



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 10:11 pm GMT

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

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

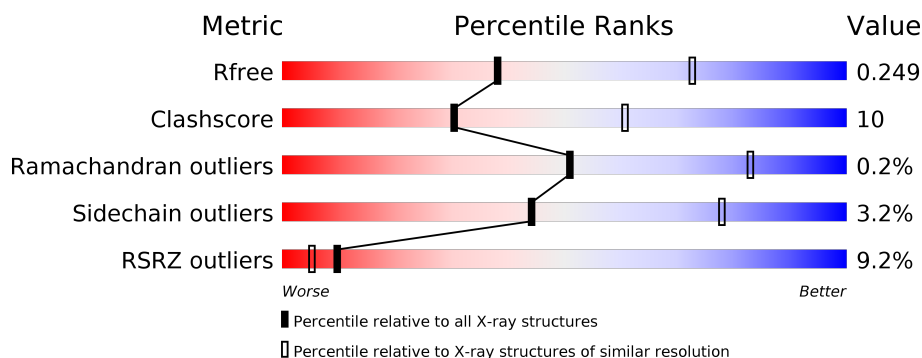
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



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

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

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

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

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Mol	Chain	Length	Quality of chain
16	9	196	

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

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

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

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

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

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

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

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

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

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 71157 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			
1	a	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			
3	c	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			

- Molecule 4 is a protein called Uncharacterized protein.

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

- Molecule 5 is a protein called Putative uncharacterized protein.

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

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

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

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

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

- Molecule 8 is a protein called Putative uncharacterized protein.

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

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

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

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

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

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

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

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

- Molecule 12 is a protein called Putative uncharacterized protein.

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

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

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

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

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

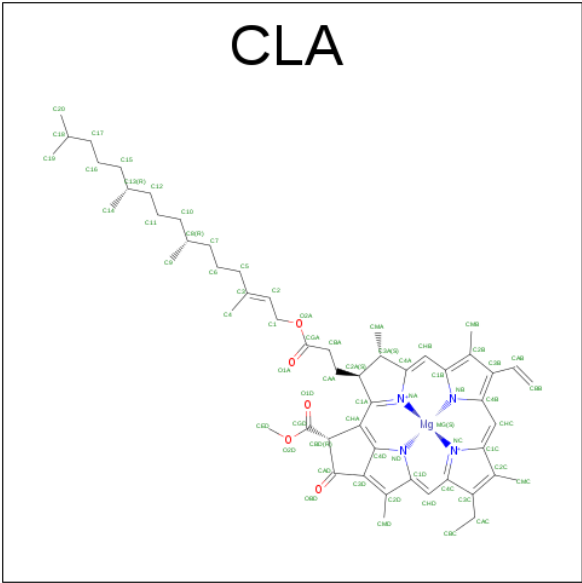
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

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

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

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

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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

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

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

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

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

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

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

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

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

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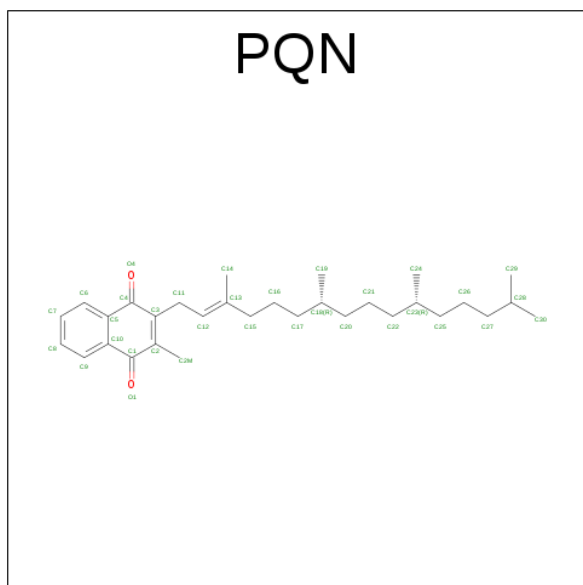
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5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

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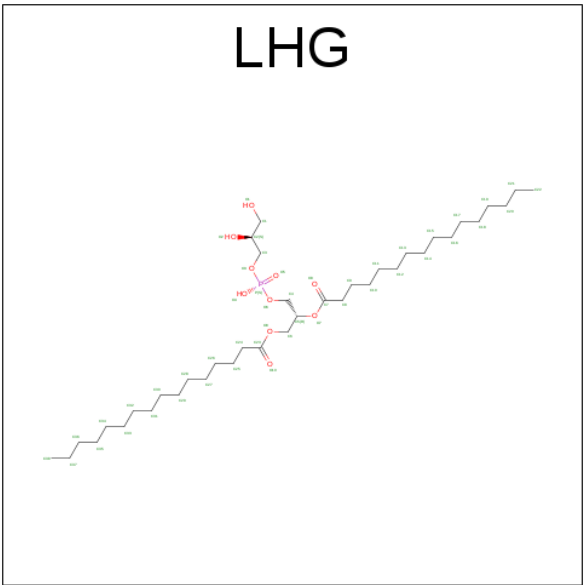
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	9	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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



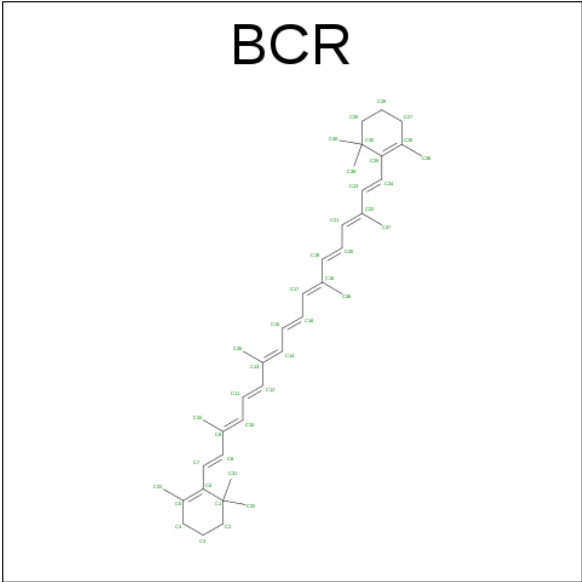
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			33	31	2		
18	B	1	Total	C	O	0	0
			33	31	2		
18	a	1	Total	C	O	0	0
			33	31	2		
18	b	1	Total	C	O	0	0
			33	31	2		

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



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

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

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

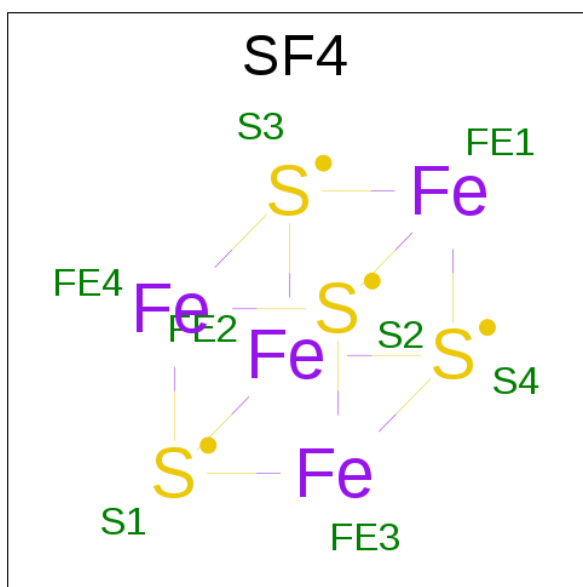
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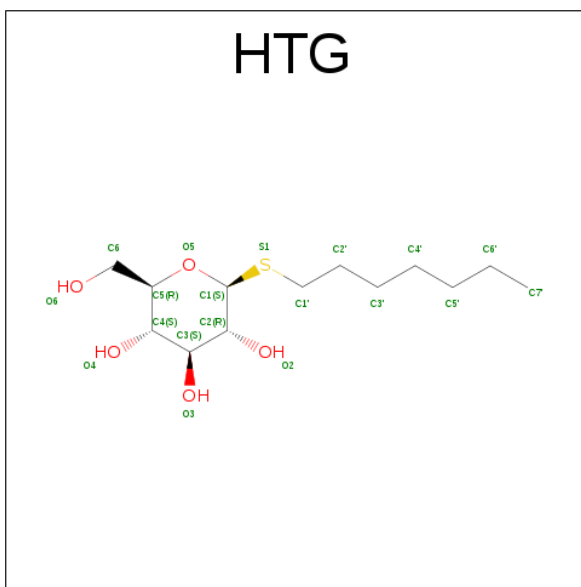
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	f	1	Total C 40 40	0	0
20	g	1	Total C 40 40	0	0
20	i	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	k	1	Total C 40 40	0	0
20	l	1	Total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

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



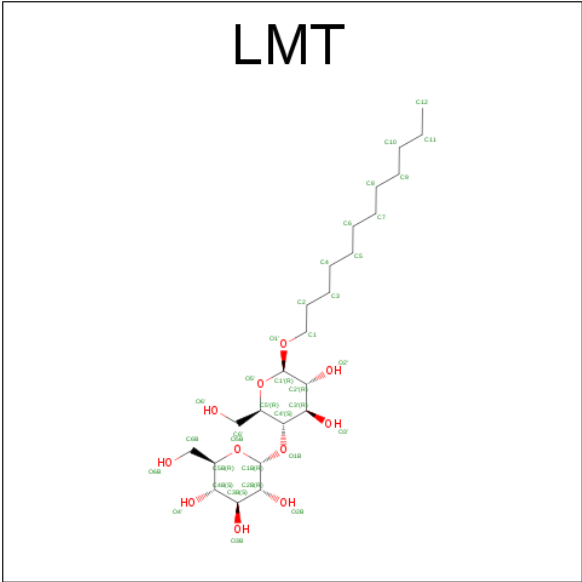
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	a	1	Total	Fe	S	0	0
			8	4	4		
21	c	1	Total	Fe	S	0	0
			8	4	4		
21	c	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 22 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



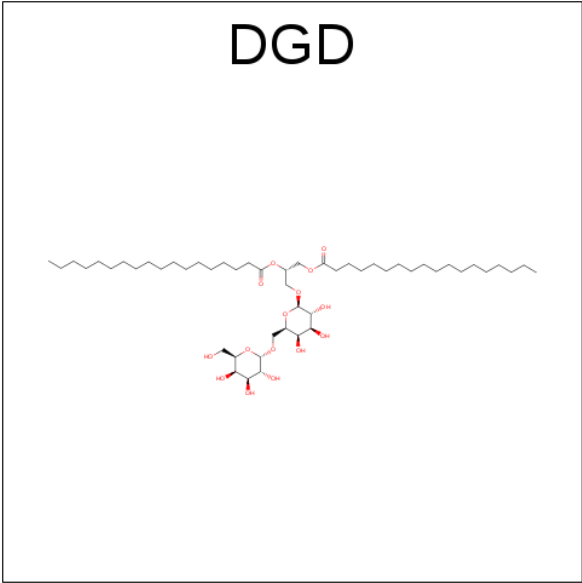
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	S	0	0
			19	13	5	1		
22	F	1	Total	C	O	S	0	0
			19	13	5	1		
22	J	1	Total	C	O	S	0	0
			19	13	5	1		
22	a	1	Total	C	O	S	0	0
			19	13	5	1		
22	f	1	Total	C	O	S	0	0
			19	13	5	1		
22	j	1	Total	C	O	S	0	0
			19	13	5	1		

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



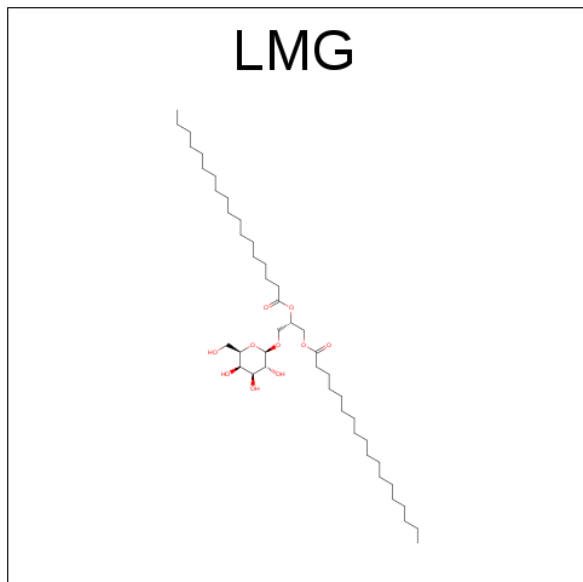
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



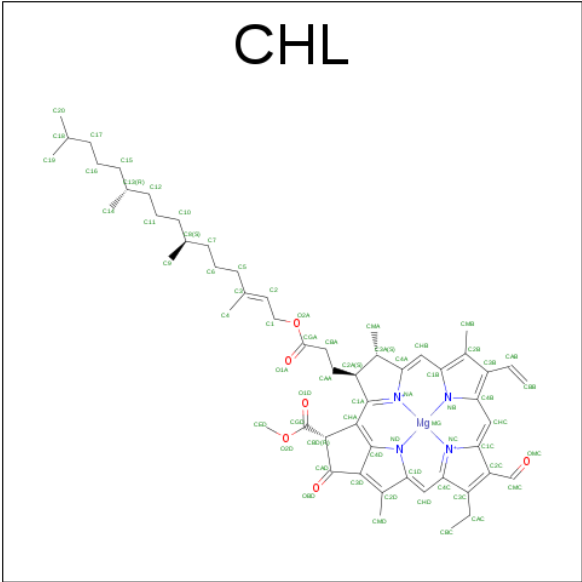
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			66	51	15		
24	b	1	Total	C	O	0	0
			66	51	15		

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



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

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



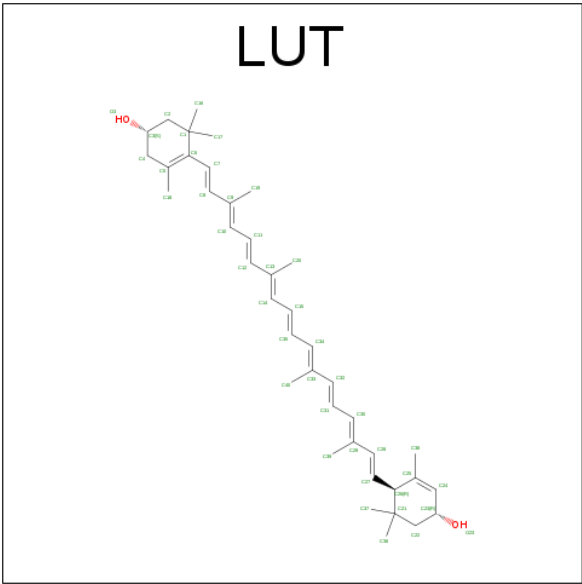
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	1	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	1	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
26	2	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	2	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
26	2	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	2	1	Total 43	C 34	Mg 1	N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

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

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



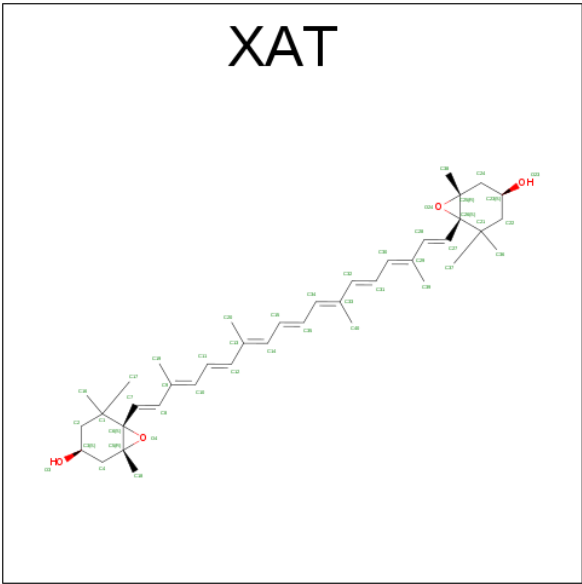
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		

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

- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



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

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

- Molecule 29 is water.

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

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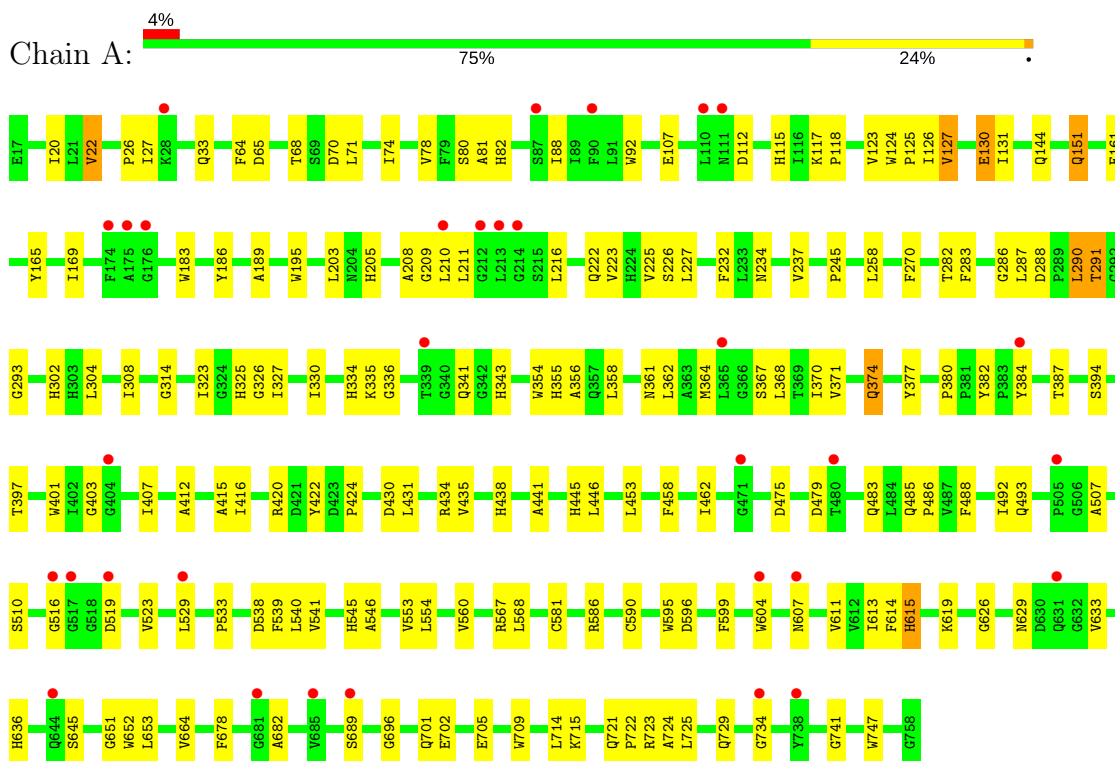
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	d	1	Total 1	O 1	0	0
29	f	4	Total 4	O 4	0	0
29	h	1	Total 1	O 1	0	0
29	l	3	Total 3	O 3	0	0
29	6	3	Total 3	O 3	0	0
29	7	6	Total 6	O 6	0	0
29	8	3	Total 3	O 3	0	0
29	9	5	Total 5	O 5	0	0

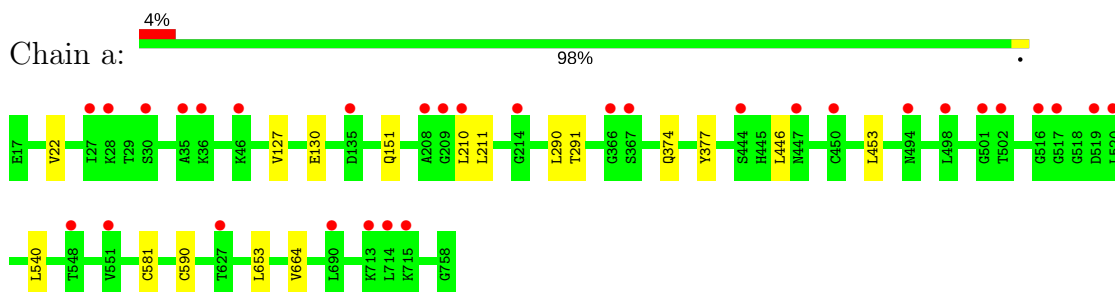
### 3 Residue-property plots

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

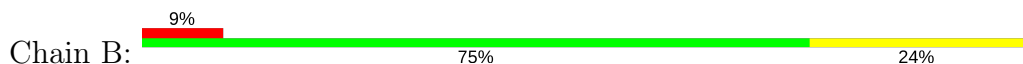
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

