



wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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

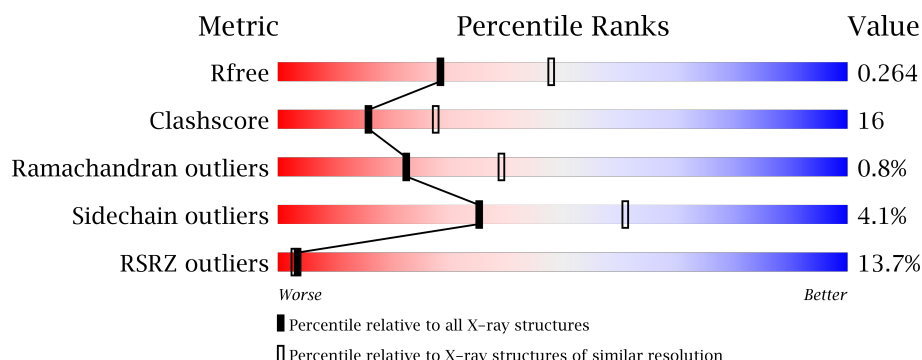
1 Overall quality at a glance ⓘ

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.



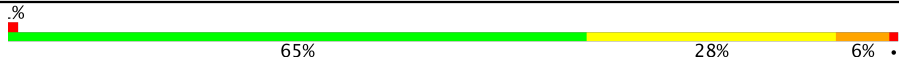

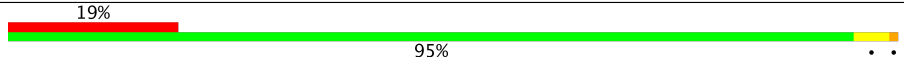
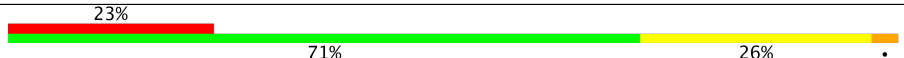
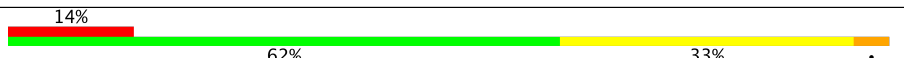
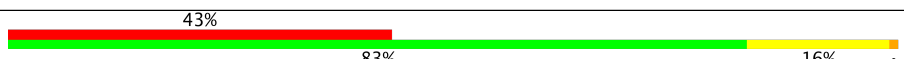
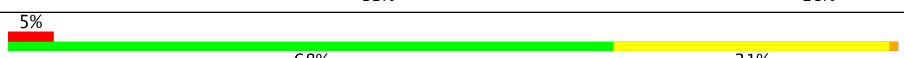

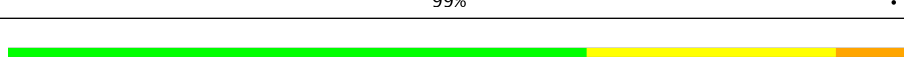

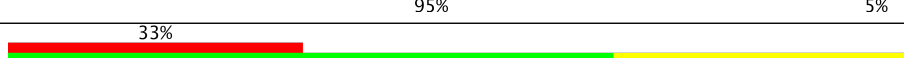

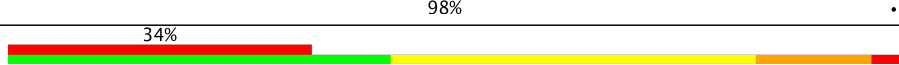
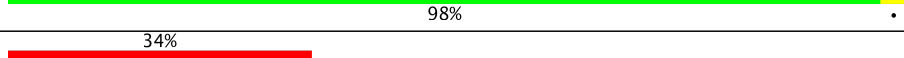


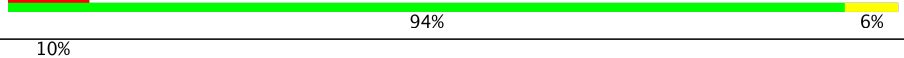

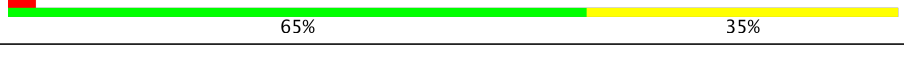
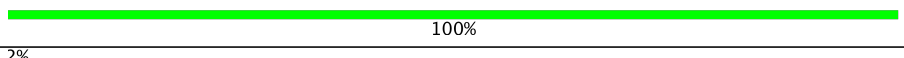
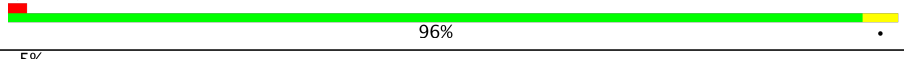
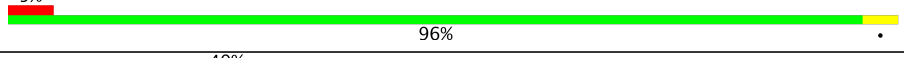
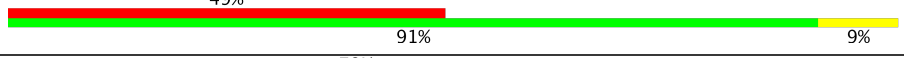


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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			

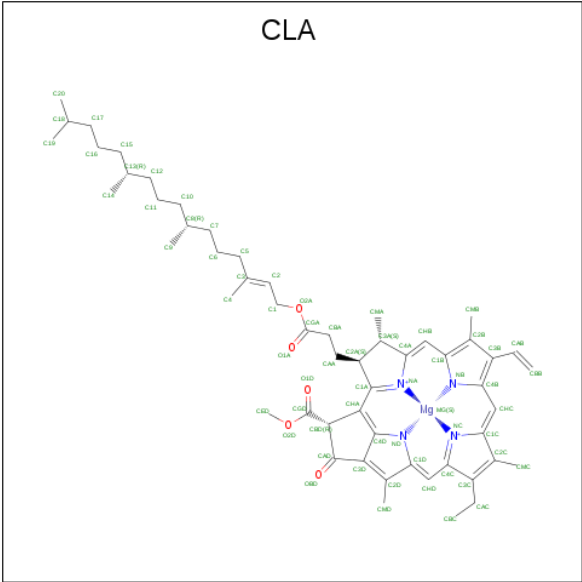
- Molecule 19 is a protein called Photosystem I reaction center subunit PsaK 2.

