBA	2.55	119.32	111.90
21	B	823	CLA	O2A-CGA-CBA	2.55	119.32	111.90
21	b	1822	CLA	O2A-CGA-CBA	2.55	119.32	111.90
21	b	1832	CLA	CMA-C3A-C4A	2.55	118.63	111.77
25	2	851	LHG	O8-C23-C24	2.55	119.33	111.90
21	1	801	CLA	C2A-C1A-CHA	2.55	128.44	123.92
21	A	854	CLA	O2A-CGA-CBA	2.56	119.34	111.90
21	J	1101	CLA	C1-O2A-CGA	2.56	122.91	116.77
21	b	1831	CLA	CMA-C3A-C4A	2.56	118.65	111.77
24	7	1102	BCR	C40-C30-C29	2.56	118.89	108.80
21	A	814	CLA	O2A-CGA-CBA	2.56	119.34	111.90
21	a	804	CLA	O2A-CGA-CBA	2.56	119.35	111.90
21	B	802	CLA	CMB-C2B-C3B	2.56	129.64	124.89
21	2	805	CLA	O2A-CGA-CBA	2.56	119.36	111.90
21	B	810	CLA	O2A-CGA-CBA	2.56	119.36	111.90
21	B	824	CLA	CMA-C3A-C4A	2.56	118.67	111.77
21	B	809	CLA	O2A-CGA-CBA	2.57	119.36	111.90
21	2	802	CLA	CMB-C2B-C3B	2.57	129.66	124.89
24	a	847	BCR	C40-C30-C29	2.57	118.94	108.80
21	b	1807	CLA	O2D-CGD-CBD	2.57	115.89	111.30
21	a	830	CLA	O2A-CGA-CBA	2.57	119.38	111.90
21	6	203	CLA	CMA-C3A-C4A	2.57	118.69	111.77
21	b	1816	CLA	O2A-CGA-CBA	2.57	119.39	111.90
24	2	849	BCR	C30-C25-C24	2.57	122.96	115.73
21	B	804	CLA	O2D-CGD-CBD	2.57	115.90	111.30
24	2	849	BCR	C29-C28-C27	2.57	117.48	111.34
24	2	849	BCR	C23-C24-C25	2.58	134.47	127.25
21	f	202	CLA	CMA-C3A-C4A	2.58	118.71	111.77
21	b	1814	CLA	C1-O2A-CGA	2.58	122.97	116.77
21	A	816	CLA	CMA-C3A-C4A	2.58	118.72	111.77
21	2	827	CLA	CMA-C3A-C4A	2.58	118.72	111.77
21	a	855	CLA	O2A-CGA-CBA	2.58	119.42	111.90
21	B	804	CLA	O2A-CGA-CBA	2.59	119.42	111.90
24	a	844	BCR	C8-C9-C10	2.59	122.91	118.94
21	7	1103	CLA	CMA-C3A-C4A	2.59	118.72	111.77
21	A	829	CLA	C1-O2A-CGA	2.59	122.98	116.77
21	B	830	CLA	CMA-C3A-C4A	2.59	118.73	111.77
21	b	1835	CLA	CMA-C3A-C4A	2.59	118.73	111.77
21	L	204	CLA	CMA-C3A-C4A	2.59	118.73	111.77
21	1	818	CLA	O2A-CGA-CBA	2.59	119.43	111.90
24	2	847	BCR	C8-C9-C10	2.59	122.91	118.94
21	J	1106	CLA	O2A-CGA-CBA	2.59	119.44	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	206	BCR	C37-C22-C23	2.59	122.23	118.10
21	A	828	CLA	O2A-CGA-CBA	2.59	119.45	111.90
21	2	811	CLA	O2A-CGA-CBA	2.59	119.45	111.90
30	b	1847	ECH	C20-C19-C18	2.59	133.71	126.42
25	B	849	LHG	O8-C23-C24	2.60	119.45	111.90
21	l	205	CLA	O2A-CGA-CBA	2.60	119.45	111.90
21	a	820	CLA	CMA-C3A-C4A	2.60	118.75	111.77
24	A	843	BCR	C35-C13-C12	2.60	122.24	118.10
21	b	1823	CLA	O2A-CGA-CBA	2.60	119.47	111.90
21	A	838	CLA	CMA-C3A-C4A	2.60	118.77	111.77
21	a	838	CLA	C1-O2A-CGA	2.60	123.02	116.77
21	A	802	CLA	C1-O2A-CGA	2.60	123.02	116.77
21	a	804	CLA	CMA-C3A-C4A	2.60	118.77	111.77
21	1	837	CLA	O2A-CGA-CBA	2.61	119.48	111.90
30	b	1847	ECH	C36-C18-C19	2.61	122.25	118.10
21	1	803	CLA	CMA-C3A-C4A	2.61	118.78	111.77
21	k	1402	CLA	CMA-C3A-C4A	2.61	118.79	111.77
26	A	852	LMG	O1-C1-C2	2.61	112.50	108.23
21	A	818	CLA	O2A-CGA-CBA	2.61	119.50	111.90
24	1	858	BCR	C8-C9-C10	2.61	122.95	118.94
21	a	831	CLA	C1-O2A-CGA	2.61	123.04	116.77
21	2	823	CLA	O2A-CGA-CBA	2.61	119.51	111.90
21	2	837	CLA	O2D-CGD-CBD	2.62	115.98	111.30
21	b	1837	CLA	O2A-CGA-CBA	2.62	119.52	111.90
21	1	841	CLA	CMA-C3A-C4A	2.62	118.81	111.77
21	a	820	CLA	O2A-CGA-CBA	2.62	119.52	111.90
21	2	838	CLA	CMA-C3A-C4A	2.62	118.82	111.77
21	b	1812	CLA	C1-O2A-CGA	2.62	123.06	116.77
21	A	806	CLA	O2A-CGA-CBA	2.62	119.53	111.90
25	B	858	LHG	O8-C23-C24	2.62	119.53	111.90
21	1	814	CLA	O2A-CGA-CBA	2.63	119.54	111.90
21	a	836	CLA	C1-O2A-CGA	2.63	123.07	116.77
21	B	804	CLA	CMA-C3A-C4A	2.63	118.83	111.77
21	a	830	CLA	CMA-C3A-C4A	2.63	118.84	111.77
21	1	830	CLA	C1-O2A-CGA	2.63	123.08	116.77
21	b	1841	CLA	C1-O2A-CGA	2.63	123.08	116.77
21	A	838	CLA	C1-O2A-CGA	2.63	123.09	116.77
21	B	834	CLA	O2A-CGA-CBA	2.63	119.56	111.90
24	A	844	BCR	C8-C9-C10	2.64	122.98	118.94
24	I	102	BCR	C2-C1-C6	2.64	114.60	110.48
21	2	839	CLA	O2A-CGA-CBA	2.64	119.58	111.90
21	b	1824	CLA	CMB-C2B-C3B	2.64	129.79	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	833	CLA	O2A-CGA-CBA	2.64	119.59	111.90
21	b	1805	CLA	O2A-CGA-CBA	2.64	119.59	111.90
21	2	806	CLA	CMA-C3A-C4A	2.65	118.88	111.77
21	B	821	CLA	CMA-C3A-C4A	2.65	118.88	111.77
21	b	1804	CLA	CMA-C3A-C4A	2.65	118.89	111.77
21	a	803	CLA	O2A-CGA-CBA	2.65	119.60	111.90
21	2	815	CLA	O2A-CGA-CBA	2.65	119.61	111.90
21	B	838	CLA	C1-O2A-CGA	2.65	123.13	116.77
25	A	851	LHG	O8-C23-C24	2.65	119.61	111.90
21	a	801	CLA	C2A-C1A-CHA	2.65	128.62	123.92
24	f	201	BCR	C15-C14-C13	2.65	131.10	127.31
21	0	201	CLA	CMA-C3A-C4A	2.66	118.91	111.77
21	a	814	CLA	CMA-C3A-C4A	2.66	118.92	111.77
21	A	825	CLA	CMB-C2B-C3B	2.66	129.82	124.89
21	B	836	CLA	CMA-C3A-C4A	2.66	118.92	111.77
21	1	804	CLA	CMB-C2B-C3B	2.66	129.83	124.89
21	8	1402	CLA	CMA-C3A-C4A	2.66	118.93	111.77
21	1	829	CLA	O2A-CGA-CBA	2.66	119.65	111.90
21	0	203	CLA	O2A-CGA-CBA	2.66	119.65	111.90
26	2	850	LMG	O8-C28-C29	2.66	119.65	111.90
21	b	1843	CLA	O2A-CGA-CBA	2.66	119.65	111.90
21	1	855	CLA	O2A-CGA-CBA	2.66	119.65	111.90
21	A	825	CLA	CMA-C3A-C4A	2.67	118.94	111.77
26	a	850	LMG	O8-C28-C29	2.67	119.66	111.90
21	A	835	CLA	CMA-C3A-C4A	2.67	118.94	111.77
21	1	808	CLA	CMA-C3A-C4A	2.67	118.95	111.77
21	b	1824	CLA	O2D-CGD-CBD	2.67	116.07	111.30
21	2	818	CLA	CMA-C3A-C4A	2.68	118.96	111.77
21	K	102	CLA	CMA-C3A-C4A	2.68	118.97	111.77
21	2	818	CLA	O2A-CGA-CBA	2.68	119.70	111.90
21	1	828	CLA	O2A-CGA-CBA	2.68	119.71	111.90
21	J	1101	CLA	O2A-CGA-CBA	2.68	119.71	111.90
21	a	834	CLA	CMA-C3A-C4A	2.68	118.98	111.77
21	a	821	CLA	CMA-C3A-C4A	2.68	118.99	111.77
25	b	1802	LHG	O8-C23-C24	2.69	119.72	111.90
21	B	838	CLA	O2D-CGD-CBD	2.69	116.10	111.30
21	L	203	CLA	CMA-C3A-C4A	2.69	119.00	111.77
21	B	808	CLA	C1-O2A-CGA	2.69	123.23	116.77
25	M	7003	LHG	O8-C23-C24	2.69	119.73	111.90
21	b	1813	CLA	O2A-CGA-CBA	2.69	119.73	111.90
21	a	817	CLA	CMA-C3A-C4A	2.69	119.01	111.77
21	B	820	CLA	CMA-C3A-C4A	2.69	119.01	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	811	CLA	CMA-C3A-C4A	2.69	119.01	111.77
24	B	846	BCR	C19-C18-C17	2.69	123.08	118.94
21	B	826	CLA	O2A-CGA-CBA	2.70	119.74	111.90
21	1	827	CLA	C1-O2A-CGA	2.70	123.25	116.77
21	2	807	CLA	CMA-C3A-C4A	2.70	119.03	111.77
21	B	810	CLA	C1-O2A-CGA	2.70	123.25	116.77
21	a	816	CLA	C1-O2A-CGA	2.70	123.25	116.77
21	B	806	CLA	C1-O2A-CGA	2.70	123.25	116.77
21	B	828	CLA	O2A-CGA-CBA	2.70	119.76	111.90
24	b	1846	BCR	C37-C22-C23	2.70	122.41	118.10
21	b	1824	CLA	O2A-CGA-CBA	2.71	119.77	111.90
21	m	103	CLA	O2D-CGD-CBD	2.71	116.14	111.30
21	B	820	CLA	C1-O2A-CGA	2.71	123.28	116.77
21	a	856	CLA	C1-O2A-CGA	2.71	123.28	116.77
22	a	841	PQN	C14-C13-C15	2.71	119.99	115.29
21	A	834	CLA	O2A-CGA-CBA	2.71	119.79	111.90
21	j	1103	CLA	CMA-C3A-C4A	2.71	119.07	111.77
37	L	209	DGD	O1G-C1A-C2A	2.72	119.80	111.90
21	1	818	CLA	CMA-C3A-C4A	2.72	119.08	111.77
21	a	818	CLA	O2A-CGA-CBA	2.72	119.81	111.90
21	l	204	CLA	CMA-C3A-C4A	2.72	119.08	111.77
21	B	819	CLA	CMA-C3A-C4A	2.72	119.09	111.77
21	A	808	CLA	CMA-C3A-C4A	2.72	119.09	111.77
24	j	1102	BCR	C8-C9-C10	2.73	123.13	118.94
21	b	1820	CLA	O2A-CGA-CBA	2.73	119.84	111.90
21	b	1824	CLA	CMA-C3A-C4A	2.73	119.11	111.77
21	a	807	CLA	O2A-CGA-CBA	2.73	119.85	111.90
21	A	823	CLA	O2D-CGD-CBD	2.73	116.18	111.30
21	1	830	CLA	O2A-CGA-CBA	2.74	119.86	111.90
21	b	1813	CLA	O2D-CGD-CBD	2.74	116.19	111.30
21	J	1105	CLA	C1-O2A-CGA	2.74	123.34	116.77
21	b	1836	CLA	C1-O2A-CGA	2.74	123.34	116.77
25	9	101	LHG	O8-C23-C24	2.74	119.87	111.90
24	A	848	BCR	C8-C7-C6	2.74	134.92	127.25
25	b	1803	LHG	O8-C23-C24	2.74	119.88	111.90
21	2	836	CLA	CMA-C3A-C4A	2.74	119.14	111.77
24	6	205	BCR	C12-C13-C14	2.74	123.15	118.94
21	A	821	CLA	CMA-C3A-C4A	2.74	119.15	111.77
21	b	1834	CLA	O2D-CGD-CBD	2.75	116.21	111.30
21	A	802	CLA	C1C-NC-C4C	2.75	108.64	107.06
21	a	837	CLA	O2A-CGA-CBA	2.75	119.89	111.90
21	7	1101	CLA	O2A-CGA-CBA	2.75	119.90	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1810	CLA	C1-O2A-CGA	2.75	123.37	116.77
21	2	827	CLA	O2A-CGA-CBA	2.75	119.91	111.90
21	2	831	CLA	CMA-C3A-C4A	2.75	119.17	111.77
21	1	835	CLA	CMA-C3A-C4A	2.75	119.17	111.77
21	B	835	CLA	CMA-C3A-C4A	2.76	119.18	111.77
25	B	857	LHG	O8-C23-C24	2.76	119.92	111.90
21	1	813	CLA	O2D-CGD-CBD	2.76	116.23	111.30
21	B	817	CLA	O2A-CGA-CBA	2.76	119.94	111.90
21	A	822	CLA	CMA-C3A-C4A	2.76	119.20	111.77
21	b	1840	CLA	O2A-CGA-CBA	2.76	119.94	111.90
21	K	103	CLA	CMA-C3A-C4A	2.77	119.22	111.77
21	b	1838	CLA	CMA-C3A-C4A	2.78	119.23	111.77
21	1	801	CLA	O2A-CGA-CBA	2.78	119.98	111.90
25	l	209	LHG	O8-C23-C24	2.78	119.98	111.90
21	a	814	CLA	O2A-CGA-CBA	2.78	119.98	111.90
21	f	203	CLA	CMA-C3A-C4A	2.78	119.24	111.77
21	A	811	CLA	CMA-C3A-C4A	2.78	119.24	111.77
21	2	807	CLA	O2A-CGA-CBA	2.78	120.00	111.90
21	2	828	CLA	O2A-CGA-CBA	2.78	120.00	111.90
25	L	210	LHG	O8-C23-C24	2.78	120.00	111.90
21	B	833	CLA	C1-O2A-CGA	2.79	123.45	116.77
21	a	855	CLA	CMB-C2B-C3B	2.79	130.06	124.89
21	B	838	CLA	CMA-C3A-C4A	2.79	119.26	111.77
21	j	1101	CLA	CMA-C3A-C4A	2.79	119.27	111.77
21	1	855	CLA	CMA-C3A-C4A	2.79	119.27	111.77
21	B	811	CLA	CMA-C3A-C4A	2.79	119.27	111.77
21	a	812	CLA	CMA-C3A-C4A	2.79	119.28	111.77
21	b	1808	CLA	C1-O2A-CGA	2.79	123.47	116.77
21	b	1827	CLA	CMA-C3A-C4A	2.79	119.28	111.77
25	l	210	LHG	O8-C23-C24	2.79	120.03	111.90
21	B	813	CLA	CMA-C3A-C4A	2.79	119.28	111.77
21	a	839	CLA	CMA-C3A-C4A	2.80	119.29	111.77
21	1	836	CLA	CMA-C3A-C4A	2.80	119.29	111.77
21	B	816	CLA	CMA-C3A-C4A	2.80	119.30	111.77
21	2	829	CLA	O2A-CGA-CBA	2.80	120.06	111.90
21	1	830	CLA	CMA-C3A-C4A	2.80	119.31	111.77
21	a	807	CLA	CMA-C3A-C4A	2.81	119.31	111.77
21	B	818	CLA	CMA-C3A-C4A	2.81	119.32	111.77
21	b	1825	CLA	O2A-CGA-CBA	2.81	120.07	111.90
21	1	809	CLA	CMA-C3A-C4A	2.81	119.32	111.77
21	2	810	CLA	CMA-C3A-C4A	2.81	119.33	111.77
21	b	1801	CLA	O2A-CGA-CBA	2.81	120.08	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	808	CLA	O2A-CGA-CBA	2.81	120.08	111.90
25	l	208	LHG	O8-C23-C24	2.81	120.08	111.90
21	A	820	CLA	CMB-C2B-C3B	2.81	130.11	124.89
21	b	1843	CLA	CMA-C3A-C4A	2.82	119.34	111.77
30	2	846	ECH	C37-C22-C21	2.82	126.87	122.92
21	A	836	CLA	CMA-C3A-C4A	2.82	119.36	111.77
21	k	1402	CLA	O2A-CGA-CBA	2.82	120.11	111.90
36	L	201	EQ3	C35-C13-C12	2.83	122.60	118.10
21	1	838	CLA	CMA-C3A-C4A	2.83	119.37	111.77
21	2	820	CLA	CMA-C3A-C4A	2.83	119.38	111.77
25	a	853	LHG	O8-C23-C24	2.84	120.15	111.90
21	2	806	CLA	O2A-CGA-CBA	2.84	120.15	111.90
21	A	814	CLA	CMA-C3A-C4A	2.84	119.39	111.77
21	B	805	CLA	O2D-CGD-CBD	2.84	116.37	111.30
21	B	812	CLA	CMA-C3A-C4A	2.84	119.41	111.77
25	1	850	LHG	O8-C23-C24	2.84	120.17	111.90
24	a	859	BCR	C8-C9-C10	2.84	123.30	118.94
25	I	104	LHG	O8-C23-C24	2.85	120.18	111.90
26	B	850	LMG	O8-C28-C29	2.85	120.18	111.90
21	A	840	CLA	CMA-C3A-C4A	2.85	119.42	111.77
21	b	1826	CLA	O2A-CGA-CBA	2.85	120.19	111.90
21	B	805	CLA	O2A-CGA-CBA	2.85	120.19	111.90
24	f	201	BCR	C19-C18-C17	2.85	123.31	118.94
21	b	1842	CLA	O2A-CGA-CBA	2.85	120.19	111.90
21	1	823	CLA	CMA-C3A-C4A	2.85	119.44	111.77
21	A	819	CLA	O2D-CGD-CBD	2.86	116.40	111.30
21	1	817	CLA	CMA-C3A-C4A	2.86	119.45	111.77
21	2	841	CLA	CMA-C3A-C4A	2.86	119.45	111.77
26	A	852	LMG	O8-C28-C29	2.86	120.22	111.90
25	B	855	LHG	O8-C23-C24	2.86	120.24	111.90
21	B	839	CLA	O2A-CGA-CBA	2.87	120.25	111.90
26	1	853	LMG	O8-C28-C29	2.87	120.25	111.90
21	2	805	CLA	O2D-CGD-CBD	2.87	116.43	111.30
24	I	102	BCR	C35-C13-C12	2.87	122.67	118.10
21	1	829	CLA	CMA-C3A-C4A	2.87	119.49	111.77
21	2	834	CLA	CMA-C3A-C4A	2.87	119.49	111.77
21	a	826	CLA	O2A-CGA-CBA	2.87	120.26	111.90
21	B	815	CLA	CMA-C3A-C4A	2.87	119.50	111.77
24	9	102	BCR	C30-C25-C24	2.87	123.81	115.73
21	1	839	CLA	CMA-C3A-C4A	2.87	119.50	111.77
21	A	829	CLA	O2A-CGA-CBA	2.87	120.26	111.90
22	2	843	PQN	C14-C13-C15	2.88	120.28	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	824	CLA	CMA-C3A-C4A	2.88	119.51	111.77
21	7	1104	CLA	CMA-C3A-C4A	2.88	119.52	111.77
24	F	201	BCR	C19-C18-C17	2.88	123.36	118.94
26	2	852	LMG	O8-C28-C29	2.89	120.30	111.90
21	a	809	CLA	CMA-C3A-C4A	2.89	119.54	111.77
24	A	845	BCR	C19-C18-C17	2.89	123.38	118.94
28	2	854	45D	C21-C15-C17	2.89	119.90	115.48
21	a	827	CLA	CMA-C3A-C4A	2.89	119.55	111.77
21	1	819	CLA	O2D-CGD-CBD	2.89	116.47	111.30
24	I	102	BCR	C15-C14-C13	2.90	131.44	127.31
21	B	814	CLA	CMA-C3A-C4A	2.90	119.56	111.77
21	A	802	CLA	CMB-C2B-C3B	2.90	130.26	124.89
21	A	806	CLA	CMA-C3A-C4A	2.90	119.56	111.77
21	B	822	CLA	CMA-C3A-C4A	2.90	119.56	111.77
24	2	847	BCR	C15-C14-C13	2.90	131.45	127.31
21	1	841	CLA	O2A-CGA-CBA	2.90	120.34	111.90
21	2	817	CLA	CMA-C3A-C4A	2.91	119.58	111.77
21	b	1820	CLA	CMA-C3A-C4A	2.91	119.59	111.77
21	b	1829	CLA	CMA-C3A-C4A	2.91	119.60	111.77
21	a	816	CLA	O2A-CGA-CBA	2.91	120.38	111.90
21	a	818	CLA	CMA-C3A-C4A	2.92	119.61	111.77
25	a	849	LHG	O8-C23-C24	2.92	120.39	111.90
21	a	826	CLA	CMA-C3A-C4A	2.92	119.61	111.77
21	A	801	CLA	C2A-C1A-CHA	2.92	129.09	123.92
26	b	1855	LMG	O8-C28-C29	2.92	120.40	111.90
21	B	826	CLA	CMA-C3A-C4A	2.92	119.63	111.77
21	b	1826	CLA	O2D-CGD-CBD	2.92	116.52	111.30
21	2	811	CLA	O2D-CGD-CBD	2.92	116.52	111.30
21	b	1841	CLA	CMA-C3A-C4A	2.93	119.64	111.77
21	A	809	CLA	CMA-C3A-C4A	2.93	119.64	111.77
26	K	101	LMG	O8-C28-C29	2.93	120.42	111.90
21	B	817	CLA	CMA-C3A-C4A	2.93	119.65	111.77
21	1	826	CLA	CMA-C3A-C4A	2.93	119.65	111.77
26	b	1853	LMG	O8-C28-C29	2.93	120.43	111.90
21	2	809	CLA	C1-O2A-CGA	2.93	123.81	116.77
21	a	815	CLA	CMA-C3A-C4A	2.93	119.66	111.77
21	1	825	CLA	CMA-C3A-C4A	2.94	119.67	111.77
21	k	1401	CLA	O2D-CGD-CBD	2.94	116.55	111.30
21	b	1813	CLA	CMA-C3A-C4A	2.94	119.67	111.77
25	b	1852	LHG	O8-C23-C24	2.94	120.46	111.90
24	9	102	BCR	C12-C13-C14	2.94	123.45	118.94
21	1	801	CLA	O2D-CGD-CBD	2.94	116.56	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	827	CLA	C1-O2A-CGA	2.94	123.84	116.77
21	a	816	CLA	CMA-C3A-C4A	2.95	119.69	111.77
21	2	824	CLA	O2A-CGA-CBA	2.95	120.47	111.90
21	b	1823	CLA	CMA-C3A-C4A	2.95	119.70	111.77
22	B	841	PQN	C14-C13-C15	2.95	120.41	115.29
21	A	836	CLA	O2D-CGD-CBD	2.95	116.57	111.30
25	2	801	LHG	O8-C23-C24	2.95	120.49	111.90
21	2	840	CLA	CMA-C3A-C4A	2.95	119.71	111.77
21	2	810	CLA	O2A-CGA-CBA	2.95	120.49	111.90
21	A	813	CLA	O2A-CGA-CBA	2.95	120.49	111.90
21	B	802	CLA	C1-O2A-CGA	2.96	123.88	116.77
21	2	820	CLA	C1-O2A-CGA	2.96	123.88	116.77
21	b	1815	CLA	C1-O2A-CGA	2.96	123.89	116.77
24	f	204	BCR	C2-C1-C6	2.97	115.11	110.48
21	1	827	CLA	CMA-C3A-C4A	2.97	119.75	111.77
26	K	105	LMG	O8-C28-C29	2.97	120.55	111.90
21	k	1401	CLA	CMA-C3A-C4A	2.97	119.76	111.77
21	a	824	CLA	CMA-C3A-C4A	2.98	119.77	111.77
24	2	849	BCR	C19-C18-C17	2.98	123.51	118.94
21	a	840	CLA	CMA-C3A-C4A	2.98	119.78	111.77
21	2	830	CLA	CMA-C3A-C4A	2.98	119.79	111.77
21	F	203	CLA	CMA-C3A-C4A	2.98	119.79	111.77
21	b	1808	CLA	O2A-CGA-CBA	2.98	120.58	111.90
21	A	807	CLA	O2A-CGA-CBA	2.99	120.59	111.90
21	b	1816	CLA	CMA-C3A-C4A	2.99	119.80	111.77
21	b	1831	CLA	O2D-CGD-CBD	2.99	116.64	111.30
21	2	841	CLA	O2A-CGA-CBA	2.99	120.59	111.90
21	K	103	CLA	O2A-CGA-CBA	2.99	120.60	111.90
25	m	101	LHG	O8-C23-C24	2.99	120.60	111.90
21	a	829	CLA	CMA-C3A-C4A	2.99	119.81	111.77
21	7	1101	CLA	CMA-C3A-C4A	2.99	119.81	111.77
21	b	1837	CLA	CMA-C3A-C4A	3.00	119.82	111.77
26	0	206	LMG	C3-C4-C5	3.00	115.50	110.22
21	1	840	CLA	CMA-C3A-C4A	3.00	119.83	111.77
21	b	1822	CLA	O2D-CGD-CBD	3.00	116.65	111.30
26	0	206	LMG	O8-C28-C29	3.00	120.62	111.90
21	A	809	CLA	O2D-CGD-CBD	3.00	116.66	111.30
21	2	824	CLA	CMA-C3A-C4A	3.00	119.83	111.77
21	1	814	CLA	CMA-C3A-C4A	3.00	119.84	111.77
34	b	1858	C7Z	C28-C29-C30	3.00	123.55	118.94
24	A	848	BCR	C8-C9-C10	3.00	123.55	118.94
21	I	101	CLA	CAC-C3C-C2C	3.01	132.70	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1805	CLA	CMA-C3A-C4A	3.01	119.85	111.77
21	B	828	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	b	1841	CLA	O2D-CGD-CBD	3.01	116.67	111.30
21	B	834	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	J	1106	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	A	815	CLA	CMA-C3A-C4A	3.01	119.86	111.77
21	1	826	CLA	O2A-CGA-CBA	3.01	120.67	111.90
21	a	838	CLA	CMA-C3A-C4A	3.01	119.87	111.77
21	a	824	CLA	O2D-CGD-CBD	3.02	116.69	111.30
21	A	823	CLA	CMA-C3A-C4A	3.02	119.88	111.77
21	I	101	CLA	CMA-C3A-C4A	3.02	119.88	111.77
21	b	1811	CLA	O2A-CGA-CBA	3.02	120.69	111.90
21	a	823	CLA	CMA-C3A-C4A	3.02	119.90	111.77
21	2	838	CLA	O2D-CGD-CBD	3.03	116.70	111.30
21	1	807	CLA	CMA-C3A-C4A	3.03	119.90	111.77
25	I	103	LHG	O8-C23-C24	3.03	120.72	111.90
21	1	816	CLA	CMA-C3A-C4A	3.03	119.92	111.77
21	B	817	CLA	O2D-CGD-CBD	3.03	116.72	111.30
21	1	812	CLA	CMA-C3A-C4A	3.04	119.94	111.77
21	B	801	CLA	O2D-CGD-CBD	3.05	116.74	111.30
21	b	1830	CLA	O2A-CGA-CBA	3.05	120.77	111.90
21	2	836	CLA	O2D-CGD-CBD	3.05	116.75	111.30
21	1	838	CLA	O2A-CGA-CBA	3.05	120.78	111.90
21	A	828	CLA	O2D-CGD-CBD	3.06	116.77	111.30
21	1	824	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	2	822	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	1	822	CLA	CMA-C3A-C4A	3.06	120.00	111.77
21	A	810	CLA	O2A-CGA-CBA	3.06	120.81	111.90
21	A	822	CLA	O2D-CGD-CBD	3.06	116.77	111.30
21	1	837	CLA	CMA-C3A-C4A	3.06	120.01	111.77
21	2	813	CLA	CMA-C3A-C4A	3.06	120.01	111.77
21	2	828	CLA	CMA-C3A-C4A	3.07	120.01	111.77
21	1	815	CLA	CMA-C3A-C4A	3.07	120.01	111.77
21	a	828	CLA	CMA-C3A-C4A	3.07	120.02	111.77
21	j	1105	CLA	CMA-C3A-C4A	3.07	120.02	111.77
21	B	823	CLA	CMA-C3A-C4A	3.07	120.03	111.77
26	B	848	LMG	O8-C28-C29	3.07	120.84	111.90
21	b	1829	CLA	O2D-CGD-CBD	3.07	116.79	111.30
21	J	1105	CLA	CMA-C3A-C4A	3.08	120.05	111.77
21	7	1105	CLA	CMA-C3A-C4A	3.08	120.06	111.77
21	2	814	CLA	CMA-C3A-C4A	3.08	120.06	111.77
25	1	852	LHG	O8-C23-C24	3.09	120.88	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1830	CLA	O2D-CGD-CBD	3.09	116.82	111.30
26	b	1855	LMG	O1-C1-C2	3.10	113.29	108.23
21	6	204	CLA	CMA-C3A-C4A	3.10	120.10	111.77
21	b	1825	CLA	CMA-C3A-C4A	3.10	120.11	111.77
21	2	812	CLA	O2D-CGD-CBD	3.10	116.85	111.30
21	1	828	CLA	CMA-C3A-C4A	3.11	120.12	111.77
30	b	1847	ECH	C21-C20-C19	3.11	132.78	123.23
21	1	824	CLA	O2D-CGD-CBD	3.11	116.86	111.30
21	B	806	CLA	O2A-CGA-CBA	3.12	120.96	111.90
25	a	851	LHG	O8-C23-C24	3.12	120.97	111.90
21	2	812	CLA	O2A-CGA-CBA	3.12	120.97	111.90
21	2	823	CLA	CMA-C3A-C4A	3.12	120.16	111.77
25	B	851	LHG	O8-C23-C24	3.12	120.99	111.90
21	2	825	CLA	CMA-C3A-C4A	3.12	120.17	111.77
21	b	1815	CLA	CMA-C3A-C4A	3.13	120.18	111.77
21	2	839	CLA	CMA-C3A-C4A	3.13	120.19	111.77
21	a	836	CLA	O2A-CGA-CBA	3.13	121.02	111.90
21	1	804	CLA	O2A-CGA-CBA	3.13	121.02	111.90
21	2	829	CLA	O2D-CGD-CBD	3.14	116.90	111.30
24	f	204	BCR	C15-C14-C13	3.14	131.79	127.31
21	B	840	CLA	CMA-C3A-C4A	3.14	120.22	111.77
21	a	835	CLA	CMA-C3A-C4A	3.15	120.23	111.77
21	8	1401	CLA	CMA-C3A-C4A	3.15	120.23	111.77
21	A	855	CLA	O2D-CGD-CBD	3.15	116.92	111.30
21	2	816	CLA	CMA-C3A-C4A	3.15	120.25	111.77
21	k	1402	CLA	O2D-CGD-CBD	3.16	116.94	111.30
21	6	201	CLA	CMA-C3A-C4A	3.16	120.25	111.77
26	a	852	LMG	O8-C28-C29	3.16	121.09	111.90
21	1	810	CLA	CMA-C3A-C4A	3.17	120.28	111.77
21	1	811	CLA	O2D-CGD-CBD	3.17	116.97	111.30
21	a	856	CLA	O2A-CGA-CBA	3.18	121.15	111.90
21	b	1806	CLA	O2D-CGD-CBD	3.18	116.98	111.30
26	A	850	LMG	O8-C28-C29	3.18	121.15	111.90
21	b	1840	CLA	O2D-CGD-CBD	3.18	116.98	111.30
22	1	842	PQN	C14-C13-C15	3.18	120.81	115.29
21	b	1812	CLA	O2D-CGD-CBD	3.19	116.99	111.30
21	A	839	CLA	CMA-C3A-C4A	3.19	120.35	111.77
21	a	819	CLA	O2D-CGD-CBD	3.19	117.00	111.30
21	2	837	CLA	CMA-C3A-C4A	3.19	120.35	111.77
21	2	827	CLA	O2D-CGD-CBD	3.19	117.00	111.30
21	a	819	CLA	CMA-C3A-C4A	3.20	120.38	111.77
21	B	823	CLA	O2D-CGD-CBD	3.20	117.02	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	837	CLA	O2D-CGD-CBD	3.21	117.03	111.30
21	A	803	CLA	O2A-CGA-CBA	3.21	121.23	111.90
21	b	1813	CLA	C1-O2A-CGA	3.21	124.47	116.77