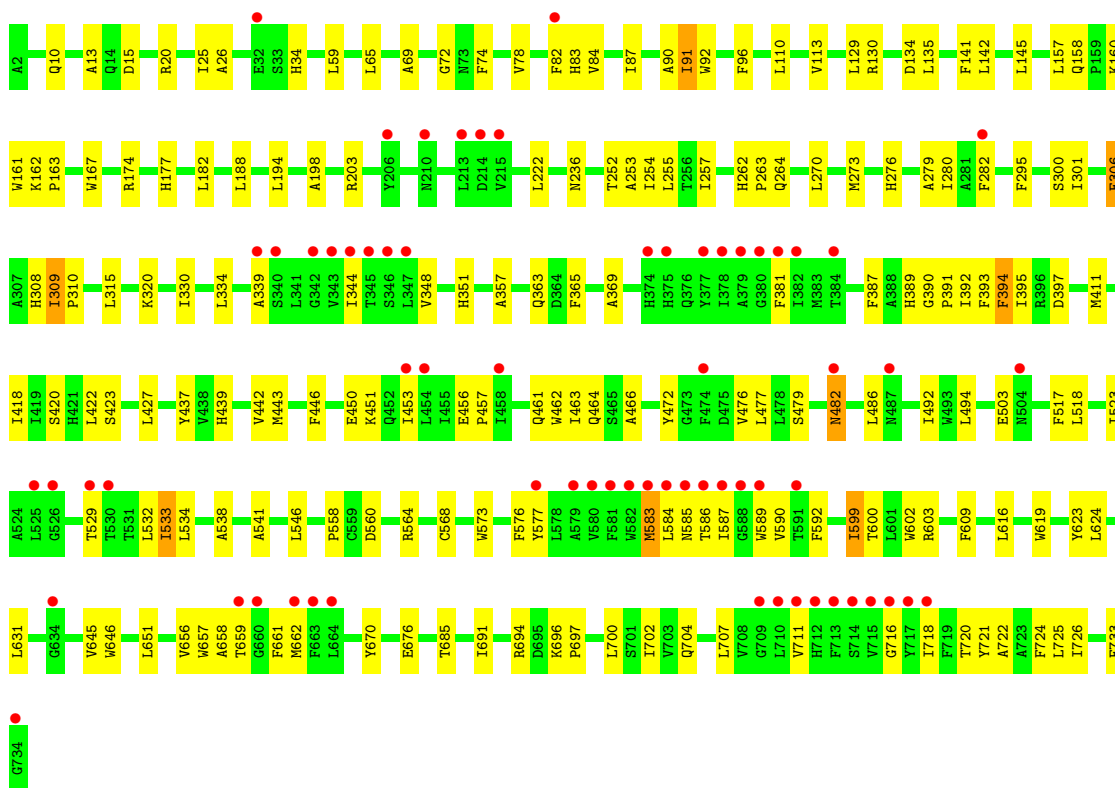


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

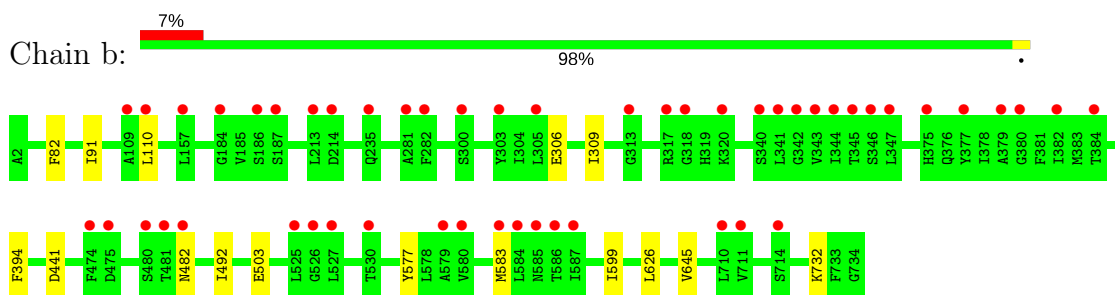


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

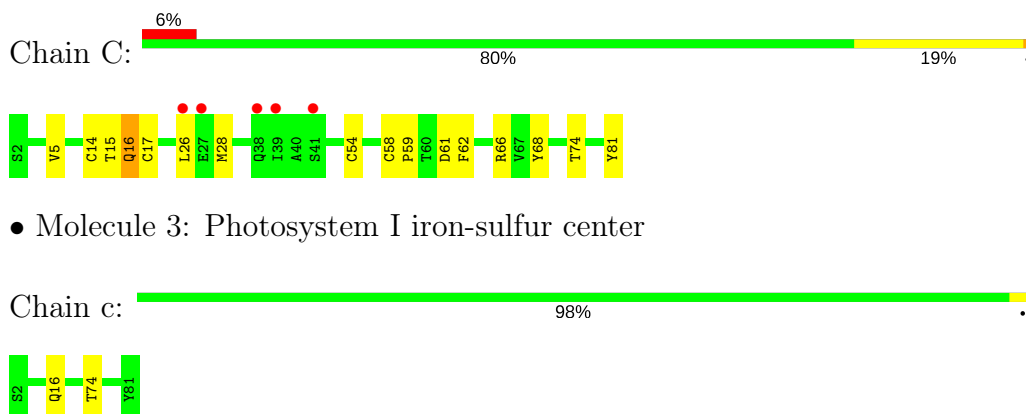




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

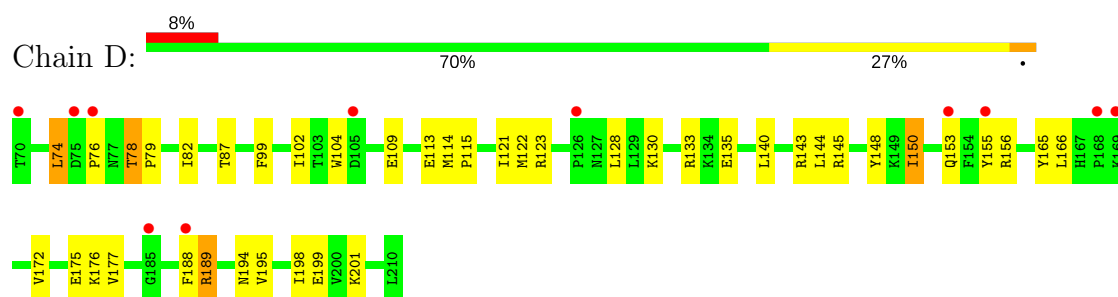


- Molecule 3: Photosystem I iron-sulfur center

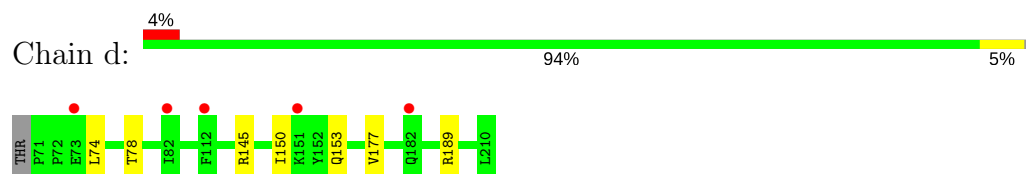


- Molecule 3: Photosystem I iron-sulfur center

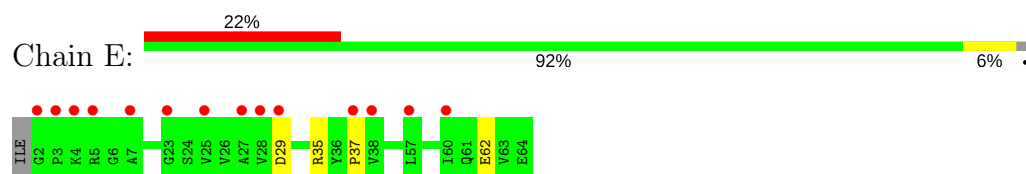
- Molecule 4: Uncharacterized protein



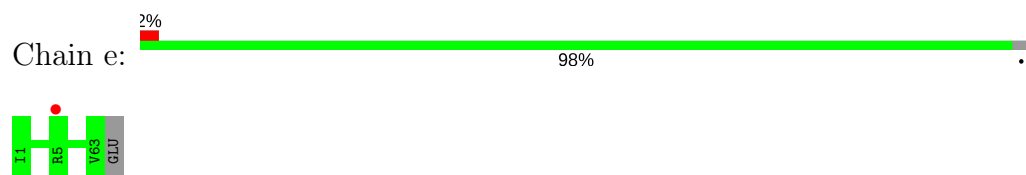
- Molecule 4: Uncharacterized protein



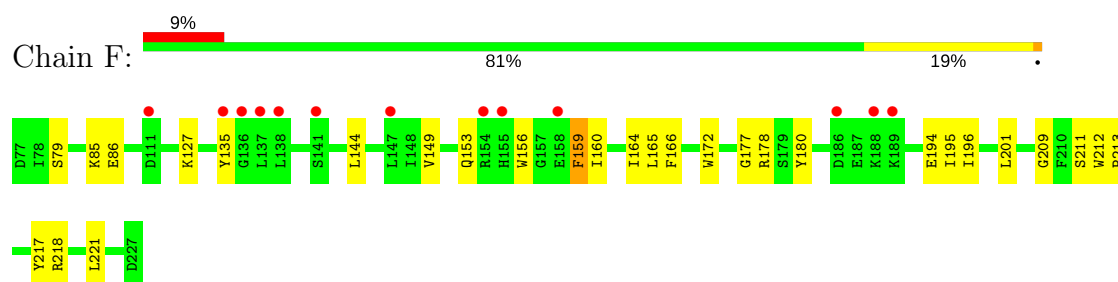
- Molecule 5: Putative uncharacterized protein



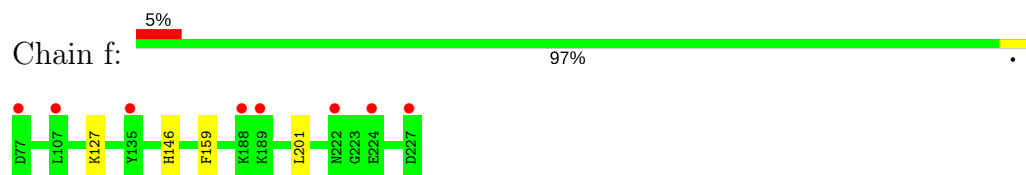
- Molecule 5: Putative uncharacterized protein



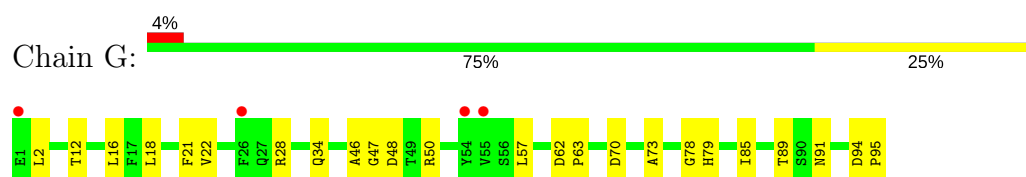
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



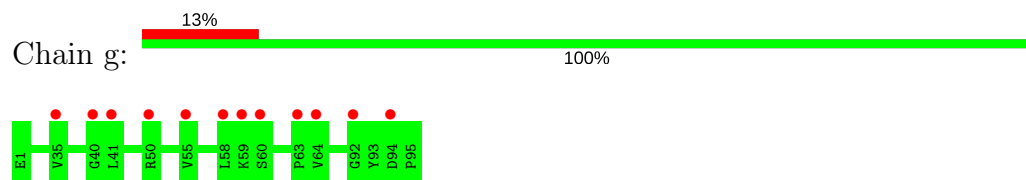
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



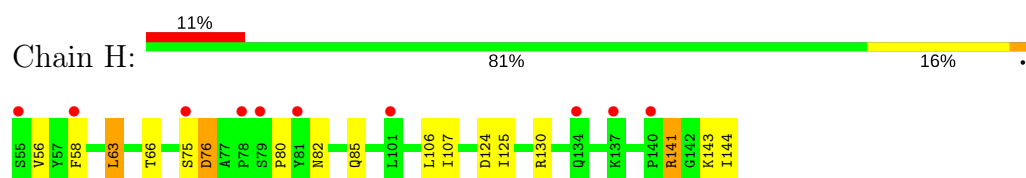
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



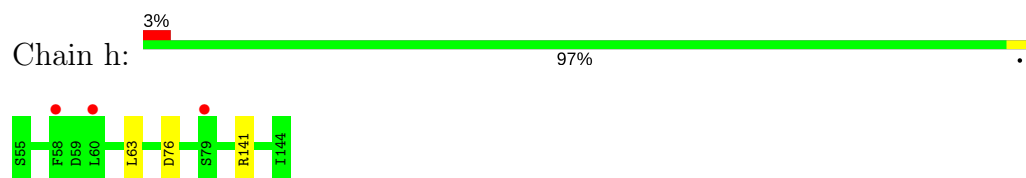
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



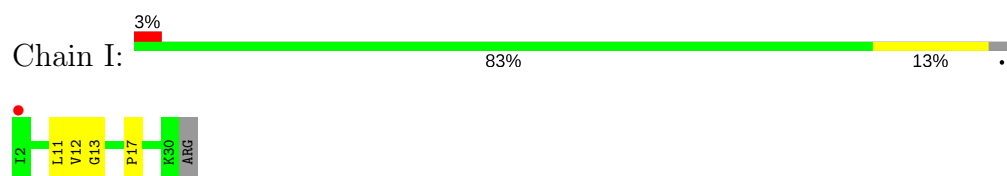
- Molecule 8: Putative uncharacterized protein



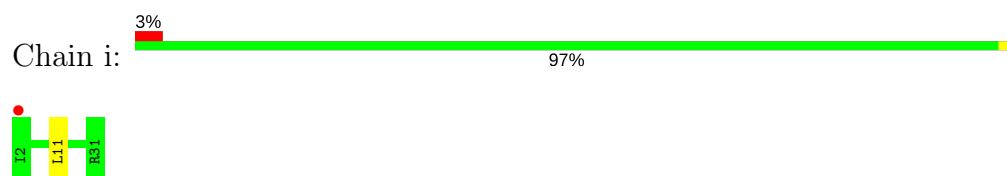
- Molecule 8: Putative uncharacterized protein



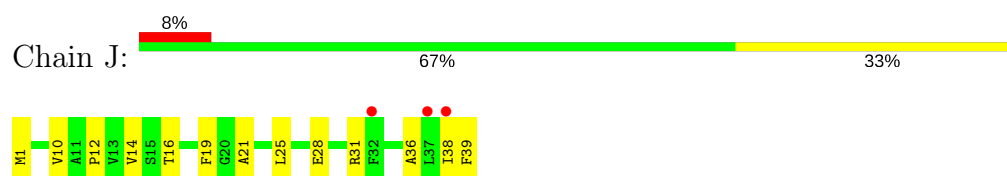
- Molecule 9: Photosystem I reaction center subunit VIII



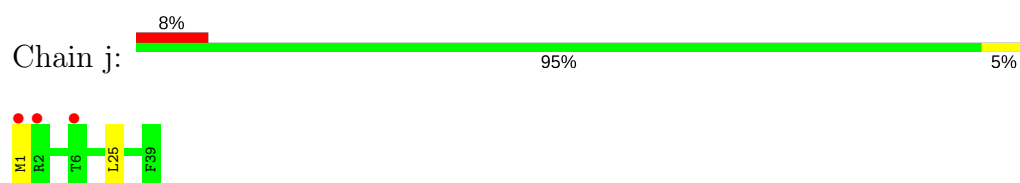
- Molecule 9: Photosystem I reaction center subunit VIII



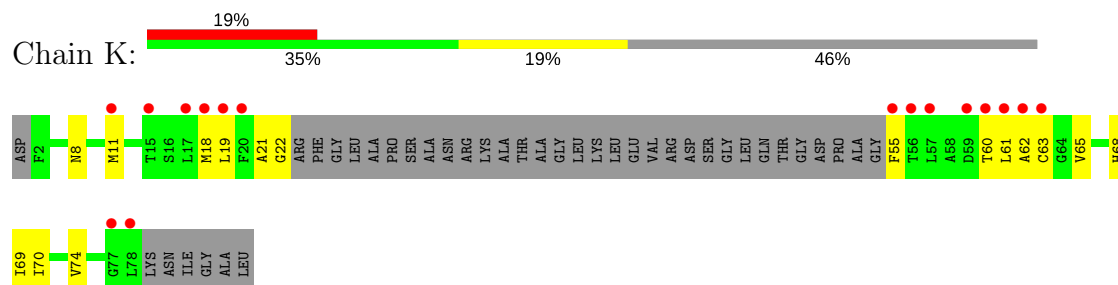
- Molecule 10: Photosystem I reaction center subunit IX



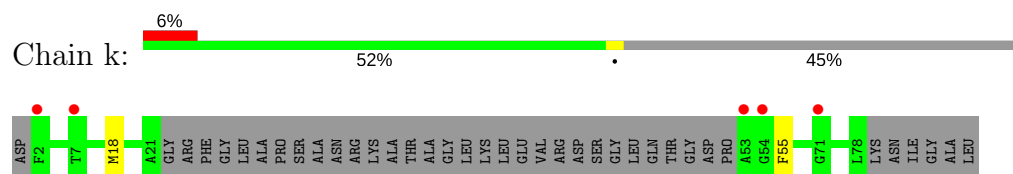
- Molecule 10: Photosystem I reaction center subunit IX



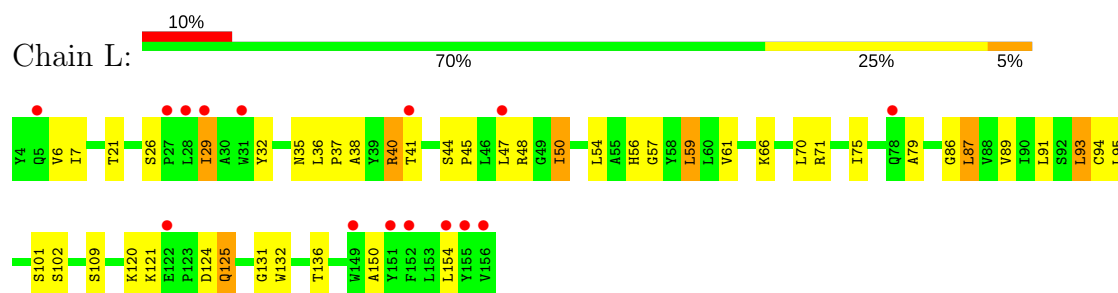
• Molecule 11: Photosystem I reaction center subunit X psaK



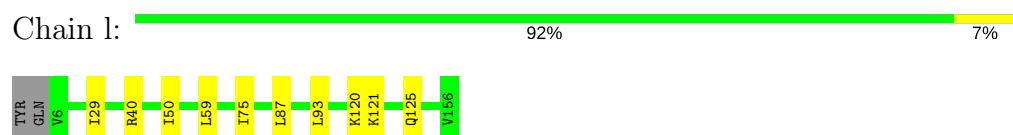
• Molecule 11: Photosystem I reaction center subunit X psaK