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
			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 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	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 60	C 50	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	A	1	Total 58	C 48	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

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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 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 58	C 48	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 50	C 40	Mg 1	N 4	O 5	0	0
21	a	1	Total 57	C 47	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 59	C 49	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 50	C 40	Mg 1	N 4	O 5	0	0
21	a	1	Total 52	C 42	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 60	C 50	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 55	C 45	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
			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 55	C 45	Mg 1	N 4	O 5	0	0
21	k	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	k	1	Total 49	C 39	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	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	m	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
21	1	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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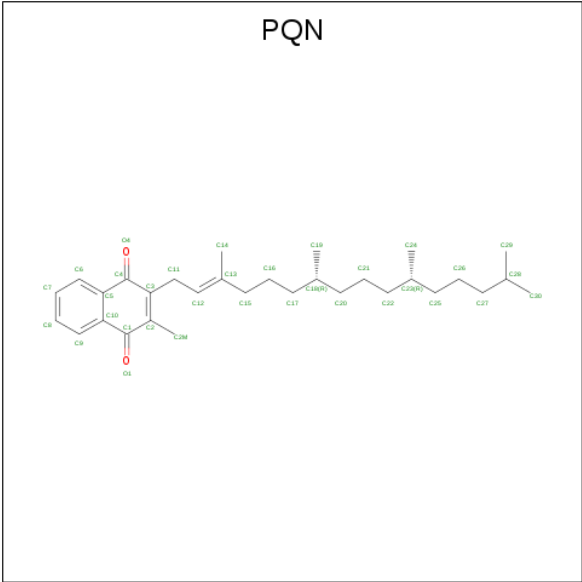
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5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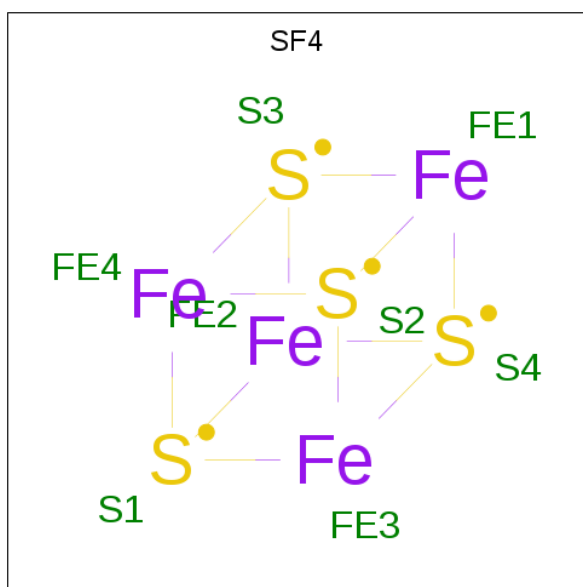
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



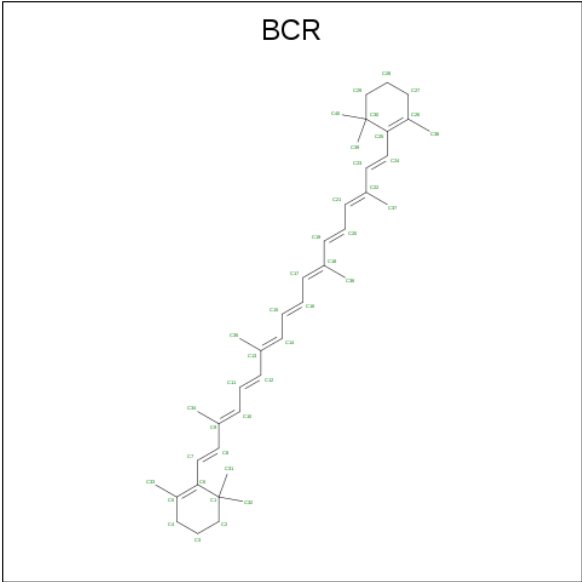
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			33	31	2		
22	B	1	Total	C	O	0	0
			33	31	2		
22	a	1	Total	C	O	0	0
			33	31	2		
22	b	1	Total	C	O	0	0
			33	31	2		
22	1	1	Total	C	O	0	0
			33	31	2		
22	2	1	Total	C	O	0	0
			33	31	2		

- 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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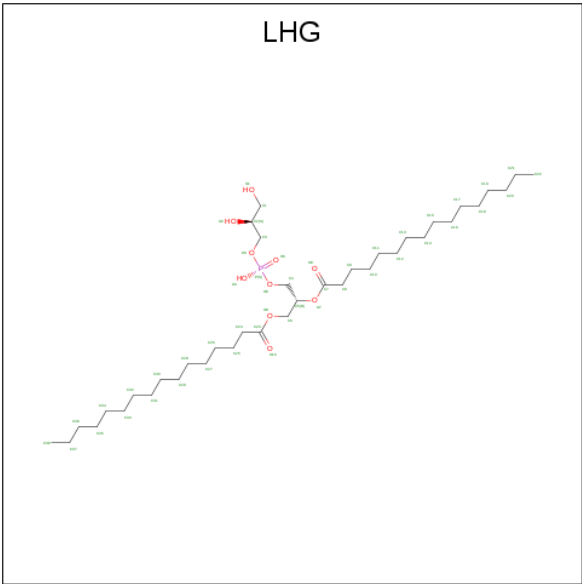
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	2	1	Total 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).



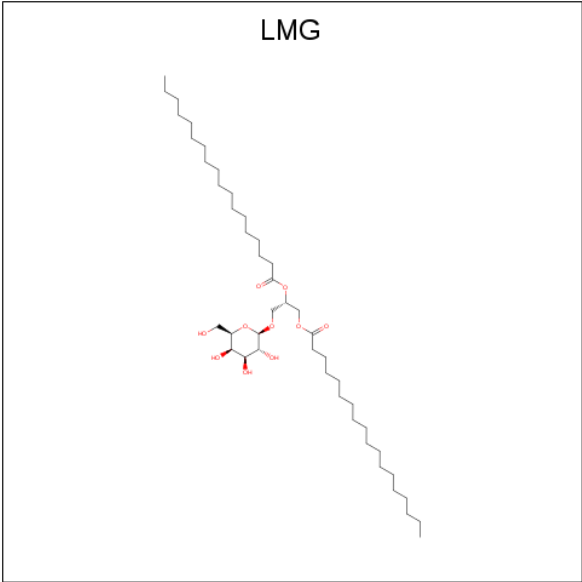
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 49 38 10 1	0	0
25	A	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	B	1	Total C O P 49 38 10 1	0	0
25	I	1	Total C O P 49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