21	2	828	CLA	O2D-CGD-CBD	3.21	117.04	111.30
21	a	809	CLA	O2D-CGD-CBD	3.21	117.04	111.30
21	A	815	CLA	O2D-CGD-CBD	3.21	117.04	111.30
21	a	810	CLA	CMA-C3A-C4A	3.22	120.42	111.77
21	a	836	CLA	CMA-C3A-C4A	3.22	120.42	111.77
26	0	206	LMG	O6-C5-C4	3.22	115.59	109.66
21	2	809	CLA	O2A-CGA-CBA	3.22	121.27	111.90
21	B	827	CLA	O2A-CGA-CBA	3.22	121.27	111.90
21	A	805	CLA	O2D-CGD-CBD	3.23	117.06	111.30
21	2	842	CLA	CMA-C3A-C4A	3.23	120.44	111.77
21	b	1804	CLA	O2D-CGD-CBD	3.23	117.06	111.30
21	a	811	CLA	CMA-C3A-C4A	3.23	120.45	111.77
21	a	838	CLA	O2D-CGD-CBD	3.23	117.07	111.30
21	1	838	CLA	O2D-CGD-CBD	3.23	117.08	111.30
26	0	206	LMG	C1-O6-C5	3.24	119.81	113.72
21	2	830	CLA	O2D-CGD-CBD	3.24	117.09	111.30
21	b	1839	CLA	O2D-CGD-CBD	3.25	117.10	111.30
21	0	202	CLA	CMA-C3A-C4A	3.25	120.50	111.77
21	a	826	CLA	O2D-CGD-CBD	3.25	117.10	111.30
21	a	822	CLA	CMA-C3A-C4A	3.25	120.51	111.77
21	1	823	CLA	O2D-CGD-CBD	3.25	117.11	111.30
21	A	834	CLA	O2D-CGD-CBD	3.25	117.11	111.30
21	L	203	CLA	O2D-CGD-CBD	3.26	117.12	111.30
21	1	819	CLA	CMA-C3A-C4A	3.26	120.52	111.77
21	B	834	CLA	O2D-CGD-CBD	3.26	117.12	111.30
21	b	1832	CLA	C4A-NA-C1A	3.26	110.50	106.45
21	1	811	CLA	CMA-C3A-C4A	3.26	120.54	111.77
21	8	1402	CLA	O2D-CGD-CBD	3.27	117.14	111.30
21	A	813	CLA	O2D-CGD-CBD	3.27	117.14	111.30
21	a	840	CLA	O2D-CGD-CBD	3.27	117.14	111.30
21	a	825	CLA	CMA-C3A-C4A	3.27	120.56	111.77
21	a	803	CLA	O2D-CGD-CBD	3.27	117.14	111.30
21	1	829	CLA	O2D-CGD-CBD	3.27	117.14	111.30
21	1	820	CLA	O2D-CGD-CBD	3.27	117.14	111.30
21	2	841	CLA	O2D-CGD-CBD	3.27	117.15	111.30
21	1	816	CLA	O2D-CGD-CBD	3.28	117.16	111.30
26	b	1851	LMG	O8-C28-C29	3.28	121.45	111.90
35	L	211	LMT	O5B-C1B-C2B	3.28	116.63	110.30
21	B	828	CLA	O2D-CGD-CBD	3.28	117.17	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	825	CLA	O2D-CGD-CBD	3.29	117.17	111.30
22	A	841	PQN	C14-C13-C15	3.29	120.99	115.29
21	2	832	CLA	O2D-CGD-CBD	3.29	117.18	111.30
21	A	839	CLA	O2D-CGD-CBD	3.29	117.18	111.30
21	b	1821	CLA	O2D-CGD-CBD	3.30	117.19	111.30
21	a	811	CLA	O2D-CGD-CBD	3.30	117.20	111.30
21	1	817	CLA	O2D-CGD-CBD	3.30	117.20	111.30
21	B	813	CLA	O2D-CGD-CBD	3.30	117.20	111.30
21	B	807	CLA	O2D-CGD-CBD	3.31	117.21	111.30
21	I	101	CLA	O2A-CGA-CBA	3.31	121.52	111.90
21	B	818	CLA	O2D-CGD-CBD	3.31	117.21	111.30
21	B	826	CLA	O2D-CGD-CBD	3.31	117.21	111.30
21	1	832	CLA	O2D-CGD-CBD	3.31	117.21	111.30
21	B	838	CLA	C4A-NA-C1A	3.31	110.57	106.45
22	b	1844	PQN	C14-C13-C15	3.32	121.04	115.29
21	1	806	CLA	O2D-CGD-CBD	3.32	117.23	111.30
21	2	819	CLA	C4A-NA-C1A	3.32	110.58	106.45
21	A	855	CLA	O2A-CGA-CBA	3.32	121.57	111.90
24	f	204	BCR	C12-C13-C14	3.33	124.04	118.94
21	1	837	CLA	O2D-CGD-CBD	3.33	117.25	111.30
21	2	814	CLA	O2D-CGD-CBD	3.33	117.25	111.30
26	a	852	LMG	O1-C1-C2	3.33	113.67	108.23
21	7	1105	CLA	O2D-CGD-CBD	3.34	117.26	111.30
21	b	1837	CLA	O2D-CGD-CBD	3.34	117.26	111.30
21	2	834	CLA	O2D-CGD-CBD	3.34	117.27	111.30
21	1	827	CLA	O2D-CGD-CBD	3.34	117.27	111.30
21	A	804	CLA	O2D-CGD-CBD	3.35	117.28	111.30
21	A	833	CLA	C4A-NA-C1A	3.35	110.61	106.45
21	2	842	CLA	O2D-CGD-CBD	3.35	117.28	111.30
21	B	821	CLA	O2D-CGD-CBD	3.35	117.28	111.30
21	F	202	CLA	O2D-CGD-CBD	3.35	117.28	111.30
21	2	835	CLA	O2D-CGD-CBD	3.36	117.30	111.30
21	B	808	CLA	C4A-NA-C1A	3.36	110.62	106.45
21	b	1818	CLA	C4A-NA-C1A	3.36	110.62	106.45
24	b	1845	BCR	C30-C25-C24	3.36	125.17	115.73
21	f	203	CLA	O2D-CGD-CBD	3.36	117.30	111.30
21	a	814	CLA	O2D-CGD-CBD	3.36	117.30	111.30
21	1	802	CLA	O2D-CGD-CBD	3.36	117.31	111.30
21	A	818	CLA	CMA-C3A-C4A	3.37	120.82	111.77
21	a	828	CLA	O2D-CGD-CBD	3.37	117.32	111.30
21	B	819	CLA	O2D-CGD-CBD	3.37	117.33	111.30
21	2	823	CLA	O2D-CGD-CBD	3.38	117.33	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	856	45D	C05-C03-C07	3.38	115.77	110.48
21	A	816	CLA	O2D-CGD-CBD	3.38	117.34	111.30
21	A	831	CLA	O2D-CGD-CBD	3.38	117.35	111.30
25	A	849	LHG	O8-C23-C24	3.38	121.75	111.90
21	B	836	CLA	O2D-CGD-CBD	3.39	117.35	111.30
24	L	206	BCR	C15-C14-C13	3.39	132.14	127.31
21	a	835	CLA	C4A-NA-C1A	3.39	110.66	106.45
21	a	805	CLA	O2D-CGD-CBD	3.39	117.35	111.30
21	b	1809	CLA	O2D-CGD-CBD	3.39	117.36	111.30
21	B	806	CLA	O2D-CGD-CBD	3.39	117.36	111.30
21	1	828	CLA	O2D-CGD-CBD	3.39	117.36	111.30
21	0	203	CLA	O2D-CGD-CBD	3.40	117.37	111.30
21	A	837	CLA	O2D-CGD-CBD	3.40	117.37	111.30
21	a	817	CLA	O2D-CGD-CBD	3.40	117.37	111.30
21	1	803	CLA	O2D-CGD-CBD	3.40	117.38	111.30
21	b	1819	CLA	O2D-CGD-CBD	3.40	117.38	111.30
21	b	1816	CLA	O2D-CGD-CBD	3.41	117.39	111.30
21	1	826	CLA	O2D-CGD-CBD	3.41	117.39	111.30
35	L	211	LMT	C1B-C2B-C3B	3.41	116.32	109.98
21	A	808	CLA	O2D-CGD-CBD	3.41	117.40	111.30
21	2	822	CLA	O2D-CGD-CBD	3.41	117.40	111.30
21	f	202	CLA	O2D-CGD-CBD	3.42	117.40	111.30
21	7	1104	CLA	O2D-CGD-CBD	3.42	117.40	111.30
21	a	820	CLA	O2D-CGD-CBD	3.42	117.41	111.30
21	A	806	CLA	C4A-NA-C1A	3.43	110.70	106.45
21	a	813	CLA	O2D-CGD-CBD	3.43	117.43	111.30
21	a	827	CLA	O2D-CGD-CBD	3.43	117.44	111.30
21	a	806	CLA	O2D-CGD-CBD	3.43	117.44	111.30
21	2	808	CLA	O2D-CGD-CBD	3.44	117.44	111.30
21	1	809	CLA	O2D-CGD-CBD	3.44	117.45	111.30
21	2	806	CLA	O2D-CGD-CBD	3.45	117.45	111.30
21	2	831	CLA	O2D-CGD-CBD	3.45	117.46	111.30
21	1	839	CLA	O2D-CGD-CBD	3.45	117.46	111.30
21	b	1821	CLA	C1-O2A-CGA	3.45	125.05	116.77
21	a	835	CLA	O2D-CGD-CBD	3.45	117.46	111.30
21	0	202	CLA	O2D-CGD-CBD	3.45	117.47	111.30
21	b	1843	CLA	O2D-CGD-CBD	3.45	117.47	111.30
21	B	802	CLA	O2A-CGA-CBA	3.45	121.95	111.90
21	2	820	CLA	O2D-CGD-CBD	3.46	117.47	111.30
21	7	1103	CLA	O2A-C1-C2	3.46	121.30	108.40
21	A	820	CLA	O2D-CGD-CBD	3.46	117.48	111.30
21	A	818	CLA	O2D-CGD-CBD	3.46	117.48	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	824	CLA	O2D-CGD-CBD	3.46	117.48	111.30
21	B	833	CLA	O2D-CGD-CBD	3.46	117.48	111.30
21	1	810	CLA	O2D-CGD-CBD	3.46	117.49	111.30
21	A	835	CLA	C4A-NA-C1A	3.46	110.75	106.45
28	2	854	45D	C34-C36-C38	3.47	124.26	118.94
21	b	1810	CLA	O2D-CGD-CBD	3.47	117.50	111.30
21	b	1814	CLA	O2D-CGD-CBD	3.47	117.50	111.30
21	B	815	CLA	O2D-CGD-CBD	3.47	117.50	111.30
21	0	201	CLA	O2D-CGD-CBD	3.47	117.51	111.30
21	L	204	CLA	O2D-CGD-CBD	3.48	117.51	111.30
21	1	826	CLA	C4A-NA-C1A	3.48	110.77	106.45
21	A	802	CLA	O2D-CGD-CBD	3.48	117.52	111.30
21	1	841	CLA	O2D-CGD-CBD	3.48	117.52	111.30
21	2	819	CLA	O2D-CGD-CBD	3.48	117.52	111.30
24	1	856	BCR	C15-C14-C13	3.48	132.28	127.31
21	b	1828	CLA	O2D-CGD-CBD	3.48	117.53	111.30
21	a	834	CLA	O2D-CGD-CBD	3.49	117.53	111.30
21	B	832	CLA	O2D-CGD-CBD	3.49	117.54	111.30
21	B	802	CLA	O2D-CGD-CBD	3.49	117.54	111.30
21	b	1823	CLA	O2D-CGD-CBD	3.50	117.55	111.30
21	a	829	CLA	O2D-CGD-CBD	3.50	117.55	111.30
21	b	1820	CLA	O2D-CGD-CBD	3.50	117.56	111.30
21	1	814	CLA	O2D-CGD-CBD	3.50	117.56	111.30
21	A	821	CLA	C4A-NA-C1A	3.50	110.80	106.45
21	B	820	CLA	O2D-CGD-CBD	3.50	117.56	111.30
21	1	831	CLA	C4A-NA-C1A	3.50	110.80	106.45
21	a	833	CLA	O2D-CGD-CBD	3.50	117.56	111.30
21	1	818	CLA	O2D-CGD-CBD	3.51	117.56	111.30
21	B	814	CLA	O2D-CGD-CBD	3.51	117.56	111.30
24	6	202	BCR	C15-C14-C13	3.51	132.32	127.31
24	A	847	BCR	C15-C14-C13	3.52	132.33	127.31
21	a	815	CLA	O2D-CGD-CBD	3.52	117.59	111.30
21	B	822	CLA	O2D-CGD-CBD	3.52	117.59	111.30
21	b	1836	CLA	O2D-CGD-CBD	3.52	117.59	111.30
21	a	832	CLA	O2D-CGD-CBD	3.52	117.59	111.30
21	2	840	CLA	C4A-NA-C1A	3.52	110.83	106.45
21	A	854	CLA	O2D-CGD-CBD	3.52	117.60	111.30
21	a	833	CLA	C4A-NA-C1A	3.53	110.83	106.45
21	l	205	CLA	C4A-NA-C1A	3.53	110.83	106.45
21	1	836	CLA	C4A-NA-C1A	3.53	110.83	106.45
21	j	1104	CLA	CMA-C3A-C4A	3.53	121.26	111.77
21	b	1815	CLA	O2D-CGD-CBD	3.53	117.61	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	844	BCR	C15-C14-C13	3.54	132.36	127.31
21	A	820	CLA	C4A-NA-C1A	3.54	110.84	106.45
21	1	840	CLA	O2D-CGD-CBD	3.54	117.63	111.30
21	A	832	CLA	C4A-NA-C1A	3.54	110.85	106.45
21	6	201	CLA	O2D-CGD-CBD	3.54	117.63	111.30
21	6	203	CLA	C4A-NA-C1A	3.55	110.86	106.45
21	J	1101	CLA	C4A-NA-C1A	3.55	110.86	106.45
21	f	202	CLA	C4A-NA-C1A	3.55	110.86	106.45
21	b	1810	CLA	C4A-NA-C1A	3.56	110.87	106.45
21	a	816	CLA	O2D-CGD-CBD	3.56	117.66	111.30
21	a	831	CLA	C4A-NA-C1A	3.56	110.88	106.45
21	b	1825	CLA	O2D-CGD-CBD	3.56	117.67	111.30
21	a	818	CLA	O2D-CGD-CBD	3.57	117.67	111.30
21	A	814	CLA	C4A-NA-C1A	3.57	110.88	106.45
21	A	832	CLA	O2D-CGD-CBD	3.57	117.68	111.30
21	B	822	CLA	C4A-NA-C1A	3.57	110.89	106.45
21	a	810	CLA	O2D-CGD-CBD	3.57	117.68	111.30
21	A	827	CLA	O2D-CGD-CBD	3.57	117.68	111.30
21	b	1831	CLA	C4A-NA-C1A	3.57	110.89	106.45
21	b	1842	CLA	O2D-CGD-CBD	3.58	117.69	111.30
21	J	1101	CLA	O2D-CGD-CBD	3.58	117.69	111.30
21	A	818	CLA	C4A-NA-C1A	3.58	110.89	106.45
21	b	1811	CLA	C4A-NA-C1A	3.58	110.90	106.45
21	2	821	CLA	O2D-CGD-CBD	3.58	117.70	111.30
21	B	810	CLA	O2D-CGD-CBD	3.58	117.70	111.30
21	b	1820	CLA	C4A-NA-C1A	3.58	110.90	106.45
21	A	828	CLA	C4A-NA-C1A	3.58	110.90	106.45
21	A	830	CLA	C4A-NA-C1A	3.58	110.90	106.45
21	A	815	CLA	C4A-NA-C1A	3.59	110.91	106.45
21	A	810	CLA	O2D-CGD-CBD	3.59	117.71	111.30
21	2	830	CLA	C4A-NA-C1A	3.59	110.91	106.45
21	B	803	CLA	O2D-CGD-CBD	3.59	117.71	111.30
21	B	808	CLA	O2D-CGD-CBD	3.59	117.72	111.30
21	B	835	CLA	O2D-CGD-CBD	3.59	117.72	111.30
21	a	821	CLA	O2D-CGD-CBD	3.59	117.72	111.30
21	1	855	CLA	C4A-NA-C1A	3.60	110.92	106.45
21	A	806	CLA	O2D-CGD-CBD	3.60	117.72	111.30
28	A	856	45D	C21-C15-C17	3.60	120.98	115.48
21	6	203	CLA	O2A-C1-C2	3.60	121.81	108.40
21	7	1101	CLA	O2D-CGD-CBD	3.60	117.73	111.30
21	K	102	CLA	C4A-NA-C1A	3.60	110.92	106.45
21	A	829	CLA	C4A-NA-C1A	3.60	110.92	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1808	CLA	O2D-CGD-CBD	3.60	117.73	111.30
21	A	825	CLA	C4A-NA-C1A	3.60	110.92	106.45
21	A	821	CLA	O2D-CGD-CBD	3.60	117.74	111.30
21	a	856	CLA	O2D-CGD-CBD	3.61	117.74	111.30
21	b	1841	CLA	C4A-NA-C1A	3.61	110.93	106.45
21	2	817	CLA	O2D-CGD-CBD	3.61	117.75	111.30
21	b	1821	CLA	C4A-NA-C1A	3.61	110.93	106.45
21	b	1838	CLA	C4A-NA-C1A	3.61	110.93	106.45
21	J	1105	CLA	O2D-CGD-CBD	3.61	117.75	111.30
21	1	816	CLA	C4A-NA-C1A	3.61	110.94	106.45
21	A	819	CLA	C4A-NA-C1A	3.61	110.94	106.45
21	a	839	CLA	O2D-CGD-CBD	3.61	117.76	111.30
21	B	817	CLA	C4A-NA-C1A	3.61	110.94	106.45
21	a	856	CLA	C4A-NA-C1A	3.61	110.94	106.45
21	j	1105	CLA	C4A-NA-C1A	3.61	110.94	106.45
25	L	210	LHG	O7-C7-C8	3.62	119.06	111.55
21	A	823	CLA	C4A-NA-C1A	3.62	110.94	106.45
21	8	1401	CLA	O2D-CGD-CBD	3.62	117.76	111.30
21	1	830	CLA	C4A-NA-C1A	3.62	110.94	106.45
21	B	815	CLA	C4A-NA-C1A	3.62	110.94	106.45
21	0	203	CLA	C4A-NA-C1A	3.62	110.94	106.45
21	B	837	CLA	C4A-NA-C1A	3.62	110.94	106.45
21	b	1835	CLA	C4A-NA-C1A	3.62	110.94	106.45
21	A	836	CLA	C4A-NA-C1A	3.62	110.95	106.45
21	B	811	CLA	C4A-NA-C1A	3.62	110.95	106.45
21	a	820	CLA	C4A-NA-C1A	3.62	110.95	106.45
21	b	1805	CLA	O2D-CGD-CBD	3.63	117.78	111.30
21	A	831	CLA	C4A-NA-C1A	3.63	110.95	106.45
21	1	805	CLA	O2D-CGD-CBD	3.63	117.78	111.30
21	l	205	CLA	O2D-CGD-CBD	3.63	117.79	111.30
21	1	840	CLA	C4A-NA-C1A	3.64	110.97	106.45
21	b	1823	CLA	C4A-NA-C1A	3.64	110.97	106.45
21	A	833	CLA	O2D-CGD-CBD	3.64	117.80	111.30
21	K	103	CLA	C4A-NA-C1A	3.64	110.97	106.45
21	l	204	CLA	C4A-NA-C1A	3.64	110.97	106.45
21	2	839	CLA	C4A-NA-C1A	3.65	110.98	106.45
21	2	813	CLA	O2D-CGD-CBD	3.65	117.82	111.30
21	1	822	CLA	O2D-CGD-CBD	3.65	117.82	111.30
21	a	821	CLA	C4A-NA-C1A	3.65	110.98	106.45
21	A	840	CLA	O2D-CGD-CBD	3.65	117.83	111.30
21	B	827	CLA	O2D-CGD-CBD	3.65	117.83	111.30
21	a	829	CLA	C4A-NA-C1A	3.66	110.99	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1817	CLA	O2D-CGD-CBD	3.66	117.83	111.30
21	1	825	CLA	C4A-NA-C1A	3.66	110.99	106.45
21	j	1101	CLA	O2D-CGD-CBD	3.66	117.83	111.30
21	B	830	CLA	O2D-CGD-CBD	3.66	117.84	111.30
21	b	1825	CLA	C4A-NA-C1A	3.66	111.00	106.45
21	B	831	CLA	O2D-CGD-CBD	3.66	117.84	111.30
21	1	829	CLA	C4A-NA-C1A	3.66	111.00	106.45
21	b	1835	CLA	O2D-CGD-CBD	3.66	117.85	111.30
21	B	825	CLA	O2D-CGD-CBD	3.67	117.85	111.30
30	l	202	ECH	C12-C13-C14	3.67	124.57	118.94
21	2	813	CLA	C4A-NA-C1A	3.67	111.01	106.45
21	6	203	CLA	O2D-CGD-CBD	3.67	117.86	111.30
21	2	803	CLA	O2D-CGD-CBD	3.67	117.86	111.30
21	2	802	CLA	C4A-NA-C1A	3.67	111.01	106.45
21	B	829	CLA	C4A-NA-C1A	3.67	111.01	106.45
21	1	807	CLA	C4A-NA-C1A	3.68	111.02	106.45
21	0	201	CLA	C4A-NA-C1A	3.68	111.02	106.45
21	2	823	CLA	C4A-NA-C1A	3.68	111.02	106.45
21	a	807	CLA	C4A-NA-C1A	3.68	111.02	106.45
21	B	840	CLA	C4A-NA-C1A	3.68	111.02	106.45
21	1	839	CLA	C4A-NA-C1A	3.68	111.02	106.45
21	B	811	CLA	O2D-CGD-CBD	3.68	117.88	111.30
21	A	807	CLA	C4A-NA-C1A	3.68	111.02	106.45
21	1	809	CLA	C4A-NA-C1A	3.68	111.03	106.45
21	B	802	CLA	C4A-NA-C1A	3.69	111.03	106.45
21	A	812	CLA	O2D-CGD-CBD	3.69	117.89	111.30
21	2	809	CLA	O2D-CGD-CBD	3.69	117.89	111.30
21	a	837	CLA	C4A-NA-C1A	3.70	111.04	106.45
21	1	821	CLA	O2D-CGD-CBD	3.70	117.90	111.30
21	1	837	CLA	C4A-NA-C1A	3.70	111.04	106.45
21	l	201	CLA	C4A-NA-C1A	3.70	111.05	106.45
21	2	808	CLA	C4A-NA-C1A	3.70	111.05	106.45
21	a	812	CLA	O2D-CGD-CBD	3.70	117.92	111.30
21	a	855	CLA	O2D-CGD-CBD	3.71	117.92	111.30
21	A	855	CLA	C4A-NA-C1A	3.71	111.05	106.45
21	B	830	CLA	C4A-NA-C1A	3.71	111.05	106.45
21	B	813	CLA	C4A-NA-C1A	3.71	111.05	106.45
21	l	203	CLA	O2D-CGD-CBD	3.71	117.93	111.30
21	B	835	CLA	C4A-NA-C1A	3.71	111.06	106.45
21	1	812	CLA	O2D-CGD-CBD	3.71	117.93	111.30
21	1	817	CLA	C4A-NA-C1A	3.71	111.06	106.45
21	A	837	CLA	C4A-NA-C1A	3.72	111.07	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	816	CLA	C4A-NA-C1A	3.72	111.07	106.45
21	A	811	CLA	C4A-NA-C1A	3.72	111.07	106.45
21	L	205	CLA	C4A-NA-C1A	3.72	111.07	106.45
21	f	203	CLA	C4A-NA-C1A	3.72	111.07	106.45
21	2	804	CLA	O2D-CGD-CBD	3.72	117.94	111.30
21	1	819	CLA	C4A-NA-C1A	3.72	111.07	106.45
21	A	817	CLA	O2D-CGD-CBD	3.72	117.95	111.30
21	2	802	CLA	O2D-CGD-CBD	3.72	117.95	111.30
21	A	817	CLA	C4A-NA-C1A	3.72	111.07	106.45
21	B	828	CLA	C4A-NA-C1A	3.72	111.07	106.45
21	b	1839	CLA	C4A-NA-C1A	3.73	111.08	106.45
21	b	1829	CLA	C4A-NA-C1A	3.73	111.08	106.45
21	a	825	CLA	O2D-CGD-CBD	3.73	117.97	111.30
21	A	826	CLA	C4A-NA-C1A	3.73	111.09	106.45
21	a	823	CLA	C4A-NA-C1A	3.73	111.09	106.45
21	a	839	CLA	C4A-NA-C1A	3.73	111.09	106.45
21	1	813	CLA	C4A-NA-C1A	3.73	111.09	106.45
21	a	819	CLA	C4A-NA-C1A	3.74	111.09	106.45
21	2	820	CLA	C4A-NA-C1A	3.74	111.09	106.45
21	a	809	CLA	C4A-NA-C1A	3.74	111.09	106.45
21	A	811	CLA	O2D-CGD-CBD	3.74	117.98	111.30
21	1	833	CLA	C4A-NA-C1A	3.74	111.10	106.45
21	2	824	CLA	C4A-NA-C1A	3.74	111.10	106.45
21	a	822	CLA	O2D-CGD-CBD	3.74	117.99	111.30
21	B	831	CLA	C4A-NA-C1A	3.74	111.10	106.45
21	a	807	CLA	O2D-CGD-CBD	3.75	117.99	111.30
21	1	841	CLA	C4A-NA-C1A	3.75	111.10	106.45
21	B	805	CLA	C4A-NA-C1A	3.75	111.10	106.45
21	l	204	CLA	O2D-CGD-CBD	3.75	118.00	111.30
21	b	1816	CLA	C4A-NA-C1A	3.75	111.11	106.45
21	a	831	CLA	O2D-CGD-CBD	3.75	118.00	111.30
21	2	834	CLA	C4A-NA-C1A	3.75	111.11	106.45
21	7	1101	CLA	C4A-NA-C1A	3.75	111.11	106.45
21	2	840	CLA	O2D-CGD-CBD	3.75	118.00	111.30
21	a	816	CLA	C4A-NA-C1A	3.75	111.11	106.45
21	1	836	CLA	O2D-CGD-CBD	3.75	118.01	111.30
21	a	823	CLA	O2D-CGD-CBD	3.76	118.01	111.30
21	B	801	CLA	C4A-NA-C1A	3.76	111.12	106.45
21	a	825	CLA	C4A-NA-C1A	3.76	111.12	106.45
26	2	850	LMG	O7-C10-C11	3.76	119.36	111.55
21	1	838	CLA	C4A-NA-C1A	3.76	111.12	106.45
21	2	832	CLA	C4A-NA-C1A	3.76	111.12	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	1814	CLA	C4A-NA-C1A	3.76	111.12	106.45
30	2	846	ECH	C19-C18-C17	3.77	124.72	118.94
21	a	818	CLA	C4A-NA-C1A	3.77	111.13	106.45
21	b	1828	CLA	C4A-NA-C1A	3.77	111.13	106.45
21	B	826	CLA	C4A-NA-C1A	3.77	111.13	106.45
21	1	835	CLA	O2D-CGD-CBD	3.77	118.04	111.30
21	1	807	CLA	O2D-CGD-CBD	3.77	118.04	111.30
21	B	819	CLA	C4A-NA-C1A	3.77	111.14	106.45
21	0	202	CLA	C4A-NA-C1A	3.77	111.14	106.45
21	j	1105	CLA	O2D-CGD-CBD	3.78	118.05	111.30
21	a	832	CLA	C4A-NA-C1A	3.78	111.14	106.45
21	B	829	CLA	O2D-CGD-CBD	3.78	118.05	111.30
21	1	808	CLA	O2D-CGD-CBD	3.78	118.05	111.30
21	L	204	CLA	C4A-NA-C1A	3.78	111.14	106.45
21	b	1809	CLA	C4A-NA-C1A	3.78	111.14	106.45
21	2	809	CLA	C4A-NA-C1A	3.79	111.15	106.45
21	b	1833	CLA	C4A-NA-C1A	3.79	111.15	106.45
21	1	832	CLA	C4A-NA-C1A	3.79	111.15	106.45
21	a	815	CLA	C4A-NA-C1A	3.79	111.15	106.45
21	a	803	CLA	C4A-NA-C1A	3.79	111.16	106.45
21	b	1801	CLA	C4A-NA-C1A	3.79	111.16	106.45
21	j	1101	CLA	C4A-NA-C1A	3.79	111.16	106.45
21	F	202	CLA	C4A-NA-C1A	3.79	111.16	106.45
21	A	840	CLA	C4A-NA-C1A	3.79	111.16	106.45
21	L	205	CLA	O2D-CGD-CBD	3.80	118.08	111.30
21	a	837	CLA	O2D-CGD-CBD	3.80	118.08	111.30
21	2	825	CLA	C4A-NA-C1A	3.80	111.17	106.45
21	B	839	CLA	O2D-CGD-CBD	3.80	118.09	111.30
21	2	815	CLA	C4A-NA-C1A	3.80	111.17	106.45
21	F	203	CLA	C4A-NA-C1A	3.80	111.17	106.45
28	2	854	45D	C30-C32-C34	3.80	134.90	123.23
21	B	839	CLA	C4A-NA-C1A	3.80	111.17	106.45
21	b	1804	CLA	C4A-NA-C1A	3.81	111.17	106.45
21	8	1401	CLA	C4A-NA-C1A	3.81	111.18	106.45
21	A	810	CLA	C4A-NA-C1A	3.81	111.18	106.45
21	b	1815	CLA	C4A-NA-C1A	3.81	111.18	106.45
21	a	812	CLA	C4A-NA-C1A	3.81	111.18	106.45
21	b	1824	CLA	C4A-NA-C1A	3.81	111.18	106.45
25	B	855	LHG	O7-C7-C8	3.81	119.46	111.55
21	b	1840	CLA	C4A-NA-C1A	3.81	111.18	106.45
21	1	823	CLA	C4A-NA-C1A	3.81	111.18	106.45
21	a	822	CLA	C4A-NA-C1A	3.81	111.18	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	805	CLA	C4A-NA-C1A	3.81	111.18	106.45
21	1	822	CLA	C4A-NA-C1A	3.81	111.19	106.45
21	2	831	CLA	C4A-NA-C1A	3.82	111.19	106.45
21	1	808	CLA	C4A-NA-C1A	3.82	111.19	106.45
21	1	824	CLA	C4A-NA-C1A	3.82	111.19	106.45
21	a	813	CLA	C4A-NA-C1A	3.82	111.19	106.45
21	b	1842	CLA	C4A-NA-C1A	3.82	111.19	106.45
21	1	810	CLA	C4A-NA-C1A	3.82	111.19	106.45
21	A	830	CLA	O2D-CGD-CBD	3.82	118.12	111.30
21	a	806	CLA	C4A-NA-C1A	3.82	111.19	106.45
21	2	835	CLA	C4A-NA-C1A	3.82	111.20	106.45
21	2	816	CLA	C4A-NA-C1A	3.82	111.20	106.45
21	A	826	CLA	O2D-CGD-CBD	3.82	118.13	111.30
21	a	830	CLA	C4A-NA-C1A	3.82	111.20	106.45
21	b	1837	CLA	C4A-NA-C1A	3.82	111.20	106.45
21	A	802	CLA	C4A-NA-C1A	3.82	111.20	106.45
21	2	822	CLA	C4A-NA-C1A	3.83	111.20	106.45
21	A	816	CLA	C4A-NA-C1A	3.83	111.20	106.45
21	b	1822	CLA	C4A-NA-C1A	3.83	111.20	106.45
21	2	826	CLA	C4A-NA-C1A	3.83	111.21	106.45
21	A	829	CLA	O2D-CGD-CBD	3.84	118.16	111.30
21	A	807	CLA	O2D-CGD-CBD	3.84	118.16	111.30
26	B	848	LMG	O7-C10-C11	3.84	119.52	111.55
21	8	1402	CLA	C4A-NA-C1A	3.84	111.22	106.45
21	B	823	CLA	C4A-NA-C1A	3.84	111.22	106.45
21	B	821	CLA	C4A-NA-C1A	3.84	111.22	106.45
21	A	834	CLA	C4A-NA-C1A	3.85	111.22	106.45
21	A	824	CLA	O2D-CGD-CBD	3.85	118.17	111.30
21	2	837	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	2	841	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	1	818	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	B	833	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	2	815	CLA	O2D-CGD-CBD	3.85	118.18	111.30
21	a	855	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	1	815	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	a	838	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	a	827	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	2	812	CLA	C4A-NA-C1A	3.85	111.23	106.45
21	A	814	CLA	O2D-CGD-CBD	3.85	118.19	111.30
21	B	824	CLA	C4A-NA-C1A	3.85	111.24	106.45
21	B	812	CLA	C4A-NA-C1A	3.86	111.24	106.45
21	1	815	CLA	O2D-CGD-CBD	3.86	118.19	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	855	CLA	O2D-CGD-CBD	3.86	118.19	111.30
21	7	1103	CLA	C4A-NA-C1A	3.86	111.24	106.45
21	b	1819	CLA	C4A-NA-C1A	3.86	111.25	106.45
21	2	827	CLA	C4A-NA-C1A	3.87	111.25	106.45
21	A	822	CLA	C4A-NA-C1A	3.87	111.25	106.45
24	0	205	BCR	C19-C18-C17	3.87	124.88	118.94