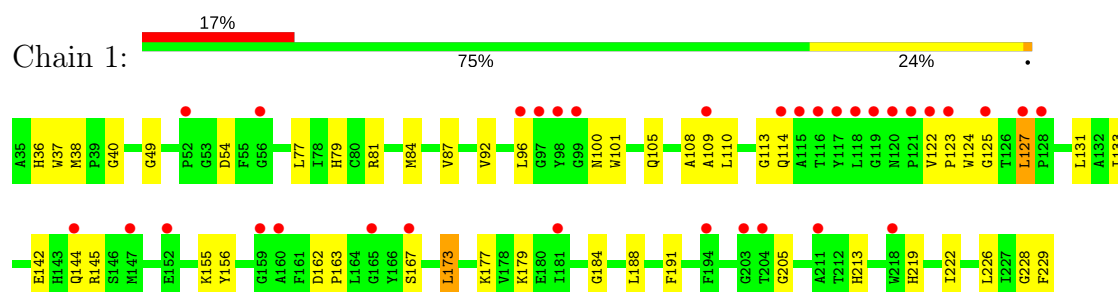
• Molecule 12: Putative uncharacterized protein



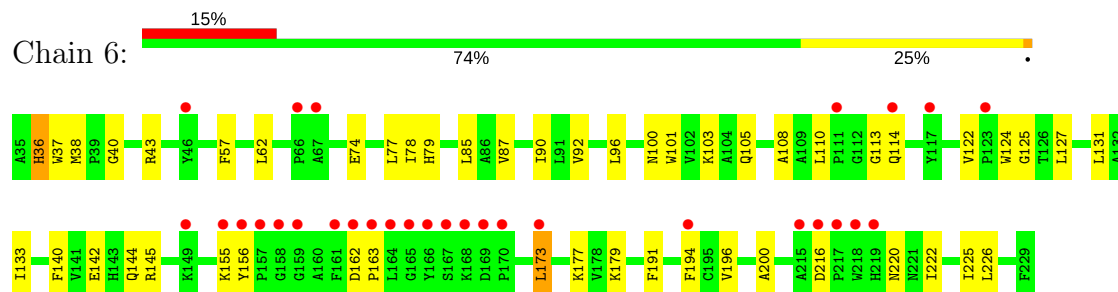
• Molecule 12: Putative uncharacterized protein



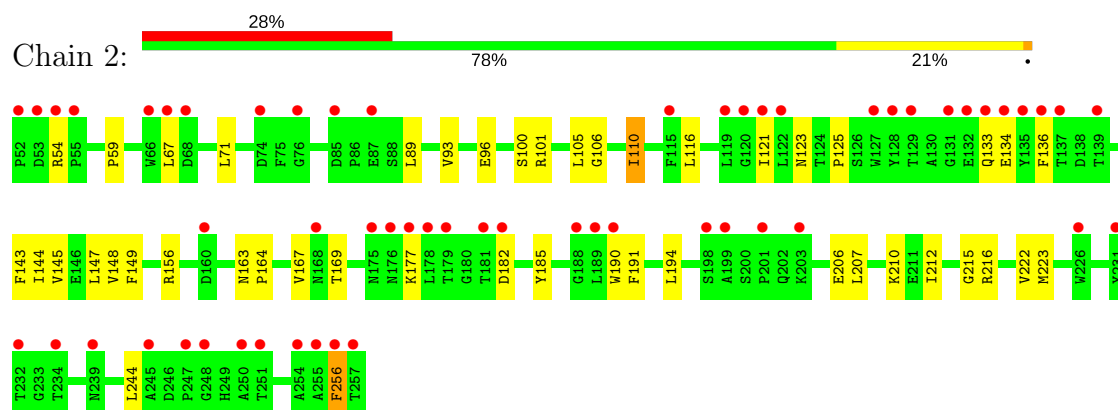
• Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



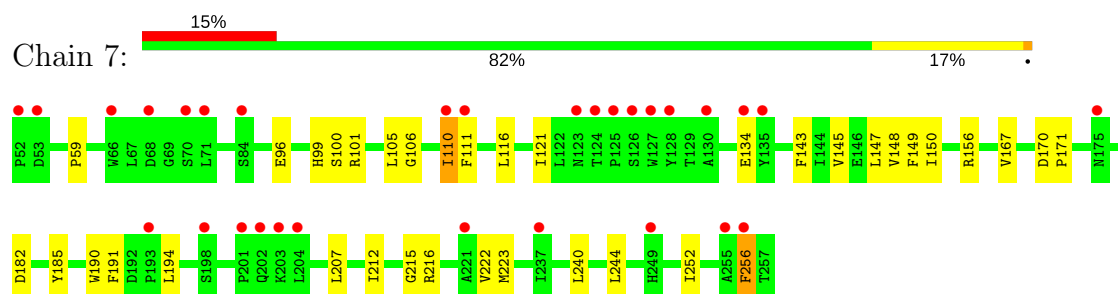
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



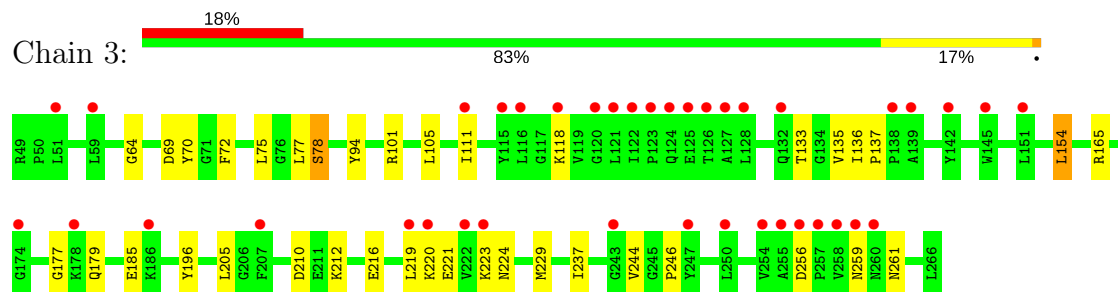
- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I



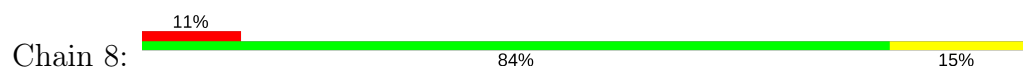
- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I



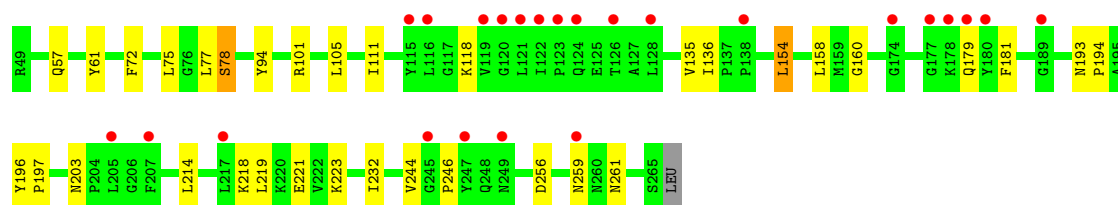
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



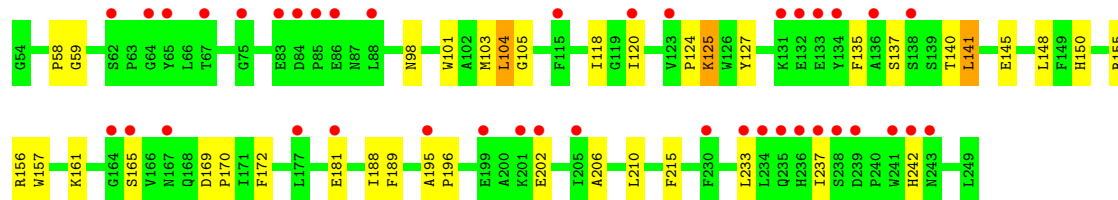
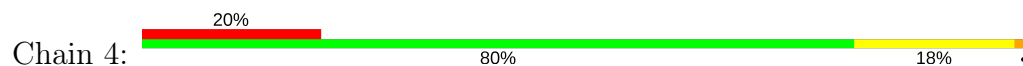
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



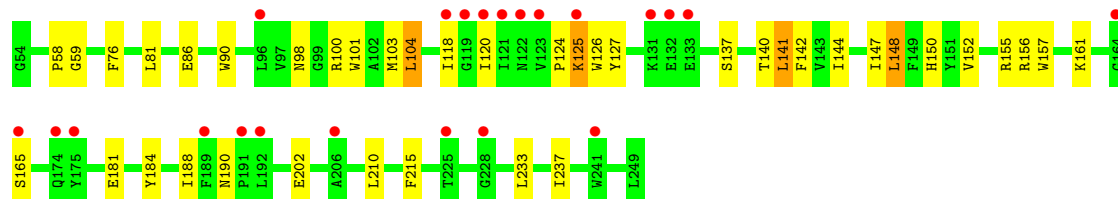
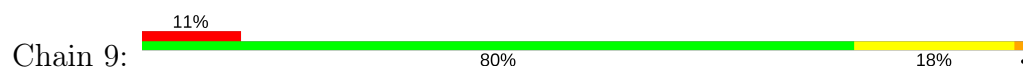




- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



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



## 4 Data and refinement statistics

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

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

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, HTG, LUT, DGD, CHL, SF4, XAT, CLA, PQN, LMT, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/6043	0.41	0/8245
1	a	0.26	0/6043	0.42	0/8245
2	B	0.25	0/6077	0.42	0/8299
2	b	0.25	0/6077	0.42	0/8299
3	C	0.22	0/624	0.41	0/846
3	c	0.23	0/624	0.43	0/846
4	D	0.23	0/1143	0.42	0/1545
4	d	0.24	0/1136	0.43	0/1534
5	E	0.21	0/517	0.39	0/701
5	e	0.21	0/516	0.39	0/700
6	F	0.23	0/1221	0.40	0/1648
6	f	0.24	0/1221	0.40	0/1648
7	G	0.24	0/759	0.39	0/1033
7	g	0.24	0/755	0.40	0/1028
8	H	0.22	0/697	0.39	0/950
8	h	0.22	0/701	0.40	0/954
9	I	0.26	0/227	0.44	0/310
9	i	0.26	0/232	0.44	0/317
10	J	0.24	0/319	0.40	0/434
10	j	0.24	0/319	0.41	0/434
11	K	0.22	0/314	0.37	0/426
11	k	0.24	0/319	0.38	0/433
12	L	0.23	0/1167	0.43	0/1596
12	l	0.25	0/1153	0.44	0/1577
13	1	0.24	0/1539	0.40	0/2099
13	6	0.23	0/1531	0.38	0/2091
14	2	0.23	0/1670	0.40	0/2288
14	7	0.23	0/1670	0.39	0/2288
15	3	0.25	0/1732	0.39	0/2352
15	8	0.25	0/1724	0.39	0/2341
16	4	0.24	0/1589	0.40	0/2168
16	9	0.23	0/1589	0.39	0/2168

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

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

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

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

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

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

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

The worst 5 of 1415 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:609:CLA:HBB1	27:4:616:LUT:H32	1.51	0.92
17:2:609:CLA:HBB1	27:2:615:LUT:H32	1.53	0.88
2:B:334:LEU:HD11	17:B:829:CLA:HBB1	1.54	0.88
17:3:309:CLA:HBB1	27:3:316:LUT:H32	1.55	0.87
13:1:179:LYS:HD3	17:1:312:CLA:HBA1	1.60	0.84

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	740/742 (100%)	710 (96%)	28 (4%)	2 (0%)	44	77
1	a	740/742 (100%)	709 (96%)	29 (4%)	2 (0%)	44	77
2	B	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	55	86
2	b	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	55	86
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
3	c	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
4	d	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
5	E	61/64 (95%)	59 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
6	F	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	25	59
6	f	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	25	59
7	G	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
7	g	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
8	H	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
8	h	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
9	I	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
9	i	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
10	J	37/39 (95%)	37 (100%)	0	0	100	100
10	j	37/39 (95%)	37 (100%)	0	0	100	100
11	K	41/84 (49%)	41 (100%)	0	0	100	100
11	k	42/84 (50%)	42 (100%)	0	0	100	100
12	L	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
12	l	149/153 (97%)	143 (96%)	6 (4%)	0	100	100
13	1	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
13	6	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
14	2	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
14	7	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
15	3	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
15	8	215/218 (99%)	204 (95%)	11 (5%)	0	100	100
16	4	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	32	67
16	9	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	32	67
All	All	6282/6434 (98%)	6041 (96%)	231 (4%)	10 (0%)	51	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	159	PHE
6	f	159	PHE
1	A	581	CYS
16	9	137	SER
16	4	137	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	602/602 (100%)	588 (98%)	14 (2%)	56	86
1	a	602/602 (100%)	587 (98%)	15 (2%)	53	84
2	B	597/597 (100%)	585 (98%)	12 (2%)	60	88
2	b	597/597 (100%)	582 (98%)	15 (2%)	53	84
3	C	69/69 (100%)	67 (97%)	2 (3%)	48	81
3	c	69/69 (100%)	67 (97%)	2 (3%)	48	81
4	D	119/120 (99%)	113 (95%)	6 (5%)	28	62
4	d	118/120 (98%)	111 (94%)	7 (6%)	23	54
5	E	55/56 (98%)	55 (100%)	0	100	100
5	e	55/56 (98%)	55 (100%)	0	100	100
6	F	123/125 (98%)	121 (98%)	2 (2%)	68	91
6	f	123/125 (98%)	120 (98%)	3 (2%)	54	85
7	G	81/81 (100%)	80 (99%)	1 (1%)	75	94
7	g	80/81 (99%)	80 (100%)	0	100	100
8	H	72/73 (99%)	69 (96%)	3 (4%)	34	68
8	h	73/73 (100%)	70 (96%)	3 (4%)	35	69
9	I	25/26 (96%)	24 (96%)	1 (4%)	36	70
9	i	25/26 (96%)	24 (96%)	1 (4%)	36	70
10	J	33/33 (100%)	31 (94%)	2 (6%)	22	53
10	j	33/33 (100%)	31 (94%)	2 (6%)	22	53
11	K	34/62 (55%)	32 (94%)	2 (6%)	23	54
11	k	34/62 (55%)	32 (94%)	2 (6%)	23	54
12	L	118/119 (99%)	108 (92%)	10 (8%)	12	35
12	l	117/119 (98%)	107 (92%)	10 (8%)	12	35
13	1	149/153 (97%)	144 (97%)	5 (3%)	42	76
13	6	147/153 (96%)	142 (97%)	5 (3%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	166/166 (100%)	158 (95%)	8 (5%)	30	63
14	7	166/166 (100%)	158 (95%)	8 (5%)	30	63
15	3	169/169 (100%)	163 (96%)	6 (4%)	40	74
15	8	168/169 (99%)	162 (96%)	6 (4%)	40	74
16	4	161/161 (100%)	154 (96%)	7 (4%)	33	67
16	9	161/161 (100%)	154 (96%)	7 (4%)	33	67
All	All	5141/5224 (98%)	4974 (97%)	167 (3%)	44	78

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	4	125	LYS
1	a	590	CYS
15	8	78	SER
16	4	148	LEU
1	a	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
14	2	123	ASN
16	4	150	HIS
16	9	150	HIS
16	4	98	ASN
16	4	168	GLN

