



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 12:13 AM GMT

PDB ID : 4Y28
Title : The structure of plant photosystem I super-complex at 2.8 angstrom resolution.
Authors : Mazor, Y.; Brovikov, A.; Nelson, N.
Deposited on : 2015-02-09
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

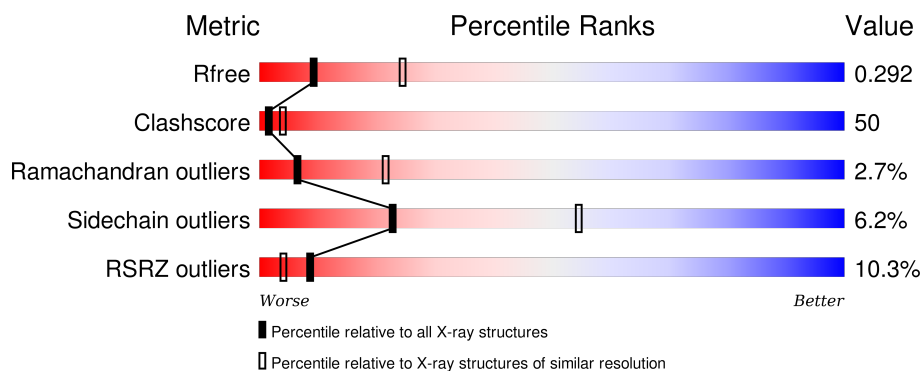
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	758	<div> <div>6%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
2	B	733	<div> <div>6%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
3	I	30	<div> <div>13%</div> <div>33%</div> <div>53%</div> <div>10%</div> <div>.</div> </div>
4	J	42	<div> <div>7%</div> <div>33%</div> <div>52%</div> <div>7%</div> <div>5%</div> <div>.</div> </div>
5	F	154	<div> <div>4%</div> <div>67%</div> <div>27%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
6	G	97	
7	L	167	
8	C	81	
9	D	147	
10	E	66	
11	H	90	
12	K	129	
13	2	269	
14	4	252	
15	1	202	
16	3	275	