21	B	827	CLA	C4A-NA-C1A	3.87	111.25	106.45
21	1	804	CLA	O2D-CGD-CBD	3.87	118.21	111.30
21	a	836	CLA	C4A-NA-C1A	3.87	111.25	106.45
21	2	842	CLA	C4A-NA-C1A	3.87	111.25	106.45
21	J	1103	CLA	C4A-NA-C1A	3.87	111.26	106.45
21	b	1832	CLA	O2D-CGD-CBD	3.87	118.22	111.30
21	b	1834	CLA	C4A-NA-C1A	3.87	111.26	106.45
21	a	826	CLA	C4A-NA-C1A	3.88	111.26	106.45
21	b	1833	CLA	O2D-CGD-CBD	3.88	118.23	111.30
21	a	817	CLA	C4A-NA-C1A	3.88	111.27	106.45
21	A	825	CLA	O2D-CGD-CBD	3.88	118.23	111.30
21	K	102	CLA	O2D-CGD-CBD	3.88	118.23	111.30
21	1	806	CLA	C4A-NA-C1A	3.88	111.27	106.45
21	L	203	CLA	C4A-NA-C1A	3.88	111.27	106.45
21	1	835	CLA	C4A-NA-C1A	3.89	111.28	106.45
21	B	825	CLA	C4A-NA-C1A	3.89	111.28	106.45
21	2	807	CLA	C4A-NA-C1A	3.89	111.28	106.45
21	J	1106	CLA	O2D-CGD-CBD	3.89	118.26	111.30
21	B	806	CLA	C4A-NA-C1A	3.90	111.29	106.45
26	K	105	LMG	C1-C2-C3	3.90	117.22	109.98
21	2	814	CLA	C4A-NA-C1A	3.90	111.29	106.45
21	m	103	CLA	C4A-NA-C1A	3.90	111.29	106.45
21	a	802	CLA	O2D-CGD-CBD	3.90	118.27	111.30
21	a	834	CLA	C4A-NA-C1A	3.90	111.29	106.45
35	l	211	LMT	O5B-C5B-C4B	3.90	116.85	109.66
21	B	809	CLA	C4A-NA-C1A	3.90	111.30	106.45
21	B	834	CLA	C4A-NA-C1A	3.91	111.30	106.45
21	l	201	CLA	O2D-CGD-CBD	3.91	118.28	111.30
21	1	812	CLA	C4A-NA-C1A	3.91	111.30	106.45
21	A	803	CLA	O2D-CGD-CBD	3.91	118.28	111.30
25	I	103	LHG	O7-C7-C8	3.91	119.67	111.55
21	J	1103	CLA	O2D-CGD-CBD	3.91	118.28	111.30
21	2	829	CLA	C4A-NA-C1A	3.91	111.31	106.45
21	A	838	CLA	C4A-NA-C1A	3.91	111.31	106.45
21	A	808	CLA	C4A-NA-C1A	3.91	111.31	106.45
21	7	1105	CLA	C4A-NA-C1A	3.92	111.32	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	838	CLA	C4A-NA-C1A	3.92	111.32	106.45
21	1	820	CLA	C4A-NA-C1A	3.92	111.32	106.45
26	A	852	LMG	O7-C10-C11	3.92	119.70	111.55
25	l	209	LHG	O7-C7-C8	3.92	119.70	111.55
21	A	854	CLA	C4A-NA-C1A	3.93	111.33	106.45
21	A	803	CLA	C4A-NA-C1A	3.93	111.33	106.45
21	A	804	CLA	C4A-NA-C1A	3.93	111.33	106.45
21	j	1104	CLA	O2D-CGD-CBD	3.93	118.33	111.30
21	1	833	CLA	O2D-CGD-CBD	3.93	118.33	111.30
21	l	203	CLA	C4A-NA-C1A	3.94	111.34	106.45
21	1	811	CLA	C4A-NA-C1A	3.94	111.34	106.45
21	b	1801	CLA	O2D-CGD-CBD	3.94	118.34	111.30
21	b	1826	CLA	C4A-NA-C1A	3.94	111.34	106.45
21	F	203	CLA	O2D-CGD-CBD	3.94	118.34	111.30
21	1	804	CLA	C4A-NA-C1A	3.94	111.35	106.45
21	b	1812	CLA	C4A-NA-C1A	3.94	111.35	106.45
21	a	805	CLA	C4A-NA-C1A	3.95	111.35	106.45
21	k	1401	CLA	C4A-NA-C1A	3.95	111.35	106.45
21	1	830	CLA	O2D-CGD-CBD	3.95	118.35	111.30
21	B	818	CLA	C4A-NA-C1A	3.95	111.35	106.45
21	1	827	CLA	C4A-NA-C1A	3.95	111.35	106.45
21	1	834	CLA	O2D-CGD-CBD	3.95	118.36	111.30
26	2	852	LMG	O7-C10-C11	3.95	119.76	111.55
21	b	1806	CLA	C4A-NA-C1A	3.95	111.36	106.45
21	B	810	CLA	C4A-NA-C1A	3.95	111.36	106.45
21	2	833	CLA	C4A-NA-C1A	3.96	111.36	106.45
21	A	812	CLA	C4A-NA-C1A	3.96	111.37	106.45
21	a	810	CLA	C4A-NA-C1A	3.96	111.37	106.45
21	b	1843	CLA	C4A-NA-C1A	3.97	111.38	106.45
21	b	1830	CLA	C4A-NA-C1A	3.97	111.39	106.45
21	1	803	CLA	C4A-NA-C1A	3.98	111.39	106.45
21	2	828	CLA	C4A-NA-C1A	3.98	111.39	106.45
21	b	1811	CLA	O2D-CGD-CBD	3.99	118.43	111.30
21	1	834	CLA	C4A-NA-C1A	4.00	111.41	106.45
25	A	849	LHG	O7-C7-C8	4.00	119.85	111.55
21	7	1103	CLA	O2D-CGD-CBD	4.00	118.44	111.30
21	A	827	CLA	C4A-NA-C1A	4.00	111.42	106.45
21	7	1104	CLA	C4A-NA-C1A	4.00	111.42	106.45
21	b	1817	CLA	C4A-NA-C1A	4.01	111.42	106.45
21	b	1805	CLA	C4A-NA-C1A	4.01	111.43	106.45
21	a	808	CLA	O2D-CGD-CBD	4.01	118.46	111.30
21	6	201	CLA	C4A-NA-C1A	4.01	111.43	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	832	CLA	C4A-NA-C1A	4.01	111.43	106.45
21	a	840	CLA	C4A-NA-C1A	4.01	111.43	106.45
26	0	206	LMG	O7-C10-C11	4.02	119.89	111.55
21	B	816	CLA	O2D-CGD-CBD	4.02	118.48	111.30
21	b	1818	CLA	O2D-CGD-CBD	4.02	118.48	111.30
21	B	814	CLA	C4A-NA-C1A	4.02	111.44	106.45
21	b	1838	CLA	O2D-CGD-CBD	4.02	118.48	111.30
21	k	1402	CLA	C4A-NA-C1A	4.02	111.45	106.45
21	J	1106	CLA	C4A-NA-C1A	4.03	111.45	106.45
26	b	1855	LMG	O7-C10-C11	4.03	119.91	111.55
25	2	801	LHG	O7-C7-C8	4.03	119.92	111.55
21	b	1813	CLA	C4A-NA-C1A	4.03	111.46	106.45
21	2	810	CLA	C4A-NA-C1A	4.03	111.46	106.45
21	2	811	CLA	C4A-NA-C1A	4.03	111.46	106.45
25	A	851	LHG	O7-C7-C8	4.04	119.93	111.55
21	A	809	CLA	C4A-NA-C1A	4.04	111.46	106.45
21	1	825	CLA	O2D-CGD-CBD	4.04	118.51	111.30
21	2	817	CLA	C4A-NA-C1A	4.04	111.46	106.45
21	A	839	CLA	C4A-NA-C1A	4.04	111.47	106.45
21	2	804	CLA	C4A-NA-C1A	4.05	111.48	106.45
21	a	824	CLA	C4A-NA-C1A	4.05	111.48	106.45
21	1	828	CLA	C4A-NA-C1A	4.06	111.49	106.45
21	B	807	CLA	C4A-NA-C1A	4.06	111.49	106.45
21	a	808	CLA	C4A-NA-C1A	4.06	111.49	106.45
21	A	824	CLA	C4A-NA-C1A	4.06	111.49	106.45
21	1	821	CLA	C4A-NA-C1A	4.07	111.50	106.45
21	2	836	CLA	C4A-NA-C1A	4.07	111.50	106.45
26	1	853	LMG	O7-C10-C11	4.07	120.00	111.55
21	2	816	CLA	O2D-CGD-CBD	4.07	118.57	111.30
21	2	821	CLA	C4A-NA-C1A	4.07	111.51	106.45
21	b	1836	CLA	C4A-NA-C1A	4.08	111.51	106.45
21	j	1104	CLA	C4A-NA-C1A	4.08	111.52	106.45
21	I	101	CLA	C4A-NA-C1A	4.09	111.53	106.45
21	a	814	CLA	C4A-NA-C1A	4.09	111.53	106.45
21	2	818	CLA	C4A-NA-C1A	4.09	111.53	106.45
21	B	820	CLA	C4A-NA-C1A	4.09	111.53	106.45
21	a	830	CLA	O2D-CGD-CBD	4.10	118.62	111.30
21	b	1827	CLA	C4A-NA-C1A	4.10	111.55	106.45
28	2	854	45D	C28-C26-C30	4.10	128.67	122.92
21	a	804	CLA	O2D-CGD-CBD	4.11	118.64	111.30
21	1	814	CLA	C4A-NA-C1A	4.11	111.56	106.45
21	a	802	CLA	C4A-NA-C1A	4.11	111.56	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	103	CLA	O2D-CGD-CBD	4.12	118.65	111.30
21	1	805	CLA	C4A-NA-C1A	4.12	111.57	106.45
21	j	1103	CLA	O2D-CGD-CBD	4.12	118.67	111.30
21	B	804	CLA	C4A-NA-C1A	4.14	111.59	106.45
21	A	813	CLA	C4A-NA-C1A	4.14	111.59	106.45
21	a	804	CLA	C4A-NA-C1A	4.14	111.59	106.45
26	a	850	LMG	O7-C10-C11	4.15	120.16	111.55
25	a	851	LHG	O7-C7-C8	4.16	120.18	111.55
21	j	1103	CLA	C4A-NA-C1A	4.16	111.62	106.45
21	2	807	CLA	O2D-CGD-CBD	4.17	118.75	111.30
21	b	1808	CLA	C4A-NA-C1A	4.17	111.63	106.45
26	1	851	LMG	O7-C10-C11	4.17	120.22	111.55
25	b	1852	LHG	O7-C7-C8	4.18	120.23	111.55
26	B	850	LMG	O7-C10-C11	4.18	120.23	111.55
25	I	104	LHG	O7-C7-C8	4.19	120.24	111.55
24	F	201	BCR	C15-C14-C13	4.19	133.29	127.31
25	9	101	LHG	O7-C7-C8	4.20	120.27	111.55
21	1	801	CLA	C4A-NA-C1A	4.22	111.68	106.45
21	B	803	CLA	C4A-NA-C1A	4.22	111.69	106.45
21	B	836	CLA	C4A-NA-C1A	4.22	111.69	106.45
21	B	809	CLA	O2D-CGD-CBD	4.23	118.86	111.30
21	2	818	CLA	O2D-CGD-CBD	4.23	118.86	111.30
21	2	810	CLA	O2D-CGD-CBD	4.23	118.86	111.30
21	J	1105	CLA	C4A-NA-C1A	4.23	111.71	106.45
21	1	831	CLA	O2D-CGD-CBD	4.24	118.87	111.30
21	1	802	CLA	C4A-NA-C1A	4.26	111.74	106.45
21	2	803	CLA	C4A-NA-C1A	4.26	111.74	106.45
25	B	851	LHG	O7-C7-C8	4.26	120.39	111.55
25	1	850	LHG	O7-C7-C8	4.26	120.40	111.55
25	l	210	LHG	O7-C7-C8	4.28	120.43	111.55
21	2	806	CLA	C4A-NA-C1A	4.28	111.76	106.45
21	a	828	CLA	C4A-NA-C1A	4.29	111.77	106.45
21	a	811	CLA	C4A-NA-C1A	4.30	111.78	106.45
21	B	824	CLA	O2D-CGD-CBD	4.31	119.00	111.30
21	6	204	CLA	C4A-NA-C1A	4.31	111.80	106.45
25	2	851	LHG	O7-C7-C8	4.32	120.52	111.55
25	1	852	LHG	O7-C7-C8	4.35	120.58	111.55
26	b	1851	LMG	O7-C10-C11	4.35	120.58	111.55
21	a	801	CLA	C4A-NA-C1A	4.38	111.89	106.45
21	2	805	CLA	C4A-NA-C1A	4.38	111.89	106.45
26	K	101	LMG	O7-C10-C11	4.39	120.66	111.55
21	A	801	CLA	C4A-NA-C1A	4.39	111.90	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	840	CLA	O2D-CGD-CBD	4.41	119.17	111.30
30	a	857	ECH	C12-C13-C14	4.41	125.71	118.94
25	b	1802	LHG	O7-C7-C8	4.41	120.72	111.55
37	L	209	DGD	O2G-C1B-C2B	4.42	120.72	111.55
25	l	208	LHG	O7-C7-C8	4.42	120.73	111.55
26	A	850	LMG	O7-C10-C11	4.43	120.75	111.55
25	B	849	LHG	O7-C7-C8	4.43	120.75	111.55
25	a	849	LHG	O7-C7-C8	4.46	120.80	111.55
25	B	857	LHG	O7-C7-C8	4.49	120.87	111.55
25	B	858	LHG	O7-C7-C8	4.49	120.88	111.55
21	b	1807	CLA	C4A-NA-C1A	4.49	112.03	106.45
25	m	101	LHG	O7-C7-C8	4.52	120.94	111.55
26	b	1853	LMG	O7-C10-C11	4.55	120.99	111.55
21	b	1827	CLA	O2D-CGD-CBD	4.56	119.45	111.30
21	2	826	CLA	O2D-CGD-CBD	4.68	119.66	111.30
21	6	204	CLA	O2D-CGD-CBD	4.75	119.78	111.30
21	2	833	CLA	O2D-CGD-CBD	4.80	119.88	111.30
26	K	105	LMG	O7-C10-C11	4.97	121.88	111.55
21	B	812	CLA	O2D-CGD-CBD	5.02	120.27	111.30
25	a	853	LHG	O7-C7-C8	5.06	122.05	111.55
26	a	852	LMG	O7-C10-C11	5.14	122.23	111.55
21	a	836	CLA	O2D-CGD-CBD	5.16	120.53	111.30
21	a	834	CLA	O2A-C1-C2	5.18	121.44	109.02
25	b	1803	LHG	O7-C7-C8	5.30	122.56	111.55
21	A	801	CLA	O2D-CGD-CBD	5.60	121.31	111.30
28	2	854	45D	C20-C24-C26	5.62	134.65	126.21
24	2	849	BCR	C20-C19-C18	5.65	142.28	126.42
25	M	7003	LHG	O7-C7-C8	5.72	123.43	111.55
21	k	1402	CLA	O2A-C1-C2	5.81	122.93	109.02
28	2	854	45D	C28-C26-C24	5.83	127.38	118.10
24	0	205	BCR	C20-C19-C18	5.97	143.19	126.42
24	9	102	BCR	C20-C19-C18	5.98	143.22	126.42
24	a	848	BCR	C20-C19-C18	6.36	144.29	126.42
24	A	845	BCR	C20-C19-C18	6.64	145.07	126.42
24	6	202	BCR	C20-C19-C18	6.69	145.21	126.42
24	1	845	BCR	C20-C19-C18	6.77	145.44	126.42
24	1	858	BCR	C20-C19-C18	6.78	145.47	126.42
24	a	859	BCR	C20-C19-C18	6.80	145.52	126.42
24	b	1848	BCR	C20-C19-C18	6.80	145.53	126.42
24	B	842	BCR	C20-C19-C18	6.84	145.64	126.42
24	f	201	BCR	C20-C19-C18	6.89	145.78	126.42
24	1	846	BCR	C20-C19-C18	7.02	146.14	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	l	207	BCR	C20-C19-C18	7.03	146.17	126.42
24	F	201	BCR	C20-C19-C18	7.09	146.33	126.42
24	J	1102	BCR	C20-C19-C18	7.15	146.50	126.42
24	2	844	BCR	C20-C19-C18	7.17	146.57	126.42
24	b	1845	BCR	C20-C19-C18	7.19	146.62	126.42
24	8	1403	BCR	C20-C19-C18	7.34	147.02	126.42
28	2	854	45D	C32-C30-C26	7.39	137.86	127.31
24	1	844	BCR	C20-C19-C18	7.45	147.33	126.42
24	a	846	BCR	C20-C19-C18	7.49	147.45	126.42
24	f	204	BCR	C20-C19-C18	7.58	147.70	126.42
24	B	845	BCR	C20-C19-C18	7.58	147.70	126.42
24	A	843	BCR	C20-C19-C18	7.62	147.82	126.42
24	1	848	BCR	C20-C19-C18	7.64	147.87	126.42
24	L	207	BCR	C20-C19-C18	7.73	148.14	126.42
24	A	844	BCR	C20-C19-C18	7.79	148.31	126.42
24	A	847	BCR	C20-C19-C18	7.81	148.37	126.42
24	6	205	BCR	C20-C19-C18	7.85	148.47	126.42
24	k	1403	BCR	C20-C19-C18	7.91	148.65	126.42
24	J	1107	BCR	C20-C19-C18	7.96	148.79	126.42
24	7	1102	BCR	C20-C19-C18	7.99	148.87	126.42
24	a	845	BCR	C20-C19-C18	7.99	148.87	126.42
24	K	104	BCR	C20-C19-C18	8.01	148.91	126.42
24	I	102	BCR	C21-C20-C19	8.02	147.84	123.23
24	1	849	BCR	C20-C19-C18	8.03	148.99	126.42
24	l	206	BCR	C20-C19-C18	8.07	149.09	126.42
24	L	206	BCR	C20-C19-C18	8.22	149.50	126.42
24	a	843	BCR	C20-C19-C18	8.32	149.78	126.42
24	b	1846	BCR	C20-C19-C18	8.43	150.10	126.42
24	A	848	BCR	C20-C19-C18	8.44	150.13	126.42
24	2	845	BCR	C20-C19-C18	8.46	150.19	126.42
24	l	206	BCR	C11-C10-C9	8.49	139.43	127.31
24	L	206	BCR	C16-C15-C14	8.53	141.66	123.46
24	B	846	BCR	C20-C19-C18	8.61	150.60	126.42
24	0	204	BCR	C20-C19-C18	8.64	150.68	126.42
24	A	846	BCR	C20-C19-C18	8.65	150.71	126.42
24	a	844	BCR	C20-C19-C18	8.71	150.88	126.42
24	A	847	BCR	C11-C10-C9	8.77	139.83	127.31
24	B	843	BCR	C20-C19-C18	8.81	151.17	126.42
24	j	1102	BCR	C20-C19-C18	8.82	151.19	126.42
24	A	846	BCR	C11-C10-C9	8.84	139.92	127.31
24	1	847	BCR	C20-C19-C18	8.86	151.31	126.42
24	B	847	BCR	C20-C19-C18	8.87	151.33	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	856	BCR	C20-C19-C18	8.88	151.35	126.42
24	a	847	BCR	C20-C19-C18	8.92	151.49	126.42
24	b	1849	BCR	C20-C19-C18	8.94	151.54	126.42
24	L	206	BCR	C11-C10-C9	9.11	140.31	127.31
24	b	1850	BCR	C20-C19-C18	9.14	152.09	126.42
24	9	102	BCR	C21-C20-C19	9.22	151.50	123.23
24	2	848	BCR	C20-C19-C18	9.29	152.50	126.42
24	h	101	BCR	C21-C20-C19	9.31	151.80	123.23
24	2	847	BCR	C20-C19-C18	9.32	152.59	126.42
24	b	1850	BCR	C11-C10-C9	9.33	140.63	127.31
24	j	1102	BCR	C11-C10-C9	9.34	140.64	127.31
24	2	849	BCR	C21-C20-C19	9.35	151.93	123.23
24	A	843	BCR	C11-C10-C9	9.39	140.71	127.31
24	b	1848	BCR	C11-C10-C9	9.45	140.79	127.31
24	i	101	BCR	C21-C20-C19	9.45	152.22	123.23
24	1	845	BCR	C11-C10-C9	9.57	140.96	127.31
24	F	201	BCR	C16-C15-C14	9.59	143.93	123.46
24	B	846	BCR	C21-C20-C19	9.68	152.91	123.23
24	2	848	BCR	C21-C20-C19	9.76	153.17	123.23
24	1	856	BCR	C16-C15-C14	9.86	144.51	123.46
24	0	205	BCR	C16-C15-C14	9.87	144.52	123.46
24	b	1849	BCR	C21-C20-C19	9.89	153.57	123.23
24	8	1403	BCR	C11-C10-C9	9.95	141.52	127.31
24	1	856	BCR	C11-C10-C9	10.09	141.71	127.31
24	a	846	BCR	C11-C10-C9	10.23	141.91	127.31
24	A	847	BCR	C16-C15-C14	10.26	145.37	123.46
24	l	206	BCR	C16-C15-C14	10.27	145.38	123.46
24	a	848	BCR	C21-C20-C19	10.28	154.78	123.23
24	0	204	BCR	C11-C10-C9	10.36	142.09	127.31
24	1	848	BCR	C11-C10-C9	10.39	142.13	127.31
24	A	846	BCR	C16-C15-C14	10.40	145.67	123.46
24	b	1846	BCR	C21-C20-C19	10.48	155.38	123.23
24	B	843	BCR	C11-C10-C9	10.50	142.29	127.31
24	J	1102	BCR	C11-C10-C9	10.50	142.30	127.31
24	i	101	BCR	C20-C19-C18	10.51	155.95	126.42
24	K	104	BCR	C11-C10-C9	10.54	142.36	127.31
24	1	849	BCR	C11-C10-C9	10.55	142.36	127.31
24	B	842	BCR	C11-C10-C9	10.55	142.37	127.31
24	A	844	BCR	C11-C10-C9	10.63	142.48	127.31
24	a	847	BCR	C21-C20-C19	10.72	156.13	123.23
24	f	201	BCR	C16-C15-C14	10.72	146.35	123.46
24	7	1102	BCR	C11-C10-C9	10.76	142.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	847	BCR	C11-C10-C9	10.79	142.70	127.31
24	I	102	BCR	C20-C19-C18	10.84	156.86	126.42
24	A	846	BCR	C21-C20-C19	10.84	156.49	123.23
24	k	1403	BCR	C11-C10-C9	10.84	142.79	127.31
24	L	206	BCR	C21-C20-C19	10.87	156.58	123.23
24	6	202	BCR	C16-C15-C14	10.87	146.67	123.46
24	f	204	BCR	C16-C15-C14	10.88	146.68	123.46
24	J	1102	BCR	C16-C15-C14	10.89	146.71	123.46
24	h	101	BCR	C20-C19-C18	10.89	157.01	126.42
24	B	843	BCR	C21-C20-C19	10.90	156.68	123.23
24	1	846	BCR	C11-C10-C9	10.93	142.91	127.31
24	A	845	BCR	C16-C15-C14	10.96	146.86	123.46
24	L	207	BCR	C16-C15-C14	11.01	146.97	123.46
24	a	859	BCR	C16-C15-C14	11.02	146.98	123.46
24	A	844	BCR	C16-C15-C14	11.03	147.00	123.46
24	a	846	BCR	C16-C15-C14	11.03	147.00	123.46
24	A	845	BCR	C11-C10-C9	11.04	143.06	127.31
24	l	207	BCR	C16-C15-C14	11.05	147.04	123.46
24	0	204	BCR	C21-C20-C19	11.14	157.40	123.23
24	1	856	BCR	C21-C20-C19	11.16	157.46	123.23
24	b	1850	BCR	C21-C20-C19	11.19	157.56	123.23
24	j	1102	BCR	C21-C20-C19	11.21	157.62	123.23
24	I	102	BCR	C11-C10-C9	11.21	143.31	127.31
24	L	207	BCR	C11-C10-C9	11.23	143.34	127.31
24	I	102	BCR	C16-C15-C14	11.27	147.53	123.46
24	b	1845	BCR	C16-C15-C14	11.28	147.53	123.46
24	K	104	BCR	C21-C20-C19	11.28	157.84	123.23
24	A	843	BCR	C16-C15-C14	11.29	147.56	123.46
24	2	849	BCR	C16-C15-C14	11.35	147.68	123.46
24	2	844	BCR	C11-C10-C9	11.40	143.58	127.31
24	B	845	BCR	C16-C15-C14	11.43	147.86	123.46
24	2	845	BCR	C21-C20-C19	11.44	158.31	123.23
24	a	845	BCR	C11-C10-C9	11.46	143.67	127.31
24	l	206	BCR	C21-C20-C19	11.47	158.41	123.23
24	L	207	BCR	C21-C20-C19	11.48	158.44	123.23
24	A	844	BCR	C21-C20-C19	11.48	158.45	123.23
24	1	844	BCR	C21-C20-C19	11.50	158.52	123.23
24	a	859	BCR	C11-C10-C9	11.53	143.76	127.31
24	h	101	BCR	C11-C10-C9	11.54	143.78	127.31
24	B	847	BCR	C11-C10-C9	11.55	143.80	127.31
24	a	843	BCR	C11-C10-C9	11.56	143.80	127.31
24	a	847	BCR	C11-C10-C9	11.56	143.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	1848	BCR	C16-C15-C14	11.56	148.14	123.46
24	J	1107	BCR	C21-C20-C19	11.56	158.71	123.23
24	1	847	BCR	C21-C20-C19	11.58	158.76	123.23
24	b	1846	BCR	C16-C15-C14	11.63	148.28	123.46
24	B	845	BCR	C11-C10-C9	11.63	143.91	127.31
24	2	848	BCR	C16-C15-C14	11.64	148.32	123.46
24	A	847	BCR	C21-C20-C19	11.67	159.04	123.23
24	a	844	BCR	C21-C20-C19	11.71	159.17	123.23
24	b	1846	BCR	C11-C10-C9	11.74	144.06	127.31
24	1	858	BCR	C16-C15-C14	11.76	148.56	123.46
24	0	204	BCR	C16-C15-C14	11.78	148.60	123.46
24	F	201	BCR	C11-C10-C9	11.81	144.17	127.31
24	k	1403	BCR	C21-C20-C19	11.81	159.47	123.23
24	1	858	BCR	C11-C10-C9	11.89	144.28	127.31
24	f	204	BCR	C11-C10-C9	11.89	144.28	127.31
24	a	845	BCR	C21-C20-C19	11.92	159.81	123.23
24	2	845	BCR	C11-C10-C9	11.93	144.33	127.31
24	J	1107	BCR	C16-C15-C14	11.94	148.94	123.46
24	A	848	BCR	C21-C20-C19	11.95	159.90	123.23
24	f	201	BCR	C11-C10-C9	12.00	144.43	127.31
24	1	844	BCR	C11-C10-C9	12.02	144.46	127.31
24	i	101	BCR	C11-C10-C9	12.02	144.46	127.31
24	J	1107	BCR	C11-C10-C9	12.05	144.50	127.31
24	6	205	BCR	C16-C15-C14	12.07	149.22	123.46
24	1	848	BCR	C21-C20-C19	12.11	160.39	123.23
24	9	102	BCR	C11-C10-C9	12.14	144.64	127.31
24	j	1102	BCR	C16-C15-C14	12.19	149.49	123.46
24	a	843	BCR	C21-C20-C19	12.22	160.72	123.23
24	b	1845	BCR	C21-C20-C19	12.23	160.77	123.23
24	7	1102	BCR	C21-C20-C19	12.26	160.85	123.23
24	K	104	BCR	C16-C15-C14	12.28	149.68	123.46
24	a	844	BCR	C11-C10-C9	12.37	144.96	127.31
24	a	848	BCR	C11-C10-C9	12.39	145.00	127.31
24	a	846	BCR	C21-C20-C19	12.40	161.27	123.23
24	2	844	BCR	C16-C15-C14	12.40	149.93	123.46
24	1	849	BCR	C21-C20-C19	12.43	161.36	123.23
24	l	207	BCR	C11-C10-C9	12.44	145.06	127.31
24	B	846	BCR	C16-C15-C14	12.47	150.07	123.46
24	f	204	BCR	C21-C20-C19	12.51	161.62	123.23
24	B	842	BCR	C21-C20-C19	12.53	161.66	123.23
24	B	842	BCR	C16-C15-C14	12.53	150.20	123.46
24	k	1403	BCR	C16-C15-C14	12.53	150.21	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	845	BCR	C21-C20-C19	12.53	161.68	123.23
24	6	205	BCR	C21-C20-C19	12.61	161.91	123.23
24	1	846	BCR	C16-C15-C14	12.62	150.40	123.46
24	b	1845	BCR	C11-C10-C9	12.65	145.36	127.31
24	F	201	BCR	C21-C20-C19	12.69	162.17	123.23
24	A	843	BCR	C21-C20-C19	12.70	162.20	123.23
24	1	858	BCR	C21-C20-C19	12.71	162.22	123.23
24	b	1849	BCR	C11-C10-C9	12.74	145.50	127.31
24	J	1102	BCR	C21-C20-C19	12.74	162.33	123.23
24	l	207	BCR	C21-C20-C19	12.80	162.49	123.23
24	b	1849	BCR	C16-C15-C14	12.82	150.83	123.46
24	1	848	BCR	C16-C15-C14	12.85	150.90	123.46
24	8	1403	BCR	C21-C20-C19	12.93	162.90	123.23
24	2	844	BCR	C21-C20-C19	12.94	162.92	123.23
24	2	848	BCR	C11-C10-C9	12.95	145.79	127.31
24	7	1102	BCR	C16-C15-C14	12.95	151.11	123.46
24	0	205	BCR	C11-C10-C9	12.96	145.81	127.31
24	6	205	BCR	C11-C10-C9	12.96	145.81	127.31
24	6	202	BCR	C11-C10-C9	12.96	145.81	127.31
24	A	845	BCR	C21-C20-C19	12.98	163.04	123.23
24	f	201	BCR	C21-C20-C19	13.01	163.16	123.23
24	a	859	BCR	C21-C20-C19	13.05	163.28	123.23
24	a	845	BCR	C16-C15-C14	13.08	151.38	123.46
24	1	845	BCR	C16-C15-C14	13.08	151.38	123.46
24	B	846	BCR	C11-C10-C9	13.08	145.98	127.31
24	B	847	BCR	C21-C20-C19	13.14	163.53	123.23
24	8	1403	BCR	C16-C15-C14	13.16	151.55	123.46
24	B	843	BCR	C16-C15-C14	13.19	151.62	123.46
24	2	847	BCR	C11-C10-C9	13.20	146.15	127.31
24	1	846	BCR	C21-C20-C19	13.24	163.86	123.23
24	0	205	BCR	C21-C20-C19	13.25	163.88	123.23
24	1	844	BCR	C16-C15-C14	13.29	151.83	123.46
24	1	845	BCR	C21-C20-C19	13.41	164.37	123.23
24	6	202	BCR	C21-C20-C19	13.45	164.48	123.23
24	2	847	BCR	C21-C20-C19	13.49	164.61	123.23
24	a	847	BCR	C16-C15-C14	13.50	152.28	123.46
24	2	847	BCR	C16-C15-C14	13.52	152.32	123.46
24	B	847	BCR	C16-C15-C14	13.52	152.32	123.46
24	1	847	BCR	C16-C15-C14	13.54	152.36	123.46
24	b	1848	BCR	C21-C20-C19	13.59	164.93	123.23
24	9	102	BCR	C16-C15-C14	13.67	152.63	123.46
24	2	845	BCR	C16-C15-C14	13.71	152.73	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	101	BCR	C16-C15-C14	13.79	152.91	123.46
24	A	848	BCR	C16-C15-C14	14.04	153.42	123.46
24	A	848	BCR	C11-C10-C9	14.06	147.38	127.31
24	2	849	BCR	C11-C10-C9	14.19	147.57	127.31
24	a	843	BCR	C16-C15-C14	14.23	153.83	123.46
24	i	101	BCR	C16-C15-C14	14.33	154.06	123.46
24	1	849	BCR	C16-C15-C14	14.80	155.06	123.46
24	a	844	BCR	C16-C15-C14	14.91	155.29	123.46
24	b	1850	BCR	C16-C15-C14	15.59	156.75	123.46
24	a	848	BCR	C16-C15-C14	16.01	157.64	123.46