### 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

414 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	CHL	2	607	29	49,59,74	4.14	26 (53%)	33,96,114	3.19	16 (48%)
17	CLA	2	608	14	41,58,73	2.30	12 (29%)	47,95,113	2.48	22 (46%)
17	CLA	2	609	14	51,68,73	2.07	12 (23%)	59,107,113	2.14	23 (38%)
17	CLA	2	610	19	32,49,73	2.49	12 (37%)	37,84,113	2.79	19 (51%)
17	CLA	2	611	14	43,60,73	2.25	12 (27%)	49,97,113	2.43	20 (40%)
17	CLA	2	612	14	56,73,73	1.97	12 (21%)	65,113,113	2.09	18 (27%)
17	CLA	2	613	14	34,51,73	2.41	11 (32%)	39,86,113	2.52	16 (41%)
26	CHL	2	614	14	41,51,74	4.43	23 (56%)	24,86,114	3.46	13 (54%)
27	LUT	2	615	-	41,43,43	0.74	0	50,60,60	1.61	11 (22%)
28	XAT	2	616	-	39,47,47	0.85	0	54,74,74	2.62	19 (35%)
20	BCR	2	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.85	18 (32%)
19	LHG	2	618	17	36,36,48	1.06	2 (5%)	37,42,54	1.21	4 (10%)
17	CLA	3	301	-	37,54,73	2.41	12 (32%)	43,90,113	2.47	17 (39%)
17	CLA	3	302	15	51,68,73	2.04	12 (23%)	59,107,113	2.17	22 (37%)
17	CLA	3	303	15	41,58,73	2.29	12 (29%)	47,95,113	2.49	19 (40%)
17	CLA	3	304	29	33,53,73	2.42	11 (33%)	37,89,113	2.58	18 (48%)
17	CLA	3	305	29	33,50,73	2.43	11 (33%)	38,85,113	2.61	18 (47%)
17	CLA	3	306	15	38,55,73	2.41	12 (31%)	44,91,113	2.44	18 (40%)
26	CHL	3	307	29	45,55,74	4.29	24 (53%)	29,91,114	3.29	12 (41%)
17	CLA	3	308	15	41,58,73	2.29	12 (29%)	47,95,113	2.41	20 (42%)
17	CLA	3	309	15	41,58,73	2.30	12 (29%)	47,95,113	2.37	22 (46%)
17	CLA	3	310	19	29,45,73	2.46	11 (37%)	33,78,113	2.71	16 (48%)
17	CLA	3	311	-	43,60,73	2.26	12 (27%)	49,97,113	2.43	21 (42%)
17	CLA	3	312	15	46,63,73	2.18	12 (26%)	53,101,113	2.29	20 (37%)
17	CLA	3	313	15	33,53,73	2.47	11 (33%)	37,89,113	2.61	18 (48%)
17	CLA	3	314	15	37,54,73	2.40	12 (32%)	43,90,113	2.53	17 (39%)
17	CLA	3	315	-	17,32,73	2.99	10 (58%)	24,54,113	4.44	19 (79%)
27	LUT	3	316	-	41,43,43	0.74	0	50,60,60	1.62	13 (26%)
28	XAT	3	317	-	39,47,47	0.86	0	54,74,74	2.69	19 (35%)
20	BCR	3	318	-	41,41,41	1.04	1 (2%)	56,56,56	1.88	14 (25%)
19	LHG	3	319	17	19,19,48	1.09	1 (5%)	19,24,54	1.04	1 (5%)
17	CLA	4	601	16	37,54,73	2.39	12 (32%)	43,90,113	2.51	17 (39%)
17	CLA	4	602	16	51,68,73	2.06	12 (23%)	59,107,113	2.15	23 (38%)
17	CLA	4	603	16	37,54,73	2.34	12 (32%)	43,90,113	2.57	18 (41%)
17	CLA	4	604	29	41,58,73	2.28	12 (29%)	47,95,113	2.45	22 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	CHL	4	605	29	54,64,74	3.94	24 (44%)	39,102,114	3.06	18 (46%)
26	CHL	4	606	29	49,59,74	4.11	24 (48%)	33,96,114	3.10	18 (54%)
26	CHL	4	607	29	49,59,74	4.11	24 (48%)	33,96,114	3.12	15 (45%)
17	CLA	4	608	16	41,58,73	2.30	12 (29%)	47,95,113	2.46	20 (42%)
17	CLA	4	609	16	51,68,73	2.04	12 (23%)	59,107,113	2.14	22 (37%)
17	CLA	4	610	29	46,63,73	2.17	12 (26%)	53,101,113	2.26	21 (39%)
17	CLA	4	611	16	43,60,73	2.22	12 (27%)	49,97,113	2.42	19 (38%)
17	CLA	4	612	16	47,64,73	2.16	12 (25%)	54,102,113	2.30	20 (37%)
17	CLA	4	613	16	33,53,73	2.44	11 (33%)	37,89,113	2.62	18 (48%)
17	CLA	4	614	16	41,58,73	2.29	12 (29%)	47,95,113	2.48	21 (44%)
26	CHL	4	615	16	41,51,74	4.41	23 (56%)	24,86,114	3.47	13 (54%)
27	LUT	4	616	-	41,43,43	0.75	0	50,60,60	1.65	14 (28%)
28	XAT	4	617	-	39,47,47	0.86	0	54,74,74	2.60	18 (33%)
20	BCR	4	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.79	15 (26%)
25	LMG	4	619	-	44,44,55	0.99	2 (4%)	52,52,63	1.03	3 (5%)
25	LMG	4	620	-	44,44,55	1.01	3 (6%)	52,52,63	1.21	5 (9%)
19	LHG	6	301	17	22,22,48	1.15	2 (9%)	23,28,54	1.28	2 (8%)
25	LMG	6	302	-	40,40,55	1.04	2 (5%)	48,48,63	1.12	3 (6%)
26	CHL	6	303	13	59,69,74	3.73	24 (40%)	45,108,114	2.77	17 (37%)
17	CLA	6	304	13	56,73,73	1.96	12 (21%)	65,113,113	2.08	20 (30%)
17	CLA	6	305	13	56,73,73	1.95	12 (21%)	65,113,113	2.14	20 (30%)
17	CLA	6	306	29	42,59,73	2.27	12 (28%)	48,96,113	2.46	21 (43%)
17	CLA	6	307	-	33,50,73	2.44	11 (33%)	38,85,113	2.54	17 (44%)
26	CHL	6	308	13	45,55,74	4.26	24 (53%)	29,91,114	3.31	15 (51%)
17	CLA	6	309	29	37,54,73	2.41	12 (32%)	43,90,113	2.41	15 (34%)
17	CLA	6	310	13	56,73,73	1.97	12 (21%)	65,113,113	2.10	18 (27%)
17	CLA	6	311	13	51,68,73	2.06	12 (23%)	59,107,113	2.13	23 (38%)
17	CLA	6	312	19	32,49,73	2.50	12 (37%)	37,84,113	2.80	19 (51%)
17	CLA	6	313	13	43,60,73	2.25	12 (27%)	49,97,113	2.43	20 (40%)
17	CLA	6	314	13	51,68,73	2.05	12 (23%)	59,107,113	2.20	19 (32%)
17	CLA	6	315	13	46,63,73	2.17	12 (26%)	53,101,113	2.34	21 (39%)
17	CLA	6	316	13	37,54,73	2.41	12 (32%)	43,90,113	2.44	17 (39%)
27	LUT	6	317	-	41,43,43	0.75	0	50,60,60	1.66	13 (26%)
28	XAT	6	318	-	39,47,47	0.88	0	54,74,74	2.62	19 (35%)
20	BCR	6	319	-	41,41,41	1.05	1 (2%)	56,56,56	1.88	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	LHG	6	320	17	48,48,48	0.93	2 (4%)	49,54,54	1.12	4 (8%)
27	LUT	6	321	-	41,43,43	0.73	0	50,60,60	1.74	10 (20%)
26	CHL	7	601	14	59,69,74	3.74	25 (42%)	45,108,114	2.91	19 (42%)
17	CLA	7	602	14	56,73,73	1.94	12 (21%)	65,113,113	2.06	20 (30%)
17	CLA	7	603	14	42,59,73	2.24	12 (28%)	48,96,113	2.45	20 (41%)
17	CLA	7	604	29	51,68,73	2.05	12 (23%)	59,107,113	2.19	22 (37%)
26	CHL	7	605	29	41,51,74	4.40	23 (56%)	24,86,114	3.53	13 (54%)
26	CHL	7	606	-	46,56,74	4.22	25 (54%)	30,92,114	3.30	15 (50%)
26	CHL	7	607	29	49,59,74	4.09	24 (48%)	33,96,114	3.13	16 (48%)
17	CLA	7	608	14	41,58,73	2.28	12 (29%)	47,95,113	2.42	22 (46%)
17	CLA	7	609	14	51,68,73	2.06	12 (23%)	59,107,113	2.12	22 (37%)
17	CLA	7	610	19	32,49,73	2.50	12 (37%)	37,84,113	2.79	18 (48%)
17	CLA	7	611	14	43,60,73	2.24	12 (27%)	49,97,113	2.45	21 (42%)
17	CLA	7	612	14	56,73,73	1.97	12 (21%)	65,113,113	2.11	19 (29%)
17	CLA	7	613	14	34,51,73	2.39	11 (32%)	39,86,113	2.50	17 (43%)
26	CHL	7	614	14	41,51,74	4.42	23 (56%)	24,86,114	3.57	15 (62%)
27	LUT	7	615	-	41,43,43	0.74	0	50,60,60	1.56	11 (22%)
28	XAT	7	616	-	39,47,47	0.84	0	54,74,74	2.60	19 (35%)
20	BCR	7	617	-	41,41,41	1.07	1 (2%)	56,56,56	2.08	13 (23%)
19	LHG	7	618	17	36,36,48	1.06	2 (5%)	37,42,54	1.22	3 (8%)
17	CLA	8	301	15	51,68,73	2.07	12 (23%)	59,107,113	2.14	22 (37%)
17	CLA	8	302	15	41,58,73	2.27	12 (29%)	47,95,113	2.52	20 (42%)
17	CLA	8	303	29	33,53,73	2.42	11 (33%)	37,89,113	2.61	17 (45%)
17	CLA	8	304	29	33,50,73	2.44	11 (33%)	38,85,113	2.51	18 (47%)
17	CLA	8	305	15	38,55,73	2.40	12 (31%)	44,91,113	2.43	18 (40%)
26	CHL	8	306	29	45,55,74	4.26	24 (53%)	29,91,114	3.25	16 (55%)
17	CLA	8	307	15	41,58,73	2.29	12 (29%)	47,95,113	2.34	20 (42%)
17	CLA	8	308	15	41,58,73	2.31	12 (29%)	47,95,113	2.35	21 (44%)
17	CLA	8	309	-	43,60,73	2.27	12 (27%)	49,97,113	2.40	19 (38%)
17	CLA	8	310	15	46,63,73	2.17	12 (26%)	53,101,113	2.29	19 (35%)
17	CLA	8	311	15	33,53,73	2.46	11 (33%)	37,89,113	2.63	19 (51%)
17	CLA	8	312	15	37,54,73	2.39	12 (32%)	43,90,113	2.51	18 (41%)
17	CLA	8	313	-	17,32,73	3.00	10 (58%)	24,54,113	4.44	19 (79%)
27	LUT	8	314	-	41,43,43	0.73	0	50,60,60	1.52	11 (22%)
28	XAT	8	315	-	39,47,47	0.86	0	54,74,74	2.72	21 (38%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	BCR	8	316	-	41,41,41	1.05	1 (2%)	56,56,56	1.92	15 (26%)
17	CLA	9	601	16	37,54,73	2.38	12 (32%)	43,90,113	2.49	19 (44%)
17	CLA	9	602	16	51,68,73	2.04	12 (23%)	59,107,113	2.20	23 (38%)
17	CLA	9	603	16	37,54,73	2.35	12 (32%)	43,90,113	2.53	18 (41%)
17	CLA	9	604	29	41,58,73	2.28	12 (29%)	47,95,113	2.43	21 (44%)
26	CHL	9	605	29	54,64,74	3.91	24 (44%)	39,102,114	3.08	19 (48%)
26	CHL	9	606	29	49,59,74	4.09	24 (48%)	33,96,114	3.21	16 (48%)
26	CHL	9	607	29	49,59,74	4.09	25 (51%)	33,96,114	3.16	14 (42%)
17	CLA	9	608	16	41,58,73	2.28	12 (29%)	47,95,113	2.50	20 (42%)
17	CLA	9	609	16	51,68,73	2.05	12 (23%)	59,107,113	2.14	22 (37%)
17	CLA	9	610	29	32,49,73	2.50	12 (37%)	37,84,113	2.72	18 (48%)
17	CLA	9	611	16	43,60,73	2.25	12 (27%)	49,97,113	2.47	20 (40%)
17	CLA	9	612	16	47,64,73	2.16	12 (25%)	54,102,113	2.25	19 (35%)
17	CLA	9	613	16	33,53,73	2.44	11 (33%)	37,89,113	2.61	18 (48%)
17	CLA	9	614	16	38,55,73	2.36	12 (31%)	44,91,113	2.47	19 (43%)
26	CHL	9	615	16	41,51,74	4.44	23 (56%)	24,86,114	3.58	14 (58%)
27	LUT	9	616	-	41,43,43	0.74	0	50,60,60	1.61	11 (22%)
28	XAT	9	617	-	39,47,47	0.84	0	54,74,74	2.62	17 (31%)
20	BCR	9	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.80	16 (28%)
25	LMG	9	619	-	50,50,55	0.92	2 (4%)	58,58,63	1.01	3 (5%)
17	CLA	A	801	1	56,73,73	1.93	12 (21%)	65,113,113	2.24	23 (35%)
17	CLA	A	802	1	56,73,73	1.97	12 (21%)	65,113,113	2.00	18 (27%)
17	CLA	A	803	29	56,73,73	1.92	12 (21%)	65,113,113	2.22	22 (33%)
17	CLA	A	804	1	56,73,73	1.93	12 (21%)	65,113,113	2.18	21 (32%)
17	CLA	A	805	1	46,63,73	2.16	12 (26%)	53,101,113	2.43	22 (41%)
17	CLA	A	806	1	56,73,73	1.96	12 (21%)	65,113,113	2.05	21 (32%)
17	CLA	A	807	1	56,73,73	1.95	12 (21%)	65,113,113	2.14	19 (29%)
17	CLA	A	808	1	56,73,73	1.99	12 (21%)	65,113,113	2.14	19 (29%)
17	CLA	A	809	1	56,73,73	1.96	12 (21%)	65,113,113	2.16	20 (30%)
17	CLA	A	810	1	56,73,73	1.94	12 (21%)	65,113,113	2.18	19 (29%)
17	CLA	A	811	1	56,73,73	1.95	12 (21%)	65,113,113	2.08	20 (30%)
17	CLA	A	812	1	56,73,73	1.95	12 (21%)	65,113,113	2.10	21 (32%)
17	CLA	A	813	1	45,62,73	2.19	12 (26%)	51,99,113	2.27	20 (39%)
17	CLA	A	814	1	56,73,73	1.95	12 (21%)	65,113,113	2.16	20 (30%)
17	CLA	A	815	1	33,53,73	2.42	11 (33%)	37,89,113	2.54	17 (45%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	A	816	1	41,58,73	2.29	12 (29%)	47,95,113	2.44	19 (40%)
17	CLA	A	817	29	33,53,73	2.43	11 (33%)	37,89,113	2.57	15 (40%)
17	CLA	A	818	1	56,73,73	1.97	12 (21%)	65,113,113	2.17	21 (32%)
17	CLA	A	819	1	56,73,73	1.95	12 (21%)	65,113,113	2.12	21 (32%)
17	CLA	A	820	1	56,73,73	1.95	12 (21%)	65,113,113	2.07	20 (30%)
17	CLA	A	821	1	33,53,73	2.42	11 (33%)	37,89,113	2.82	18 (48%)
17	CLA	A	822	29	56,73,73	1.95	12 (21%)	65,113,113	2.04	20 (30%)
17	CLA	A	823	1	40,57,73	2.33	12 (30%)	46,93,113	2.45	18 (39%)
17	CLA	A	824	1	42,59,73	2.27	12 (28%)	48,96,113	2.47	20 (41%)
17	CLA	A	825	1	46,63,73	2.19	12 (26%)	53,101,113	2.34	19 (35%)
17	CLA	A	826	29	56,73,73	1.93	12 (21%)	65,113,113	2.18	17 (26%)
17	CLA	A	827	29	56,73,73	1.97	12 (21%)	65,113,113	2.02	19 (29%)
17	CLA	A	828	1	56,73,73	1.93	12 (21%)	65,113,113	2.13	19 (29%)
17	CLA	A	829	1	56,73,73	1.91	12 (21%)	65,113,113	2.11	20 (30%)
17	CLA	A	830	1	56,73,73	1.99	12 (21%)	65,113,113	2.16	20 (30%)
17	CLA	A	831	1	56,73,73	1.93	12 (21%)	65,113,113	2.21	19 (29%)
17	CLA	A	832	1	41,58,73	2.28	12 (29%)	47,95,113	2.53	21 (44%)
17	CLA	A	833	1	56,73,73	1.95	12 (21%)	65,113,113	2.08	20 (30%)
17	CLA	A	834	1	56,73,73	1.94	12 (21%)	65,113,113	2.21	19 (29%)
17	CLA	A	835	1	56,73,73	1.95	12 (21%)	65,113,113	2.20	22 (33%)
17	CLA	A	836	1	41,58,73	2.28	12 (29%)	47,95,113	2.55	20 (42%)
17	CLA	A	837	1	33,53,73	2.46	11 (33%)	37,89,113	2.63	18 (48%)
17	CLA	A	838	1	42,59,73	2.24	12 (28%)	48,96,113	2.43	19 (39%)
17	CLA	A	839	1	56,73,73	1.93	12 (21%)	65,113,113	2.17	19 (29%)
17	CLA	A	840	1	56,73,73	1.96	12 (21%)	65,113,113	2.16	20 (30%)
17	CLA	A	841	1	56,73,73	1.99	11 (19%)	65,113,113	2.05	16 (24%)
17	CLA	A	842	1	56,73,73	1.96	12 (21%)	65,113,113	2.09	20 (30%)
17	CLA	A	843	29	56,73,73	1.92	12 (21%)	65,113,113	2.11	19 (29%)
18	PQN	A	844	-	34,34,34	1.41	2 (5%)	43,45,45	1.16	4 (9%)
17	CLA	A	845	19	43,60,73	2.26	12 (27%)	49,97,113	2.41	18 (36%)
19	LHG	A	846	-	48,48,48	0.92	2 (4%)	49,54,54	1.11	3 (6%)
19	LHG	A	847	17	26,26,48	1.26	2 (7%)	27,32,54	1.33	3 (11%)
20	BCR	A	848	-	41,41,41	1.01	1 (2%)	56,56,56	1.81	14 (25%)
20	BCR	A	849	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	13 (23%)
20	BCR	A	850	-	41,41,41	1.03	1 (2%)	56,56,56	1.94	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	BCR	A	851	-	41,41,41	1.04	1 (2%)	56,56,56	2.02	14 (25%)
20	BCR	A	852	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	14 (25%)
21	SF4	A	853	1,2	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	A	854	29	56,73,73	1.94	12 (21%)	65,113,113	2.41	24 (36%)
22	HTG	A	855	-	19,19,19	1.01	2 (10%)	23,24,24	0.73	0
20	BCR	A	856	-	41,41,41	1.01	1 (2%)	56,56,56	2.03	16 (28%)
20	BCR	B	801	-	41,41,41	1.03	1 (2%)	56,56,56	1.47	8 (14%)
17	CLA	B	802	2	56,73,73	1.95	12 (21%)	65,113,113	2.14	22 (33%)
17	CLA	B	803	2	56,73,73	1.96	12 (21%)	65,113,113	1.92	21 (32%)
17	CLA	B	804	2	33,53,73	2.41	11 (33%)	37,89,113	2.69	18 (48%)
17	CLA	B	805	2	56,73,73	1.93	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	B	806	2	56,73,73	1.95	12 (21%)	65,113,113	2.04	19 (29%)
17	CLA	B	807	2	56,73,73	1.98	12 (21%)	65,113,113	2.15	23 (35%)
17	CLA	B	808	2	56,73,73	1.96	12 (21%)	65,113,113	2.22	23 (35%)
17	CLA	B	809	2	56,73,73	1.91	12 (21%)	65,113,113	2.11	18 (27%)
17	CLA	B	810	2	56,73,73	1.95	12 (21%)	65,113,113	2.14	22 (33%)
17	CLA	B	811	2	45,62,73	2.02	12 (26%)	56,100,113	2.38	21 (37%)
17	CLA	B	812	2	46,63,73	2.18	12 (26%)	53,101,113	2.24	18 (33%)
17	CLA	B	813	2	56,73,73	1.94	12 (21%)	65,113,113	2.11	20 (30%)
17	CLA	B	814	2	56,73,73	1.93	12 (21%)	65,113,113	2.06	22 (33%)
17	CLA	B	815	2	51,68,73	2.06	12 (23%)	59,107,113	2.21	20 (33%)
17	CLA	B	816	2	46,63,73	2.15	12 (26%)	53,101,113	2.33	21 (39%)
17	CLA	B	817	2	50,67,73	2.05	12 (24%)	57,105,113	2.26	22 (38%)
17	CLA	B	818	2	51,68,73	2.05	12 (23%)	59,107,113	2.24	19 (32%)
17	CLA	B	819	29	56,73,73	1.95	12 (21%)	65,113,113	2.13	23 (35%)
17	CLA	B	820	2	41,58,73	2.31	12 (29%)	47,95,113	2.41	19 (40%)
17	CLA	B	821	2	37,54,73	2.40	12 (32%)	43,90,113	2.57	17 (39%)
17	CLA	B	822	2	46,63,73	2.18	12 (26%)	53,101,113	2.24	20 (37%)
17	CLA	B	823	2	51,68,73	2.06	12 (23%)	59,107,113	2.19	22 (37%)
17	CLA	B	824	29	56,73,73	1.93	12 (21%)	65,113,113	2.11	20 (30%)
17	CLA	B	825	29	56,73,73	1.95	12 (21%)	65,113,113	2.13	23 (35%)
17	CLA	B	826	2	56,73,73	1.94	12 (21%)	65,113,113	2.18	19 (29%)
17	CLA	B	827	2	56,73,73	1.94	12 (21%)	65,113,113	2.15	21 (32%)
17	CLA	B	828	2	56,73,73	1.97	12 (21%)	65,113,113	2.08	19 (29%)
17	CLA	B	829	2	56,73,73	1.94	12 (21%)	65,113,113	2.25	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	B	830	2	41,58,73	2.27	12 (29%)	47,95,113	2.44	19 (40%)
17	CLA	B	831	2	40,57,73	2.30	12 (30%)	46,93,113	2.35	18 (39%)
17	CLA	B	832	2	56,73,73	1.95	12 (21%)	65,113,113	2.03	19 (29%)
17	CLA	B	833	2	49,66,73	2.08	12 (24%)	56,104,113	2.28	18 (32%)
17	CLA	B	834	2	56,73,73	1.98	12 (21%)	65,113,113	2.04	19 (29%)
17	CLA	B	835	29	33,53,73	2.42	11 (33%)	37,89,113	2.52	18 (48%)
17	CLA	B	836	2	51,68,73	2.08	12 (23%)	59,107,113	2.27	18 (30%)
17	CLA	B	837	2	56,73,73	1.95	12 (21%)	65,113,113	2.13	22 (33%)
17	CLA	B	838	2	38,55,73	2.34	12 (31%)	44,91,113	2.53	18 (40%)
17	CLA	B	839	29	56,73,73	1.96	12 (21%)	65,113,113	2.13	18 (27%)
17	CLA	B	840	2	56,73,73	1.96	12 (21%)	65,113,113	2.10	19 (29%)
17	CLA	B	841	19	56,73,73	1.96	12 (21%)	65,113,113	2.15	20 (30%)
18	PQN	B	842	-	34,34,34	1.40	2 (5%)	43,45,45	1.08	2 (4%)
20	BCR	B	843	-	41,41,41	1.03	1 (2%)	56,56,56	1.87	13 (23%)
20	BCR	B	844	-	41,41,41	1.02	1 (2%)	56,56,56	1.97	13 (23%)
20	BCR	B	845	-	41,41,41	0.99	1 (2%)	56,56,56	2.01	17 (30%)
20	BCR	B	846	-	41,41,41	1.02	1 (2%)	56,56,56	1.75	18 (32%)
20	BCR	B	847	-	41,41,41	1.04	1 (2%)	56,56,56	1.73	15 (26%)
20	BCR	B	848	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	13 (23%)
23	LMT	B	849	-	36,36,36	0.48	0	47,47,47	0.99	3 (6%)
24	DGD	B	850	-	67,67,67	0.85	2 (2%)	81,81,81	0.96	5 (6%)
21	SF4	C	101	3	0,12,12	0.00	-	0,24,24	0.00	-