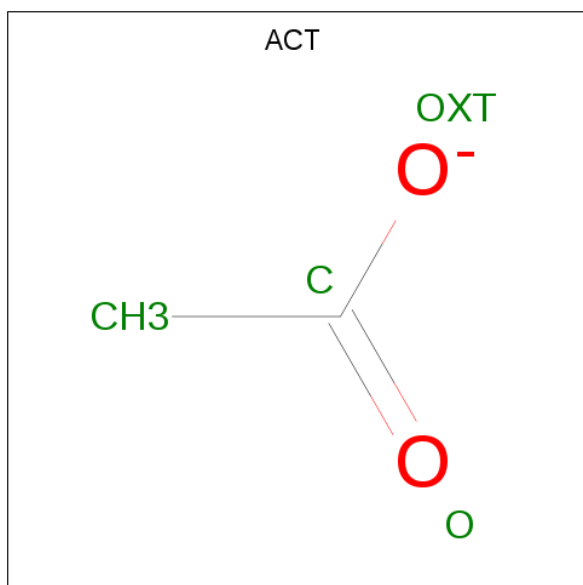
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			50	40	10		
26	A	1	Total	C	O	0	0
			48	38	10		
26	B	1	Total	C	O	0	0
			55	45	10		
26	B	1	Total	C	O	0	0
			55	45	10		
26	K	1	Total	C	O	0	0
			55	45	10		
26	K	1	Total	C	O	0	0
			55	45	10		
26	a	1	Total	C	O	0	0
			50	40	10		
26	a	1	Total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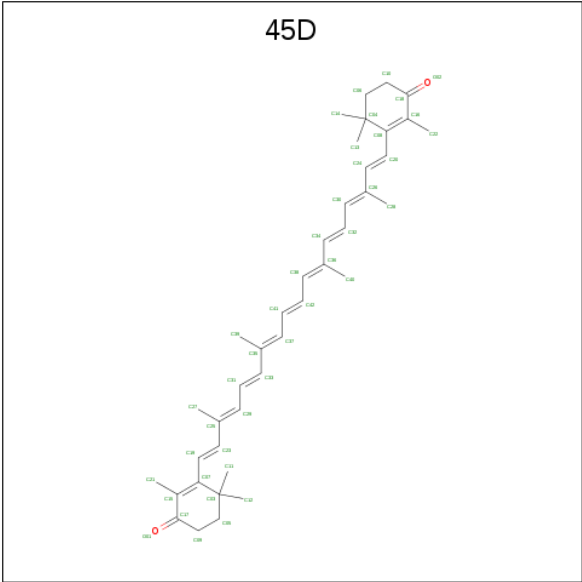
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	2	1	Total	C	O	0	0
			55	45	10		
26	0	1	Total	C	O	0	0
			55	45	10		

- 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: $C_{40}H_{52}O_2$).

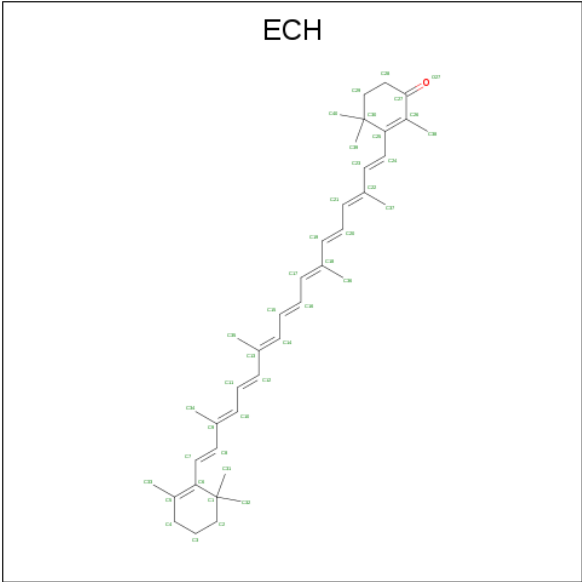


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			42	40	2		
28	2	1	Total	C	O	0	0
			42	40	2		

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

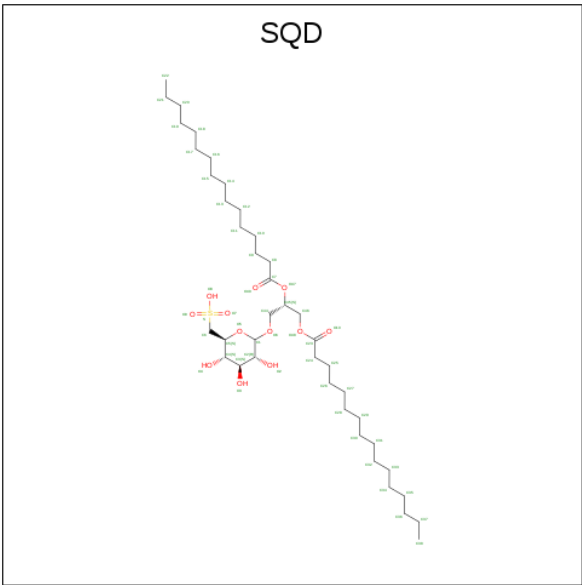
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	1	1	Total	Cl	0	0
			1	1		
29	A	1	Total	Cl	0	0
			1	1		
29	a	1	Total	Cl	0	0
			1	1		

- 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		

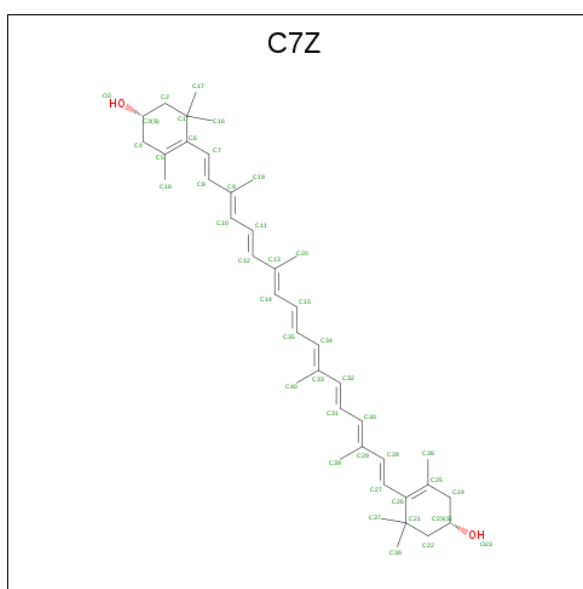
- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

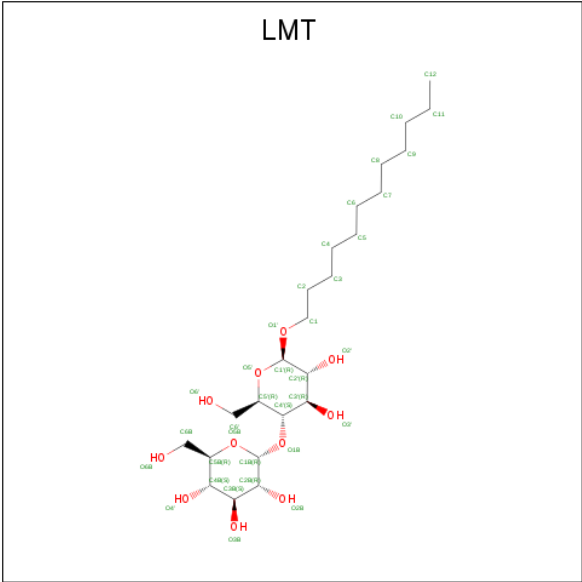
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Mg	0	0
			1	1		
33	b	1	Total	Mg	0	0
			1	1		

- 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).