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	CL0	A	1011	X	-	-	-
18	CLA	1	1001	X	-	X	-
18	CLA	1	1002	X	-	X	-
18	CLA	1	1003	X	-	X	-
18	CLA	1	1004	X	-	X	-
18	CLA	1	1005	X	-	-	-
18	CLA	1	1006	X	-	-	-
18	CLA	1	1007	X	-	-	-
18	CLA	1	1008	X	-	X	-
18	CLA	1	1011	X	-	-	-
18	CLA	1	1012	X	-	-	-
18	CLA	1	1013	X	-	-	-
18	CLA	1	1014	X	-	-	-
18	CLA	2	2001	X	-	X	-
18	CLA	2	2002	X	-	X	-
18	CLA	2	2003	X	-	X	-
18	CLA	2	2004	X	-	X	-
18	CLA	2	2005	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	2006	X	-	X	-
18	CLA	2	2007	X	-	X	-
18	CLA	2	2008	X	-	-	-
18	CLA	2	2009	X	-	-	-
18	CLA	2	2012	X	-	X	X
18	CLA	2	2016	X	-	X	-
18	CLA	2	2019	X	-	-	-
18	CLA	3	3001	X	-	X	-
18	CLA	3	3002	X	-	-	-
18	CLA	3	3003	X	-	X	-
18	CLA	3	3004	X	-	-	-
18	CLA	3	3005	X	-	-	-
18	CLA	3	3006	X	-	X	-
18	CLA	3	3007	X	-	-	-
18	CLA	3	3008	X	-	-	X
18	CLA	3	3010	X	-	X	-
18	CLA	3	3012	X	-	X	-
18	CLA	3	3013	X	-	X	-
18	CLA	3	3017	X	-	-	-
18	CLA	3	3018	X	-	-	-
18	CLA	3	3019	X	-	-	-
18	CLA	4	4001	X	-	X	-
18	CLA	4	4002	X	-	-	-
18	CLA	4	4003	X	-	-	-
18	CLA	4	4004	X	-	-	-
18	CLA	4	4005	X	-	-	-
18	CLA	4	4006	X	-	X	-
18	CLA	4	4007	X	-	-	-
18	CLA	4	4008	X	-	-	-
18	CLA	4	4009	X	-	-	-
18	CLA	4	4012	X	-	X	-
18	CLA	4	4016	X	-	X	-
18	CLA	4	4017	X	-	-	-
18	CLA	A	1013	X	-	-	-
18	CLA	A	1022	X	-	-	-
18	CLA	A	1101	X	-	-	-
18	CLA	A	1102	X	-	-	-
18	CLA	A	1103	X	-	-	-
18	CLA	A	1104	X	-	-	-
18	CLA	A	1105	X	-	-	-
18	CLA	A	1106	X	-	-	-
18	CLA	A	1107	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	1108	X	-	-	-
18	CLA	A	1109	X	-	-	-
18	CLA	A	1110	X	-	-	-
18	CLA	A	1111	X	-	-	-
18	CLA	A	1112	X	-	-	-
18	CLA	A	1113	X	-	-	-
18	CLA	A	1114	X	-	-	-
18	CLA	A	1115	X	-	-	-
18	CLA	A	1116	X	-	-	-
18	CLA	A	1117	X	-	-	X
18	CLA	A	1118	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1120	X	-	-	-
18	CLA	A	1121	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	-	-
18	CLA	A	1124	X	-	-	-
18	CLA	A	1125	X	-	-	-
18	CLA	A	1126	X	-	-	-
18	CLA	A	1127	X	-	-	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1130	X	-	-	-
18	CLA	A	1131	X	-	-	-
18	CLA	A	1132	X	-	-	-
18	CLA	A	1133	X	-	-	-
18	CLA	A	1134	X	-	-	-
18	CLA	A	1135	X	-	-	-
18	CLA	A	1136	X	-	-	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1138	X	-	-	-
18	CLA	A	1139	X	-	-	-
18	CLA	A	1140	X	-	-	X
18	CLA	A	1151	X	-	-	-
18	CLA	A	1237	X	-	-	-
18	CLA	B	1012	X	-	-	-
18	CLA	B	1021	X	-	-	-
18	CLA	B	1023	X	-	-	-
18	CLA	B	1201	X	-	-	-
18	CLA	B	1202	X	-	-	-
18	CLA	B	1203	X	-	-	-
18	CLA	B	1204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1205	X	-	-	-
18	CLA	B	1206	X	-	-	-
18	CLA	B	1207	X	-	-	-
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	-	-
18	CLA	B	1210	X	-	-	-
18	CLA	B	1211	X	-	-	-
18	CLA	B	1212	X	-	-	-
18	CLA	B	1213	X	-	-	-
18	CLA	B	1214	X	-	-	-
18	CLA	B	1215	X	-	-	-
18	CLA	B	1216	X	-	-	-
18	CLA	B	1217	X	-	-	-
18	CLA	B	1218	X	-	-	-
18	CLA	B	1219	X	-	-	-
18	CLA	B	1220	X	-	-	-
18	CLA	B	1221	X	-	-	-
18	CLA	B	1222	X	-	-	X
18	CLA	B	1223	X	-	-	-
18	CLA	B	1224	X	-	-	-
18	CLA	B	1225	X	-	-	-
18	CLA	B	1226	X	-	-	-
18	CLA	B	1227	X	-	-	-
18	CLA	B	1228	X	-	-	-
18	CLA	B	1229	X	-	-	-
18	CLA	B	1230	X	-	-	-
18	CLA	B	1231	X	-	-	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	X	-	-	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1236	X	-	-	-
18	CLA	B	1238	X	-	-	-
18	CLA	B	1239	X	-	-	-
18	CLA	B	1240	X	-	-	-
18	CLA	F	1301	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	G	1001	X	-	X	-
18	CLA	G	1002	X	-	X	-
18	CLA	G	1003	X	-	X	-
18	CLA	H	1000	X	-	-	-
18	CLA	J	1302	X	-	-	X
18	CLA	K	1001	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	L	1501	X	-	-	-
18	CLA	L	1502	X	-	-	-
18	CLA	L	1503	X	-	-	-
22	BCR	3	3503	-	-	X	-
22	BCR	A	6003	-	-	-	X
22	BCR	A	6007	-	-	-	X
22	BCR	B	6004	-	-	-	X
22	BCR	B	6005	-	-	-	X
22	BCR	B	6009	-	-	-	X
22	BCR	G	2011	-	-	X	-
22	BCR	J	6012	-	-	-	X
22	BCR	J	6013	-	-	-	X
22	BCR	L	6019	-	-	X	X
22	BCR	L	6020	-	-	-	X
27	LUT	1	1501	X	-	X	-
27	LUT	1	1502	X	-	-	-
27	LUT	2	2501	X	-	X	-
27	LUT	2	2502	X	-	X	X
27	LUT	3	3501	X	-	X	X
27	LUT	3	3502	X	-	X	X
27	LUT	4	4501	X	-	X	-
27	LUT	4	4502	X	-	X	-
27	LUT	4	4503	X	-	X	X
27	LUT	I	6018	X	-	-	-
28	CHL	1	1009	-	-	X	-
28	CHL	3	3011	-	-	X	X
29	ZEX	4	4505	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35653 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
			Total	C	N	O	S			
1	A	742	5852	3833	997	1004	18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	LEU	engineered mutation	UNP P05310
A	22	LEU	VAL	engineered mutation	UNP P05310
A	117	ARG	GLY	engineered mutation	UNP P05310
A	220	GLY	ARG	engineered mutation	UNP P05310