21	SF4	C	102	3	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	F	301	29	56,73,73	1.97	12 (21%)	65,113,113	2.12	18 (27%)
22	HTG	F	302	-	19,19,19	0.99	2 (10%)	23,24,24	0.63	0
17	CLA	F	303	29	33,53,73	2.42	11 (33%)	37,89,113	2.60	16 (43%)
17	CLA	F	304	6	46,63,73	2.17	12 (26%)	53,101,113	2.26	22 (41%)
20	BCR	F	305	-	41,41,41	1.02	1 (2%)	56,56,56	1.73	17 (30%)
17	CLA	G	101	29	33,53,73	2.42	11 (33%)	37,89,113	2.60	16 (43%)
25	LMG	G	102	-	44,44,55	0.99	2 (4%)	52,52,63	1.01	3 (5%)
17	CLA	G	103	7	41,58,73	2.30	12 (29%)	47,95,113	2.42	19 (40%)
17	CLA	G	104	7	37,54,73	2.40	12 (32%)	43,90,113	2.41	17 (39%)
20	BCR	G	105	-	41,41,41	1.03	1 (2%)	56,56,56	1.85	16 (28%)
20	BCR	I	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.92	16 (28%)
22	HTG	J	3001	-	19,19,19	1.04	2 (10%)	23,24,24	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	J	3002	10	33,50,73	2.47	11 (33%)	38,85,113	2.61	18 (47%)
20	BCR	J	3003	-	41,41,41	1.01	1 (2%)	56,56,56	1.76	14 (25%)
20	BCR	K	4001	-	41,41,41	1.03	1 (2%)	56,56,56	1.79	11 (19%)
17	CLA	K	4002	-	33,53,73	2.45	11 (33%)	37,89,113	2.61	17 (45%)
17	CLA	K	4003	11	37,54,73	2.42	12 (32%)	43,90,113	2.53	18 (41%)
20	BCR	K	4004	-	41,41,41	1.02	1 (2%)	56,56,56	1.81	13 (23%)
20	BCR	L	201	-	41,41,41	1.04	1 (2%)	56,56,56	1.87	14 (25%)
17	CLA	L	202	12	56,73,73	1.95	12 (21%)	65,113,113	2.09	20 (30%)
17	CLA	L	203	12	56,73,73	1.96	12 (21%)	65,113,113	2.06	22 (33%)
17	CLA	L	204	29	41,58,73	2.29	12 (29%)	47,95,113	2.42	20 (42%)
20	BCR	L	205	-	41,41,41	1.01	1 (2%)	56,56,56	1.66	11 (19%)
20	BCR	L	206	-	41,41,41	1.04	1 (2%)	56,56,56	1.84	12 (21%)
17	CLA	a	801	1	56,73,73	1.95	12 (21%)	65,113,113	2.28	22 (33%)
17	CLA	a	802	1	56,73,73	1.97	12 (21%)	65,113,113	2.03	24 (36%)
17	CLA	a	803	29	56,73,73	1.91	12 (21%)	65,113,113	2.24	20 (30%)
17	CLA	a	804	1	56,73,73	1.97	12 (21%)	65,113,113	2.15	21 (32%)
17	CLA	a	805	1	46,63,73	2.15	12 (26%)	53,101,113	2.32	20 (37%)
17	CLA	a	806	1	56,73,73	1.96	12 (21%)	65,113,113	2.18	22 (33%)
17	CLA	a	807	1	56,73,73	1.95	12 (21%)	65,113,113	2.18	22 (33%)
17	CLA	a	808	1	56,73,73	1.96	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	a	809	1	56,73,73	1.96	11 (19%)	65,113,113	2.14	19 (29%)
17	CLA	a	810	1	56,73,73	1.96	12 (21%)	65,113,113	2.15	20 (30%)
17	CLA	a	811	1	56,73,73	1.96	12 (21%)	65,113,113	2.11	22 (33%)
17	CLA	a	812	1	56,73,73	1.96	12 (21%)	65,113,113	2.08	21 (32%)
17	CLA	a	813	1	45,62,73	2.23	12 (26%)	51,99,113	2.32	19 (37%)
17	CLA	a	814	1	56,73,73	1.96	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	a	815	1	33,53,73	2.45	11 (33%)	37,89,113	2.51	16 (43%)
17	CLA	a	816	1	41,58,73	2.30	12 (29%)	47,95,113	2.40	19 (40%)
17	CLA	a	817	29	33,53,73	2.42	11 (33%)	37,89,113	2.67	16 (43%)
17	CLA	a	818	1	56,73,73	1.98	12 (21%)	65,113,113	2.20	21 (32%)
17	CLA	a	819	1	56,73,73	1.99	12 (21%)	65,113,113	2.01	19 (29%)
17	CLA	a	820	1	56,73,73	1.98	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	a	821	1	33,53,73	2.40	10 (30%)	37,89,113	2.86	17 (45%)
17	CLA	a	822	29	56,73,73	1.95	12 (21%)	65,113,113	2.06	20 (30%)
17	CLA	a	823	1	40,57,73	2.33	12 (30%)	46,93,113	2.44	18 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	a	824	1	42,59,73	2.26	12 (28%)	48,96,113	2.48	18 (37%)
17	CLA	a	825	1	46,63,73	2.18	12 (26%)	53,101,113	2.28	19 (35%)
17	CLA	a	826	29	56,73,73	1.94	12 (21%)	65,113,113	2.17	18 (27%)
17	CLA	a	827	29	56,73,73	1.96	12 (21%)	65,113,113	2.03	19 (29%)
17	CLA	a	828	1	56,73,73	1.92	12 (21%)	65,113,113	2.17	19 (29%)
17	CLA	a	829	1	56,73,73	1.93	12 (21%)	65,113,113	2.14	19 (29%)
17	CLA	a	830	1	56,73,73	1.99	12 (21%)	65,113,113	2.16	19 (29%)
17	CLA	a	831	1	56,73,73	1.92	12 (21%)	65,113,113	2.21	21 (32%)
17	CLA	a	832	1	41,58,73	2.29	12 (29%)	47,95,113	2.56	21 (44%)
17	CLA	a	833	1	56,73,73	1.96	12 (21%)	65,113,113	2.06	19 (29%)
17	CLA	a	834	1	56,73,73	1.94	12 (21%)	65,113,113	2.13	20 (30%)
17	CLA	a	835	1	56,73,73	1.95	12 (21%)	65,113,113	2.19	22 (33%)
17	CLA	a	836	1	41,58,73	2.27	12 (29%)	47,95,113	2.53	20 (42%)
17	CLA	a	837	1	33,53,73	2.44	11 (33%)	37,89,113	2.71	18 (48%)
17	CLA	a	838	1	42,59,73	2.25	11 (26%)	48,96,113	2.43	22 (45%)
17	CLA	a	839	1	56,73,73	1.95	12 (21%)	65,113,113	2.14	18 (27%)
17	CLA	a	840	1	56,73,73	1.96	12 (21%)	65,113,113	2.19	20 (30%)
17	CLA	a	841	1	56,73,73	1.96	12 (21%)	65,113,113	2.06	20 (30%)
17	CLA	a	842	29	56,73,73	1.97	12 (21%)	65,113,113	2.10	19 (29%)
17	CLA	a	843	1	56,73,73	1.93	12 (21%)	65,113,113	2.10	21 (32%)
17	CLA	a	844	29	56,73,73	1.91	12 (21%)	65,113,113	2.15	18 (27%)
18	PQN	a	845	-	34,34,34	1.43	2 (5%)	43,45,45	1.04	4 (9%)
17	CLA	a	846	19	43,60,73	2.26	12 (27%)	49,97,113	2.40	18 (36%)
19	LHG	a	847	-	48,48,48	0.92	2 (4%)	49,54,54	1.11	3 (6%)
19	LHG	a	848	17	26,26,48	1.24	2 (7%)	27,32,54	1.38	3 (11%)
20	BCR	a	849	-	41,41,41	1.03	1 (2%)	56,56,56	1.95	12 (21%)
20	BCR	a	850	-	41,41,41	0.99	1 (2%)	56,56,56	1.86	15 (26%)
20	BCR	a	851	-	41,41,41	1.01	1 (2%)	56,56,56	1.72	16 (28%)
20	BCR	a	852	-	41,41,41	1.02	1 (2%)	56,56,56	1.93	17 (30%)
20	BCR	a	853	-	41,41,41	1.03	1 (2%)	56,56,56	1.93	14 (25%)
20	BCR	a	854	-	41,41,41	1.02	1 (2%)	56,56,56	1.73	12 (21%)
21	SF4	a	855	1,2	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	a	856	29	56,73,73	1.92	12 (21%)	65,113,113	2.38	23 (35%)
22	HTG	a	857	-	19,19,19	1.03	2 (10%)	23,24,24	0.56	0
20	BCR	b	801	-	41,41,41	1.01	1 (2%)	56,56,56	1.42	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	b	802	2	56,73,73	1.94	12 (21%)	65,113,113	2.13	22 (33%)
17	CLA	b	803	2	56,73,73	1.96	12 (21%)	65,113,113	1.92	19 (29%)
17	CLA	b	804	2	33,53,73	2.40	11 (33%)	37,89,113	2.75	17 (45%)
17	CLA	b	805	2	56,73,73	1.93	12 (21%)	65,113,113	2.14	20 (30%)
17	CLA	b	806	2	56,73,73	1.95	12 (21%)	65,113,113	2.01	19 (29%)
17	CLA	b	807	2	56,73,73	1.98	12 (21%)	65,113,113	2.12	19 (29%)
17	CLA	b	808	2	56,73,73	1.94	12 (21%)	65,113,113	2.26	23 (35%)
17	CLA	b	809	2	56,73,73	1.88	12 (21%)	65,113,113	2.14	19 (29%)
17	CLA	b	810	2	56,73,73	1.96	12 (21%)	65,113,113	2.09	19 (29%)
17	CLA	b	811	2	45,62,73	2.01	12 (26%)	56,100,113	2.44	22 (39%)
17	CLA	b	812	2	46,63,73	2.18	12 (26%)	53,101,113	2.29	20 (37%)
17	CLA	b	813	2	56,73,73	1.94	12 (21%)	65,113,113	2.12	18 (27%)
17	CLA	b	814	2	56,73,73	1.95	12 (21%)	65,113,113	2.07	20 (30%)
17	CLA	b	815	2	46,63,73	2.15	12 (26%)	53,101,113	2.39	21 (39%)
17	CLA	b	816	2	46,63,73	2.15	12 (26%)	53,101,113	2.33	21 (39%)
17	CLA	b	817	2	50,67,73	2.07	12 (24%)	57,105,113	2.23	22 (38%)
17	CLA	b	818	2	51,68,73	2.03	12 (23%)	59,107,113	2.27	19 (32%)
17	CLA	b	819	29	56,73,73	1.95	12 (21%)	65,113,113	2.11	19 (29%)
17	CLA	b	820	2	41,58,73	2.29	12 (29%)	47,95,113	2.48	21 (44%)
17	CLA	b	821	2	37,54,73	2.39	12 (32%)	43,90,113	2.53	16 (37%)
17	CLA	b	822	2	46,63,73	2.17	12 (26%)	53,101,113	2.25	19 (35%)
17	CLA	b	823	2	51,68,73	2.05	12 (23%)	59,107,113	2.14	18 (30%)
17	CLA	b	824	29	56,73,73	1.95	12 (21%)	65,113,113	2.16	21 (32%)
17	CLA	b	825	29	56,73,73	1.95	12 (21%)	65,113,113	2.07	21 (32%)
17	CLA	b	826	2	56,73,73	1.93	12 (21%)	65,113,113	2.14	20 (30%)
17	CLA	b	827	2	56,73,73	1.94	12 (21%)	65,113,113	2.13	19 (29%)
17	CLA	b	828	2	56,73,73	1.96	12 (21%)	65,113,113	2.07	19 (29%)
17	CLA	b	829	2	56,73,73	1.89	12 (21%)	65,113,113	2.30	20 (30%)
17	CLA	b	830	2	41,58,73	2.29	12 (29%)	47,95,113	2.45	22 (46%)
17	CLA	b	831	2	40,57,73	2.30	12 (30%)	46,93,113	2.38	17 (36%)
17	CLA	b	832	2	56,73,73	1.94	12 (21%)	65,113,113	2.08	21 (32%)
17	CLA	b	833	2	49,66,73	2.10	12 (24%)	56,104,113	2.34	19 (33%)
17	CLA	b	834	2	56,73,73	1.97	12 (21%)	65,113,113	2.17	20 (30%)
17	CLA	b	835	29	33,53,73	2.42	11 (33%)	37,89,113	2.57	18 (48%)
17	CLA	b	836	2	51,68,73	2.06	12 (23%)	59,107,113	2.32	19 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	b	837	2	56,73,73	1.95	12 (21%)	65,113,113	2.11	23 (35%)
17	CLA	b	838	2	38,55,73	2.41	12 (31%)	44,91,113	2.50	19 (43%)
17	CLA	b	839	29	56,73,73	1.98	12 (21%)	65,113,113	2.13	17 (26%)
17	CLA	b	840	2	56,73,73	1.96	12 (21%)	65,113,113	2.16	18 (27%)
17	CLA	b	841	19	56,73,73	1.96	12 (21%)	65,113,113	2.15	21 (32%)
18	PQN	b	842	-	34,34,34	1.42	2 (5%)	43,45,45	1.02	2 (4%)
20	BCR	b	843	-	41,41,41	1.04	1 (2%)	56,56,56	1.92	14 (25%)
20	BCR	b	844	-	41,41,41	1.01	1 (2%)	56,56,56	2.07	14 (25%)
20	BCR	b	845	-	41,41,41	1.03	1 (2%)	56,56,56	1.94	14 (25%)
20	BCR	b	846	-	41,41,41	1.06	1 (2%)	56,56,56	1.65	13 (23%)
20	BCR	b	847	-	41,41,41	1.03	1 (2%)	56,56,56	1.82	15 (26%)
20	BCR	b	848	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	10 (17%)
24	DGD	b	849	-	67,67,67	0.85	2 (2%)	81,81,81	1.03	4 (4%)
21	SF4	c	101	3	0,12,12	0.00	-	0,24,24	0.00	-
21	SF4	c	102	3	0,12,12	0.00	-	0,24,24	0.00	-
22	HTG	f	7001	-	19,19,19	1.03	2 (10%)	23,24,24	0.59	0
17	CLA	f	7002	29	33,53,73	2.41	11 (33%)	37,89,113	2.60	18 (48%)
17	CLA	f	7003	6	46,63,73	2.18	12 (26%)	53,101,113	2.32	21 (39%)
20	BCR	f	7004	-	41,41,41	1.01	1 (2%)	56,56,56	1.74	17 (30%)
17	CLA	g	101	-	32,49,73	2.47	12 (37%)	37,84,113	2.75	17 (45%)
17	CLA	g	102	7	41,58,73	2.30	12 (29%)	47,95,113	2.49	21 (44%)
17	CLA	g	103	7	37,54,73	2.39	12 (32%)	43,90,113	2.47	17 (39%)
20	BCR	g	104	-	41,41,41	1.03	1 (2%)	56,56,56	1.89	16 (28%)
20	BCR	i	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.59	11 (19%)
22	HTG	j	3001	-	19,19,19	1.09	2 (10%)	23,24,24	0.60	0
17	CLA	j	3002	10	33,50,73	2.47	11 (33%)	38,85,113	2.60	18 (47%)
20	BCR	j	3003	-	41,41,41	1.00	1 (2%)	56,56,56	1.71	15 (26%)
20	BCR	j	3004	-	41,41,41	1.03	1 (2%)	56,56,56	2.15	18 (32%)
17	CLA	k	1401	-	33,53,73	2.44	11 (33%)	37,89,113	2.58	17 (45%)
17	CLA	k	1402	11	37,54,73	2.39	12 (32%)	43,90,113	2.44	16 (37%)
17	CLA	k	1403	-	37,54,73	2.42	12 (32%)	43,90,113	2.50	18 (41%)
20	BCR	k	1404	-	41,41,41	1.02	1 (2%)	56,56,56	1.78	12 (21%)
20	BCR	l	201	-	41,41,41	1.02	1 (2%)	56,56,56	1.84	15 (26%)
17	CLA	l	202	12	56,73,73	1.96	12 (21%)	65,113,113	2.10	20 (30%)
17	CLA	l	203	12	56,73,73	1.96	12 (21%)	65,113,113	2.09	22 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	1	204	29	41,58,73	2.28	12 (29%)	47,95,113	2.43	22 (46%)
20	BCR	1	205	-	41,41,41	1.00	1 (2%)	56,56,56	1.59	10 (17%)
20	BCR	1	206	-	41,41,41	1.04	1 (2%)	56,56,56	1.79	11 (19%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	2	609	14	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	2	610	19	2/2/15/25	0/8/106/135	0/0/9/9
17	CLA	2	611	14	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	2	612	14	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	2	613	14	3/3/15/25	0/11/109/135	0/0/9/9
26	CHL	2	614	14	-	0/14/150/177	0/0/9/9
27	LUT	2	615	-	-	0/29/67/67	0/2/2/2
28	XAT	2	616	-	-	0/31/93/93	0/2/4/4
20	BCR	2	617	-	-	0/29/63/63	0/2/2/2
19	LHG	2	618	17	-	0/41/41/53	0/0/0/0
17	CLA	3	301	-	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	3	302	15	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	3	303	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	3	304	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	3	305	29	3/3/15/25	0/10/108/135	0/0/9/9
17	CLA	3	306	15	3/3/16/25	0/16/114/135	0/0/9/9
26	CHL	3	307	29	-	0/19/155/177	0/0/9/9
17	CLA	3	308	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	3	309	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	3	310	19	3/3/13/25	0/2/96/135	0/0/9/9
17	CLA	3	311	-	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	3	312	15	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	3	313	15	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	3	314	15	2/2/16/25	0/15/113/135	0/0/9/9
17	CLA	3	315	-	3/3/7/25	0/0/66/135	0/0/8/9
27	LUT	3	316	-	-	0/29/67/67	0/2/2/2
28	XAT	3	317	-	-	0/31/93/93	0/2/4/4
20	BCR	3	318	-	-	0/29/63/63	0/2/2/2
19	LHG	3	319	17	-	0/23/23/53	0/0/0/0
17	CLA	4	601	16	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	4	602	16	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	4	603	16	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	4	604	29	3/3/17/25	0/19/117/135	0/0/9/9
26	CHL	4	605	29	1/1/28/36	0/29/165/177	0/0/9/9
26	CHL	4	606	29	-	0/23/159/177	0/0/9/9
26	CHL	4	607	29	-	0/23/159/177	0/0/9/9
17	CLA	4	608	16	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	609	16	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	4	610	29	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	4	611	16	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	4	612	16	3/3/18/25	0/27/125/135	0/0/9/9
17	CLA	4	613	16	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	4	614	16	3/3/17/25	0/19/117/135	0/0/9/9
26	CHL	4	615	16	-	0/14/150/177	0/0/9/9
27	LUT	4	616	-	-	0/29/67/67	0/2/2/2
28	XAT	4	617	-	-	0/31/93/93	0/2/4/4
20	BCR	4	618	-	-	0/29/63/63	0/2/2/2
25	LMG	4	619	-	-	0/39/59/70	0/1/1/1
25	LMG	4	620	-	-	0/39/59/70	0/1/1/1
19	LHG	6	301	17	-	0/26/26/53	0/0/0/0
25	LMG	6	302	-	-	0/35/55/70	0/1/1/1
26	CHL	6	303	13	1/1/29/36	1/35/171/177	0/0/9/9
17	CLA	6	304	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	6	305	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	6	306	29	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	6	307	-	3/3/15/25	0/10/108/135	0/0/9/9
26	CHL	6	308	13	-	0/19/155/177	0/0/9/9
17	CLA	6	309	29	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	6	310	13	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	6	311	13	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	6	312	19	3/3/15/25	0/8/106/135	0/0/9/9
17	CLA	6	313	13	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	6	314	13	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	6	315	13	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	6	316	13	3/3/16/25	0/15/113/135	0/0/9/9
27	LUT	6	317	-	-	0/29/67/67	0/2/2/2
28	XAT	6	318	-	-	0/31/93/93	0/2/4/4
20	BCR	6	319	-	-	0/29/63/63	0/2/2/2
19	LHG	6	320	17	-	0/53/53/53	0/0/0/0
27	LUT	6	321	-	-	0/29/67/67	0/2/2/2
26	CHL	7	601	14	1/1/29/36	1/35/171/177	0/0/9/9
17	CLA	7	602	14	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	7	603	14	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	7	604	29	3/3/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	7	605	29	-	0/14/150/177	0/0/9/9
26	CHL	7	606	-	-	0/20/156/177	0/0/9/9
26	CHL	7	607	29	-	0/23/159/177	0/0/9/9
17	CLA	7	608	14	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	7	609	14	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	7	610	19	3/3/15/25	0/8/106/135	0/0/9/9
17	CLA	7	611	14	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	7	612	14	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	7	613	14	2/2/15/25	0/11/109/135	0/0/9/9
26	CHL	7	614	14	-	0/14/150/177	0/0/9/9
27	LUT	7	615	-	-	0/29/67/67	0/2/2/2
28	XAT	7	616	-	-	0/31/93/93	0/2/4/4
20	BCR	7	617	-	-	0/29/63/63	0/2/2/2
19	LHG	7	618	17	-	0/41/41/53	0/0/0/0
17	CLA	8	301	15	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	8	302	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	8	303	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	8	304	29	3/3/15/25	0/10/108/135	0/0/9/9
17	CLA	8	305	15	3/3/16/25	0/16/114/135	0/0/9/9
26	CHL	8	306	29	-	0/19/155/177	0/0/9/9
17	CLA	8	307	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	8	308	15	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	8	309	-	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	8	310	15	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	8	311	15	2/2/16/25	0/11/111/135	0/0/9/9