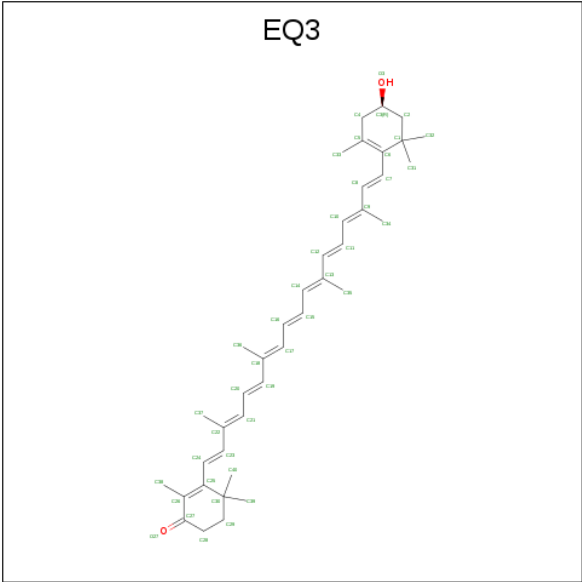
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			42	40	2		
34	F	1	Total	C	O	0	0
			42	40	2		
34	b	1	Total	C	O	0	0
			42	40	2		
34	2	1	Total	C	O	0	0
			42	40	2		

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



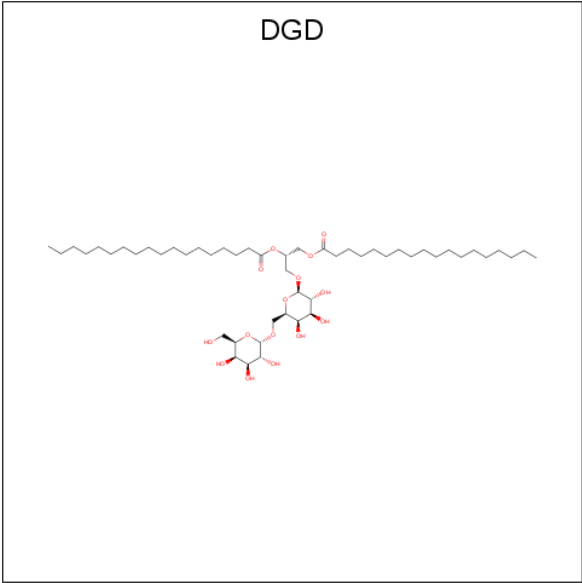
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	J	1	Total	C	O	0	0
			35	24	11		
35	L	1	Total	C	O	0	0
			35	24	11		
35	l	1	Total	C	O	0	0
			35	24	11		
35	1	1	Total	C	O	0	0
			35	24	11		
35	0	1	Total	C	O	0	0
			35	24	11		

- 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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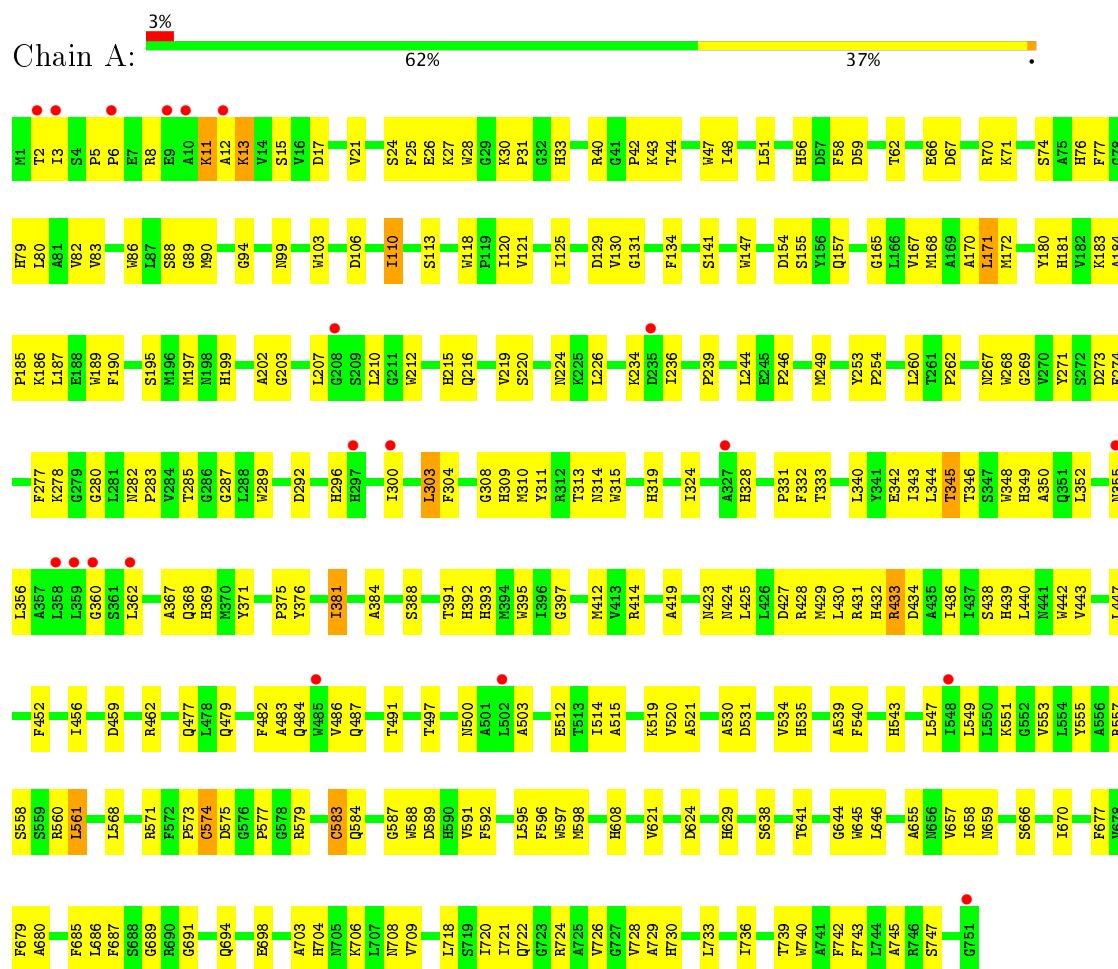
Continued from previous page...