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	732	5856	3851	995	996	14	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	LEU	ILE	engineered mutation	UNP P05311
B	115	ILE	ASN	engineered mutation	UNP P05311
B	273	MET	VAL	engineered mutation	UNP P05311
B	471	SER	THR	engineered mutation	UNP P05311
B	476	VAL	ILE	engineered mutation	UNP P05311
B	477	LEU	PRO	engineered mutation	UNP P05311
B	635	TYR	ILE	engineered mutation	UNP P05311

- Molecule 3 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	29	Total	C	N	O	S	0	0	0
			224	155	35	33	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	41	Total	C	N	O	S	0	0	0
			321	217	50	54				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	150	Total	C	N	O	S	0	0	0
			1187	770	207	208	2			

- Molecule 6 is a protein called photosystem I reaction center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	91	Total	C	N	O	S	0	0	0
			689	444	117	128				

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	160	Total	C	N	O	S	0	0	0
			1197	791	190	215	1			

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	0
			1116	720	192	201	3			

- Molecule 10 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	E	66	Total	C	N	O	0	0	0
			530	337	93	100			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	H	84	Total	C	N	O	0	0	0
			642	425	97	120			

- Molecule 12 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	57	Total	C	N	O	S	0	0	0
			379	241	64	71	3			

- Molecule 13 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	2	207	Total	C	N	O	S	0	0	0
			1613	1057	263	289	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	133	LEU	ASN	engineered mutation	UNP Q41038

- Molecule 14 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	4	198	Total	C	N	O	S	0	0	0
			1544	1007	252	282	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	128	ASP	ALA	engineered mutation	UNP Q9SQL2

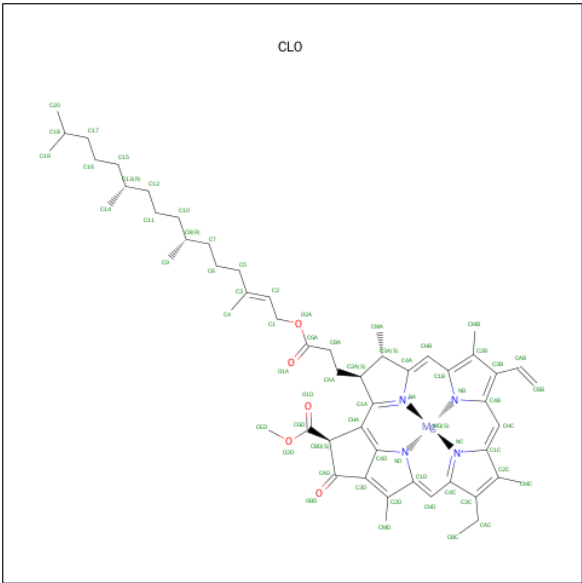
- Molecule 15 is a protein called Light-harvesting complex I chlorophyll A/B-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	194	Total	C	N	O	S	0	0	0
			1513	986	254	268	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