17	CLA	8	312	15	2/2/16/25	0/15/113/135	0/0/9/9
17	CLA	8	313	-	3/3/7/25	0/0/66/135	0/0/8/9
27	LUT	8	314	-	-	0/29/67/67	0/2/2/2
28	XAT	8	315	-	-	0/31/93/93	0/2/4/4
20	BCR	8	316	-	-	0/29/63/63	0/2/2/2
17	CLA	9	601	16	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	9	602	16	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	9	603	16	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	9	604	29	3/3/17/25	0/19/117/135	0/0/9/9
26	CHL	9	605	29	1/1/28/36	0/29/165/177	0/0/9/9
26	CHL	9	606	29	-	0/23/159/177	0/0/9/9
26	CHL	9	607	29	-	0/23/159/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	9	608	16	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	9	609	16	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	9	610	29	3/3/15/25	0/8/106/135	0/0/9/9
17	CLA	9	611	16	3/3/17/25	0/22/120/135	0/0/9/9
17	CLA	9	612	16	3/3/18/25	0/27/125/135	0/0/9/9
17	CLA	9	613	16	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	9	614	16	3/3/16/25	0/16/114/135	0/0/9/9
26	CHL	9	615	16	-	0/14/150/177	0/0/9/9
27	LUT	9	616	-	-	0/29/67/67	0/2/2/2
28	XAT	9	617	-	-	0/31/93/93	0/2/4/4
20	BCR	9	618	-	-	0/29/63/63	0/2/2/2
25	LMG	9	619	-	-	0/45/65/70	0/1/1/1
17	CLA	A	801	1	4/4/20/25	0/37/135/135	0/0/9/9
17	CLA	A	802	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	803	29	1/1/20/25	0/37/135/135	0/0/9/9
17	CLA	A	804	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	805	1	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	A	806	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	807	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	808	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	809	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	810	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	811	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	812	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	813	1	3/3/17/25	0/24/122/135	0/0/9/9
17	CLA	A	814	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	815	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	A	816	1	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	A	817	29	2/2/16/25	0/11/111/135	0/0/9/9
17	CLA	A	818	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	819	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	820	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	821	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	A	822	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	823	1	3/3/16/25	0/18/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	824	1	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	A	825	1	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	A	826	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	827	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	828	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	829	1	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	A	830	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	831	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	832	1	2/2/17/25	0/19/117/135	0/0/9/9
17	CLA	A	833	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	834	1	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	A	835	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	836	1	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	A	837	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	A	838	1	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	A	839	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	840	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	841	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	842	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	A	843	29	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	A	844	-	-	0/23/43/43	0/2/2/2
17	CLA	A	845	19	3/3/17/25	0/22/120/135	0/0/9/9
19	LHG	A	846	-	-	0/53/53/53	0/0/0/0
19	LHG	A	847	17	-	0/31/31/53	0/0/0/0
20	BCR	A	848	-	-	0/29/63/63	0/2/2/2
20	BCR	A	849	-	-	0/29/63/63	0/2/2/2
20	BCR	A	850	-	-	0/29/63/63	0/2/2/2
20	BCR	A	851	-	-	0/29/63/63	0/2/2/2
20	BCR	A	852	-	-	0/29/63/63	0/2/2/2
21	SF4	A	853	1,2	-	0/0/48/48	0/6/5/5
17	CLA	A	854	29	1/1/20/25	0/37/135/135	0/0/9/9
22	HTG	A	855	-	-	0/10/30/30	0/1/1/1
20	BCR	A	856	-	-	0/29/63/63	0/2/2/2
20	BCR	B	801	-	-	0/29/63/63	0/2/2/2
17	CLA	B	802	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	803	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	804	2	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	805	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	806	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	807	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	808	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	809	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	810	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	811	2	3/3/18/25	0/25/121/135	0/0/9/9
17	CLA	B	812	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	B	813	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	814	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	815	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	B	816	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	B	817	2	3/3/18/25	0/30/128/135	0/0/9/9
17	CLA	B	818	2	2/2/19/25	0/31/129/135	0/0/9/9
17	CLA	B	819	29	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	820	2	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	B	821	2	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	B	822	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	B	823	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	B	824	29	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	825	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	826	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	827	2	1/1/20/25	0/37/135/135	0/0/9/9
17	CLA	B	828	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	829	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	830	2	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	B	831	2	3/3/16/25	0/18/116/135	0/0/9/9
17	CLA	B	832	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	833	2	3/3/18/25	0/29/127/135	0/0/9/9
17	CLA	B	834	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	835	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	B	836	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	B	837	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	838	2	2/2/16/25	0/16/114/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	839	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	B	840	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	B	841	19	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	B	842	-	-	0/23/43/43	0/2/2/2
20	BCR	B	843	-	-	0/29/63/63	0/2/2/2
20	BCR	B	844	-	-	0/29/63/63	0/2/2/2
20	BCR	B	845	-	-	0/29/63/63	0/2/2/2
20	BCR	B	846	-	-	0/29/63/63	0/2/2/2
20	BCR	B	847	-	-	0/29/63/63	0/2/2/2
20	BCR	B	848	-	-	0/29/63/63	0/2/2/2
23	LMT	B	849	-	-	0/21/61/61	0/2/2/2
24	DGD	B	850	-	-	0/55/95/95	0/2/2/2
21	SF4	C	101	3	-	0/0/48/48	0/6/5/5
21	SF4	C	102	3	-	0/0/48/48	0/6/5/5
17	CLA	F	301	29	3/3/20/25	0/37/135/135	0/0/9/9
22	HTG	F	302	-	-	0/10/30/30	0/1/1/1
17	CLA	F	303	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	F	304	6	3/3/18/25	0/25/123/135	0/0/9/9
20	BCR	F	305	-	-	0/29/63/63	0/2/2/2
17	CLA	G	101	29	3/3/16/25	0/11/111/135	0/0/9/9
25	LMG	G	102	-	-	0/39/59/70	0/1/1/1
17	CLA	G	103	7	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	G	104	7	3/3/16/25	0/15/113/135	0/0/9/9
20	BCR	G	105	-	-	0/29/63/63	0/2/2/2
20	BCR	I	101	-	-	0/29/63/63	0/2/2/2
22	HTG	J	3001	-	-	0/10/30/30	0/1/1/1
17	CLA	J	3002	10	3/3/15/25	0/10/108/135	0/0/9/9
20	BCR	J	3003	-	-	0/29/63/63	0/2/2/2
20	BCR	K	4001	-	-	0/29/63/63	0/2/2/2
17	CLA	K	4002	-	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	K	4003	11	3/3/16/25	0/15/113/135	0/0/9/9
20	BCR	K	4004	-	-	0/29/63/63	0/2/2/2
20	BCR	L	201	-	-	0/29/63/63	0/2/2/2
17	CLA	L	202	12	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	L	203	12	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	L	204	29	3/3/17/25	0/19/117/135	0/0/9/9
20	BCR	L	205	-	-	0/29/63/63	0/2/2/2
20	BCR	L	206	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	801	1	4/4/20/25	0/37/135/135	0/0/9/9
17	CLA	a	802	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	803	29	1/1/20/25	0/37/135/135	0/0/9/9
17	CLA	a	804	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	805	1	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	a	806	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	807	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	808	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	809	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	810	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	811	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	812	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	813	1	3/3/17/25	0/24/122/135	0/0/9/9
17	CLA	a	814	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	815	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	a	816	1	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	a	817	29	2/2/16/25	0/11/111/135	0/0/9/9
17	CLA	a	818	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	819	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	820	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	821	1	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	a	822	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	823	1	3/3/16/25	0/18/116/135	0/0/9/9
17	CLA	a	824	1	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	a	825	1	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	a	826	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	827	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	828	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	829	1	1/1/20/25	0/37/135/135	0/0/9/9
17	CLA	a	830	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	831	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	832	1	2/2/17/25	0/19/117/135	0/0/9/9
17	CLA	a	833	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	834	1	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	835	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	836	1	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	a	837	1	2/2/16/25	0/11/111/135	0/0/9/9
17	CLA	a	838	1	3/3/17/25	0/21/119/135	0/0/9/9
17	CLA	a	839	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	840	1	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	a	841	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	842	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	843	1	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	a	844	29	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	a	845	-	-	0/23/43/43	0/2/2/2
17	CLA	a	846	19	3/3/17/25	0/22/120/135	0/0/9/9
19	LHG	a	847	-	-	0/53/53/53	0/0/0/0
19	LHG	a	848	17	-	0/31/31/53	0/0/0/0
20	BCR	a	849	-	-	0/29/63/63	0/2/2/2
20	BCR	a	850	-	-	0/29/63/63	0/2/2/2
20	BCR	a	851	-	-	0/29/63/63	0/2/2/2
20	BCR	a	852	-	-	0/29/63/63	0/2/2/2
20	BCR	a	853	-	-	0/29/63/63	0/2/2/2
20	BCR	a	854	-	-	0/29/63/63	0/2/2/2
21	SF4	a	855	1,2	-	0/0/48/48	0/6/5/5
17	CLA	a	856	29	1/1/20/25	0/37/135/135	0/0/9/9
22	HTG	a	857	-	-	0/10/30/30	0/1/1/1
20	BCR	b	801	-	-	0/29/63/63	0/2/2/2
17	CLA	b	802	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	b	803	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	804	2	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	b	805	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	806	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	807	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	808	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	809	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	810	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	811	2	3/3/18/25	0/25/121/135	0/0/9/9
17	CLA	b	812	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	b	813	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	814	2	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	815	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	b	816	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	b	817	2	3/3/18/25	0/30/128/135	0/0/9/9
17	CLA	b	818	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	b	819	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	820	2	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	b	821	2	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	b	822	2	3/3/18/25	0/25/123/135	0/0/9/9
17	CLA	b	823	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	b	824	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	825	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	826	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	827	2	2/2/20/25	0/37/135/135	0/0/9/9
17	CLA	b	828	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	829	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	830	2	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	b	831	2	2/2/16/25	0/18/116/135	0/0/9/9
17	CLA	b	832	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	833	2	3/3/18/25	0/29/127/135	0/0/9/9
17	CLA	b	834	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	835	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	b	836	2	3/3/19/25	0/31/129/135	0/0/9/9
17	CLA	b	837	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	838	2	3/3/16/25	0/16/114/135	0/0/9/9
17	CLA	b	839	29	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	840	2	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	b	841	19	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	b	842	-	-	0/23/43/43	0/2/2/2
20	BCR	b	843	-	-	0/29/63/63	0/2/2/2
20	BCR	b	844	-	-	0/29/63/63	0/2/2/2
20	BCR	b	845	-	-	0/29/63/63	0/2/2/2
20	BCR	b	846	-	-	0/29/63/63	0/2/2/2
20	BCR	b	847	-	-	0/29/63/63	0/2/2/2
20	BCR	b	848	-	-	0/29/63/63	0/2/2/2
24	DGD	b	849	-	-	0/55/95/95	0/2/2/2
21	SF4	c	101	3	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	SF4	c	102	3	-	0/0/48/48	0/6/5/5
22	HTG	f	7001	-	-	0/10/30/30	0/1/1/1
17	CLA	f	7002	29	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	f	7003	6	1/1/18/25	0/25/123/135	0/0/9/9
20	BCR	f	7004	-	-	0/29/63/63	0/2/2/2
17	CLA	g	101	-	2/2/15/25	0/8/106/135	0/0/9/9
17	CLA	g	102	7	3/3/17/25	0/19/117/135	0/0/9/9
17	CLA	g	103	7	3/3/16/25	0/15/113/135	0/0/9/9
20	BCR	g	104	-	-	0/29/63/63	0/2/2/2
20	BCR	i	101	-	-	0/29/63/63	0/2/2/2
22	HTG	j	3001	-	-	0/10/30/30	0/1/1/1
17	CLA	j	3002	10	3/3/15/25	0/10/108/135	0/0/9/9
20	BCR	j	3003	-	-	0/29/63/63	0/2/2/2
20	BCR	j	3004	-	-	0/29/63/63	0/2/2/2
17	CLA	k	1401	-	3/3/16/25	0/11/111/135	0/0/9/9
17	CLA	k	1402	11	3/3/16/25	0/15/113/135	0/0/9/9
17	CLA	k	1403	-	3/3/16/25	0/15/113/135	0/0/9/9
20	BCR	k	1404	-	-	0/29/63/63	0/2/2/2
20	BCR	l	201	-	-	0/29/63/63	0/2/2/2
17	CLA	l	202	12	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	l	203	12	3/3/20/25	0/37/135/135	0/0/9/9
17	CLA	l	204	29	3/3/17/25	0/19/117/135	0/0/9/9
20	BCR	l	205	-	-	0/29/63/63	0/2/2/2
20	BCR	l	206	-	-	0/29/63/63	0/2/2/2