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

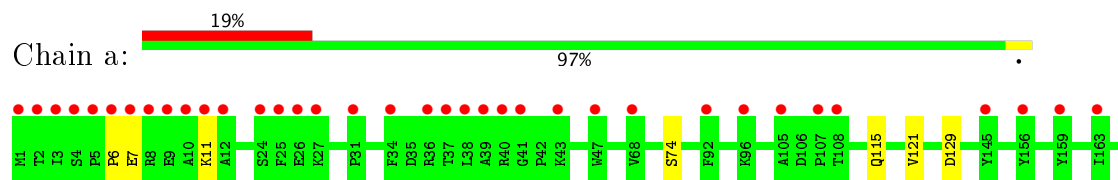
3 Residue-property plots

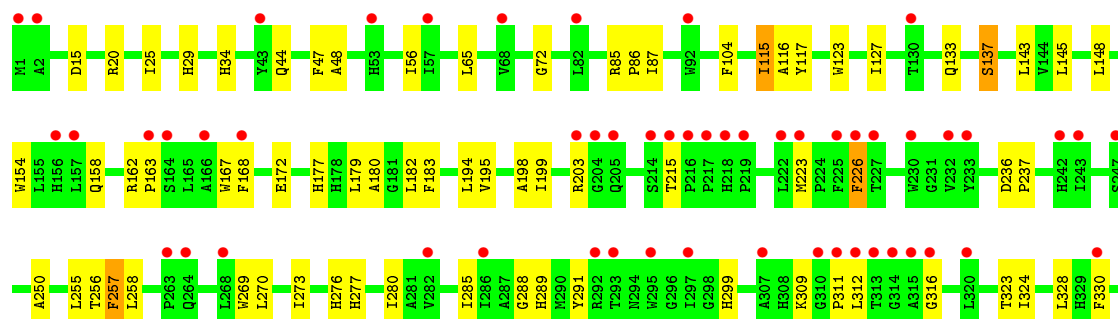
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

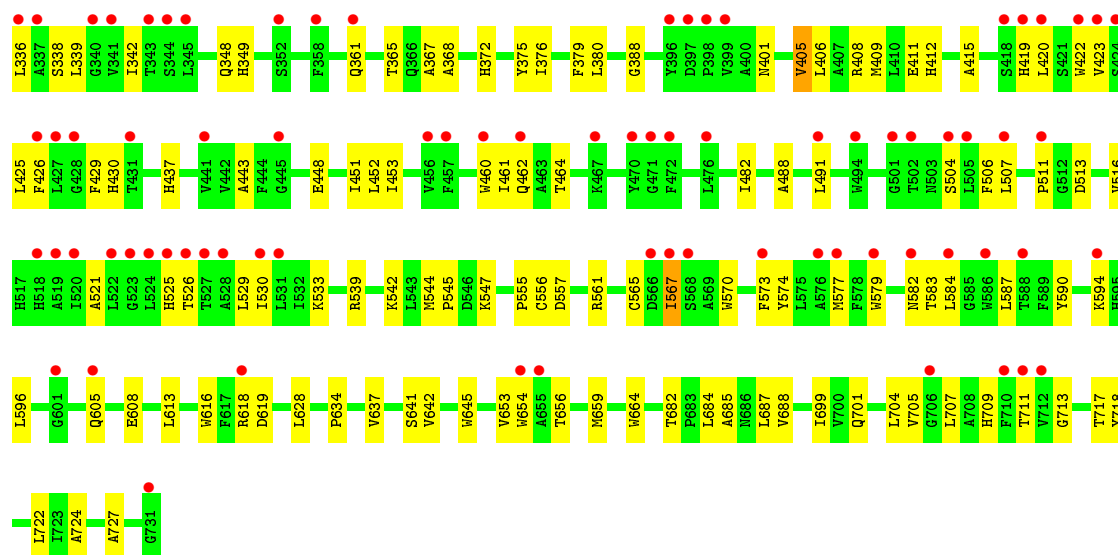
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



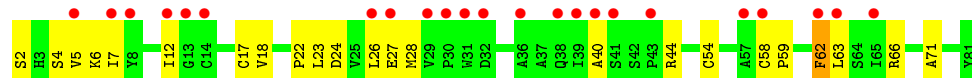




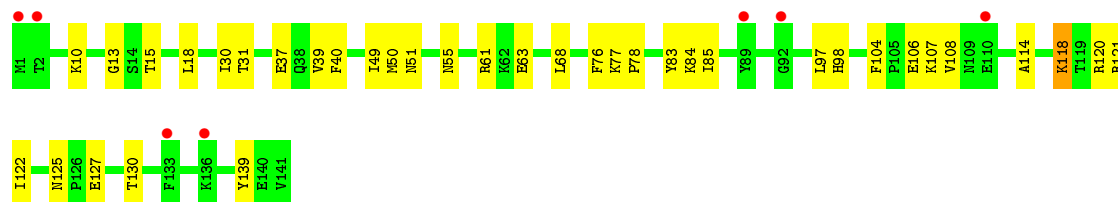
• Molecule 3: Photosystem I iron-sulfur center



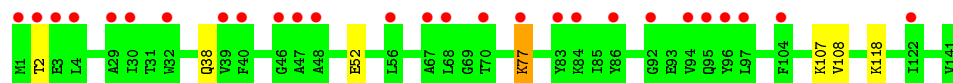
• Molecule 3: Photosystem I iron-sulfur center



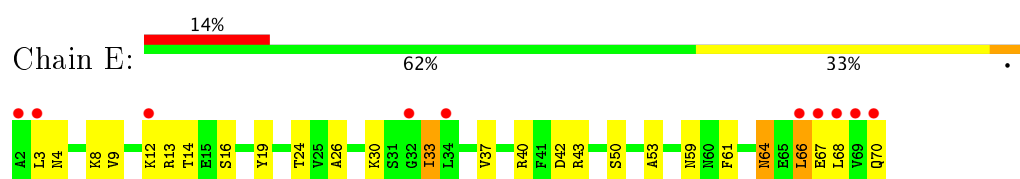
• Molecule 4: Photosystem I reaction center subunit II



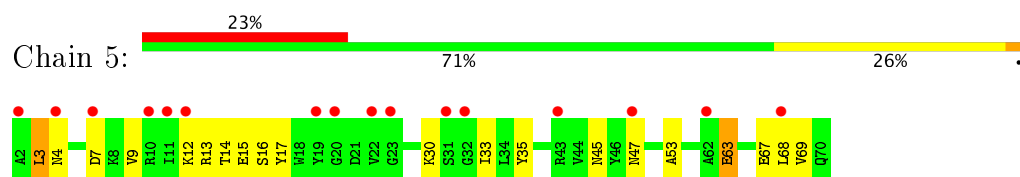
• Molecule 4: Photosystem I reaction center subunit II