All (798) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1	813	CLA	NC
21	1	813	CLA	ND
21	1	813	CLA	NA
21	A	855	CLA	NC
21	A	855	CLA	ND
21	A	855	CLA	NA
21	2	825	CLA	NC
21	2	825	CLA	ND
21	2	825	CLA	NA
21	1	837	CLA	NC
21	1	837	CLA	ND
21	1	837	CLA	NA
21	2	806	CLA	NC
21	2	806	CLA	ND
21	2	806	CLA	NA
21	1	828	CLA	NC
21	1	828	CLA	ND
21	1	828	CLA	NA
21	a	816	CLA	NC
21	a	816	CLA	ND
21	a	816	CLA	NA
21	a	833	CLA	NC
21	a	833	CLA	NA
21	2	835	CLA	NC
21	2	835	CLA	ND
21	2	835	CLA	NA
21	A	826	CLA	NC
21	A	826	CLA	NA

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Mol	Chain	Res	Type	Atom
21	1	805	CLA	ND
21	1	805	CLA	NA
21	A	807	CLA	NC
21	A	807	CLA	ND
21	A	807	CLA	NA
21	b	1805	CLA	NC
21	b	1805	CLA	ND
21	b	1805	CLA	NA
21	b	1836	CLA	NC
21	b	1836	CLA	ND
21	b	1836	CLA	NA
21	1	806	CLA	NC
21	1	806	CLA	ND
21	1	806	CLA	NA
21	J	1106	CLA	NC
21	J	1106	CLA	ND
21	J	1106	CLA	NA
21	a	810	CLA	NC
21	a	810	CLA	ND
21	a	810	CLA	NA
21	A	832	CLA	NC
21	A	832	CLA	ND
21	A	832	CLA	NA
21	1	819	CLA	NC
21	1	819	CLA	ND
21	1	819	CLA	NA
21	2	837	CLA	NC
21	2	837	CLA	ND
21	2	837	CLA	NA
21	a	819	CLA	NC
21	a	819	CLA	ND
21	a	819	CLA	NA
21	A	835	CLA	NA
21	2	820	CLA	NC
21	2	820	CLA	ND
21	2	820	CLA	NA
21	B	804	CLA	NC
21	B	804	CLA	ND
21	B	804	CLA	NA
21	K	103	CLA	NA
21	7	1105	CLA	NC
21	7	1105	CLA	ND