The worst 5 of 4063 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	601	CHL	C3D-C4D	-14.22	1.38	1.54
26	4	606	CHL	C3D-C4D	-14.18	1.38	1.54
26	1	307	CHL	C3D-C4D	-14.09	1.38	1.54
26	2	601	CHL	C3D-C4D	-14.07	1.38	1.54
26	9	615	CHL	C3D-C4D	-14.03	1.38	1.54

The worst 5 of 7028 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	307	CHL	C1C-C2C-C3C	-9.14	102.40	111.52
26	9	607	CHL	C1C-C2C-C3C	-9.04	102.51	111.52
26	8	306	CHL	C1C-C2C-C3C	-8.95	102.60	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	607	CHL	C1C-C2C-C3C	-8.92	102.63	111.52
26	7	614	CHL	C1C-C2C-C3C	-8.83	102.72	111.52

5 of 824 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	9	609	CLA	NC
17	9	609	CLA	ND
17	9	609	CLA	NA
17	a	812	CLA	NC
17	a	812	CLA	ND

All (2) torsion outliers are listed below:

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

There are no ring outliers.

267 monomers are involved in 1072 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	302	CHL	11	0
17	1	303	CLA	3	0
17	1	304	CLA	5	0
17	1	306	CLA	4	0
26	1	307	CHL	2	0
17	1	308	CLA	5	0
17	1	309	CLA	4	0
17	1	310	CLA	2	0
17	1	311	CLA	2	0
17	1	312	CLA	2	0
17	1	313	CLA	8	0
17	1	314	CLA	3	0
17	1	315	CLA	2	0
27	1	316	LUT	8	0
28	1	317	XAT	7	0
20	1	318	BCR	4	0
19	1	319	LHG	3	0
27	1	320	LUT	3	0
26	2	601	CHL	8	0

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	4	610	CLA	6	0
17	4	611	CLA	3	0
17	4	613	CLA	3	0
17	4	614	CLA	1	0
26	4	615	CHL	1	0
27	4	616	LUT	5	0
28	4	617	XAT	5	0
20	4	618	BCR	9	0
25	4	619	LMG	4	0
25	4	620	LMG	4	0
25	6	302	LMG	3	0
26	6	303	CHL	9	0
17	6	304	CLA	4	0
17	6	305	CLA	4	0
17	6	306	CLA	3	0
17	6	307	CLA	4	0
26	6	308	CHL	3	0
17	6	309	CLA	1	0
17	6	310	CLA	2	0
17	6	311	CLA	4	0
17	6	312	CLA	1	0
17	6	313	CLA	3	0
17	6	314	CLA	5	0
17	6	315	CLA	3	0
17	6	316	CLA	1	0
27	6	317	LUT	9	0
28	6	318	XAT	8	0
20	6	319	BCR	7	0
19	6	320	LHG	5	0
27	6	321	LUT	5	0
26	7	601	CHL	5	0
17	7	602	CLA	6	0
17	7	604	CLA	6	0
26	7	605	CHL	5	0
26	7	606	CHL	2	0
26	7	607	CHL	5	0
17	7	608	CLA	5	0
17	7	609	CLA	8	0
17	7	611	CLA	2	0
17	7	612	CLA	4	0
17	7	613	CLA	2	0
26	7	614	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	7	615	LUT	9	0
28	7	616	XAT	6	0
20	7	617	BCR	14	0
19	7	618	LHG	2	0
17	8	301	CLA	6	0
17	8	302	CLA	2	0
17	8	303	CLA	3	0
17	8	304	CLA	1	0
17	8	305	CLA	2	0
26	8	306	CHL	3	0
17	8	307	CLA	6	0
17	8	308	CLA	6	0
17	8	309	CLA	3	0
17	8	310	CLA	1	0
17	8	311	CLA	1	0
17	8	312	CLA	2	0
27	8	314	LUT	7	0
28	8	315	XAT	7	0
20	8	316	BCR	7	0
17	9	601	CLA	3	0
17	9	602	CLA	5	0
17	9	603	CLA	1	0
17	9	604	CLA	4	0
26	9	605	CHL	4	0
26	9	606	CHL	3	0
26	9	607	CHL	4	0
17	9	608	CLA	8	0
17	9	609	CLA	6	0
17	9	610	CLA	2	0
17	9	611	CLA	5	0
17	9	612	CLA	1	0
17	9	614	CLA	4	0
26	9	615	CHL	1	0
27	9	616	LUT	5	0
28	9	617	XAT	8	0
20	9	618	BCR	7	0
25	9	619	LMG	2	0
17	A	801	CLA	7	0
17	A	802	CLA	7	0
17	A	803	CLA	10	0
17	A	804	CLA	11	0
17	A	805	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	806	CLA	13	0
17	A	807	CLA	13	0
17	A	808	CLA	4	0
17	A	809	CLA	12	0
17	A	810	CLA	8	0
17	A	811	CLA	8	0
17	A	812	CLA	10	0
17	A	813	CLA	6	0
17	A	814	CLA	7	0
17	A	815	CLA	3	0
17	A	816	CLA	6	0
17	A	817	CLA	1	0
17	A	818	CLA	9	0
17	A	819	CLA	6	0
17	A	820	CLA	8	0
17	A	821	CLA	3	0
17	A	822	CLA	6	0
17	A	823	CLA	2	0
17	A	824	CLA	4	0
17	A	825	CLA	7	0
17	A	826	CLA	8	0
17	A	827	CLA	6	0
17	A	828	CLA	3	0
17	A	829	CLA	17	0
17	A	830	CLA	9	0
17	A	831	CLA	11	0
17	A	832	CLA	4	0
17	A	833	CLA	9	0
17	A	834	CLA	10	0
17	A	835	CLA	8	0
17	A	836	CLA	4	0
17	A	837	CLA	3	0
17	A	838	CLA	3	0
17	A	839	CLA	11	0
17	A	840	CLA	6	0
17	A	841	CLA	11	0
17	A	842	CLA	12	0
17	A	843	CLA	18	0
18	A	844	PQN	5	0
17	A	845	CLA	3	0
19	A	846	LHG	4	0
19	A	847	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	848	BCR	4	0
20	A	849	BCR	7	0
20	A	850	BCR	5	0
20	A	851	BCR	9	0
20	A	852	BCR	9	0
17	A	854	CLA	7	0
20	A	856	BCR	5	0
20	B	801	BCR	6	0
17	B	802	CLA	9	0
17	B	803	CLA	7	0
17	B	804	CLA	6	0
17	B	805	CLA	5	0
17	B	806	CLA	11	0
17	B	807	CLA	7	0
17	B	808	CLA	8	0
17	B	809	CLA	6	0
17	B	810	CLA	6	0
17	B	811	CLA	6	0
17	B	812	CLA	5	0
17	B	813	CLA	11	0
17	B	814	CLA	4	0
17	B	815	CLA	8	0
17	B	816	CLA	7	0
17	B	817	CLA	7	0
17	B	818	CLA	7	0
17	B	819	CLA	4	0
17	B	820	CLA	2	0
17	B	821	CLA	1	0
17	B	822	CLA	4	0
17	B	823	CLA	5	0
17	B	824	CLA	10	0
17	B	825	CLA	12	0
17	B	826	CLA	3	0
17	B	827	CLA	10	0
17	B	828	CLA	6	0
17	B	829	CLA	13	0
17	B	830	CLA	6	0
17	B	831	CLA	10	0
17	B	832	CLA	10	0
17	B	833	CLA	7	0
17	B	834	CLA	2	0
17	B	835	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	836	CLA	10	0
17	B	837	CLA	8	0
17	B	838	CLA	8	0
17	B	839	CLA	14	0
17	B	840	CLA	9	0
17	B	841	CLA	9	0
18	B	842	PQN	2	0
20	B	843	BCR	8	0
20	B	844	BCR	8	0
20	B	845	BCR	8	0
20	B	846	BCR	10	0
20	B	847	BCR	5	0
20	B	848	BCR	5	0
23	B	849	LMT	2	0
24	B	850	DGD	2	0
17	F	301	CLA	4	0
22	F	302	HTG	2	0
17	F	303	CLA	3	0
17	F	304	CLA	4	0
20	F	305	BCR	6	0
17	G	101	CLA	3	0
25	G	102	LMG	2	0
17	G	103	CLA	5	0
17	G	104	CLA	4	0
20	G	105	BCR	5	0
20	I	101	BCR	7	0
17	J	3002	CLA	2	0
20	J	3003	BCR	6	0
20	K	4001	BCR	4	0
17	K	4002	CLA	3	0
17	K	4003	CLA	3	0
20	K	4004	BCR	2	0
20	L	201	BCR	4	0
17	L	202	CLA	7	0
17	L	203	CLA	7	0
17	L	204	CLA	5	0
20	L	205	BCR	5	0
20	L	206	BCR	5	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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