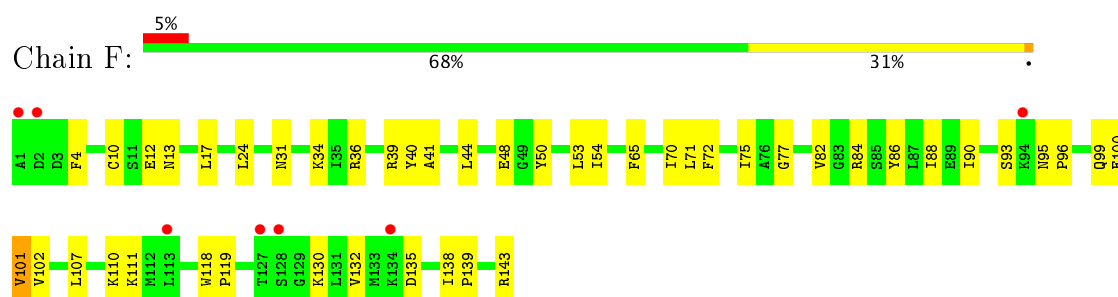
• Molecule 5: Photosystem I reaction center subunit IV



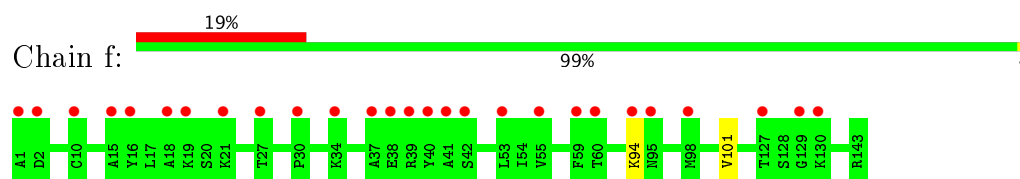
- Molecule 5: Photosystem I reaction center subunit IV



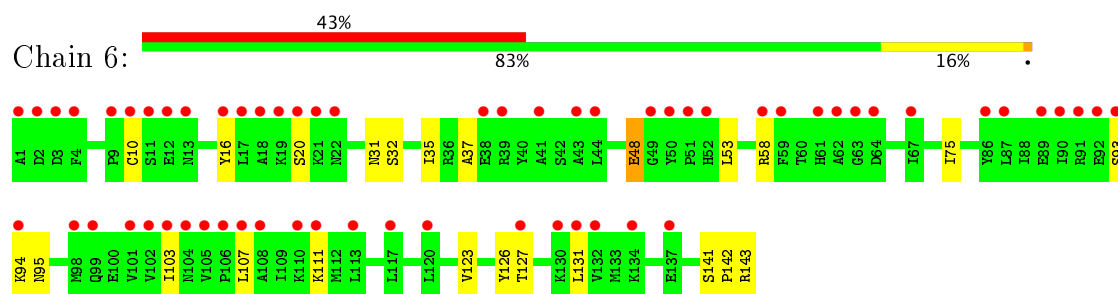
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



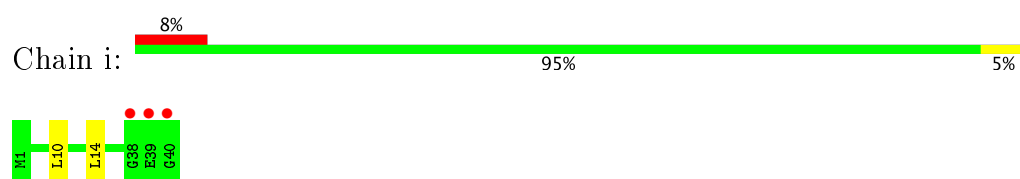
- Molecule 6: Photosystem I reaction center subunit III



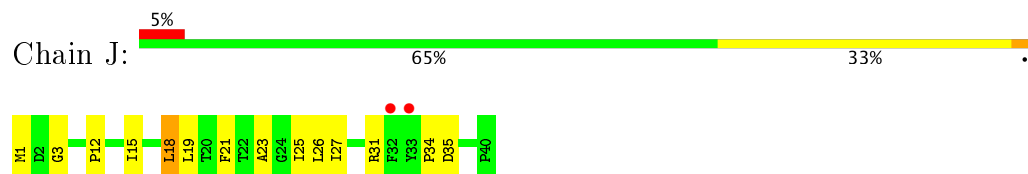
- Molecule 7: Photosystem I reaction center subunit VIII



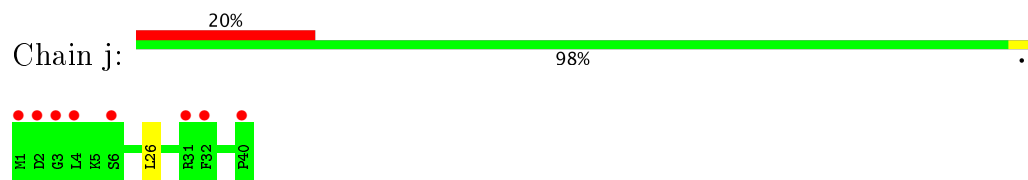
- Molecule 7: Photosystem I reaction center subunit VIII



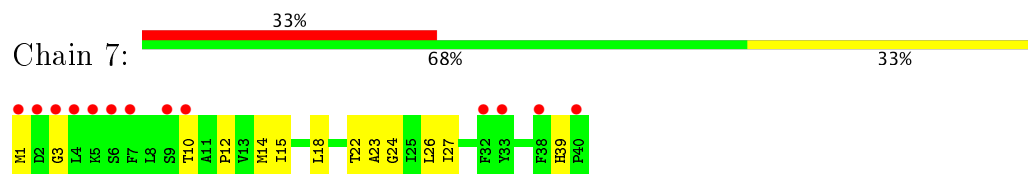
- Molecule 8: Photosystem I reaction center subunit IX



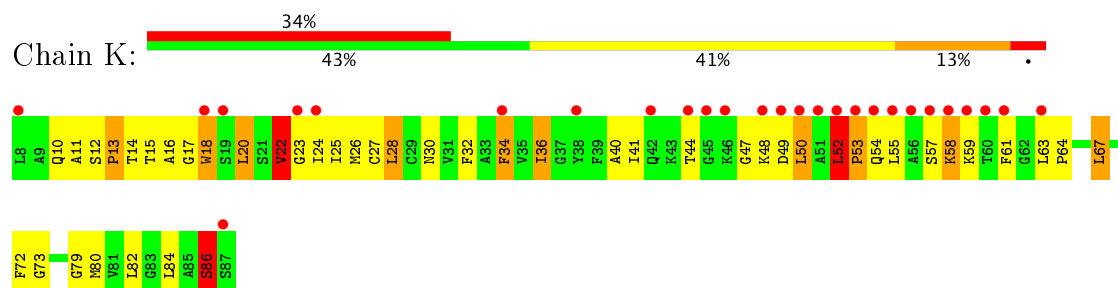
- Molecule 8: Photosystem I reaction center subunit IX