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Mol	Chain	Res	Type	Atom
21	7	1105	CLA	NA
21	F	202	CLA	NC
21	F	202	CLA	ND
21	F	202	CLA	NA
21	a	824	CLA	NC
21	a	824	CLA	ND
21	a	824	CLA	NA
21	A	809	CLA	NC
21	A	809	CLA	ND
21	A	809	CLA	NA
21	2	810	CLA	NC
21	2	810	CLA	ND
21	2	810	CLA	NA
21	b	1829	CLA	ND
21	b	1829	CLA	NA
21	2	842	CLA	NC
21	2	842	CLA	NA
21	a	823	CLA	NC
21	a	823	CLA	ND
21	a	823	CLA	NA
21	B	827	CLA	NC
21	B	827	CLA	ND
21	B	827	CLA	NA
21	2	841	CLA	NC
21	2	841	CLA	ND
21	2	841	CLA	NA
21	b	1826	CLA	NC
21	b	1826	CLA	ND
21	b	1826	CLA	NA
21	1	833	CLA	NC
21	1	833	CLA	ND
21	1	833	CLA	NA
21	1	830	CLA	NC
21	1	830	CLA	ND
21	1	830	CLA	NA
21	B	816	CLA	NC
21	B	816	CLA	ND
21	B	816	CLA	NA
21	A	854	CLA	NA
21	A	854	CLA	ND
21	b	1828	CLA	NC
21	b	1828	CLA	ND