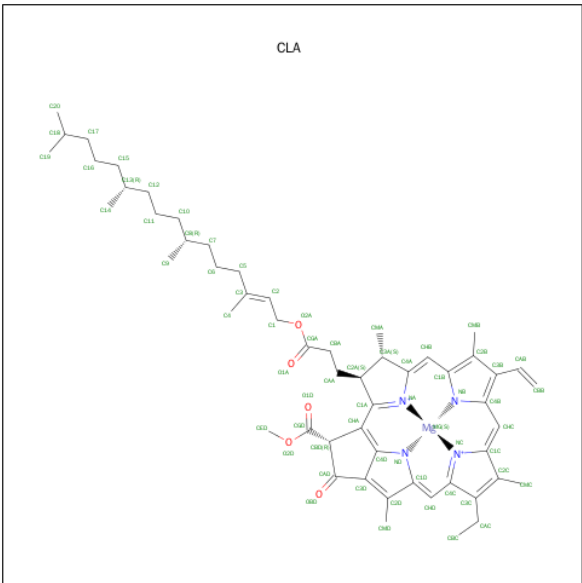
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	3	215	1619	1053	263	298	5	0	0	0

- Molecule 17 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	H	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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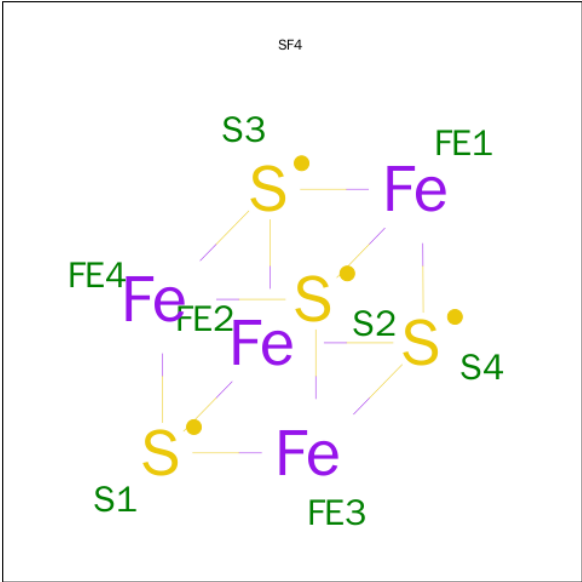
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	2	1	Total 27	C 22	Mg 1	N 4	0	0
18	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	4	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	4	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	4	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	1	1	Total 60	C 50	Mg 1	N 4 O 5	0	0
18	1	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	1	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	1	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
18	1	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	1	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	1	1	Total 46	C 36	Mg 1	N 4 O 5	0	0

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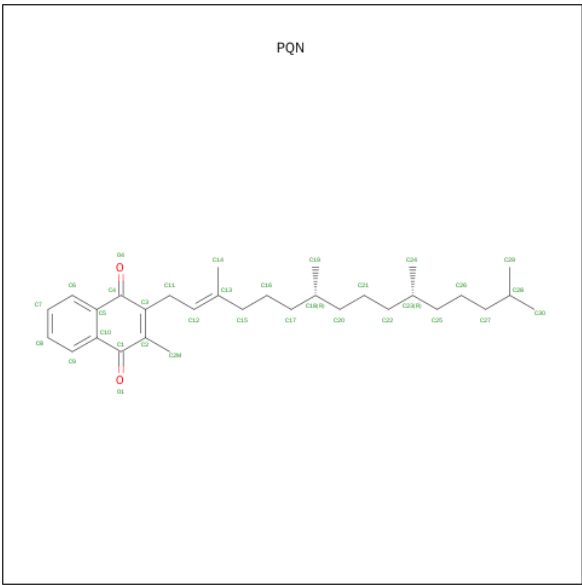
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N		0	0
			27	22	1	4			