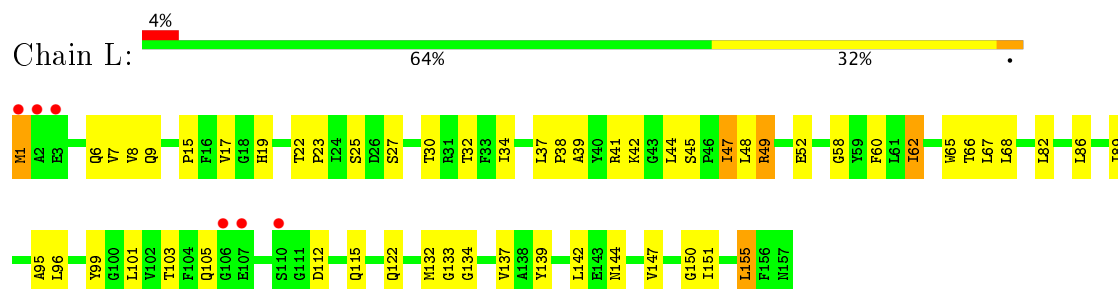
- Molecule 8: Photosystem I reaction center subunit IX



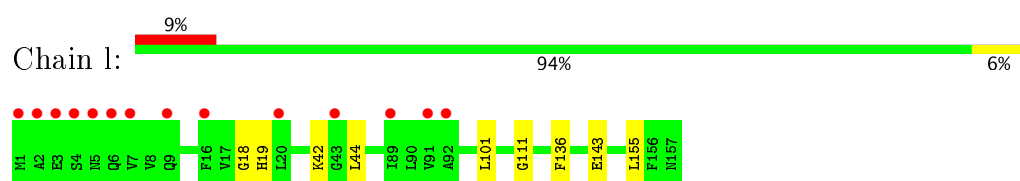
- Molecule 9: Photosystem I reaction center subunit PsaK 2



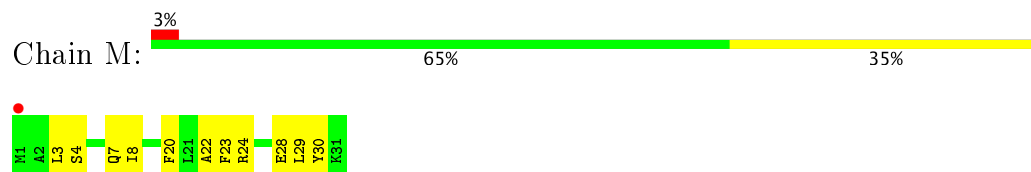
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII

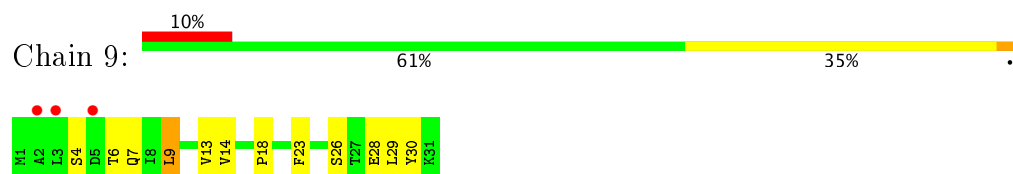


- Molecule 11: Photosystem I reaction center subunit XII

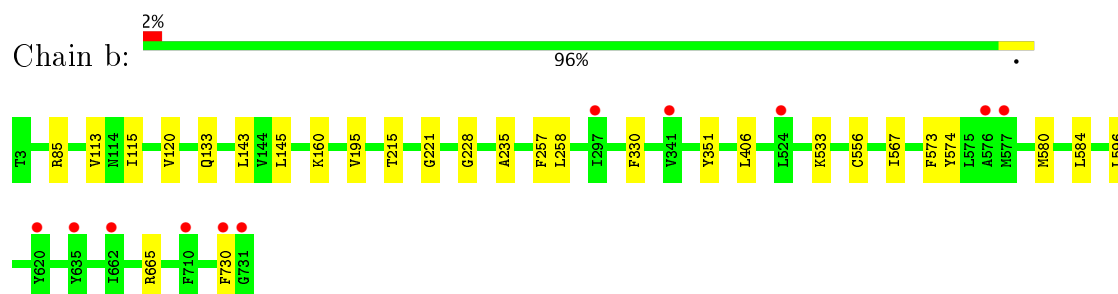


There are no outlier residues recorded for this chain.

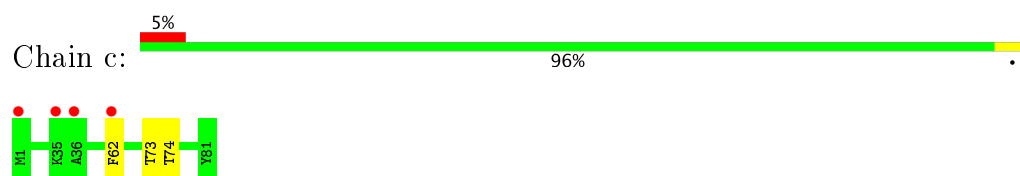
- Molecule 11: Photosystem I reaction center subunit XII



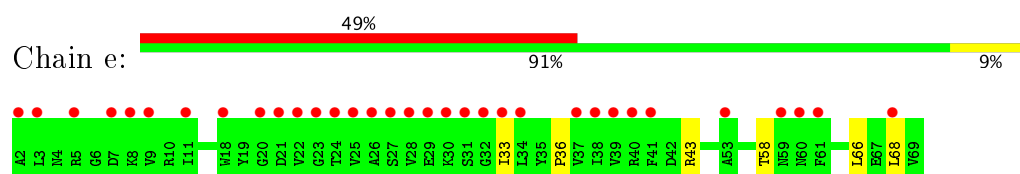
- Molecule 12: Photosystem I P700 chlorophyll a apoprotein A2



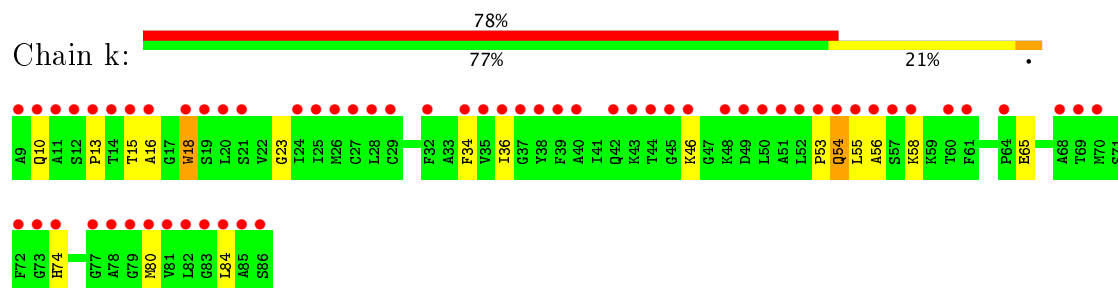
- Molecule 13: Photosystem I iron-sulfur center