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Mol	Chain	Res	Type	Atom
21	b	1828	CLA	NA
21	b	1813	CLA	NC
21	b	1813	CLA	NA
21	B	839	CLA	NC
21	B	839	CLA	ND
21	B	839	CLA	NA
21	A	838	CLA	NC
21	A	838	CLA	ND
21	A	838	CLA	NA
21	2	809	CLA	NC
21	2	809	CLA	ND
21	2	809	CLA	NA
21	J	1105	CLA	NC
21	J	1105	CLA	ND
21	J	1105	CLA	NA
21	B	818	CLA	NC
21	B	818	CLA	ND
21	B	818	CLA	NA
21	b	1804	CLA	NC
21	b	1804	CLA	ND
21	b	1804	CLA	NA
21	B	824	CLA	NC
21	B	824	CLA	ND
21	B	824	CLA	NA
21	a	825	CLA	ND
21	a	825	CLA	NA
21	A	827	CLA	NC
21	A	827	CLA	ND
21	A	827	CLA	NA
21	b	1814	CLA	NC
21	b	1814	CLA	ND
21	b	1814	CLA	NA
21	2	807	CLA	ND
21	2	807	CLA	NA
21	a	829	CLA	NC
21	a	829	CLA	ND
21	a	829	CLA	NA
21	A	817	CLA	NC
21	A	817	CLA	ND
21	A	817	CLA	NA
21	A	828	CLA	NC
21	A	828	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	828	CLA	NA
21	k	1401	CLA	NC
21	k	1401	CLA	ND
21	k	1401	CLA	NA
21	1	808	CLA	NC
21	1	808	CLA	ND
21	1	808	CLA	NA
21	a	809	CLA	NC
21	a	809	CLA	ND
21	a	809	CLA	NA
21	7	1103	CLA	NC
21	7	1103	CLA	ND
21	7	1103	CLA	NA
21	b	1822	CLA	NC
21	b	1822	CLA	ND
21	b	1822	CLA	NA
21	A	818	CLA	NC
21	A	818	CLA	ND
21	A	818	CLA	NA
21	B	825	CLA	NC
21	B	825	CLA	ND
21	B	825	CLA	NA
21	1	818	CLA	NC
21	1	818	CLA	ND
21	1	818	CLA	NA
21	L	205	CLA	NC
21	L	205	CLA	NA
21	B	808	CLA	ND
21	B	808	CLA	NA
21	B	819	CLA	NC
21	B	819	CLA	ND
21	B	819	CLA	NA
21	A	824	CLA	ND
21	A	824	CLA	NA
21	b	1811	CLA	NC
21	b	1811	CLA	NA
21	b	1811	CLA	ND
21	J	1103	CLA	NC
21	J	1103	CLA	ND
21	J	1103	CLA	NA
21	b	1820	CLA	NC
21	b	1820	CLA	ND

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Mol	Chain	Res	Type	Atom
21	b	1820	CLA	NA
21	B	826	CLA	NC
21	B	826	CLA	ND
21	B	826	CLA	NA
21	6	203	CLA	NC
21	6	203	CLA	ND
21	6	203	CLA	NA
21	b	1808	CLA	ND
21	b	1808	CLA	NA
21	a	856	CLA	NC
21	a	856	CLA	ND
21	a	856	CLA	NA
21	b	1807	CLA	NC
21	b	1807	CLA	ND
21	b	1807	CLA	NA
21	a	837	CLA	NC
21	a	837	CLA	ND
21	a	837	CLA	NA
21	1	810	CLA	NC
21	1	810	CLA	ND
21	1	810	CLA	NA
21	b	1835	CLA	NC
21	b	1835	CLA	ND
21	b	1835	CLA	NA
21	A	834	CLA	NC
21	A	834	CLA	ND
21	A	834	CLA	NA
21	2	827	CLA	NC
21	2	827	CLA	ND
21	2	827	CLA	NA
21	A	811	CLA	NC
21	A	811	CLA	ND
21	A	811	CLA	NA
21	A	801	CLA	NC
21	A	801	CLA	ND
21	A	801	CLA	NA
21	B	805	CLA	NC
21	B	805	CLA	ND
21	B	805	CLA	NA
21	2	815	CLA	NC
21	2	815	CLA	NA
21	B	817	CLA	NC

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Mol	Chain	Res	Type	Atom
21	B	817	CLA	ND
21	B	817	CLA	NA
21	a	805	CLA	ND
21	a	805	CLA	NA
21	8	1402	CLA	NC
21	8	1402	CLA	ND
21	8	1402	CLA	NA
21	B	811	CLA	NC
21	B	811	CLA	ND
21	B	811	CLA	NA
21	b	1840	CLA	NC
21	b	1840	CLA	ND
21	b	1840	CLA	NA
21	B	821	CLA	NC
21	B	821	CLA	ND
21	B	821	CLA	NA
21	j	1101	CLA	NC
21	j	1101	CLA	NA
21	2	839	CLA	NC
21	2	839	CLA	ND
21	2	839	CLA	NA
21	B	832	CLA	NC
21	B	832	CLA	ND
21	B	832	CLA	NA
21	A	803	CLA	NC
21	A	803	CLA	ND
21	A	803	CLA	NA
21	b	1819	CLA	NC
21	b	1819	CLA	ND
21	b	1819	CLA	NA
21	A	823	CLA	NC
21	A	823	CLA	ND
21	A	823	CLA	NA
21	A	825	CLA	NC
21	A	825	CLA	ND
21	A	825	CLA	NA
21	1	815	CLA	NC
21	1	815	CLA	ND
21	1	815	CLA	NA
21	2	831	CLA	NC
21	2	831	CLA	ND
21	2	831	CLA	NA

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Mol	Chain	Res	Type	Atom
21	B	814	CLA	NC
21	B	814	CLA	ND
21	B	814	CLA	NA
21	a	838	CLA	NC
21	a	838	CLA	ND
21	a	838	CLA	NA
21	a	815	CLA	NC
21	a	815	CLA	ND
21	a	815	CLA	NA
21	2	802	CLA	NC
21	2	802	CLA	ND
21	2	802	CLA	NA
21	l	201	CLA	NC
21	l	201	CLA	ND
21	l	201	CLA	NA
21	K	102	CLA	NC
21	K	102	CLA	ND
21	K	102	CLA	NA
21	1	836	CLA	NA
21	1	839	CLA	NC
21	1	839	CLA	ND
21	1	839	CLA	NA
21	a	807	CLA	NC
21	a	807	CLA	ND
21	a	807	CLA	NA
21	B	807	CLA	ND
21	B	807	CLA	NA
21	A	839	CLA	NC
21	A	839	CLA	ND
21	A	839	CLA	NA
21	b	1833	CLA	NC
21	b	1833	CLA	ND
21	b	1833	CLA	NA
21	B	806	CLA	ND
21	B	806	CLA	NA
21	b	1809	CLA	NC
21	b	1809	CLA	ND
21	b	1809	CLA	NA
21	7	1101	CLA	NA
21	2	833	CLA	NC
21	2	833	CLA	ND
21	2	833	CLA	NA

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Mol	Chain	Res	Type	Atom
21	b	1817	CLA	NC
21	b	1817	CLA	ND
21	b	1817	CLA	NA
21	a	832	CLA	NC
21	a	832	CLA	ND
21	a	832	CLA	NA
21	B	812	CLA	NC
21	B	812	CLA	NA
21	1	814	CLA	NC
21	1	814	CLA	ND
21	1	814	CLA	NA
21	k	1402	CLA	NC
21	k	1402	CLA	ND
21	k	1402	CLA	NA
21	m	103	CLA	NC
21	m	103	CLA	ND
21	m	103	CLA	NA
21	A	805	CLA	ND
21	A	805	CLA	NA
21	b	1806	CLA	NC
21	b	1806	CLA	ND
21	b	1806	CLA	NA
21	1	817	CLA	NC
21	1	817	CLA	ND
21	1	817	CLA	NA
21	1	802	CLA	NC
21	1	802	CLA	ND
21	1	802	CLA	NA
21	2	813	CLA	NC
21	2	813	CLA	ND
21	2	813	CLA	NA
21	a	840	CLA	NC
21	a	840	CLA	ND
21	a	840	CLA	NA
21	a	820	CLA	NC
21	a	820	CLA	ND
21	a	820	CLA	NA
21	B	831	CLA	NC
21	B	831	CLA	ND
21	B	831	CLA	NA
21	1	829	CLA	NC
21	1	829	CLA	ND

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Mol	Chain	Res	Type	Atom
21	1	829	CLA	NA
21	A	833	CLA	NC
21	A	833	CLA	ND
21	A	833	CLA	NA
21	2	814	CLA	NA
21	A	808	CLA	NC
21	A	808	CLA	ND
21	A	808	CLA	NA
21	1	816	CLA	NC
21	1	816	CLA	ND
21	1	816	CLA	NA
21	B	838	CLA	NC
21	B	838	CLA	ND
21	B	838	CLA	NA
21	A	814	CLA	NC
21	A	814	CLA	ND
21	A	814	CLA	NA
21	b	1810	CLA	NC
21	b	1810	CLA	ND
21	b	1810	CLA	NA
21	b	1801	CLA	NC
21	b	1801	CLA	ND
21	b	1801	CLA	NA
21	b	1837	CLA	NC
21	b	1837	CLA	ND
21	b	1837	CLA	NA
21	2	830	CLA	NC
21	2	830	CLA	ND
21	2	830	CLA	NA
21	B	802	CLA	NC
21	B	802	CLA	ND
21	B	802	CLA	NA
21	a	835	CLA	ND
21	a	835	CLA	NA
21	A	812	CLA	NC
21	A	812	CLA	ND
21	A	812	CLA	NA
21	A	813	CLA	NC
21	A	813	CLA	ND
21	A	813	CLA	NA
21	B	829	CLA	NC
21	B	829	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	829	CLA	NA
21	B	823	CLA	NC
21	B	823	CLA	ND
21	B	823	CLA	NA
21	b	1843	CLA	NC
21	b	1843	CLA	ND
21	b	1843	CLA	NA
21	a	834	CLA	NC
21	a	834	CLA	ND
21	a	834	CLA	NA
21	1	823	CLA	NC
21	1	823	CLA	ND
21	1	823	CLA	NA
21	1	807	CLA	NC
21	1	807	CLA	ND
21	1	807	CLA	NA
21	1	820	CLA	NC
21	1	820	CLA	ND
21	1	820	CLA	NA
21	1	825	CLA	NA
21	2	817	CLA	NC
21	2	817	CLA	ND
21	2	817	CLA	NA
21	2	818	CLA	NC
21	2	818	CLA	ND
21	2	818	CLA	NA
21	A	819	CLA	NC
21	A	819	CLA	ND
21	A	819	CLA	NA
21	B	809	CLA	NC
21	B	809	CLA	NA
21	B	809	CLA	ND
21	A	804	CLA	NC
21	A	804	CLA	ND
21	A	804	CLA	NA
21	a	827	CLA	NC
21	a	827	CLA	ND
21	a	827	CLA	NA
21	2	822	CLA	NC
21	2	822	CLA	ND
21	2	822	CLA	NA
21	b	1839	CLA	NC

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Mol	Chain	Res	Type	Atom
21	b	1839	CLA	ND
21	b	1839	CLA	NA
21	a	802	CLA	NC
21	a	802	CLA	ND
21	a	802	CLA	NA
21	1	821	CLA	NC
21	1	821	CLA	ND
21	1	821	CLA	NA
21	1	838	CLA	NC
21	1	838	CLA	ND
21	1	838	CLA	NA
21	A	830	CLA	NC
21	A	830	CLA	NA
21	6	204	CLA	NC
21	6	204	CLA	ND
21	6	204	CLA	NA
21	2	836	CLA	ND
21	2	836	CLA	NA
21	a	812	CLA	NC
21	a	812	CLA	ND
21	a	812	CLA	NA
21	B	836	CLA	NC
21	B	836	CLA	ND
21	B	836	CLA	NA
21	B	840	CLA	NC
21	B	840	CLA	ND
21	B	840	CLA	NA
21	0	201	CLA	NC
21	0	201	CLA	ND
21	0	201	CLA	NA
21	2	829	CLA	NC
21	2	829	CLA	ND
21	2	829	CLA	NA
21	b	1823	CLA	NC
21	b	1823	CLA	ND
21	b	1823	CLA	NA
21	A	815	CLA	NC
21	A	815	CLA	ND
21	A	815	CLA	NA
21	2	808	CLA	NC
21	2	808	CLA	ND
21	2	808	CLA	NA

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Mol	Chain	Res	Type	Atom
21	6	201	CLA	NC
21	6	201	CLA	ND
21	6	201	CLA	NA
21	a	855	CLA	NC
21	a	855	CLA	ND
21	a	855	CLA	NA
21	2	826	CLA	NC
21	2	826	CLA	ND
21	2	826	CLA	NA
21	F	203	CLA	NC
21	F	203	CLA	ND
21	F	203	CLA	NA
21	a	831	CLA	NC
21	a	831	CLA	ND
21	a	831	CLA	NA
21	1	840	CLA	NC
21	1	840	CLA	ND
21	1	840	CLA	NA
21	A	837	CLA	NC
21	A	837	CLA	ND
21	A	837	CLA	NA
21	l	204	CLA	NC
21	l	204	CLA	ND
21	l	204	CLA	NA
21	1	824	CLA	NC
21	1	824	CLA	ND
21	1	824	CLA	NA
21	B	828	CLA	NC
21	B	828	CLA	ND
21	B	828	CLA	NA
21	b	1841	CLA	NC
21	b	1841	CLA	ND
21	b	1841	CLA	NA
21	b	1842	CLA	NC
21	b	1842	CLA	ND
21	b	1842	CLA	NA
21	2	832	CLA	NC
21	2	832	CLA	ND
21	2	832	CLA	NA
21	b	1821	CLA	NC
21	b	1821	CLA	ND
21	b	1821	CLA	NA

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Mol	Chain	Res	Type	Atom
21	2	816	CLA	NC
21	2	816	CLA	ND
21	2	816	CLA	NA
21	0	203	CLA	NC
21	0	203	CLA	ND
21	0	203	CLA	NA
21	a	822	CLA	NC
21	a	822	CLA	NA
21	2	824	CLA	NC
21	2	824	CLA	NA
21	2	819	CLA	NC
21	2	819	CLA	ND
21	2	819	CLA	NA
21	b	1834	CLA	NC
21	b	1834	CLA	ND
21	b	1834	CLA	NA
21	1	834	CLA	NC
21	1	834	CLA	ND
21	1	834	CLA	NA
21	J	1101	CLA	NA
21	j	1103	CLA	NC
21	j	1103	CLA	ND
21	j	1103	CLA	NA
21	a	817	CLA	NC
21	a	817	CLA	NA
21	b	1827	CLA	NC
21	b	1827	CLA	ND
21	b	1827	CLA	NA
21	a	821	CLA	NC
21	a	821	CLA	ND
21	a	821	CLA	NA
21	l	203	CLA	NC
21	l	203	CLA	ND
21	l	203	CLA	NA
21	b	1824	CLA	NC
21	b	1824	CLA	ND
21	b	1824	CLA	NA
21	2	838	CLA	NC
21	2	838	CLA	ND
21	2	838	CLA	NA
21	b	1815	CLA	NC
21	b	1815	CLA	NA

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Mol	Chain	Res	Type	Atom
21	2	803	CLA	NA
21	2	803	CLA	ND
21	f	202	CLA	NC
21	f	202	CLA	ND
21	f	202	CLA	NA
21	b	1816	CLA	NC
21	b	1816	CLA	NA
21	a	801	CLA	NC
21	a	801	CLA	ND
21	a	801	CLA	NA
21	2	804	CLA	NC
21	2	804	CLA	ND
21	2	804	CLA	NA
21	b	1832	CLA	NC
21	b	1832	CLA	ND
21	b	1832	CLA	NA
21	b	1838	CLA	NC
21	b	1838	CLA	ND
21	b	1838	CLA	NA
21	B	835	CLA	NA
21	B	834	CLA	NC
21	B	834	CLA	ND
21	B	834	CLA	NA
21	j	1105	CLA	NC
21	j	1105	CLA	ND
21	j	1105	CLA	NA
21	2	821	CLA	NC
21	2	821	CLA	NA
21	2	821	CLA	ND
21	2	812	CLA	NC
21	2	812	CLA	NA
21	B	830	CLA	NC
21	B	830	CLA	NA
21	2	811	CLA	NC
21	2	811	CLA	ND
21	2	811	CLA	NA
21	7	1104	CLA	ND
21	7	1104	CLA	NA
21	a	818	CLA	ND
21	a	818	CLA	NA
21	1	812	CLA	NC
21	1	812	CLA	ND

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Mol	Chain	Res	Type	Atom
21	1	812	CLA	NA
21	B	822	CLA	NC
21	B	822	CLA	NA
21	B	813	CLA	NC
21	B	813	CLA	NA
21	a	839	CLA	NC
21	a	839	CLA	ND
21	a	839	CLA	NA
21	A	829	CLA	NC
21	A	829	CLA	ND
21	A	829	CLA	NA
21	A	836	CLA	NC
21	A	836	CLA	ND
21	A	836	CLA	NA
21	1	826	CLA	NC
21	1	826	CLA	ND
21	1	826	CLA	NA
21	b	1825	CLA	NC
21	b	1825	CLA	ND
21	b	1825	CLA	NA
21	1	827	CLA	NC
21	1	827	CLA	ND
21	1	827	CLA	NA
21	2	840	CLA	NC
21	2	840	CLA	ND
21	2	840	CLA	NA
21	1	803	CLA	NC
21	1	803	CLA	ND
21	1	803	CLA	NA
21	1	832	CLA	NC
21	1	832	CLA	ND
21	1	832	CLA	NA
21	1	855	CLA	NC
21	1	855	CLA	ND
21	1	855	CLA	NA
21	L	204	CLA	NC
21	L	204	CLA	ND
21	L	204	CLA	NA
21	1	835	CLA	NC
21	1	835	CLA	ND
21	1	835	CLA	NA
21	B	820	CLA	NC

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Mol	Chain	Res	Type	Atom
21	B	820	CLA	ND
21	B	820	CLA	NA
21	A	822	CLA	NC
21	A	822	CLA	ND
21	A	822	CLA	NA
21	L	203	CLA	NC
21	L	203	CLA	ND
21	L	203	CLA	NA
21	A	806	CLA	NC
21	A	806	CLA	ND
21	A	806	CLA	NA
21	f	203	CLA	NC
21	f	203	CLA	ND
21	f	203	CLA	NA
21	A	831	CLA	NC
21	A	831	CLA	ND
21	A	831	CLA	NA
21	1	822	CLA	NC
21	1	822	CLA	ND
21	1	822	CLA	NA
21	1	811	CLA	NC
21	1	811	CLA	ND
21	1	811	CLA	NA
21	a	804	CLA	NC
21	a	804	CLA	ND
21	a	804	CLA	NA
21	b	1818	CLA	NC
21	b	1818	CLA	NA
21	a	814	CLA	NC
21	a	814	CLA	ND
21	a	814	CLA	NA
21	a	803	CLA	ND
21	a	803	CLA	NA
21	8	1401	CLA	NC
21	8	1401	CLA	ND
21	8	1401	CLA	NA
21	j	1104	CLA	NC
21	j	1104	CLA	ND
21	j	1104	CLA	NA
21	B	815	CLA	NC
21	B	815	CLA	ND
21	B	815	CLA	NA

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Mol	Chain	Res	Type	Atom
21	2	805	CLA	NC
21	2	805	CLA	ND
21	2	805	CLA	NA
21	A	821	CLA	NC
21	A	821	CLA	ND
21	A	821	CLA	NA
21	A	840	CLA	NC
21	A	840	CLA	ND
21	A	840	CLA	NA
21	1	801	CLA	NC
21	1	801	CLA	ND
21	1	801	CLA	NA
21	A	810	CLA	NC
21	A	810	CLA	ND
21	A	810	CLA	NA
21	a	806	CLA	NC
21	a	806	CLA	ND
21	a	806	CLA	NA
21	a	811	CLA	NC
21	a	811	CLA	ND
21	a	811	CLA	NA
21	1	809	CLA	NC
21	1	809	CLA	ND
21	1	809	CLA	NA
21	b	1830	CLA	NC
21	b	1830	CLA	ND
21	b	1830	CLA	NA
21	1	804	CLA	NC
21	1	804	CLA	ND
21	1	804	CLA	NA
21	A	820	CLA	NC
21	A	820	CLA	ND
21	A	820	CLA	NA
21	B	837	CLA	NC
21	B	837	CLA	ND
21	B	837	CLA	NA
21	a	808	CLA	NC
21	a	808	CLA	ND
21	a	808	CLA	NA
21	2	823	CLA	NC
21	2	823	CLA	ND
21	2	823	CLA	NA

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Mol	Chain	Res	Type	Atom
21	a	826	CLA	NC
21	a	826	CLA	ND
21	a	826	CLA	NA
21	a	836	CLA	NC
21	a	836	CLA	ND
21	a	836	CLA	NA
21	B	801	CLA	NC
21	B	801	CLA	ND
21	B	801	CLA	NA
21	B	833	CLA	NA
21	a	830	CLA	NC
21	a	830	CLA	ND
21	a	830	CLA	NA
21	A	816	CLA	NC
21	A	816	CLA	ND
21	A	816	CLA	NA
21	a	813	CLA	NC
21	a	813	CLA	ND
21	a	813	CLA	NA
21	1	841	CLA	NC
21	1	841	CLA	ND
21	1	841	CLA	NA
21	b	1831	CLA	NC
21	b	1831	CLA	ND
21	b	1831	CLA	NA
21	2	834	CLA	NC
21	2	834	CLA	ND
21	2	834	CLA	NA
21	B	810	CLA	NC
21	B	810	CLA	ND
21	B	810	CLA	NA
21	2	828	CLA	NC
21	2	828	CLA	NA
21	1	831	CLA	NC
21	1	831	CLA	ND
21	1	831	CLA	NA
21	b	1812	CLA	NC
21	b	1812	CLA	ND
21	b	1812	CLA	NA
21	A	802	CLA	NC
21	A	802	CLA	ND
21	A	802	CLA	NA

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Mol	Chain	Res	Type	Atom
21	l	205	CLA	NC
21	l	205	CLA	ND
21	l	205	CLA	NA
21	0	202	CLA	NC
21	0	202	CLA	ND
21	0	202	CLA	NA
21	I	101	CLA	NC
21	I	101	CLA	NA
21	a	828	CLA	NC
21	a	828	CLA	NA
21	a	828	CLA	ND
21	B	803	CLA	NC
21	B	803	CLA	ND
21	B	803	CLA	NA

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	h	101	BCR	C11-C10-C9-C34
24	h	101	BCR	C11-C10-C9-C8
24	6	202	BCR	C11-C10-C9-C8
24	6	202	BCR	C11-C10-C9-C34
24	2	848	BCR	C11-C10-C9-C8
24	2	848	BCR	C11-C10-C9-C34
24	i	101	BCR	C11-C10-C9-C8
24	1	858	BCR	C11-C10-C9-C8
24	b	1849	BCR	C11-C10-C9-C8
24	i	101	BCR	C11-C10-C9-C34
24	9	102	BCR	C10-C11-C12-C13
24	b	1849	BCR	C11-C10-C9-C34
24	1	858	BCR	C11-C10-C9-C34
24	6	205	BCR	C10-C11-C12-C13
24	f	204	BCR	C10-C11-C12-C13
26	K	105	LMG	C7-O1-C1-O6
25	B	851	LHG	C5-O7-C7-C8
25	a	853	LHG	C5-O7-C7-O9
25	a	853	LHG	C5-O7-C7-C8
26	K	101	LMG	C8-O7-C10-O9
26	K	101	LMG	C8-O7-C10-C11
25	b	1803	LHG	C5-O7-C7-O9
25	M	7003	LHG	C5-O7-C7-O9
25	b	1803	LHG	C5-O7-C7-C8

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Mol	Chain	Res	Type	Atoms
25	M	7003	LHG	C5-O7-C7-C8

There are no ring outliers.