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

The worst 5 of 585 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	3	259	ASN	8.7
9	i	2	ILE	8.2
15	8	121	LEU	7.2
5	E	2	GLY	7.0
14	2	121	ILE	6.8

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
20	BCR	2	617	40/40	0.67	0.77	20.87	125,133,163,164	0
27	LUT	6	321	42/42	0.75	0.49	7.93	107,113,133,134	0
20	BCR	7	617	40/40	0.70	0.63	7.51	112,119,127,128	0
20	BCR	L	206	40/40	0.48	0.80	6.13	146,151,156,156	0
17	CLA	A	824	51/65	0.84	0.38	6.02	77,89,118,118	0
20	BCR	l	206	40/40	0.77	0.52	5.60	77,82,93,93	0
17	CLA	6	316	46/65	0.82	0.30	5.14	152,162,171,203	0
19	LHG	6	320	49/49	0.89	0.32	4.34	90,100,111,113	0
20	BCR	a	852	40/40	0.86	0.33	4.33	40,62,120,120	0
17	CLA	g	102	50/65	0.92	0.33	4.18	92,107,123,124	0
22	HTG	f	7001	19/19	0.86	0.33	3.92	49,104,107,108	0
17	CLA	3	301	46/65	0.80	0.78	3.83	142,149,154,175	0
20	BCR	K	4004	40/40	0.49	0.62	3.56	94,115,138,138	0
20	BCR	A	850	40/40	0.84	0.30	3.53	53,72,112,112	0
17	CLA	A	845	52/65	0.85	0.41	3.49	90,115,146,149	0
20	BCR	6	319	40/40	0.82	0.47	3.10	104,124,138,140	0
17	CLA	l	202	65/65	0.87	0.40	2.83	57,88,111,113	0
20	BCR	1	318	40/40	0.77	0.50	2.72	94,105,126,127	0
20	BCR	4	618	40/40	0.85	0.30	2.63	79,86,89,90	0
17	CLA	a	824	51/65	0.91	0.23	2.51	61,74,91,93	0
19	LHG	1	319	49/49	0.90	0.27	2.49	77,84,109,109	0
18	PQN	B	842	33/33	0.94	0.44	2.43	46,56,63,63	0
20	BCR	l	205	40/40	0.93	0.24	2.34	39,46,52,54	0
17	CLA	B	809	65/65	0.93	0.23	2.23	41,50,81,82	0
17	CLA	9	609	60/65	0.91	0.37	2.19	72,93,107,108	0
20	BCR	9	618	40/40	0.90	0.29	2.14	86,92,100,101	0
27	LUT	7	615	42/42	0.88	0.47	2.06	72,83,97,98	0
20	BCR	B	844	40/40	0.87	0.28	2.02	50,53,85,87	0
17	CLA	a	811	65/65	0.93	0.20	2.01	42,59,94,96	0
17	CLA	A	811	65/65	0.94	0.26	1.99	54,69,89,90	0
17	CLA	a	809	65/65	0.95	0.20	1.98	36,39,53,57	0
20	BCR	A	856	40/40	0.81	0.25	1.91	65,71,85,85	0
20	BCR	g	104	40/40	0.86	0.40	1.83	57,102,117,118	0
20	BCR	K	4001	40/40	0.59	0.41	1.75	91,94,96,96	0
20	BCR	L	205	40/40	0.92	0.21	1.72	51,61,70,71	0
20	BCR	8	316	40/40	0.87	0.36	1.69	66,71,88,90	0
17	CLA	7	611	52/65	0.91	0.33	1.66	87,104,123,126	0
17	CLA	G	103	50/65	0.91	0.23	1.66	61,80,91,93	0
27	LUT	1	320	42/42	0.87	0.22	1.64	71,79,90,91	0
17	CLA	a	819	65/65	0.93	0.22	1.60	38,54,96,99	0
27	LUT	8	314	42/42	0.91	0.39	1.56	57,73,82,84	0
20	BCR	G	105	40/40	0.85	0.30	1.53	63,71,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	BCR	A	849	40/40	0.93	0.44	1.50	54,62,83,84	0
17	CLA	1	309	65/65	0.86	0.25	1.50	71,79,106,108	0
28	XAT	3	317	44/44	0.87	0.26	1.47	61,74,100,101	0
28	XAT	8	315	44/44	0.90	0.23	1.47	64,69,80,83	0
20	BCR	B	848	40/40	0.94	0.33	1.45	40,45,51,52	0
19	LHG	a	848	27/49	0.73	0.33	1.44	74,95,125,127	0
17	CLA	a	816	50/65	0.93	0.23	1.44	43,52,94,96	0
20	BCR	j	3004	40/40	0.88	0.24	1.44	56,71,82,84	0
17	CLA	8	310	55/65	0.92	0.33	1.44	74,88,99,104	0
17	CLA	2	608	50/65	0.91	0.18	1.42	65,69,108,111	0
25	LMG	6	302	40/55	0.75	0.34	1.41	116,148,163,164	0
17	CLA	K	4002	45/65	0.76	0.46	1.41	115,123,125,154	0
17	CLA	8	311	45/65	0.89	0.34	1.40	100,110,122,161	0
27	LUT	9	616	42/42	0.89	0.38	1.39	68,79,103,104	0
17	CLA	9	614	47/65	0.94	0.23	1.38	62,75,97,99	0
17	CLA	a	846	52/65	0.88	0.32	1.37	86,102,115,140	0
19	LHG	2	618	37/49	0.94	0.30	1.31	80,91,127,130	0
17	CLA	7	603	51/65	0.95	0.19	1.30	52,60,97,98	0
18	PQN	A	844	33/33	0.96	0.24	1.26	42,45,57,58	0
17	CLA	1	308	65/65	0.92	0.37	1.22	57,92,120,121	0
17	CLA	B	808	65/65	0.95	0.25	1.19	41,45,70,73	0
20	BCR	I	101	40/40	0.90	0.23	1.14	54,60,65,65	0
20	BCR	j	3003	40/40	0.92	0.22	1.11	42,52,59,61	0
17	CLA	B	810	65/65	0.92	0.22	1.10	59,77,84,86	0
17	CLA	A	835	65/65	0.92	0.23	1.10	58,67,75,81	0
17	CLA	G	104	46/65	0.93	0.31	1.09	70,93,100,111	0
17	CLA	B	807	65/65	0.93	0.21	1.07	51,66,113,117	0
22	HTG	j	3001	19/19	0.93	0.37	1.07	61,71,80,84	0
28	XAT	6	318	44/44	0.92	0.24	1.04	71,81,94,95	0
17	CLA	b	832	65/65	0.93	0.22	1.04	36,55,70,79	0
17	CLA	a	829	65/65	0.95	0.23	1.04	35,41,56,58	0
17	CLA	A	809	65/65	0.95	0.19	1.03	44,51,63,65	0
26	CHL	2	601	61/66	0.92	0.32	1.02	68,99,113,115	0
17	CLA	b	811	54/65	0.88	0.29	1.02	50,74,114,114	0
17	CLA	B	827	65/65	0.92	0.40	1.02	49,61,78,80	0
17	CLA	b	834	65/65	0.93	0.21	1.02	61,74,105,106	0
17	CLA	B	839	65/65	0.93	0.25	1.02	53,60,69,72	0
17	CLA	7	608	50/65	0.91	0.20	1.01	60,65,93,96	0
27	LUT	4	616	42/42	0.85	0.31	0.99	71,90,94,95	0
26	CHL	9	615	43/66	0.87	0.34	0.98	90,144,147,148	0
26	CHL	7	614	43/66	0.92	0.29	0.97	105,120,127,139	0
25	LMG	4	619	44/55	0.80	0.35	0.95	82,92,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	3	303	50/65	0.95	0.21	0.94	60,67,75,76	0
17	CLA	6	310	65/65	0.89	0.25	0.91	80,90,121,126	0
17	CLA	7	609	60/65	0.93	0.27	0.90	64,86,97,97	0
17	CLA	4	603	46/65	0.95	0.19	0.89	54,62,69,72	0
17	CLA	A	814	65/65	0.92	0.31	0.88	50,59,67,68	0
17	CLA	a	833	65/65	0.94	0.25	0.88	39,46,98,102	0
17	CLA	6	307	42/65	0.91	0.27	0.88	112,126,137,139	0
17	CLA	6	314	60/65	0.93	0.23	0.87	66,109,124,125	0
17	CLA	A	837	45/65	0.86	0.28	0.86	84,95,103,165	0
17	CLA	4	614	50/65	0.94	0.20	0.85	60,68,90,91	0
20	BCR	B	846	40/40	0.91	0.23	0.84	49,53,70,70	0
20	BCR	3	318	40/40	0.92	0.23	0.83	77,83,105,108	0
17	CLA	B	838	47/65	0.95	0.30	0.83	43,48,65,68	0
20	BCR	b	844	40/40	0.83	0.32	0.83	52,67,91,93	0
27	LUT	2	615	42/42	0.90	0.27	0.82	77,84,89,89	0
17	CLA	B	817	59/65	0.91	0.22	0.79	46,53,59,64	0
17	CLA	7	613	43/65	0.93	0.23	0.79	73,78,82,86	0
28	XAT	7	616	44/44	0.89	0.33	0.78	57,64,73,74	0
17	CLA	B	805	65/65	0.93	0.25	0.77	45,47,53,60	0
17	CLA	L	202	65/65	0.84	0.37	0.76	83,111,131,132	0
17	CLA	A	843	65/65	0.94	0.26	0.74	48,64,79,81	0
20	BCR	k	1404	40/40	0.87	0.26	0.71	49,89,103,104	0
27	LUT	6	317	42/42	0.66	0.43	0.70	86,93,118,120	0
28	XAT	1	317	44/44	0.93	0.21	0.69	63,68,93,96	0
17	CLA	1	313	65/65	0.92	0.21	0.69	81,88,108,112	0
20	BCR	B	847	40/40	0.90	0.31	0.68	44,49,52,53	0
24	DGD	b	849	66/66	0.86	0.27	0.68	41,64,90,91	0
24	DGD	B	850	66/66	0.80	0.33	0.68	52,71,93,102	0
17	CLA	a	808	65/65	0.95	0.20	0.67	54,63,86,87	0
17	CLA	B	819	65/65	0.96	0.23	0.67	46,53,80,83	0
17	CLA	b	827	65/65	0.95	0.28	0.67	40,53,83,83	0
17	CLA	g	101	41/65	0.86	0.21	0.66	146,164,166,167	0
17	CLA	8	308	50/65	0.91	0.33	0.64	75,81,87,88	0
20	BCR	a	849	40/40	0.87	0.26	0.62	56,63,75,76	0
26	CHL	9	607	51/66	0.92	0.27	0.60	67,77,98,99	0
17	CLA	a	842	65/65	0.94	0.21	0.60	47,59,96,98	0
25	LMG	9	619	50/55	0.84	0.28	0.59	68,88,96,98	0
17	CLA	A	806	65/65	0.91	0.29	0.59	46,51,59,59	0
17	CLA	B	840	65/65	0.93	0.33	0.59	41,50,72,78	0
17	CLA	B	824	65/65	0.91	0.27	0.58	48,53,70,74	0
20	BCR	B	843	40/40	0.91	0.23	0.57	54,64,72,72	0
17	CLA	B	803	65/65	0.94	0.33	0.57	39,50,61,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	LHG	1	301	23/49	0.95	0.20	0.57	63,84,93,94	0
20	BCR	l	201	40/40	0.93	0.21	0.57	38,46,54,54	0
17	CLA	A	823	49/65	0.89	0.25	0.56	66,79,104,105	0
20	BCR	A	851	40/40	0.88	0.28	0.56	43,66,78,79	0
17	CLA	7	604	60/65	0.87	0.34	0.55	92,101,106,109	0
17	CLA	a	843	65/65	0.95	0.24	0.55	35,39,60,65	0
19	LHG	a	847	49/49	0.96	0.21	0.55	35,41,47,48	0
20	BCR	L	201	40/40	0.94	0.18	0.55	51,59,72,73	0
17	CLA	2	612	65/65	0.90	0.32	0.55	70,93,113,118	0
20	BCR	b	846	40/40	0.92	0.22	0.54	48,56,76,77	0
17	CLA	b	810	65/65	0.95	0.17	0.54	39,49,59,62	0
17	CLA	k	1401	45/65	0.88	0.34	0.54	75,83,94,96	0
17	CLA	b	837	65/65	0.95	0.21	0.53	46,57,69,70	0
26	CHL	6	308	47/66	0.92	0.23	0.53	103,135,146,149	0
17	CLA	A	801	65/65	0.94	0.27	0.52	40,44,49,53	0
17	CLA	B	832	65/65	0.95	0.23	0.52	43,48,73,76	0
17	CLA	a	813	54/65	0.93	0.19	0.51	43,51,60,70	0
17	CLA	k	1402	46/65	0.90	0.26	0.50	62,78,100,106	0
17	CLA	6	306	51/65	0.92	0.24	0.49	118,123,130,131	0
17	CLA	A	834	65/65	0.90	0.24	0.48	49,60,71,75	0
28	XAT	9	617	44/44	0.85	0.23	0.48	72,81,97,98	0
20	BCR	A	848	40/40	0.89	0.32	0.47	50,59,95,95	0
17	CLA	B	818	60/65	0.91	0.26	0.47	45,50,57,61	0
17	CLA	a	814	65/65	0.94	0.24	0.46	39,47,64,67	0
20	BCR	b	801	40/40	0.92	0.20	0.46	36,43,52,55	0
17	CLA	K	4003	46/65	0.83	0.29	0.44	81,119,128,130	0
25	LMG	4	620	44/55	0.69	0.42	0.43	89,97,111,113	0
17	CLA	b	817	59/65	0.92	0.24	0.43	56,59,67,68	0
17	CLA	a	840	65/65	0.92	0.32	0.42	36,41,87,89	0
17	CLA	A	819	65/65	0.95	0.21	0.42	54,65,117,120	0
26	CHL	2	606	48/66	0.86	0.45	0.41	89,97,105,107	0
17	CLA	4	604	50/65	0.90	0.30	0.40	75,84,111,114	0
17	CLA	A	829	65/65	0.95	0.23	0.39	42,46,55,58	0
17	CLA	a	806	65/65	0.95	0.21	0.39	37,39,49,51	0
17	CLA	A	830	65/65	0.95	0.28	0.39	45,53,58,61	0
20	BCR	F	305	40/40	0.95	0.20	0.39	46,51,58,60	0
17	CLA	A	804	65/65	0.92	0.23	0.38	46,58,70,71	0
17	CLA	9	603	46/65	0.95	0.17	0.38	62,64,77,78	0
17	CLA	b	809	65/65	0.94	0.20	0.38	39,50,72,75	0
26	CHL	6	303	61/66	0.93	0.20	0.38	78,91,102,103	0
17	CLA	f	7003	55/65	0.93	0.24	0.37	68,87,121,122	0
17	CLA	6	311	60/65	0.91	0.46	0.37	81,99,115,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	BCR	b	845	40/40	0.88	0.24	0.36	46,67,106,106	0
17	CLA	A	841	65/65	0.95	0.19	0.36	44,50,55,60	0
28	XAT	4	617	44/44	0.93	0.19	0.36	63,72,87,88	0
17	CLA	l	203	65/65	0.93	0.20	0.35	40,51,71,73	0
17	CLA	B	834	65/65	0.90	0.21	0.35	46,58,90,90	0
17	CLA	b	833	58/65	0.93	0.20	0.35	48,63,77,78	0
17	CLA	8	301	60/65	0.96	0.17	0.34	56,64,68,72	0
17	CLA	9	612	56/65	0.91	0.24	0.34	68,77,89,92	0
17	CLA	6	315	55/65	0.93	0.28	0.34	105,114,131,131	0
20	BCR	a	851	40/40	0.95	0.32	0.34	37,53,66,67	0
17	CLA	3	313	45/65	0.87	0.41	0.32	85,97,102,106	0
17	CLA	a	839	65/65	0.93	0.24	0.32	36,43,65,69	0
17	CLA	B	828	65/65	0.95	0.29	0.31	43,48,58,61	0
17	CLA	A	803	65/65	0.95	0.27	0.31	39,44,54,59	0
17	CLA	2	604	60/65	0.88	0.34	0.31	100,111,118,119	0
17	CLA	3	302	60/65	0.88	0.20	0.31	67,79,85,95	0
17	CLA	A	826	65/65	0.93	0.23	0.29	47,57,65,66	0
26	CHL	7	606	48/66	0.90	0.29	0.29	71,87,104,105	0
17	CLA	a	810	65/65	0.95	0.19	0.29	44,59,94,95	0
20	BCR	f	7004	40/40	0.93	0.20	0.28	55,62,66,66	0
17	CLA	7	612	65/65	0.94	0.24	0.27	56,66,87,89	0
17	CLA	9	602	60/65	0.94	0.18	0.27	60,67,74,86	0
17	CLA	4	609	60/65	0.88	0.31	0.26	69,86,106,111	0
17	CLA	a	841	65/65	0.95	0.21	0.26	55,62,65,67	0
17	CLA	2	610	41/65	0.90	0.21	0.26	80,94,108,110	0
17	CLA	B	811	54/65	0.90	0.21	0.26	58,74,103,104	0
17	CLA	b	839	65/65	0.96	0.18	0.25	38,44,50,53	0
17	CLA	9	608	50/65	0.94	0.18	0.25	72,78,103,105	0
17	CLA	B	841	65/65	0.94	0.19	0.25	49,56,63,68	0
22	HTG	F	302	19/19	0.84	0.32	0.24	43,98,105,107	0
17	CLA	4	608	50/65	0.94	0.17	0.24	56,66,76,86	0
17	CLA	a	835	65/65	0.96	0.19	0.24	36,43,48,49	0
17	CLA	F	303	45/65	0.95	0.20	0.23	51,60,71,76	0
28	XAT	2	616	44/44	0.92	0.25	0.23	69,79,86,87	0
17	CLA	F	301	65/65	0.94	0.19	0.23	48,55,83,87	0
17	CLA	A	818	65/65	0.92	0.22	0.23	58,71,95,97	0
20	BCR	B	801	40/40	0.95	0.21	0.22	43,46,54,55	0
17	CLA	A	813	54/65	0.93	0.21	0.22	60,68,77,95	0
17	CLA	L	203	65/65	0.91	0.23	0.21	64,74,87,89	0
17	CLA	B	802	65/65	0.92	0.30	0.20	40,44,50,52	0
17	CLA	b	818	60/65	0.95	0.28	0.20	44,47,53,56	0
17	CLA	B	813	65/65	0.91	0.23	0.20	47,51,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	b	807	65/65	0.91	0.22	0.19	42,51,102,104	0
17	CLA	B	820	50/65	0.95	0.20	0.19	53,69,95,100	0
17	CLA	1	303	65/65	0.90	0.24	0.19	60,67,83,90	0
17	CLA	B	837	65/65	0.94	0.23	0.18	49,55,61,65	0
18	PQN	a	845	33/33	0.96	0.22	0.18	35,48,54,58	0
17	CLA	b	802	65/65	0.95	0.24	0.17	36,41,45,52	0
17	CLA	3	308	50/65	0.94	0.21	0.16	76,86,93,104	0
17	CLA	b	820	50/65	0.91	0.21	0.16	65,72,77,82	0
17	CLA	b	835	45/65	0.93	0.16	0.16	86,92,94,96	0
17	CLA	b	815	55/65	0.92	0.28	0.15	62,78,93,94	0
17	CLA	B	821	46/65	0.88	0.23	0.15	51,60,72,80	0
17	CLA	A	816	50/65	0.95	0.20	0.15	52,70,108,108	0
17	CLA	6	304	65/65	0.94	0.20	0.15	66,79,104,106	0
27	LUT	3	316	42/42	0.92	0.25	0.15	74,78,97,99	0
17	CLA	b	812	55/65	0.91	0.22	0.14	59,70,103,104	0
17	CLA	b	828	65/65	0.96	0.29	0.14	41,47,56,56	0
17	CLA	B	822	55/65	0.93	0.23	0.13	48,58,82,83	0
18	PQN	b	842	33/33	0.96	0.22	0.13	36,41,49,50	0
17	CLA	a	826	65/65	0.94	0.22	0.13	39,43,48,56	0
17	CLA	b	813	65/65	0.94	0.23	0.12	44,57,67,69	0
17	CLA	a	818	65/65	0.95	0.21	0.12	45,53,81,83	0
20	BCR	a	850	40/40	0.96	0.23	0.12	39,48,79,81	0
26	CHL	7	605	43/66	0.87	0.27	0.11	85,89,93,99	0
17	CLA	1	314	55/65	0.89	0.23	0.11	78,93,105,110	0
17	CLA	B	814	65/65	0.91	0.20	0.10	50,57,80,82	0
17	CLA	1	310	60/65	0.90	0.25	0.10	63,80,90,92	0
17	CLA	b	836	60/65	0.94	0.23	0.10	43,53,106,107	0
17	CLA	a	834	65/65	0.94	0.24	0.10	37,44,48,50	0
17	CLA	6	309	46/65	0.90	0.30	0.10	92,99,106,137	0
17	CLA	A	802	65/65	0.95	0.29	0.10	41,45,51,53	0
17	CLA	a	815	45/65	0.94	0.19	0.10	41,54,63,63	0
17	CLA	B	826	65/65	0.95	0.28	0.09	44,50,56,64	0
17	CLA	9	604	50/65	0.89	0.23	0.09	105,116,125,126	0
17	CLA	b	830	50/65	0.90	0.21	0.09	46,59,70,74	0
17	CLA	b	840	65/65	0.94	0.23	0.09	36,41,59,67	0
17	CLA	A	832	50/65	0.90	0.24	0.06	52,70,98,99	0
17	CLA	a	804	65/65	0.91	0.21	0.06	36,52,71,73	0
17	CLA	a	825	55/65	0.96	0.18	0.06	39,44,58,68	0
17	CLA	A	820	65/65	0.94	0.22	0.06	46,50,57,58	0
22	HTG	J	3001	19/19	0.85	0.18	0.05	73,76,78,82	0
17	CLA	B	823	60/65	0.92	0.20	0.05	46,57,84,84	0
17	CLA	A	815	45/65	0.95	0.19	0.04	54,59,65,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	CHL	7	607	51/66	0.94	0.20	0.04	64,70,92,98	0
17	CLA	A	831	65/65	0.93	0.21	0.03	43,52,59,61	0
17	CLA	B	816	55/65	0.93	0.20	0.03	60,67,73,91	0
17	CLA	A	854	65/65	0.95	0.31	0.03	40,44,57,59	0
17	CLA	8	307	50/65	0.96	0.18	0.02	52,65,91,93	0
17	CLA	A	833	65/65	0.93	0.22	0.02	54,61,101,102	0
17	CLA	B	825	65/65	0.92	0.35	0.01	42,50,83,88	0
17	CLA	4	601	46/65	0.92	0.20	0.00	84,92,95,111	0
17	CLA	a	817	45/65	0.92	0.20	-0.01	64,73,78,79	0
17	CLA	J	3002	42/65	0.91	0.17	-0.01	92,105,119,148	0
17	CLA	4	610	55/65	0.89	0.28	-0.01	72,88,94,122	0
17	CLA	A	805	55/65	0.90	0.23	-0.01	45,54,89,89	0
17	CLA	a	802	65/65	0.95	0.27	-0.03	35,42,56,62	0
17	CLA	A	827	65/65	0.92	0.27	-0.04	40,60,97,98	0
17	CLA	B	829	65/65	0.89	0.26	-0.05	42,50,76,77	0
17	CLA	2	609	60/65	0.88	0.23	-0.05	73,87,98,101	0
19	LHG	A	847	27/49	0.83	0.26	-0.06	68,88,113,113	0
26	CHL	2	614	43/66	0.88	0.33	-0.06	116,134,143,145	0
26	CHL	1	302	61/66	0.94	0.21	-0.06	64,74,101,105	0
17	CLA	b	805	65/65	0.94	0.21	-0.06	42,45,52,58	0
17	CLA	9	613	45/65	0.91	0.20	-0.07	87,105,115,137	0
17	CLA	7	602	65/65	0.91	0.20	-0.08	62,70,88,93	0
17	CLA	b	826	65/65	0.95	0.27	-0.11	48,55,59,62	0
17	CLA	a	856	65/65	0.94	0.26	-0.11	36,41,56,59	0
17	CLA	A	808	65/65	0.92	0.18	-0.11	52,61,113,115	0
17	CLA	a	828	65/65	0.95	0.22	-0.11	37,44,67,72	0
17	CLA	a	805	55/65	0.94	0.18	-0.11	38,43,76,78	0
17	CLA	a	820	65/65	0.98	0.20	-0.12	38,43,48,50	0
17	CLA	B	804	45/65	0.94	0.18	-0.12	44,50,68,77	0
25	LMG	G	102	44/55	0.83	0.21	-0.12	72,95,110,113	0
20	BCR	b	847	40/40	0.91	0.24	-0.12	40,49,69,70	0
26	CHL	4	605	56/66	0.91	0.26	-0.12	69,88,96,102	0
17	CLA	a	831	65/65	0.96	0.19	-0.13	36,43,54,56	0
17	CLA	a	807	65/65	0.95	0.22	-0.13	35,41,50,54	0
17	CLA	B	830	50/65	0.94	0.17	-0.13	45,56,75,75	0
17	CLA	B	836	60/65	0.92	0.22	-0.13	43,46,97,97	0
17	CLA	b	841	65/65	0.88	0.20	-0.14	64,80,92,94	0
17	CLA	2	603	65/65	0.94	0.16	-0.14	64,72,106,108	0
17	CLA	b	814	65/65	0.90	0.18	-0.14	47,55,69,71	0
17	CLA	2	602	65/65	0.93	0.22	-0.15	66,73,80,83	0
17	CLA	b	829	65/65	0.93	0.23	-0.15	39,54,67,69	0
17	CLA	a	801	65/65	0.96	0.21	-0.15	35,39,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	A	836	50/65	0.92	0.18	-0.16	60,73,80,86	0
17	CLA	A	810	65/65	0.93	0.19	-0.16	43,51,85,89	0
17	CLA	a	844	65/65	0.96	0.23	-0.16	38,49,59,64	0
17	CLA	b	824	65/65	0.88	0.27	-0.16	45,51,69,72	0
17	CLA	b	808	65/65	0.95	0.18	-0.16	39,47,53,59	0
17	CLA	B	806	65/65	0.94	0.26	-0.17	43,52,60,64	0
20	BCR	B	845	40/40	0.90	0.18	-0.18	47,63,102,102	0
17	CLA	a	832	50/65	0.94	0.20	-0.18	41,54,78,83	0
17	CLA	6	312	41/65	0.92	0.20	-0.19	90,102,109,129	0
17	CLA	A	817	45/65	0.92	0.22	-0.19	66,75,86,92	0
26	CHL	2	607	51/66	0.93	0.22	-0.20	66,75,117,118	0
17	CLA	8	302	50/65	0.95	0.16	-0.20	46,54,73,74	0
17	CLA	A	828	65/65	0.94	0.22	-0.21	49,61,79,84	0
17	CLA	b	821	46/65	0.93	0.18	-0.21	58,69,90,118	0
17	CLA	a	838	51/65	0.95	0.19	-0.21	36,40,63,68	0
26	CHL	3	307	47/66	0.95	0.17	-0.21	72,77,94,97	0
17	CLA	G	101	45/65	0.93	0.21	-0.21	74,79,85,89	0
20	BCR	J	3003	40/40	0.92	0.21	-0.21	45,54,67,68	0
17	CLA	1	305	52/65	0.92	0.23	-0.22	76,101,105,108	0
17	CLA	b	816	55/65	0.93	0.19	-0.22	57,65,72,75	0
20	BCR	b	843	40/40	0.93	0.20	-0.23	54,60,68,69	0
19	LHG	A	846	49/49	0.94	0.21	-0.25	44,49,58,59	0
17	CLA	b	831	49/65	0.91	0.23	-0.25	51,55,71,71	0
17	CLA	a	823	49/65	0.92	0.18	-0.26	60,67,102,104	0
17	CLA	a	830	65/65	0.97	0.21	-0.26	36,40,47,49	0
17	CLA	3	309	50/65	0.91	0.23	-0.28	76,95,104,107	0
17	CLA	a	803	65/65	0.96	0.22	-0.28	35,38,50,53	0
17	CLA	a	812	65/65	0.93	0.23	-0.28	47,59,70,77	0
17	CLA	b	806	65/65	0.95	0.26	-0.28	39,43,52,65	0
17	CLA	B	812	55/65	0.95	0.21	-0.28	53,62,106,107	0
19	LHG	7	618	37/49	0.90	0.25	-0.29	83,95,102,104	0
17	CLA	b	823	60/65	0.92	0.23	-0.30	50,60,92,94	0
17	CLA	8	303	45/65	0.92	0.26	-0.31	75,92,99,133	0
17	CLA	A	807	65/65	0.96	0.27	-0.31	44,47,58,69	0
21	SF4	A	853	8/8	0.99	0.18	-0.31	43,44,48,51	0
17	CLA	9	601	46/65	0.93	0.18	-0.32	81,91,95,110	0
26	CHL	7	601	61/66	0.93	0.20	-0.33	62,74,93,95	0
17	CLA	8	304	42/65	0.93	0.18	-0.33	59,72,78,80	0
17	CLA	b	838	47/65	0.95	0.22	-0.34	38,44,54,64	0
17	CLA	2	611	52/65	0.94	0.17	-0.34	68,83,119,128	0
17	CLA	b	804	45/65	0.96	0.14	-0.34	42,52,68,75	0
17	CLA	a	836	50/65	0.91	0.17	-0.35	42,54,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	4	602	60/65	0.92	0.19	-0.35	54,67,73,74	0
17	CLA	j	3002	42/65	0.91	0.15	-0.35	91,94,96,97	0
17	CLA	a	821	45/65	0.94	0.19	-0.35	51,62,70,87	0
26	CHL	8	306	47/66	0.94	0.21	-0.36	60,64,79,84	0
26	CHL	2	605	43/66	0.86	0.27	-0.37	77,89,100,106	0
17	CLA	g	103	46/65	0.90	0.28	-0.37	87,99,103,116	0
17	CLA	B	815	60/65	0.89	0.22	-0.38	60,72,100,102	0
26	CHL	4	606	51/66	0.90	0.21	-0.38	71,81,109,110	0
17	CLA	k	1403	46/65	0.85	0.21	-0.39	89,95,103,110	0
17	CLA	L	204	50/65	0.92	0.19	-0.41	76,84,109,109	0
17	CLA	4	613	45/65	0.91	0.25	-0.42	92,103,108,160	0
17	CLA	a	837	45/65	0.93	0.18	-0.43	57,65,74,77	0
17	CLA	l	204	50/65	0.93	0.18	-0.43	46,59,100,104	0
17	CLA	A	842	65/65	0.95	0.23	-0.44	42,45,56,65	0
27	LUT	1	316	42/42	0.92	0.19	-0.44	69,74,100,101	0
20	BCR	A	852	40/40	0.96	0.23	-0.45	42,44,49,50	0
17	CLA	f	7002	45/65	0.96	0.16	-0.45	54,59,76,77	0
17	CLA	B	833	58/65	0.93	0.18	-0.46	43,52,79,80	0
21	SF4	C	101	8/8	0.99	0.14	-0.47	47,49,53,57	0
17	CLA	A	839	65/65	0.92	0.19	-0.49	54,60,80,83	0
17	CLA	A	822	65/65	0.95	0.20	-0.50	49,67,76,79	0
20	BCR	a	854	40/40	0.97	0.20	-0.51	35,40,47,47	0
17	CLA	8	305	47/65	0.95	0.15	-0.51	61,71,78,79	0
17	CLA	A	812	65/65	0.90	0.21	-0.51	49,63,74,82	0
17	CLA	a	827	65/65	0.95	0.27	-0.52	35,41,82,85	0
17	CLA	b	822	55/65	0.93	0.16	-0.52	46,60,80,83	0
21	SF4	a	855	8/8	0.98	0.20	-0.53	37,37,43,43	0
17	CLA	4	612	56/65	0.91	0.19	-0.54	63,78,87,88	0
17	CLA	A	821	45/65	0.93	0.21	-0.54	69,74,88,109	0
17	CLA	1	315	46/65	0.93	0.15	-0.55	76,87,93,132	0
26	CHL	1	307	48/66	0.91	0.19	-0.56	75,95,109,110	0
26	CHL	4	607	51/66	0.93	0.20	-0.56	57,73,82,85	0
17	CLA	b	819	65/65	0.94	0.24	-0.57	50,57,92,95	0
17	CLA	A	840	65/65	0.95	0.23	-0.58	48,55,95,96	0
17	CLA	b	803	65/65	0.97	0.27	-0.60	35,40,47,49	0
17	CLA	1	311	41/65	0.95	0.17	-0.61	67,74,81,82	0
26	CHL	4	615	43/66	0.92	0.19	-0.62	61,74,87,89	0
21	SF4	c	101	8/8	0.99	0.16	-0.63	41,46,54,56	0
26	CHL	9	606	51/66	0.92	0.19	-0.64	86,106,118,119	0
20	BCR	a	853	40/40	0.93	0.26	-0.65	44,48,66,67	0
17	CLA	1	306	52/65	0.92	0.17	-0.65	90,99,109,111	0
17	CLA	A	838	51/65	0.95	0.17	-0.65	45,60,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	F	304	55/65	0.90	0.21	-0.67	52,69,95,95	0
17	CLA	B	831	49/65	0.96	0.18	-0.68	45,53,62,65	0
17	CLA	b	825	65/65	0.92	0.32	-0.70	38,55,82,83	0
19	LHG	6	301	23/49	0.93	0.15	-0.71	67,101,110,111	0
26	CHL	9	605	56/66	0.92	0.18	-0.71	80,94,97,126	0
17	CLA	3	304	45/65	0.90	0.21	-0.71	109,122,133,162	0
17	CLA	A	825	55/65	0.93	0.16	-0.74	58,67,74,78	0
20	BCR	b	848	40/40	0.94	0.20	-0.76	37,42,45,47	0
17	CLA	B	835	45/65	0.92	0.17	-0.81	57,66,70,72	0
21	SF4	c	102	8/8	0.99	0.12	-0.82	41,50,62,77	0
17	CLA	3	306	47/65	0.94	0.18	-0.87	67,79,90,91	0
17	CLA	a	822	65/65	0.95	0.17	-0.91	42,46,53,57	0
17	CLA	3	312	55/65	0.93	0.15	-0.91	86,107,114,117	0
17	CLA	3	305	42/65	0.93	0.20	-0.93	67,78,84,90	0
17	CLA	7	610	41/65	0.95	0.19	-1.23	74,82,94,99	0
17	CLA	9	610	41/65	0.95	0.25	-1.25	99,103,113,114	0
21	SF4	C	102	8/8	0.99	0.09	-1.70	51,62,72,84	0
17	CLA	2	613	43/65	0.88	0.23	-2.46	80,88,94,95	0
17	CLA	6	305	65/65	0.89	0.23	-	83,87,104,110	0
17	CLA	8	313	25/65	0.83	0.28	-	102,110,116,146	0
17	CLA	3	311	52/65	0.89	0.41	-	129,142,154,157	0
22	HTG	A	855	19/19	0.96	0.15	-	68,72,74,75	0
17	CLA	4	611	52/65	0.91	0.28	-	71,88,123,125	0
17	CLA	9	611	52/65	0.90	0.36	-	76,89,102,103	0
17	CLA	1	312	52/65	0.93	0.20	-	70,76,99,100	0
19	LHG	3	319	20/49	0.79	0.50	-	152,157,193,194	0
17	CLA	8	309	52/65	0.61	0.51	-	155,164,169,259	0
17	CLA	3	315	25/65	0.87	0.26	-	112,115,121,157	0
17	CLA	3	314	46/65	0.92	0.18	-	73,78,101,103	0
17	CLA	6	313	52/65	0.88	0.23	-	83,94,119,120	0
22	HTG	a	857	19/19	0.93	0.25	-	53,70,79,81	0
17	CLA	8	312	46/65	0.95	0.15	-	57,66,99,103	0
20	BCR	i	101	40/40	0.93	0.17	-	36,45,49,50	0
17	CLA	1	304	65/65	0.94	0.21	-	63,70,95,97	0
17	CLA	3	310	37/65	0.82	0.63	-	179,186,191,221	0
23	LMT	B	849	35/35	0.80	0.33	-	80,97,102,103	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.