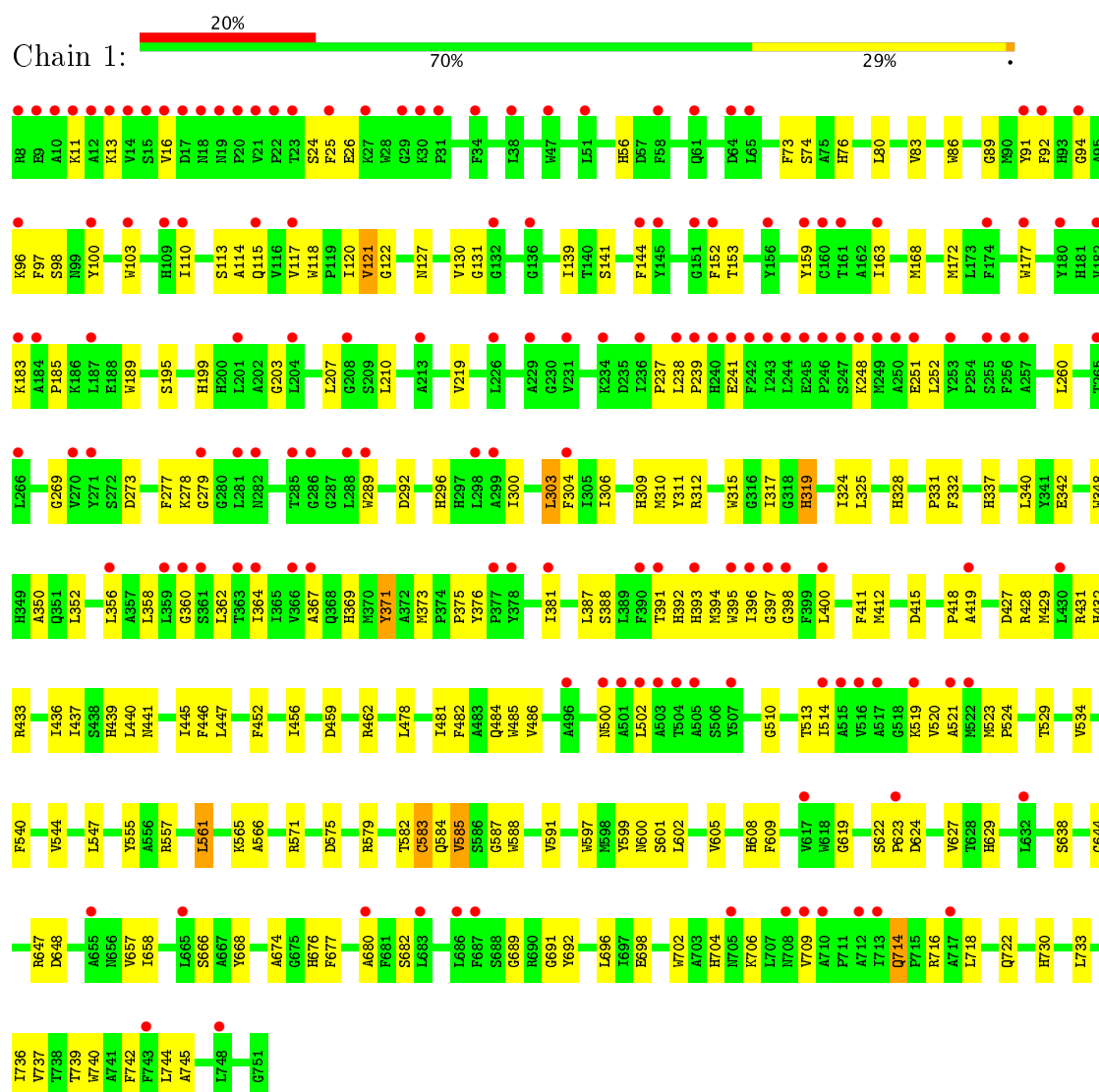
- Molecule 14: Photosystem I reaction center subunit IV



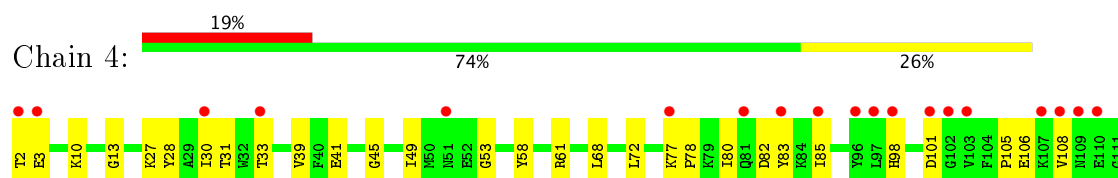
• Molecule 15: Photosystem I reaction center subunit PsaK 2

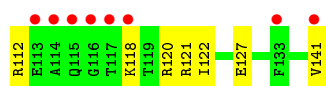


• Molecule 16: Photosystem I P700 chlorophyll a apoprotein A1

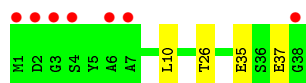
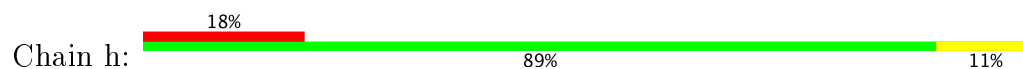


• Molecule 17: Photosystem I reaction center subunit II

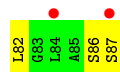
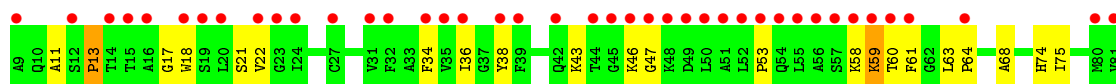




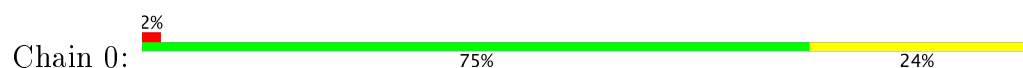
- Molecule 18: Photosystem I reaction center subunit VIII



- 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.

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	b	120	VAL
4	d	52	GLU
6	6	127	THR
12	b	145	LEU
12	b	567	ILE

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
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 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

The worst 5 of 2697 bond angle outliers are listed below:

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

5 of 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

5 of 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

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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%)

The worst 5 of 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

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.