274 monomers are involved in 1402 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	0	201	CLA	6	0
21	0	202	CLA	8	0
21	0	203	CLA	7	0
24	0	204	BCR	2	0
24	0	205	BCR	6	0
26	0	206	LMG	4	0
31	0	207	SQD	2	0
35	0	208	LMT	4	0
21	1	801	CLA	3	0
21	1	802	CLA	6	0
21	1	803	CLA	6	0
21	1	804	CLA	5	0
21	1	805	CLA	8	0
21	1	806	CLA	4	0
21	1	807	CLA	4	0
21	1	808	CLA	4	0
21	1	809	CLA	9	0
21	1	810	CLA	2	0
21	1	811	CLA	8	0
21	1	812	CLA	3	0
21	1	813	CLA	17	0
21	1	814	CLA	1	0
21	1	815	CLA	2	0
21	1	817	CLA	4	0
21	1	818	CLA	10	0
21	1	819	CLA	5	0
21	1	820	CLA	6	0
21	1	821	CLA	9	0
21	1	822	CLA	2	0
21	1	823	CLA	4	0
21	1	824	CLA	5	0
21	1	825	CLA	5	0
21	1	826	CLA	3	0
21	1	827	CLA	5	0
21	1	828	CLA	12	0
21	1	829	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	830	CLA	10	0
21	1	831	CLA	5	0
21	1	832	CLA	3	0
21	1	833	CLA	6	0
21	1	834	CLA	5	0
21	1	835	CLA	6	0
21	1	836	CLA	7	0
21	1	837	CLA	6	0
21	1	838	CLA	3	0
21	1	839	CLA	6	0
21	1	840	CLA	7	0
21	1	841	CLA	5	0
22	1	842	PQN	5	0
24	1	844	BCR	7	0
24	1	845	BCR	6	0
24	1	846	BCR	7	0
24	1	847	BCR	6	0
24	1	848	BCR	3	0
24	1	849	BCR	2	0
25	1	850	LHG	4	0
26	1	851	LMG	1	0
25	1	852	LHG	3	0
26	1	853	LMG	4	0
21	1	855	CLA	8	0
24	1	856	BCR	7	0
24	1	858	BCR	5	0
25	2	801	LHG	3	0
21	2	802	CLA	4	0
21	2	803	CLA	14	0
21	2	804	CLA	7	0
21	2	805	CLA	8	0
21	2	806	CLA	7	0
21	2	807	CLA	6	0
21	2	808	CLA	13	0
21	2	809	CLA	6	0
21	2	810	CLA	12	0
21	2	811	CLA	8	0
21	2	812	CLA	1	0
21	2	813	CLA	4	0
21	2	814	CLA	1	0
21	2	815	CLA	7	0
21	2	816	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	817	CLA	2	0
21	2	818	CLA	3	0
21	2	819	CLA	8	0
21	2	820	CLA	4	0
21	2	821	CLA	6	0
21	2	822	CLA	1	0
21	2	823	CLA	5	0
21	2	824	CLA	3	0
21	2	825	CLA	3	0
21	2	826	CLA	10	0
21	2	827	CLA	9	0
21	2	828	CLA	5	0
21	2	829	CLA	6	0
21	2	830	CLA	8	0
21	2	831	CLA	5	0
21	2	832	CLA	6	0
21	2	833	CLA	7	0
21	2	834	CLA	8	0
21	2	835	CLA	2	0
21	2	836	CLA	1	0
21	2	837	CLA	5	0
21	2	838	CLA	3	0
21	2	839	CLA	7	0
21	2	840	CLA	4	0
21	2	841	CLA	5	0
21	2	842	CLA	3	0
22	2	843	PQN	4	0
24	2	844	BCR	1	0
24	2	845	BCR	6	0
30	2	846	ECH	2	0
24	2	847	BCR	7	0
24	2	848	BCR	9	0
24	2	849	BCR	4	0
26	2	850	LMG	6	0
25	2	851	LHG	6	0
26	2	852	LMG	5	0
28	2	854	45D	8	0
23	3	102	SF4	1	0
21	6	201	CLA	8	0
24	6	202	BCR	7	0
21	6	203	CLA	6	0
21	6	204	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	6	205	BCR	1	0
25	6	206	LHG	1	0
21	7	1101	CLA	10	0
24	7	1102	BCR	7	0
21	7	1103	CLA	4	0
21	7	1104	CLA	1	0
21	7	1105	CLA	1	0
21	8	1401	CLA	5	0
21	8	1402	CLA	2	0
24	8	1403	BCR	3	0
25	9	101	LHG	4	0
24	9	102	BCR	5	0
21	A	801	CLA	10	0
21	A	802	CLA	13	0
21	A	803	CLA	7	0
21	A	804	CLA	15	0
21	A	805	CLA	14	0
21	A	806	CLA	12	0
21	A	807	CLA	11	0
21	A	808	CLA	15	0
21	A	809	CLA	7	0
21	A	810	CLA	13	0
21	A	811	CLA	12	0
21	A	812	CLA	7	0
21	A	813	CLA	21	0
21	A	814	CLA	8	0
21	A	815	CLA	4	0
21	A	816	CLA	4	0
21	A	817	CLA	11	0
21	A	818	CLA	11	0
21	A	819	CLA	19	0
21	A	820	CLA	15	0
21	A	821	CLA	11	0
21	A	822	CLA	5	0
21	A	823	CLA	9	0
21	A	824	CLA	13	0
21	A	825	CLA	16	0
21	A	826	CLA	9	0
21	A	827	CLA	19	0
21	A	828	CLA	18	0
21	A	829	CLA	18	0
21	A	830	CLA	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	831	CLA	15	0
21	A	832	CLA	4	0
21	A	833	CLA	17	0
21	A	834	CLA	10	0
21	A	835	CLA	22	0
21	A	836	CLA	14	0
21	A	837	CLA	14	0
21	A	838	CLA	9	0
21	A	839	CLA	13	0
21	A	840	CLA	11	0
22	A	841	PQN	7	0
24	A	843	BCR	11	0
24	A	844	BCR	14	0
24	A	845	BCR	6	0
24	A	846	BCR	9	0
24	A	847	BCR	9	0
24	A	848	BCR	5	0
25	A	849	LHG	10	0
26	A	850	LMG	9	0
25	A	851	LHG	14	0
26	A	852	LMG	4	0
27	A	853	ACT	1	0
21	A	854	CLA	10	0
21	A	855	CLA	7	0
28	A	856	45D	5	0
21	B	801	CLA	5	0
21	B	802	CLA	6	0
21	B	803	CLA	6	0
21	B	804	CLA	7	0
21	B	805	CLA	6	0
21	B	806	CLA	2	0
21	B	807	CLA	10	0
21	B	808	CLA	6	0
21	B	809	CLA	12	0
21	B	810	CLA	7	0
21	B	811	CLA	3	0
21	B	812	CLA	5	0
21	B	813	CLA	5	0
21	B	814	CLA	6	0
21	B	815	CLA	6	0
21	B	816	CLA	9	0
21	B	817	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	818	CLA	5	0
21	B	819	CLA	9	0
21	B	820	CLA	9	0
21	B	821	CLA	4	0
21	B	822	CLA	8	0
21	B	823	CLA	6	0
21	B	824	CLA	9	0
21	B	825	CLA	11	0
21	B	826	CLA	6	0
21	B	827	CLA	13	0
21	B	828	CLA	11	0
21	B	829	CLA	6	0
21	B	830	CLA	8	0
21	B	831	CLA	4	0
21	B	832	CLA	5	0
21	B	833	CLA	4	0
21	B	834	CLA	2	0
21	B	835	CLA	11	0
21	B	836	CLA	7	0
21	B	837	CLA	10	0
21	B	838	CLA	3	0
21	B	839	CLA	5	0
21	B	840	CLA	7	0
22	B	841	PQN	2	0
24	B	842	BCR	6	0
24	B	843	BCR	6	0
30	B	844	ECH	3	0
24	B	845	BCR	8	0
24	B	846	BCR	10	0
24	B	847	BCR	9	0
26	B	848	LMG	7	0
25	B	849	LHG	9	0
26	B	850	LMG	2	0
25	B	851	LHG	3	0
31	B	852	SQD	6	0
25	B	855	LHG	2	0
25	B	857	LHG	1	0
25	B	858	LHG	4	0
23	C	101	SF4	1	0
23	C	102	SF4	5	0
24	F	201	BCR	7	0
21	F	202	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	203	CLA	6	0
31	F	205	SQD	9	0
21	I	101	CLA	10	0
24	I	102	BCR	6	0
25	I	103	LHG	6	0
25	I	104	LHG	2	0
21	J	1101	CLA	18	0
24	J	1102	BCR	15	0
21	J	1103	CLA	12	0
21	J	1105	CLA	4	0
21	J	1106	CLA	1	0
24	J	1107	BCR	7	0
26	K	101	LMG	6	0
21	K	102	CLA	8	0
21	K	103	CLA	5	0
24	K	104	BCR	4	0
26	K	105	LMG	10	0
21	L	203	CLA	11	0
21	L	204	CLA	13	0
21	L	205	CLA	10	0
24	L	206	BCR	5	0
24	L	207	BCR	8	0
31	L	208	SQD	3	0
37	L	209	DGD	5	0
25	L	210	LHG	5	0
35	L	211	LMT	2	0
30	M	7002	ECH	2	0
25	M	7003	LHG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	751/751 (100%)	-0.19	20 (2%) 55 58	29, 47, 72, 134	0
1	a	751/751 (100%)	0.97	139 (18%) 1 1	48, 95, 149, 209	0
2	2	731/731 (100%)	0.85	131 (17%) 2 1	43, 101, 146, 169	0
2	B	731/731 (100%)	0.06	42 (5%) 24 25	29, 56, 90, 152	0
3	3	80/80 (100%)	1.51	23 (28%) 1 0	54, 84, 110, 119	0
3	C	80/80 (100%)	-0.47	1 (1%) 77 78	33, 45, 59, 81	0
4	D	141/141 (100%)	-0.25	7 (4%) 30 31	30, 44, 70, 120	0
4	d	141/141 (100%)	0.81	27 (19%) 1 1	56, 82, 106, 136	0
5	5	69/69 (100%)	1.53	16 (23%) 1 0	75, 109, 122, 128	0
5	E	69/69 (100%)	0.59	10 (14%) 3 2	45, 62, 91, 97	0
6	6	143/143 (100%)	2.12	61 (42%) 0 0	114, 141, 158, 189	0
6	F	143/143 (100%)	-0.03	7 (4%) 30 32	56, 78, 94, 130	0
6	f	143/143 (100%)	0.86	27 (18%) 1 1	60, 97, 112, 132	0
7	I	40/40 (100%)	-0.02	0 100 100	36, 49, 87, 107	0
7	i	40/40 (100%)	0.48	3 (7%) 15 15	41, 49, 103, 132	0
8	7	40/40 (100%)	1.28	13 (32%) 0 0	109, 128, 152, 165	0
8	J	40/40 (100%)	-0.13	2 (5%) 30 31	54, 69, 95, 101	0
8	j	40/40 (100%)	0.81	8 (20%) 1 1	87, 98, 117, 132	0
9	K	80/80 (100%)	1.71	27 (33%) 0 0	53, 72, 127, 146	38 (47%)
10	L	157/157 (100%)	-0.03	6 (3%) 41 43	36, 43, 64, 131	0
10	l	157/157 (100%)	0.36	14 (8%) 10 10	45, 60, 107, 184	0
11	9	31/31 (100%)	0.30	3 (9%) 8 8	78, 86, 98, 111	0
11	M	31/31 (100%)	-0.30	1 (3%) 48 51	49, 58, 66, 96	0
11	m	31/31 (100%)	-0.58	0 100 100	38, 43, 55, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	b	729/729 (100%)	-0.11	11 (1%) 74 75	39, 54, 75, 93	0
13	c	81/81 (100%)	0.25	4 (4%) 30 32	54, 69, 83, 96	0
14	e	68/68 (100%)	2.09	33 (48%) 0 0	63, 79, 100, 108	0
15	k	78/78 (100%)	4.53	61 (78%) 0 0	140, 160, 200, 208	38 (48%)
16	1	744/744 (100%)	1.08	152 (20%) 1 1	42, 90, 121, 151	0
17	4	140/140 (100%)	0.68	27 (19%) 1 1	51, 76, 105, 120	0
18	h	38/38 (100%)	0.60	7 (18%) 1 1	54, 68, 95, 96	0
19	8	79/79 (100%)	3.23	43 (54%) 0 0	103, 127, 168, 172	39 (49%)
20	0	154/154 (100%)	-0.26	3 (1%) 67 69	38, 51, 73, 108	0
All	All	6771/6771 (100%)	0.56	929 (13%) 3 3	29, 70, 138, 209	115 (1%)

All (929) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	4	SER	15.2
15	k	81	VAL	14.5
15	k	15	THR	13.6
1	a	6	PRO	12.8
1	a	5	PRO	12.1
9	K	52	LEU	11.8
15	k	14	THR	11.7
19	8	55	LEU	11.5
16	1	239	PRO	11.4
1	a	256	PHE	11.2
15	k	38	TYR	11.1
1	a	3	ILE	11.1
1	a	268	TRP	10.9
2	2	1	MET	10.8
16	1	12	ALA	10.8
19	8	56	ALA	10.7
15	k	50	LEU	10.5
15	k	12	SER	10.5
1	a	271	TYR	10.4
15	k	18	TRP	10.2
15	k	39	PHE	10.1
19	8	58	LYS	10.1
7	i	39	GLU	10.0
19	8	48	LYS	9.8
16	1	243	ILE	9.7

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Mol	Chain	Res	Type	RSRZ
15	k	11	ALA	9.5
1	a	257	ALA	9.5
19	8	39	PHE	9.4
1	a	244	LEU	9.3
19	8	15	THR	9.3
19	8	57	SER	9.2
19	8	38	TYR	9.2
6	6	1	ALA	9.2
6	6	90	ILE	8.8
2	B	1	MET	8.8
1	a	265	THR	8.7
1	a	751	GLY	8.5
15	k	56	ALA	8.5
19	8	50	LEU	8.4
15	k	53	PRO	8.3
15	k	55	LEU	8.3
6	6	92	GLU	8.1
3	3	65	ILE	8.0
6	6	103	ILE	8.0
2	2	314	GLY	8.0
19	8	18	TRP	8.0
2	2	312	LEU	7.9
9	K	56	ALA	7.8
19	8	87	SER	7.7
15	k	13	PRO	7.5
16	1	246	PRO	7.5
15	k	19	SER	7.5
4	d	1	MET	7.5
15	k	16	ALA	7.4
1	a	2	THR	7.4
6	6	102	VAL	7.4
4	d	2	THR	7.4
16	1	286	GLY	7.3
16	1	11	LYS	7.3
6	6	106	PRO	7.2
10	1	2	ALA	7.2
2	2	225	PHE	7.1
5	5	31	SER	7.0
7	i	40	GLY	7.0
15	k	36	ILE	7.0
5	E	32	GLY	7.0
15	k	60	THR	6.9

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Mol	Chain	Res	Type	RSRZ
19	8	14	THR	6.9
1	a	7	GLU	6.9
16	1	244	LEU	6.9
1	a	270	VAL	6.9
6	6	99	GLN	6.9
1	a	243	ILE	6.9
6	6	89	GLU	6.8
3	3	30	PRO	6.8
1	a	519	LYS	6.8
6	6	107	LEU	6.8
16	1	279	GLY	6.8
16	1	183	LYS	6.7
16	1	30	LYS	6.7
13	c	1	MET	6.7
16	1	249	MET	6.7
15	k	44	THR	6.7
16	1	623	PRO	6.7
15	k	21	SER	6.6
6	6	101	VAL	6.6
15	k	46	LYS	6.6
1	a	231	VAL	6.6
16	1	14	VAL	6.6
1	a	274	PHE	6.6
2	2	311	PRO	6.6
2	2	310	GLY	6.6
2	2	2	ALA	6.5
19	8	60	THR	6.5
19	8	59	LYS	6.4
6	6	93	SER	6.4
15	k	70	MET	6.3
1	a	621	VAL	6.3
19	8	46	LYS	6.3
9	K	51	ALA	6.3
3	3	14	CYS	6.2
16	1	10	ALA	6.2
14	e	26	ALA	6.2
19	8	35	VAL	6.2
14	e	38	ILE	6.2
6	F	2	ASP	6.1
9	K	53	PRO	6.1
15	k	24	ILE	6.1
16	1	100	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
6	6	120	LEU	6.1
2	2	226	PHE	6.0
5	5	43	ARG	6.0
14	e	9	VAL	6.0
16	1	15	SER	6.0
12	b	730	PHE	5.9
16	1	18	ASN	5.9
5	5	19	TYR	5.9
2	2	295	TRP	5.8
1	a	266	LEU	5.8
16	1	21	VAL	5.8
16	1	31	PRO	5.8
2	2	731	GLY	5.8
19	8	9	ALA	5.8
6	6	11	SER	5.7
1	a	1	MET	5.7
16	1	16	VAL	5.7
1	a	10	ALA	5.7
14	e	30	LYS	5.7
1	a	518	GLY	5.7
2	2	215	THR	5.7
2	2	470	TYR	5.7
1	a	12	ALA	5.7
9	K	57	SER	5.6
1	a	205	LEU	5.6
16	1	51	LEU	5.6
15	k	51	ALA	5.6
16	1	238	LEU	5.6
1	a	255	SER	5.6
1	a	108	THR	5.5
16	1	515	ALA	5.4
10	l	7	VAL	5.4
14	e	31	SER	5.4
16	1	92	PHE	5.4
16	1	103	TRP	5.4
15	k	83	GLY	5.4
14	e	3	LEU	5.4
9	K	59	LYS	5.3
19	8	19	SER	5.3
15	k	79	GLY	5.3
17	4	2	THR	5.3
6	6	61	HIS	5.3