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



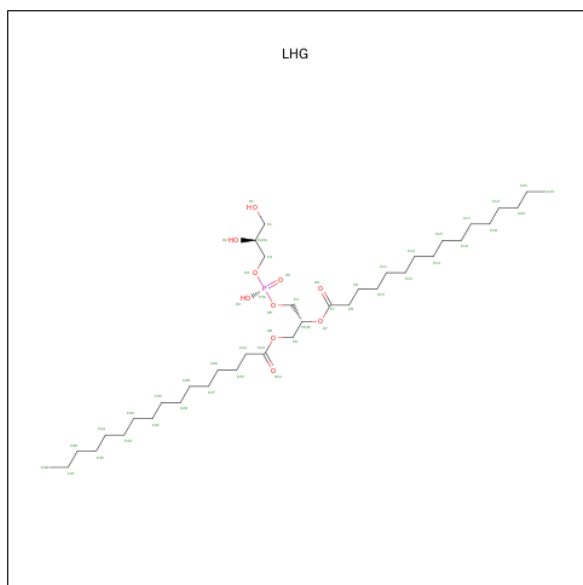
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			33	31	2		

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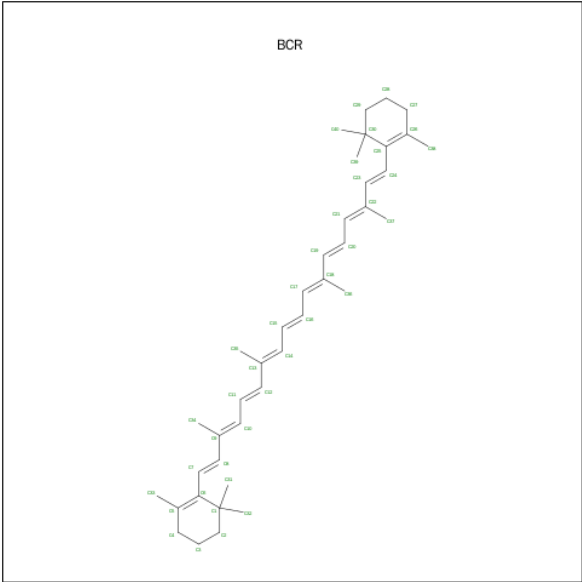
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	O	P	0	0
			40	29	10	1		
21	A	1	Total	C	O	P	0	0
			49	38	10	1		
21	B	1	Total	C	O	P	0	0
			21	10	10	1		
21	2	1	Total	C	O	P	0	0
			24	13	10	1		
21	1	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



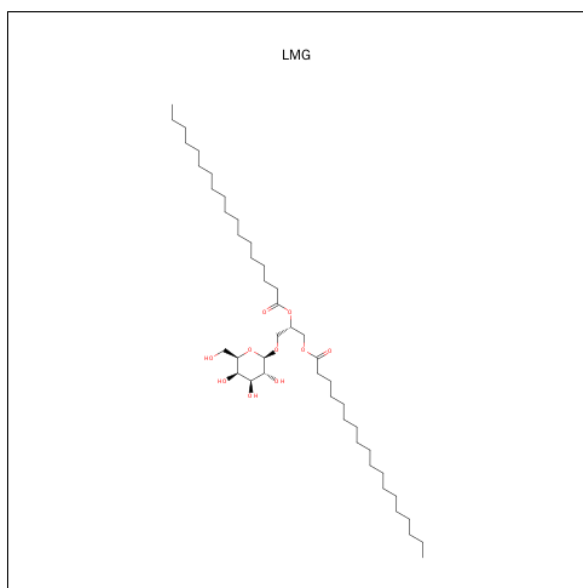
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	3	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 38 28 10	0	0
23	J	1	Total C O 55 45 10	0	0
23	F	1	Total C O 23 13 10	0	0
23	F	1	Total C O 37 27 10	0	0

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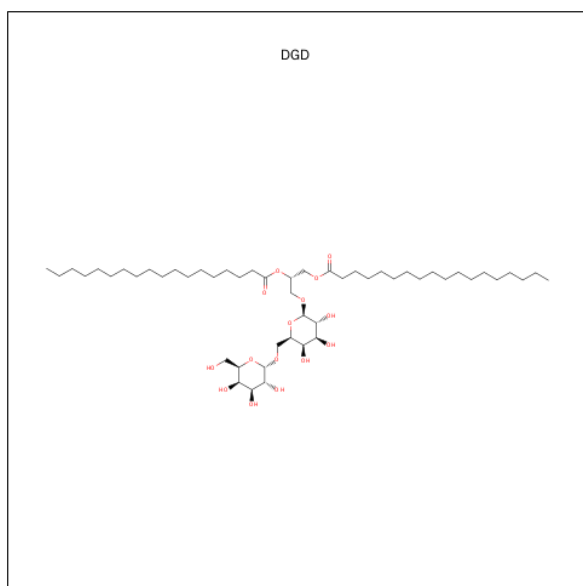
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	G	1	Total	C	O	0	0
			41	31	10		
23	2	1	Total	C	O	0	0
			35	25	10		
23	4	1	Total	C	O	0	0
			35	25	10		