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Mol	Chain	Res	Type	RSRZ
2	2	504	SER	5.3
19	8	52	LEU	5.3
14	e	23	GLY	5.2
8	7	1	MET	5.2
10	L	1	MET	5.2
9	K	45	GLY	5.2
9	K	50	LEU	5.2
19	8	84	LEU	5.2
5	5	22	VAL	5.2
16	1	505	ALA	5.1
16	1	160	CYS	5.1
16	1	256	PHE	5.1
15	k	85	ALA	5.1
11	9	2	ALA	5.1
16	1	182	VAL	5.1
6	6	4	PHE	5.1
6	6	59	PHE	5.1
2	2	524	LEU	5.1
1	A	2	THR	5.0
8	7	2	ASP	5.0
3	3	26	LEU	5.0
9	K	46	LYS	5.0
1	a	272	SER	5.0
10	l	1	MET	5.0
9	K	44	THR	5.0
15	k	57	SER	5.0
1	a	520	VAL	5.0
12	b	731	GLY	5.0
15	k	20	LEU	4.9
16	1	242	PHE	4.9
9	K	60	THR	4.9
15	k	68	ALA	4.9
16	1	184	ALA	4.9
16	1	29	GLY	4.9
19	8	44	THR	4.9
16	1	9	GLU	4.9
2	2	216	PRO	4.9
6	6	104	ASN	4.9
16	1	22	PRO	4.9
19	8	34	PHE	4.9
16	1	363	THR	4.9
5	E	66	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	4.9
4	d	68	LEU	4.9
14	e	39	VAL	4.9
6	f	16	TYR	4.8
2	2	205	GLN	4.8
15	k	86	SER	4.8
5	5	62	ALA	4.8
8	j	40	PRO	4.8
6	6	2	ASP	4.8
16	1	34	PHE	4.8
1	a	40	ARG	4.8
9	K	48	LYS	4.8
2	B	480	ASP	4.8
6	6	87	LEU	4.7
14	e	29	GLU	4.7
6	f	1	ALA	4.7
1	a	378	TYR	4.7
16	1	248	LYS	4.7
6	6	105	VAL	4.7
3	3	40	ALA	4.7
19	8	45	GLY	4.7
1	a	323	GLU	4.7
1	a	41	GLY	4.7
7	i	38	GLY	4.7
6	6	63	GLY	4.6
14	e	37	VAL	4.6
16	1	19	ASN	4.6
6	6	19	LYS	4.6
19	8	47	GLY	4.6
15	k	43	LYS	4.6
2	2	520	ILE	4.6
4	D	2	THR	4.6
2	2	456	VAL	4.6
16	1	496	ALA	4.6
16	1	8	ARG	4.6
6	6	98	MET	4.5
17	4	114	ALA	4.5
10	l	4	SER	4.5
1	a	500	ASN	4.5
14	e	60	ASN	4.5
16	1	288	LEU	4.5
1	a	47	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	a	383	TYR	4.5
16	1	231	VAL	4.5
17	4	103	VAL	4.5
2	2	579	TRP	4.5
1	a	253	TYR	4.5
16	1	709	VAL	4.5
2	2	263	PRO	4.5
1	a	267	ASN	4.5
2	2	222	LEU	4.5
3	3	57	ALA	4.4
1	a	207	LEU	4.4
1	a	249	MET	4.4
19	8	20	LEU	4.4
1	a	613	MET	4.4
6	f	59	PHE	4.4
15	k	25	ILE	4.4
2	2	166	ALA	4.4
6	6	38	GLU	4.4
19	8	36	ILE	4.4
1	a	748	LEU	4.4
15	k	10	GLN	4.4
1	a	269	GLY	4.4
2	2	286	ILE	4.3
1	a	8	ARG	4.3
1	a	38	LEU	4.3
1	A	12	ALA	4.3
8	7	9	SER	4.3
8	7	38	PHE	4.3
2	2	471	GLY	4.3
15	k	32	PHE	4.3
1	a	247	SER	4.3
16	1	266	LEU	4.3
5	5	32	GLY	4.3
2	B	342	ILE	4.3
10	l	43	GLY	4.3
15	k	35	VAL	4.3
15	k	28	LEU	4.3
16	1	180	TYR	4.3
10	l	3	GLU	4.3
14	e	40	ARG	4.3
1	A	359	LEU	4.2
4	d	56	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
15	k	72	PHE	4.2
19	8	51	ALA	4.2
2	B	244	PHE	4.2
3	3	12	ILE	4.2
9	K	55	LEU	4.2
2	2	218	HIS	4.2
3	3	13	GLY	4.2
8	j	32	PHE	4.2
14	e	33	ILE	4.2
6	6	134	LYS	4.2
2	2	441	VAL	4.2
3	3	29	VAL	4.2
15	k	29	CYS	4.2
3	3	63	LEU	4.2
16	1	396	ILE	4.1
1	a	273	ASP	4.1
2	2	217	PRO	4.1
17	4	141	VAL	4.1
16	1	270	VAL	4.1
1	a	275	LEU	4.1
1	a	9	GLU	4.1
5	5	20	GLY	4.1
9	K	42	GLN	4.1
15	k	40	ALA	4.1
5	5	23	GLY	4.1
8	7	33	TYR	4.1
3	3	41	SER	4.1
14	e	32	GLY	4.1
16	1	38	LEU	4.1
10	L	2	ALA	4.1
4	d	104	PHE	4.1
2	2	527	THR	4.0
1	a	36	ARG	4.0
10	l	5	ASN	4.0
9	K	8	LEU	4.0
16	1	504	THR	4.0
1	a	92	PHE	4.0
2	B	213	LEU	4.0
16	1	240	HIS	4.0
3	3	62	PHE	4.0
16	1	705	ASN	4.0
1	a	156	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
6	6	17	LEU	4.0
14	e	24	THR	4.0
1	a	206	GLY	4.0
2	B	243	ILE	4.0
2	2	460	TRP	4.0
2	2	232	VAL	4.0
19	8	64	PRO	4.0
5	5	10	ARG	3.9
15	k	45	GLY	3.9
6	f	94	LYS	3.9
2	2	427	LEU	3.9
6	6	131	LEU	3.9
16	1	156	TYR	3.9
16	1	234	LYS	3.9
19	8	53	PRO	3.9
2	2	501	GLY	3.9
4	d	40	PHE	3.9
8	J	32	PHE	3.9
13	c	62	PHE	3.9
1	a	254	PRO	3.9
2	2	396	TYR	3.9
14	e	8	LYS	3.9
9	K	34	PHE	3.9
1	a	37	THR	3.9
16	1	680	ALA	3.9
1	a	623	PRO	3.9
11	9	3	LEU	3.9
17	4	107	LYS	3.9
2	2	398	PRO	3.8
6	6	3	ASP	3.8
15	k	34	PHE	3.8
1	a	750	ILE	3.8
16	1	163	ILE	3.8
15	k	54	GLN	3.8
1	a	624	ASP	3.8
4	d	83	TYR	3.8
4	d	86	TYR	3.8
1	a	105	ALA	3.8
4	D	1	MET	3.8
8	j	1	MET	3.8
5	E	3	LEU	3.8
6	6	110	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
9	K	54	GLN	3.8
2	2	214	SER	3.8
15	k	37	GLY	3.8
1	A	6	PRO	3.8
1	a	263	PHE	3.8
16	1	257	ALA	3.8
15	k	58	LYS	3.8
2	2	423	VAL	3.8
1	a	107	PRO	3.8
2	B	343	THR	3.8
19	8	49	ASP	3.8
9	K	23	GLY	3.7
16	1	255	SER	3.7
2	2	472	PHE	3.7
9	K	24	ILE	3.7
16	1	360	GLY	3.7
17	4	110	GLU	3.7
2	2	528	ALA	3.7
3	3	5	VAL	3.7
6	6	21	LYS	3.7
3	3	39	ILE	3.7
2	2	424	SER	3.7
15	k	82	LEU	3.7
1	a	204	LEU	3.7
2	2	316	GLY	3.7
2	2	525	HIS	3.7
1	a	34	PHE	3.7
17	4	113	GLU	3.7
1	a	208	GLY	3.6
1	a	261	THR	3.6
19	8	24	ILE	3.6
14	e	18	TRP	3.6
14	e	27	SER	3.6
1	a	233	PRO	3.6
16	1	665	LEU	3.6
16	1	710	ALA	3.6
16	1	522	MET	3.6
1	a	39	ALA	3.6
6	6	62	ALA	3.6
15	k	78	ALA	3.6
16	1	500	ASN	3.6
18	h	38	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	a	301	ALA	3.6
1	a	617	VAL	3.6
10	L	3	GLU	3.6
5	5	7	ASP	3.6
8	7	3	GLY	3.6
16	1	250	ALA	3.6
16	1	516	VAL	3.6
6	6	91	ARG	3.5
1	a	250	ALA	3.5
16	1	285	THR	3.5
6	6	113	LEU	3.5
1	a	367	ALA	3.5
9	K	19	SER	3.5
16	1	378	TYR	3.5
17	4	77	LYS	3.5
8	7	32	PHE	3.5
1	A	3	ILE	3.5
1	a	259	GLY	3.5
16	1	514	ILE	3.5
1	a	303	LEU	3.5
6	6	50	TYR	3.5
4	d	77	LYS	3.5
15	k	61	PHE	3.4
6	6	18	ALA	3.4
2	2	341	VAL	3.4
16	1	251	GLU	3.4
16	1	201	LEU	3.4
2	2	399	VAL	3.4
16	1	177	TRP	3.4
1	a	264	PHE	3.4
6	F	113	LEU	3.4
19	8	23	GLY	3.4
10	l	6	GLN	3.4
15	k	27	CYS	3.4
2	2	82	LEU	3.4
3	3	8	TYR	3.4
1	a	258	GLN	3.4
19	8	54	GLN	3.4
6	6	94	LYS	3.4
2	2	523	GLY	3.4
6	6	51	PRO	3.4
8	j	2	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	2	522	LEU	3.3
3	3	27	GLU	3.3
2	B	2	ALA	3.3
10	1	91	VAL	3.3
19	8	81	VAL	3.3
2	2	530	ILE	3.3
9	K	61	PHE	3.3
1	a	618	TRP	3.3
6	6	86	TYR	3.3
19	8	32	PHE	3.3
16	1	25	PHE	3.3
16	1	152	PHE	3.3
16	1	204	LEU	3.3
6	f	15	ALA	3.3
15	k	9	ALA	3.3
6	6	130	LYS	3.3
2	2	422	TRP	3.3
18	h	2	ASP	3.3
2	2	618	ARG	3.3
10	L	110	SER	3.3
4	d	30	ILE	3.3
16	1	161	THR	3.3
6	F	94	LYS	3.3
16	1	96	LYS	3.3
4	d	92	GLY	3.3
2	2	313	THR	3.3
2	2	519	ALA	3.3
6	6	132	VAL	3.3
6	6	43	ALA	3.2
14	e	5	ARG	3.2
6	6	10	CYS	3.2
15	k	80	MET	3.2
6	6	117	LEU	3.2
8	j	4	LEU	3.2
14	e	59	ASN	3.2
1	a	209	SER	3.2
1	a	619	GLY	3.2
2	B	295	TRP	3.2
6	f	37	ALA	3.2
6	f	95	ASN	3.2
16	1	17	ASP	3.2
1	a	202	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
3	3	7	ILE	3.2
16	1	393	HIS	3.2
16	1	364	ILE	3.2
1	a	286	GLY	3.2
16	1	281	LEU	3.2
16	1	359	LEU	3.2
16	1	503	ALA	3.1
17	4	83	TYR	3.1
2	B	312	LEU	3.1
4	d	4	LEU	3.1
5	5	2	ALA	3.1
1	a	242	PHE	3.1
1	a	203	GLY	3.1
16	1	47	TRP	3.1
17	4	96	TYR	3.1
6	f	2	ASP	3.1
2	2	343	THR	3.1
16	1	289	TRP	3.1
16	1	501	ALA	3.1
2	2	243	ILE	3.1
2	2	297	ILE	3.1
16	1	390	PHE	3.1
17	4	85	ILE	3.1
5	E	70	GLN	3.1
2	B	239	THR	3.1
2	2	337	ALA	3.1
6	f	129	GLY	3.1
6	6	22	ASN	3.1
6	6	41	ALA	3.1
4	d	46	GLY	3.1
2	2	526	THR	3.1
3	3	38	GLN	3.0
14	e	11	ILE	3.0
6	F	134	LYS	3.0
2	2	227	THR	3.0
4	d	47	ALA	3.0
17	4	98	HIS	3.0
3	3	43	PRO	3.0
4	d	29	ALA	3.0
8	7	6	SER	3.0
3	3	32	ASP	3.0
4	D	136	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
4	d	84	LYS	3.0
5	E	69	VAL	3.0
1	a	304	PHE	3.0
12	b	635	TYR	3.0
16	1	159	TYR	3.0
15	k	69	THR	3.0
11	M	1	MET	3.0
17	4	102	GLY	3.0
6	6	16	TYR	3.0
16	1	247	SER	3.0
16	1	507	TYR	3.0
2	B	345	LEU	3.0
2	2	476	LEU	3.0
6	f	41	ALA	3.0
16	1	367	ALA	3.0
1	a	31	PRO	3.0
1	a	300	ILE	3.0
16	1	391	THR	3.0
16	1	655	ALA	3.0
16	1	717	ALA	3.0
2	2	494	TRP	3.0
1	a	637	GLN	2.9
5	E	68	LEU	2.9
17	4	117	THR	2.9
19	8	31	VAL	2.9
1	A	300	ILE	2.9
16	1	174	PHE	2.9
19	8	61	PHE	2.9
16	1	245	GLU	2.9
2	B	495	LEU	2.9
17	4	97	LEU	2.9
2	2	230	TRP	2.9
1	a	338	LYS	2.9
16	1	712	ALA	2.9
19	8	22	VAL	2.9
1	a	163	ILE	2.9
1	a	381	ILE	2.9
1	a	11	LYS	2.9
2	2	582	ASN	2.9
2	B	339	LEU	2.9
14	e	34	LEU	2.9
1	a	145	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
6	f	19	LYS	2.9
15	k	48	LYS	2.9
14	e	20	GLY	2.9
6	f	53	LEU	2.9
2	B	338	SER	2.9
2	2	428	GLY	2.9
2	2	573	PHE	2.9
8	7	40	PRO	2.9
13	c	36	ALA	2.9
6	f	39	ARG	2.8
6	6	44	LEU	2.8
1	a	678	VAL	2.8
6	f	30	PRO	2.8
16	1	743	PHE	2.8
17	4	101	ASP	2.8
19	8	12	SER	2.8
2	2	710	PHE	2.8
6	6	127	THR	2.8
1	a	235	ASP	2.8
14	e	68	LEU	2.8
4	D	110	GLU	2.8
1	A	548	ILE	2.8
2	B	730	PHE	2.8
2	2	330	PHE	2.8
16	1	398	GLY	2.8
2	2	586	TRP	2.8
2	2	654	TRP	2.8
8	J	33	TYR	2.8
1	a	305	ILE	2.8
4	d	95	GLN	2.8
6	6	49	GLY	2.8
16	1	151	GLY	2.8
16	1	298	LEU	2.8
16	1	356	LEU	2.8
16	1	397	GLY	2.8
16	1	400	LEU	2.8
6	6	111	LYS	2.8
2	2	426	PHE	2.8
6	f	34	LYS	2.8
6	f	42	SER	2.8
4	d	39	VAL	2.7
17	4	108	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
16	1	395	TRP	2.7
2	B	377	ALA	2.7
2	B	488	ALA	2.7
1	a	201	LEU	2.7
2	2	505	LEU	2.7
2	2	361	GLN	2.7
2	2	282	VAL	2.7
14	e	22	VAL	2.7
1	a	396	ILE	2.7
2	2	268	LEU	2.7
1	a	366	VAL	2.7
16	1	94	GLY	2.7
6	f	60	THR	2.7
6	f	10	CYS	2.7
2	B	297	ILE	2.7
2	2	567	ILE	2.7
17	4	33	THR	2.7
2	B	204	GLY	2.7
2	2	420	LEU	2.7
3	C	62	PHE	2.7
4	D	133	PHE	2.7
14	e	41	PHE	2.7
8	7	7	PHE	2.7
15	k	77	GLY	2.7
2	B	215	THR	2.6
16	1	517	ALA	2.6
5	E	12	LYS	2.6
2	B	380	LEU	2.6
2	2	320	LEU	2.6
17	4	30	ILE	2.6
1	a	733	LEU	2.6
6	6	67	ILE	2.6
16	1	381	ILE	2.6
2	2	605	GLN	2.6
1	a	96	LYS	2.6
2	2	431	THR	2.6
5	5	4	ASN	2.6
8	7	10	THR	2.6
16	1	521	ALA	2.6
9	K	63	LEU	2.6
1	a	283	PRO	2.6
16	1	377	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
6	f	40	TYR	2.6
4	d	70	THR	2.6
2	2	467	LYS	2.6
16	1	683	LEU	2.6
2	2	43	TYR	2.6
2	B	344	SER	2.6
2	2	247	SER	2.6
2	B	341	VAL	2.6
2	2	307	ALA	2.6
6	f	27	THR	2.6
19	8	16	ALA	2.6
16	1	187	LEU	2.6
1	a	411	PHE	2.6
2	B	472	PHE	2.6
13	c	35	LYS	2.6
15	k	42	GLN	2.6
2	2	518	HIS	2.6
1	a	630	VAL	2.6
16	1	13	LYS	2.6
16	1	304	PHE	2.6
10	L	106	GLY	2.6
16	1	91	TYR	2.6
1	a	26	GLU	2.6
15	k	64	PRO	2.5
16	1	27	LYS	2.5
5	5	11	ILE	2.5
1	a	616	ASP	2.5
2	B	214	SER	2.5
8	j	3	GLY	2.5
17	4	116	GLY	2.5
1	A	327	ALA	2.5
1	a	229	ALA	2.5
14	e	2	ALA	2.5
1	A	358	LEU	2.5
2	B	264	GLN	2.5
2	2	336	LEU	2.5
16	1	61	GLN	2.5
2	2	223	MET	2.5
20	0	4	SER	2.5
2	B	346	VAL	2.5
6	f	55	VAL	2.5
16	1	430	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	2	344	SER	2.5
1	A	360	GLY	2.5
2	2	164	SER	2.5
6	F	128	SER	2.5
17	4	133	PHE	2.5
18	h	1	MET	2.5
3	3	58	CYS	2.5
8	7	4	LEU	2.5
10	l	9	GLN	2.5
6	6	39	ARG	2.5
2	B	499	ASN	2.5
6	6	137	GLU	2.5
18	h	4	SER	2.5
16	1	110	ILE	2.5
2	2	204	GLY	2.5
5	5	68	LEU	2.4
15	k	84	LEU	2.4
16	1	226	LEU	2.4
3	3	31	TRP	2.4
12	b	662	ILE	2.4
16	1	64	ASP	2.4
2	2	163	PRO	2.4
6	6	9	PRO	2.4
2	2	68	VAL	2.4
1	A	9	GLU	2.4
2	B	216	PRO	2.4
2	2	601	GLY	2.4
2	2	502	THR	2.4
3	3	36	ALA	2.4
2	2	712	VAL	2.4
1	a	159	TYR	2.4
1	a	611	TRP	2.4
2	2	92	TRP	2.4
6	f	98	MET	2.4
14	e	7	ASP	2.4
2	2	203	ARG	2.4
1	a	734	GLY	2.4
6	6	52	HIS	2.4
20	0	113	THR	2.4
2	2	233	TYR	2.4
15	k	26	MET	2.4
1	a	200	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
16	1	20	PRO	2.4
6	f	130	LYS	2.4
2	2	584	LEU	2.4
16	1	502	LEU	2.4
20	0	74	SER	2.4
4	d	94	VAL	2.4
6	f	38	GLU	2.4
14	e	28	VAL	2.4
1	a	27	LYS	2.4
6	6	58	ARG	2.4
8	j	31	ARG	2.4
2	B	524	LEU	2.4
16	1	713	ILE	2.3
1	a	174	PHE	2.3
4	d	67	ALA	2.3
2	2	711	THR	2.3
6	F	127	THR	2.3
6	6	20	SER	2.3
17	4	109	ASN	2.3
2	2	419	HIS	2.3
4	d	96	TYR	2.3
6	f	18	ALA	2.3
9	K	58	LYS	2.3
1	a	276	THR	2.3
1	a	362	LEU	2.3
2	2	53	HIS	2.3
1	a	284	VAL	2.3
16	1	115	GLN	2.3
19	8	42	GLN	2.3
2	2	418	SER	2.3
9	K	18	TRP	2.3
2	2	577	MET	2.3
16	1	58	PHE	2.3
1	a	521	ALA	2.3
2	B	240	ALA	2.3
2	B	259	GLY	2.3
2	B	487	GLY	2.3
2	2	352	SER	2.3
2	2	445	GLY	2.3
5	E	2	ALA	2.3
6	6	108	ALA	2.3
1	A	502	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	a	43	LYS	2.3
2	2	397	ASP	2.3
2	2	531	LEU	2.3
11	9	5	ASP	2.3
16	1	282	ASN	2.3
2	2	358	PHE	2.3
14	e	61	PHE	2.3
16	1	132	GLY	2.3
1	a	668	TYR	2.3
2	B	182	LEU	2.3
2	2	491	LEU	2.3
16	1	65	LEU	2.3
12	b	341	VAL	2.3
1	a	197	MET	2.3
2	2	706	GLY	2.3
16	1	208	GLY	2.3
1	a	199	HIS	2.3
2	2	507	LEU	2.3
5	E	67	GLU	2.3
15	k	52	LEU	2.3
16	1	271	TYR	2.3
1	a	726	VAL	2.2
12	b	710	PHE	2.2
1	a	593	LEU	2.2
16	1	253	TYR	2.2
6	6	13	ASN	2.2
1	a	723	GLY	2.2
17	4	3	GLU	2.2
2	2	594	LYS	2.2
6	f	127	THR	2.2
16	1	519	LYS	2.2
1	a	492	LEU	2.2
2	2	566	ASP	2.2
19	8	27	CYS	2.2
1	a	307	ALA	2.2
2	2	156	HIS	2.2
10	l	16	PHE	2.2
16	1	687	PHE	2.2
2	2	462	GLN	2.2
12	b	524	LEU	2.2
6	6	12	GLU	2.2
1	A	208	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
14	e	21	ASP	2.2
2	2	292	ARG	2.2
4	d	48	ALA	2.2
1	a	635	PHE	2.2
16	1	144	PHE	2.2
2	B	473	ASP	2.2
2	B	731	GLY	2.2
9	K	38	TYR	2.2
2	2	242	HIS	2.2
1	a	677	PHE	2.2
6	f	21	LYS	2.2
9	K	49	ASP	2.2
15	k	49	ASP	2.2
1	a	222	PRO	2.2
2	B	479	PRO	2.2
1	A	297	HIS	2.2
2	B	423	VAL	2.2
17	4	81	GLN	2.2
2	B	227	THR	2.2
2	2	57	ILE	2.2
1	a	684	MET	2.1
4	d	32	TRP	2.1
16	1	229	ALA	2.1
2	B	252	THR	2.1
2	2	130	THR	2.1
2	2	588	THR	2.1
4	D	92	GLY	2.1
12	b	297	ILE	2.1
1	a	25	PHE	2.1
10	L	107	GLU	2.1
16	1	241	GLU	2.1
8	7	5	LYS	2.1
1	A	355	ASN	2.1
14	e	25	VAL	2.1
1	A	751	GLY	2.1
16	1	23	THR	2.1
2	2	457	PHE	2.1
2	2	345	LEU	2.1
4	d	97	LEU	2.1
16	1	748	LEU	2.1
16	1	361	SER	2.1
4	d	3	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
5	5	47	ASN	2.1
1	a	68	VAL	2.1
10	l	92	ALA	2.1
17	4	118	LYS	2.1
16	1	708	ASN	2.1
16	1	136	GLY	2.1
1	a	729	ALA	2.1
2	2	576	ALA	2.1
18	h	7	ALA	2.1
1	a	363	THR	2.1
16	1	265	THR	2.1
1	a	548	ILE	2.1
16	1	236	ILE	2.1
1	a	747	SER	2.1
5	5	12	LYS	2.1
1	a	308	GLY	2.1
14	e	53	ALA	2.1
2	2	219	PRO	2.1
2	2	511	PRO	2.1
12	b	620	TYR	2.1
10	l	20	LEU	2.1
1	A	485	TRP	2.1
1	a	675	GLY	2.1
15	k	73	GLY	2.1
19	8	80	MET	2.1
2	2	315	ALA	2.1
12	b	576	ALA	2.1
16	1	299	ALA	2.1
2	B	431	THR	2.1
4	D	89	TYR	2.1
1	a	369	HIS	2.1
15	k	74	HIS	2.1
16	1	632	LEU	2.1
17	4	51	ASN	2.1
2	2	340	GLY	2.1
1	A	10	ALA	2.0
1	A	235	ASP	2.0
16	1	213	ALA	2.0
18	h	6	ALA	2.0
1	a	24	SER	2.0
1	a	622	SER	2.0
4	d	122	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
8	j	6	SER	2.0
10	l	89	ILE	2.0
16	1	145	TYR	2.0
1	A	362	LEU	2.0
2	2	168	PHE	2.0
17	4	115	GLN	2.0
18	h	3	GLY	2.0
2	2	655	ALA	2.0
16	1	617	VAL	2.0
2	2	264	GLN	2.0
16	1	686	LEU	2.0
12	b	577	MET	2.0
16	1	419	ALA	2.0
2	2	293	THR	2.0
16	1	109	HIS	2.0
2	2	568	SER	2.0
9	K	87	SER	2.0
16	1	117	VAL	2.0
16	1	366	VAL	2.0
2	2	157	LEU	2.0
5	E	34	LEU	2.0
6	6	64	ASP	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(\AA^2)	Q<0.9
25	LHG	B	851	49/49	0.60	0.90	22.62	84,117,143,146	0
27	ACT	M	7001	4/4	0.72	0.38	17.96	57,71,71,74	0
24	BCR	B	847	40/40	0.62	0.61	15.99	64,85,115,121	0
24	BCR	A	848	40/40	0.74	0.55	14.38	72,84,114,114	0
26	LMG	b	1855	55/55	0.63	0.61	13.41	76,97,115,116	0
37	DGD	L	209	66/66	0.72	0.33	11.83	42,87,116,121	0
24	BCR	b	1850	40/40	0.67	0.45	11.68	53,76,95,100	0
24	BCR	2	849	40/40	0.67	0.81	10.31	83,136,143,144	0
26	LMG	1	853	55/55	0.81	0.36	10.29	83,97,112,118	0
24	BCR	1	849	40/40	0.66	0.63	9.89	106,122,142,143	0
21	CLA	J	1106	65/65	0.81	0.34	9.03	93,112,125,127	0
27	ACT	A	853	4/4	0.82	0.33	7.06	28,55,63,71	0
29	CL	1	857	1/1	0.91	0.30	6.39	74,74,74,74	0
25	LHG	m	101	49/49	0.73	0.36	6.05	44,81,137,147	0
31	SQD	B	852	54/54	0.84	0.32	5.67	61,86,107,113	0
23	SF4	A	842	8/8	0.83	0.27	5.55	40,87,137,173	0
25	LHG	1	852	49/49	0.89	0.33	5.19	62,83,96,99	0
21	CLA	b	1836	65/65	0.86	0.20	5.15	50,69,93,98	0
25	LHG	a	851	49/49	0.87	0.36	5.09	76,96,106,109	0
31	SQD	f	205	54/54	0.75	0.36	4.98	42,100,123,132	0
25	LHG	M	7003	49/49	0.72	0.24	4.93	51,97,144,149	0
23	SF4	C	101	8/8	0.75	0.23	4.90	43,65,114,208	0
25	LHG	l	208	49/49	0.77	0.37	4.79	64,92,141,144	0
31	SQD	0	207	54/54	0.77	0.23	4.78	59,91,141,148	0
24	BCR	7	1102	40/40	0.79	0.33	4.22	100,112,124,125	0
21	CLA	A	814	65/65	0.87	0.31	3.96	41,64,105,111	0
26	LMG	1	851	50/55	0.78	0.31	3.90	44,94,119,120	0
26	LMG	b	1853	55/55	0.80	0.36	3.90	54,79,114,116	0
21	CLA	b	1819	65/65	0.92	0.28	3.87	39,64,89,93	0
24	BCR	1	858	40/40	0.69	0.39	3.86	78,113,122,124	0
24	BCR	A	844	40/40	0.89	0.24	3.74	33,60,75,82	0
24	BCR	2	844	40/40	0.56	0.86	3.71	105,125,145,147	0
24	BCR	1	844	40/40	0.66	0.49	3.62	90,109,136,137	0
30	ECH	2	846	41/41	0.77	0.34	3.60	65,122,132,133	0
28	45D	2	854	42/42	0.90	0.19	3.59	33,55,68,75	0
25	LHG	L	210	49/49	0.87	0.22	3.59	46,75,102,104	0
21	CLA	b	1837	65/65	0.90	0.22	3.50	64,79,121,123	0
35	LMT	L	211	35/35	0.87	0.27	3.45	55,79,90,97	0
24	BCR	1	847	40/40	0.85	0.32	3.38	55,73,127,132	0
25	LHG	9	101	49/49	0.70	0.29	3.37	65,87,148,157	0
24	BCR	a	847	40/40	0.85	0.28	3.26	51,82,109,118	0
26	LMG	a	852	55/55	0.80	0.26	3.21	85,112,130,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	7	1104	41/65	0.85	0.42	3.20	120,130,140,143	0
26	LMG	a	850	50/55	0.73	0.22	3.18	54,78,109,110	0
24	BCR	2	845	40/40	0.68	0.34	3.14	81,113,134,136	0
24	BCR	a	846	40/40	0.84	0.37	3.13	69,87,144,147	0
24	BCR	B	845	40/40	0.88	0.32	3.11	51,66,81,84	0
35	LMT	l	211	35/35	0.76	0.36	3.10	55,95,118,120	0
25	LHG	b	1802	49/49	0.76	0.27	3.09	48,72,132,139	0
21	CLA	b	1833	65/65	0.89	0.25	3.08	58,73,120,124	0
24	BCR	6	202	40/40	0.83	0.35	3.02	78,113,132,136	0
26	LMG	2	852	55/55	0.72	0.54	2.92	105,127,150,153	0
24	BCR	9	102	40/40	0.85	0.28	2.90	58,80,116,118	0
26	LMG	0	206	55/55	0.83	0.28	2.84	34,74,99,107	0
21	CLA	b	1826	65/65	0.91	0.20	2.80	48,64,100,103	0
26	LMG	A	852	48/55	0.84	0.31	2.79	37,84,102,107	0
26	LMG	A	850	50/55	0.76	0.23	2.69	40,72,99,106	0
26	LMG	B	850	55/55	0.68	0.40	2.68	71,110,133,137	0
31	SQD	F	205	54/54	0.79	0.42	2.67	66,93,129,134	0
26	LMG	K	101	55/55	0.60	0.65	2.67	72,119,146,146	0
21	CLA	A	812	65/65	0.95	0.17	2.62	31,48,81,86	0
30	ECH	m	104	41/41	0.91	0.19	2.58	23,49,80,80	0
24	BCR	l	207	40/40	0.85	0.25	2.54	57,74,97,100	0
21	CLA	6	204	43/65	0.68	0.56	2.42	116,141,171,178	0
21	CLA	B	819	65/65	0.89	0.24	2.41	65,85,101,106	0
24	BCR	f	201	40/40	0.82	0.29	2.38	59,79,88,92	0
21	CLA	a	804	65/65	0.81	0.33	2.36	68,92,118,128	0
21	CLA	B	840	65/65	0.77	0.40	2.32	76,105,133,136	0
24	BCR	B	846	40/40	0.91	0.25	2.22	22,44,56,57	0
35	LMT	J	1104	35/35	0.90	0.28	2.16	57,88,112,115	0
24	BCR	6	205	40/40	0.77	0.42	2.13	59,91,128,129	0
24	BCR	a	859	40/40	0.78	0.32	2.12	72,90,121,123	0
21	CLA	b	1825	60/65	0.93	0.22	2.10	33,66,132,132	0
24	BCR	I	102	40/40	0.94	0.21	2.08	24,45,59,67	0
25	LHG	l	209	49/49	0.77	0.36	2.03	81,111,137,138	0
24	BCR	J	1102	40/40	0.92	0.19	2.03	43,60,73,73	0
24	BCR	B	842	40/40	0.78	0.31	2.01	63,93,109,110	0
21	CLA	a	833	65/65	0.90	0.19	1.94	70,95,114,117	0
34	C7Z	2	855	42/42	0.54	0.43	1.93	100,131,150,152	0
35	LMT	0	208	35/35	0.92	0.21	1.92	51,72,84,90	0
31	SQD	m	102	54/54	0.83	0.23	1.89	33,61,95,99	0
21	CLA	a	840	55/65	0.84	0.24	1.89	83,118,128,133	0
24	BCR	F	201	40/40	0.92	0.21	1.85	35,57,80,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	B	823	57/65	0.93	0.17	1.84	53,78,101,108	0
34	C7Z	B	856	42/42	0.76	0.30	1.83	55,68,112,116	0
21	CLA	f	203	65/65	0.87	0.35	1.82	67,99,109,115	0
21	CLA	a	805	65/65	0.94	0.26	1.80	49,67,130,133	0
21	CLA	2	836	45/65	0.81	0.24	1.74	101,128,147,151	0
21	CLA	J	1105	65/65	0.80	0.32	1.73	75,95,121,137	0
21	CLA	j	1105	55/65	0.83	0.42	1.69	97,117,130,137	0
24	BCR	B	843	40/40	0.82	0.27	1.69	45,78,102,103	0
24	BCR	A	845	40/40	0.85	0.26	1.67	32,53,89,91	0
34	C7Z	b	1858	42/42	0.69	0.37	1.65	51,97,113,117	0
21	CLA	a	808	65/65	0.90	0.24	1.63	58,95,106,112	0
24	BCR	h	101	40/40	0.92	0.21	1.62	36,60,75,79	0
21	CLA	l	203	65/65	0.91	0.21	1.58	48,69,110,117	0
24	BCR	j	1102	40/40	0.88	0.26	1.58	66,95,106,110	0
36	EQ3	L	201	42/42	0.94	0.22	1.57	24,37,48,66	0
24	BCR	i	101	40/40	0.92	0.22	1.55	29,52,63,69	0
21	CLA	1	811	65/65	0.82	0.45	1.55	72,109,120,122	0
21	CLA	7	1105	41/65	0.82	0.39	1.54	133,150,155,157	0
25	LHG	B	855	49/49	0.64	0.41	1.52	73,110,175,181	0
31	SQD	L	208	51/54	0.86	0.21	1.52	42,80,104,107	0
21	CLA	A	831	65/65	0.95	0.21	1.52	27,38,59,76	0
24	BCR	A	846	40/40	0.94	0.19	1.49	31,46,106,108	0
21	CLA	a	836	65/65	0.92	0.19	1.46	44,73,87,100	0
22	PQN	1	842	33/33	0.86	0.29	1.44	67,88,108,108	0
21	CLA	B	825	55/65	0.92	0.32	1.43	50,68,84,89	0
21	CLA	B	839	65/65	0.96	0.24	1.42	11,39,59,85	0
24	BCR	1	856	40/40	0.88	0.25	1.41	60,93,104,109	0
21	CLA	B	830	55/65	0.91	0.26	1.40	67,76,102,107	0
21	CLA	B	836	65/65	0.92	0.26	1.39	45,66,92,94	0
21	CLA	b	1817	65/65	0.94	0.14	1.38	29,46,98,103	0
24	BCR	J	1107	40/40	0.91	0.18	1.37	48,69,89,91	0
21	CLA	A	817	65/65	0.94	0.26	1.37	36,53,86,90	0
21	CLA	B	838	65/65	0.95	0.19	1.35	17,35,46,56	0
21	CLA	B	802	60/65	0.95	0.17	1.35	21,39,93,95	0
25	LHG	a	853	49/49	0.71	0.25	1.34	51,107,175,183	0
21	CLA	A	818	65/65	0.95	0.29	1.34	31,46,56,59	0
22	PQN	b	1844	33/33	0.94	0.24	1.32	36,51,69,69	0
21	CLA	J	1103	65/65	0.92	0.21	1.31	29,68,110,114	0
24	BCR	b	1849	40/40	0.92	0.22	1.31	35,52,61,64	0
24	BCR	2	847	40/40	0.81	0.32	1.29	66,101,136,136	0
24	BCR	2	848	40/40	0.93	0.19	1.28	31,56,72,76	0
21	CLA	A	830	58/65	0.94	0.17	1.27	20,42,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	BCR	1	846	40/40	0.76	0.32	1.26	71,105,134,138	0
21	CLA	a	819	65/65	0.89	0.38	1.25	64,89,103,112	0
21	CLA	0	202	65/65	0.94	0.16	1.23	32,49,77,84	0
21	CLA	j	1104	65/65	0.82	0.35	1.22	77,110,125,133	0
21	CLA	2	822	52/65	0.71	0.34	1.22	99,130,138,139	0
21	CLA	l	205	65/65	0.94	0.20	1.21	31,54,99,101	0
33	MG	B	854	1/1	0.86	0.23	1.21	69,69,69,69	0
24	BCR	0	205	40/40	0.89	0.24	1.21	41,60,87,92	0
21	CLA	2	821	50/65	0.77	0.32	1.21	91,127,138,139	0
21	CLA	b	1820	65/65	0.93	0.20	1.19	33,49,89,98	0
21	CLA	A	806	65/65	0.93	0.16	1.19	44,68,92,95	0
21	CLA	F	203	65/65	0.87	0.22	1.19	70,93,105,114	0
21	CLA	a	838	65/65	0.87	0.20	1.17	64,86,103,105	0
21	CLA	l	204	65/65	0.95	0.19	1.16	30,55,103,110	0
21	CLA	1	855	65/65	0.93	0.18	1.15	30,51,61,76	0
21	CLA	B	812	65/65	0.87	0.23	1.15	67,88,123,127	0
21	CLA	B	821	65/65	0.90	0.25	1.15	62,91,123,125	0
25	LHG	A	851	49/49	0.93	0.21	1.13	29,62,101,107	0
21	CLA	B	820	65/65	0.90	0.23	1.12	64,93,113,116	0
25	LHG	B	849	49/49	0.86	0.25	1.12	73,87,96,101	0
21	CLA	A	810	65/65	0.93	0.17	1.11	36,54,65,74	0
21	CLA	B	814	65/65	0.91	0.17	1.08	45,76,102,107	0
21	CLA	2	825	45/65	0.86	0.27	1.07	114,124,128,132	0
24	BCR	k	1403	40/40	0.22	0.61	1.07	119,152,167,168	0
21	CLA	1	823	55/65	0.90	0.20	1.07	58,96,124,128	0
21	CLA	a	828	65/65	0.91	0.24	1.06	71,91,104,105	0
24	BCR	0	204	40/40	0.92	0.17	1.06	35,57,67,69	0
21	CLA	b	1818	65/65	0.93	0.17	1.05	41,53,87,97	0
21	CLA	J	1101	65/65	0.96	0.15	1.05	32,50,68,74	0
24	BCR	b	1845	40/40	0.86	0.21	1.04	36,60,76,87	0
21	CLA	B	833	65/65	0.87	0.22	1.04	66,84,101,104	0
24	BCR	l	206	40/40	0.90	0.23	1.03	29,44,54,56	0
21	CLA	1	819	65/65	0.86	0.31	1.03	57,99,112,123	0
21	CLA	2	814	45/65	0.75	0.36	1.03	104,130,139,142	0
21	CLA	A	815	65/65	0.93	0.18	1.02	56,75,111,116	0
24	BCR	8	1403	40/40	0.52	0.54	1.02	105,124,139,140	0
21	CLA	a	824	65/65	0.89	0.23	1.00	61,95,108,113	0
30	ECH	b	1847	41/41	0.91	0.16	0.99	32,47,97,99	0
21	CLA	B	837	50/65	0.93	0.27	0.99	44,63,96,101	0
21	CLA	A	803	65/65	0.95	0.14	0.99	32,49,106,120	0
21	CLA	B	811	65/65	0.93	0.16	0.99	53,76,108,111	0
25	LHG	1	850	49/49	0.90	0.23	0.99	64,84,101,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	A	808	65/65	0.93	0.17	0.96	42,56,121,124	0
25	LHG	A	849	49/49	0.95	0.18	0.96	31,47,61,64	0
21	CLA	B	832	65/65	0.95	0.19	0.93	40,60,80,85	0
22	PQN	a	841	33/33	0.91	0.24	0.92	39,65,84,87	0
24	BCR	b	1848	40/40	0.89	0.21	0.91	41,58,68,71	0
23	SF4	C	102	8/8	0.92	0.14	0.87	53,74,78,84	0
21	CLA	B	827	65/65	0.93	0.20	0.87	28,52,78,87	0
26	LMG	K	105	55/55	0.78	0.24	0.86	41,80,106,107	0
21	CLA	L	204	65/65	0.95	0.20	0.86	21,36,98,103	0
21	CLA	b	1814	60/65	0.91	0.15	0.86	36,53,91,103	0
21	CLA	B	808	65/65	0.95	0.16	0.85	32,50,67,83	0
26	LMG	2	850	55/55	0.87	0.26	0.84	55,72,93,107	0
25	LHG	B	857	49/49	0.63	0.38	0.84	90,126,165,169	0
21	CLA	1	821	65/65	0.92	0.27	0.84	53,75,92,112	0
24	BCR	A	847	40/40	0.94	0.25	0.83	17,46,78,82	0
21	CLA	B	835	65/65	0.91	0.22	0.81	39,73,95,100	0
21	CLA	B	816	65/65	0.91	0.18	0.81	58,80,112,120	0
21	CLA	a	807	58/65	0.88	0.25	0.81	78,110,122,129	0
21	CLA	b	1831	65/65	0.95	0.21	0.81	23,41,59,63	0
21	CLA	A	809	53/65	0.93	0.19	0.81	30,57,91,92	0
21	CLA	2	818	50/65	0.81	0.35	0.80	99,122,130,139	0
21	CLA	A	834	65/65	0.92	0.19	0.79	25,57,107,111	0
21	CLA	2	834	65/65	0.86	0.26	0.79	83,109,124,136	0
25	LHG	b	1852	49/49	0.90	0.23	0.78	63,80,101,105	0
24	BCR	f	204	40/40	0.88	0.22	0.78	66,81,104,107	0
21	CLA	1	824	60/65	0.93	0.18	0.78	47,75,101,106	0
21	CLA	A	828	65/65	0.93	0.24	0.77	22,42,59,64	0
21	CLA	a	825	65/65	0.83	0.30	0.76	55,105,117,121	0
21	CLA	a	813	65/65	0.86	0.28	0.76	76,106,131,133	0
24	BCR	a	845	40/40	0.72	0.39	0.75	81,121,142,146	0
21	CLA	A	835	65/65	0.94	0.17	0.75	25,42,100,107	0
24	BCR	1	848	40/40	0.89	0.24	0.75	49,69,93,95	0
21	CLA	2	824	53/65	0.81	0.23	0.74	108,125,148,156	0
21	CLA	2	819	59/65	0.84	0.25	0.74	70,109,135,159	0
21	CLA	b	1840	65/65	0.87	0.25	0.73	48,74,118,122	0
24	BCR	a	844	40/40	0.74	0.27	0.73	108,123,141,142	0
21	CLA	a	802	65/65	0.94	0.25	0.72	34,53,90,92	0
21	CLA	B	818	65/65	0.94	0.26	0.71	33,57,92,99	0
21	CLA	B	817	65/65	0.91	0.22	0.70	48,81,89,92	0
25	LHG	I	103	49/49	0.86	0.17	0.70	44,63,131,140	0
21	CLA	2	840	65/65	0.96	0.15	0.69	36,52,61,75	0
21	CLA	B	801	65/65	0.96	0.19	0.69	19,36,44,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	1	805	65/65	0.84	0.25	0.69	63,87,101,103	0
21	CLA	A	807	65/65	0.95	0.14	0.68	26,45,71,87	0
24	BCR	K	104	40/40	0.62	0.38	0.68	40,73,103,106	0
21	CLA	K	102	65/65	0.93	0.22	0.67	33,63,97,102	15
21	CLA	b	1842	65/65	0.95	0.23	0.67	36,51,62,84	0
21	CLA	0	201	65/65	0.95	0.18	0.67	37,47,74,82	0
21	CLA	a	818	60/65	0.86	0.27	0.67	79,99,109,110	0
21	CLA	a	832	65/65	0.96	0.17	0.66	36,58,68,71	0
21	CLA	b	1810	65/65	0.95	0.15	0.66	26,40,78,108	0
25	LHG	a	849	49/49	0.91	0.25	0.65	57,72,117,128	0
21	CLA	b	1843	65/65	0.89	0.23	0.65	60,88,134,154	0
21	CLA	b	1835	65/65	0.92	0.22	0.64	54,68,97,108	0
21	CLA	j	1103	65/65	0.90	0.22	0.64	53,86,120,125	0
21	CLA	1	825	65/65	0.85	0.28	0.64	49,86,107,115	0
21	CLA	1	839	60/65	0.81	0.28	0.64	84,118,134,136	0
34	C7Z	F	204	42/42	0.92	0.16	0.63	46,72,98,103	0
21	CLA	a	803	65/65	0.95	0.21	0.63	37,49,59,65	0
28	45D	A	856	42/42	0.94	0.18	0.62	31,49,61,69	0
21	CLA	m	103	65/65	0.95	0.15	0.62	30,44,81,84	0
21	CLA	B	822	65/65	0.88	0.19	0.62	73,94,125,126	0
21	CLA	A	816	65/65	0.93	0.21	0.62	41,57,69,72	0
24	BCR	b	1846	40/40	0.90	0.19	0.61	30,47,90,91	0
30	ECH	a	857	41/41	0.88	0.28	0.60	60,81,90,94	0
21	CLA	2	817	41/65	0.77	0.34	0.60	100,132,137,144	0
21	CLA	A	840	65/65	0.95	0.18	0.59	25,43,66,76	0
21	CLA	a	829	65/65	0.94	0.31	0.58	50,80,108,110	0
21	CLA	I	101	65/65	0.94	0.17	0.58	28,39,61,68	0
21	CLA	2	810	65/65	0.90	0.20	0.57	54,77,89,91	0
22	PQN	A	841	33/33	0.95	0.18	0.57	30,46,57,64	0
21	CLA	2	807	65/65	0.83	0.26	0.57	56,94,106,108	0
21	CLA	1	827	65/65	0.91	0.28	0.56	56,78,91,94	0
21	CLA	A	839	65/65	0.93	0.17	0.56	43,59,83,91	0
21	CLA	b	1807	65/65	0.95	0.23	0.55	34,51,66,80	0
21	CLA	2	815	65/65	0.88	0.23	0.55	75,107,116,119	0
21	CLA	6	203	47/65	0.84	0.22	0.54	99,128,135,136	0
22	PQN	B	841	33/33	0.97	0.17	0.54	24,35,39,48	0
21	CLA	B	831	65/65	0.91	0.20	0.54	44,66,113,122	0
21	CLA	2	829	55/65	0.93	0.21	0.53	53,70,95,110	0
24	BCR	L	206	40/40	0.95	0.17	0.53	24,38,45,52	0
21	CLA	A	833	65/65	0.92	0.19	0.52	28,48,78,81	0
21	CLA	b	1830	65/65	0.93	0.19	0.52	33,48,83,87	0
21	CLA	b	1815	65/65	0.93	0.14	0.51	40,57,100,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	PQN	2	843	33/33	0.94	0.18	0.51	42,57,70,78	0
21	CLA	A	813	65/65	0.91	0.17	0.51	39,62,94,98	0
21	CLA	2	820	60/65	0.87	0.23	0.51	73,100,112,118	0
21	CLA	a	835	65/65	0.92	0.22	0.49	42,69,151,157	0
26	LMG	B	848	55/55	0.91	0.19	0.49	36,52,81,89	0
21	CLA	a	814	65/65	0.80	0.26	0.49	74,129,135,137	0
21	CLA	2	823	65/65	0.81	0.31	0.49	91,133,158,162	0
21	CLA	b	1812	65/65	0.92	0.17	0.49	28,48,62,80	0
21	CLA	B	826	65/65	0.94	0.27	0.49	54,67,78,95	0
21	CLA	2	826	65/65	0.87	0.25	0.48	84,95,132,137	0
21	CLA	1	807	50/65	0.80	0.28	0.48	96,116,123,126	0
21	CLA	B	804	65/65	0.96	0.22	0.47	21,33,45,55	0
21	CLA	A	819	65/65	0.94	0.19	0.45	38,52,84,89	0
21	CLA	2	835	46/65	0.78	0.27	0.44	84,122,128,129	0
21	CLA	L	205	65/65	0.92	0.18	0.44	35,54,82,87	0
21	CLA	A	832	65/65	0.96	0.15	0.43	21,35,44,51	0
21	CLA	F	202	65/65	0.89	0.22	0.43	53,77,121,124	0
21	CLA	A	855	65/65	0.95	0.21	0.43	21,34,54,61	0
21	CLA	2	802	55/65	0.95	0.14	0.43	29,53,83,95	0
21	CLA	A	826	65/65	0.92	0.21	0.43	22,46,61,65	0
21	CLA	1	831	50/65	0.96	0.15	0.43	49,63,76,78	0
21	CLA	a	809	50/65	0.89	0.18	0.43	68,88,108,112	0
21	CLA	1	832	65/65	0.95	0.17	0.42	35,47,69,74	0
21	CLA	A	804	65/65	0.94	0.20	0.42	25,41,61,66	0
21	CLA	a	827	65/65	0.88	0.24	0.42	64,91,106,111	0
21	CLA	B	828	65/65	0.93	0.25	0.42	41,61,70,76	0
21	CLA	2	827	50/65	0.86	0.32	0.41	69,105,119,122	0
30	ECH	l	202	41/41	0.91	0.22	0.41	38,53,83,90	0
21	CLA	a	830	65/65	0.90	0.20	0.38	59,86,97,102	0
21	CLA	A	837	65/65	0.96	0.20	0.38	24,38,111,116	0
21	CLA	a	801	65/65	0.86	0.20	0.38	40,58,71,96	0
24	BCR	1	845	40/40	0.85	0.24	0.38	89,100,119,123	0
24	BCR	L	207	40/40	0.89	0.21	0.37	41,57,81,86	0
30	ECH	B	844	41/41	0.89	0.19	0.36	45,86,105,108	0
21	CLA	a	815	50/65	0.62	0.47	0.36	116,145,155,159	0
21	CLA	A	802	65/65	0.95	0.21	0.35	23,47,57,65	0
21	CLA	B	809	65/65	0.95	0.15	0.35	34,43,69,74	0
21	CLA	A	827	65/65	0.93	0.15	0.35	28,48,62,75	0
21	CLA	2	805	65/65	0.92	0.20	0.35	46,60,68,82	0
21	CLA	b	1828	65/65	0.90	0.25	0.34	38,54,114,118	0
21	CLA	B	810	65/65	0.96	0.15	0.33	31,43,60,72	0
30	ECH	M	7002	41/41	0.92	0.15	0.33	45,61,74,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	A	829	65/65	0.94	0.17	0.32	29,43,62,86	0
21	CLA	A	838	65/65	0.94	0.16	0.31	46,61,68,73	0
21	CLA	b	1822	65/65	0.93	0.16	0.31	41,57,91,102	0
21	CLA	B	805	65/65	0.95	0.14	0.30	37,48,80,91	0
21	CLA	b	1834	65/65	0.91	0.18	0.30	58,73,117,121	0
21	CLA	b	1804	65/65	0.94	0.15	0.29	52,68,111,119	0
24	BCR	a	843	40/40	0.72	0.34	0.29	89,142,156,156	0
21	CLA	1	841	56/65	0.94	0.15	0.28	62,76,106,112	0
26	LMG	b	1851	55/55	0.91	0.20	0.27	36,55,84,89	0
21	CLA	b	1824	65/65	0.93	0.19	0.27	46,66,101,102	0
21	CLA	b	1838	53/65	0.93	0.19	0.27	40,57,75,91	0
21	CLA	a	855	65/65	0.96	0.22	0.25	25,57,101,103	0
21	CLA	a	823	65/65	0.88	0.28	0.24	94,117,142,146	0
21	CLA	B	829	65/65	0.93	0.18	0.24	31,51,70,79	0
21	CLA	A	854	65/65	0.95	0.17	0.24	31,44,63,73	0
21	CLA	a	837	51/65	0.95	0.17	0.23	43,63,109,113	0
21	CLA	a	821	65/65	0.88	0.27	0.23	54,82,128,133	0
21	CLA	j	1101	65/65	0.87	0.21	0.23	50,83,91,100	0
21	CLA	2	803	65/65	0.90	0.26	0.22	72,88,98,101	0
21	CLA	2	811	65/65	0.91	0.17	0.18	44,66,80,88	0
21	CLA	A	824	65/65	0.92	0.18	0.18	25,38,52,60	0
21	CLA	2	806	65/65	0.93	0.16	0.18	61,77,86,90	0
21	CLA	A	805	65/65	0.93	0.21	0.18	19,41,62,64	0
21	CLA	2	816	50/65	0.90	0.16	0.17	80,110,117,123	0
21	CLA	a	811	65/65	0.89	0.20	0.17	65,102,118,124	0
21	CLA	f	202	50/65	0.91	0.15	0.17	74,93,114,116	0
21	CLA	b	1821	65/65	0.95	0.17	0.17	28,48,68,83	0
21	CLA	1	829	65/65	0.89	0.28	0.16	64,86,112,118	0
21	CLA	1	808	65/65	0.92	0.21	0.15	49,91,119,122	0
21	CLA	2	804	65/65	0.92	0.24	0.15	45,67,114,117	0
21	CLA	b	1832	65/65	0.93	0.17	0.15	26,50,71,76	0
21	CLA	A	811	65/65	0.96	0.22	0.14	30,47,124,127	0
21	CLA	a	806	65/65	0.94	0.23	0.13	40,68,105,111	0
21	CLA	1	806	65/65	0.87	0.27	0.12	65,91,99,106	0
21	CLA	A	820	65/65	0.93	0.18	0.12	27,39,52,56	0
21	CLA	b	1841	65/65	0.94	0.17	0.12	30,52,63,69	0
21	CLA	1	810	47/65	0.76	0.33	0.11	50,112,123,128	0
21	CLA	1	840	65/65	0.93	0.20	0.08	60,77,119,120	0
21	CLA	2	830	65/65	0.88	0.22	0.08	52,92,111,114	0
21	CLA	b	1809	65/65	0.96	0.19	0.08	25,45,60,64	0
21	CLA	2	812	56/65	0.96	0.14	0.08	29,46,78,86	0
21	CLA	2	808	65/65	0.90	0.26	0.07	57,88,101,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	L	203	65/65	0.95	0.18	0.07	33,51,91,94	0
21	CLA	1	802	65/65	0.85	0.28	0.06	73,91,97,104	0
21	CLA	1	830	65/65	0.90	0.21	0.05	62,79,99,113	0
21	CLA	b	1801	65/65	0.94	0.14	0.05	22,47,108,110	0
21	CLA	K	103	65/65	0.91	0.20	0.04	50,71,111,115	10
21	CLA	1	828	65/65	0.90	0.23	0.04	58,94,108,115	0
21	CLA	a	816	52/65	0.78	0.34	0.04	119,138,150,152	0
25	LHG	2	851	49/49	0.74	0.41	0.04	92,108,152,153	0
21	CLA	1	833	65/65	0.94	0.14	0.01	23,48,63,71	0
21	CLA	b	1808	65/65	0.94	0.16	-0.00	26,43,52,57	0
21	CLA	2	831	55/65	0.92	0.20	-0.01	55,70,91,97	0
21	CLA	B	806	65/65	0.92	0.16	-0.01	32,54,66,69	0
21	CLA	b	1813	65/65	0.95	0.16	-0.02	32,50,71,81	0
21	CLA	B	824	65/65	0.93	0.18	-0.03	50,62,95,98	0
21	CLA	1	838	51/65	0.93	0.18	-0.03	48,65,76,87	0
21	CLA	1	820	65/65	0.87	0.22	-0.04	79,103,130,134	0
21	CLA	A	801	65/65	0.94	0.14	-0.04	20,37,61,79	0
24	BCR	A	843	40/40	0.93	0.15	-0.06	35,52,68,68	0
21	CLA	6	201	65/65	0.80	0.28	-0.08	75,115,124,125	0
21	CLA	a	820	65/65	0.80	0.24	-0.09	102,119,142,150	0
21	CLA	1	834	65/65	0.88	0.20	-0.09	73,87,99,107	0
21	CLA	1	813	65/65	0.91	0.19	-0.09	63,85,113,118	0
21	CLA	A	823	60/65	0.92	0.16	-0.10	25,42,70,83	0
21	CLA	2	838	53/65	0.83	0.25	-0.10	82,112,122,123	0
21	CLA	B	815	55/65	0.92	0.17	-0.10	70,82,128,132	0
23	SF4	a	842	8/8	0.99	0.16	-0.10	61,65,75,77	0
21	CLA	b	1806	65/65	0.90	0.18	-0.10	36,52,66,72	0
21	CLA	b	1829	65/65	0.96	0.18	-0.11	33,55,83,86	0
21	CLA	B	813	65/65	0.91	0.16	-0.11	38,67,90,92	0
21	CLA	a	839	65/65	0.95	0.21	-0.11	48,70,93,95	0
21	CLA	1	822	65/65	0.83	0.20	-0.11	85,102,126,128	0
21	CLA	B	807	65/65	0.95	0.21	-0.11	33,50,69,75	0
21	CLA	a	826	55/65	0.93	0.20	-0.12	45,59,117,127	0
21	CLA	1	815	44/65	0.82	0.31	-0.12	83,124,133,135	0
21	CLA	1	817	65/65	0.86	0.23	-0.14	78,119,130,131	0
21	CLA	b	1816	65/65	0.94	0.14	-0.15	31,43,63,68	0
21	CLA	b	1805	65/65	0.92	0.16	-0.15	50,77,85,90	0
21	CLA	b	1827	65/65	0.95	0.15	-0.16	31,50,85,99	0
21	CLA	A	822	65/65	0.93	0.17	-0.16	28,48,130,132	0
21	CLA	l	201	65/65	0.96	0.14	-0.16	37,57,66,71	0
21	CLA	2	837	50/65	0.81	0.25	-0.16	90,107,111,113	0
21	CLA	b	1839	65/65	0.92	0.18	-0.17	45,80,93,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	B	834	50/65	0.86	0.23	-0.18	81,92,105,108	0
21	CLA	A	825	65/65	0.95	0.19	-0.18	23,35,118,122	0
21	CLA	2	828	55/65	0.91	0.26	-0.21	64,99,141,145	0
21	CLA	b	1811	65/65	0.96	0.13	-0.22	28,43,59,65	0
21	CLA	1	803	65/65	0.94	0.18	-0.23	34,62,74,74	0
21	CLA	0	203	65/65	0.94	0.15	-0.23	43,56,82,99	0
21	CLA	a	822	55/65	0.80	0.26	-0.27	98,124,129,138	0
21	CLA	1	818	65/65	0.86	0.22	-0.27	75,95,118,121	0
21	CLA	2	841	65/65	0.94	0.18	-0.27	39,57,93,104	0
21	CLA	2	809	65/65	0.93	0.17	-0.29	35,67,89,91	0
21	CLA	a	810	57/65	0.81	0.22	-0.30	91,124,129,130	0
21	CLA	2	813	60/65	0.88	0.18	-0.31	63,88,138,142	0
21	CLA	1	801	65/65	0.93	0.18	-0.31	38,62,88,103	0
21	CLA	a	856	65/65	0.93	0.16	-0.32	36,55,71,76	0
21	CLA	a	834	49/65	0.88	0.17	-0.33	73,118,128,132	0
23	SF4	1	843	8/8	0.94	0.17	-0.33	57,66,94,130	0
21	CLA	7	1103	47/65	0.86	0.18	-0.34	89,114,127,129	0
21	CLA	a	831	52/65	0.90	0.17	-0.35	64,85,95,98	0
21	CLA	a	812	59/65	0.88	0.23	-0.36	77,109,156,159	0
21	CLA	1	804	55/65	0.90	0.21	-0.36	50,81,117,120	0
21	CLA	1	836	52/65	0.93	0.17	-0.39	53,69,89,108	0
21	CLA	1	814	50/65	0.89	0.23	-0.41	83,109,122,126	0
21	CLA	A	836	65/65	0.96	0.13	-0.43	21,42,68,77	0
21	CLA	1	826	56/65	0.92	0.22	-0.45	44,66,87,93	0
21	CLA	A	821	65/65	0.93	0.13	-0.46	30,53,102,104	0
21	CLA	7	1101	65/65	0.91	0.22	-0.50	58,88,120,123	0
21	CLA	1	809	51/65	0.89	0.17	-0.51	83,102,117,121	0
21	CLA	8	1402	46/65	0.93	0.19	-0.53	103,119,135,139	5
21	CLA	1	816	45/65	0.84	0.36	-0.53	107,117,125,129	0
33	MG	b	1857	1/1	0.95	0.12	-0.60	54,54,54,54	0
21	CLA	1	835	65/65	0.81	0.23	-0.60	89,105,120,125	0
32	CA	L	202	1/1	0.98	0.08	-0.65	44,44,44,44	0
21	CLA	b	1823	51/65	0.95	0.10	-0.66	32,56,86,95	0
21	CLA	2	832	45/65	0.88	0.18	-0.66	81,94,127,131	0
21	CLA	B	803	65/65	0.95	0.14	-0.66	30,42,53,61	0
21	CLA	a	817	65/65	0.80	0.28	-0.72	89,133,152,154	0
21	CLA	1	837	65/65	0.95	0.13	-0.74	46,66,77,83	0
21	CLA	k	1402	49/65	0.77	0.26	-0.75	134,158,161,161	8
23	SF4	3	101	8/8	0.94	0.13	-0.75	65,73,110,240	0
21	CLA	1	812	50/65	0.92	0.15	-0.82	70,91,137,157	0
21	CLA	2	833	45/65	0.91	0.16	-0.85	53,67,126,132	0
21	CLA	2	839	50/65	0.87	0.27	-0.87	75,110,117,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	8	1401	45/65	0.91	0.12	-0.90	83,101,137,143	3
21	CLA	k	1401	50/65	0.80	0.24	-1.02	84,137,147,152	5
32	CA	B	853	1/1	0.98	0.10	-1.39	80,80,80,80	0
23	SF4	c	102	8/8	0.98	0.09	-1.45	57,78,82,85	0
29	CL	a	858	1/1	0.97	0.11	-1.72	53,53,53,53	0
23	SF4	3	102	8/8	0.98	0.07	-1.75	75,88,175,321	0
32	CA	L	212	1/1	0.96	0.04	-1.98	55,55,55,55	0
32	CA	2	853	1/1	0.89	0.06	-2.02	112,112,112,112	0
23	SF4	c	101	8/8	0.98	0.11	-2.24	53,57,64,76	0
32	CA	l	212	1/1	0.98	0.04	-2.51	56,56,56,56	0
29	CL	A	857	1/1	0.99	0.04	-2.65	36,36,36,36	0
32	CA	b	1856	1/1	0.96	0.06	-5.05	61,61,61,61	0
25	LHG	b	1803	49/49	0.77	0.32	-	46,85,113,121	0
24	BCR	a	848	40/40	0.74	0.53	-	98,114,155,155	0
25	LHG	l	210	49/49	0.69	0.26	-	48,75,159,163	0
31	SQD	b	1854	54/54	0.72	0.32	-	46,81,138,143	0
27	ACT	a	854	4/4	0.55	0.18	-	128,130,130,131	0
21	CLA	2	842	41/65	0.76	0.48	-	131,137,146,150	0
25	LHG	B	858	49/49	0.72	0.46	-	80,102,149,154	0
27	ACT	D	201	4/4	0.91	0.11	-	78,82,83,84	0
25	LHG	6	206	12/49	0.75	0.23	-	80,131,152,159	0
25	LHG	2	801	49/49	0.70	0.69	-	100,139,169,175	0
35	LMT	1	854	35/35	0.72	0.40	-	76,127,136,141	0
25	LHG	I	104	49/49	0.73	0.30	-	55,96,124,136	0

6.5 Other polymers

There are no such residues in this entry.