- Molecule 24 is CALCIUM ION (three-letter code: CA) (formula: Ca).

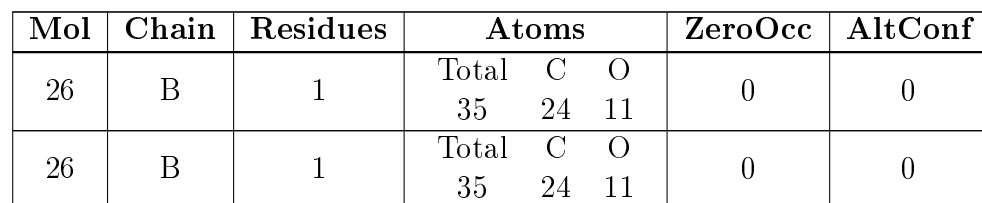
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	B	1	Total	Ca	0	0
			1	1		

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			61	46	15		

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



- LUT
-
- The chemical structure of Lutein (LUT) is shown, a tetraterpene carotenoid. It features a long conjugated polyene chain with five double bonds, terminated by a cyclohexenol ring at one end and a cyclohexene ring with an isopropylidene group at the other. The structure is labeled with atom numbers (e.g., C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C814, C815, C816, C817, C818, C819, C820, C

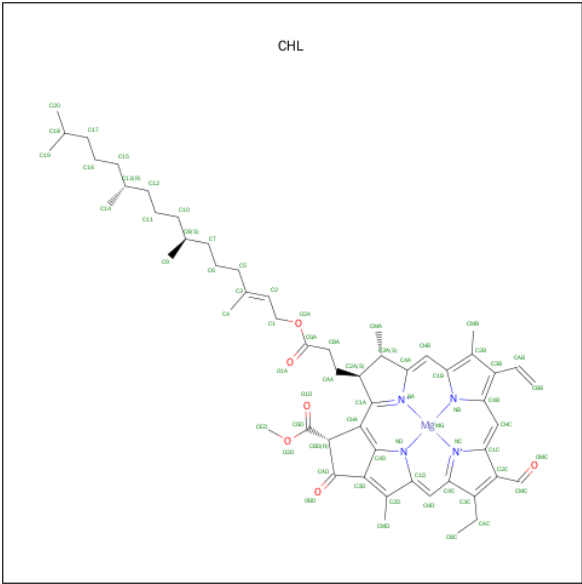
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	I	1	Total	C	O	0	0
			42	40	2		



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

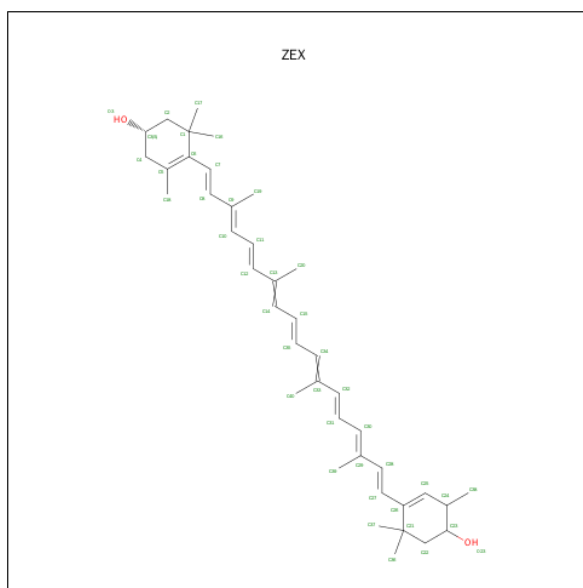
- Molecule 28 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	3	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 29 is (3S,5R,6S,3'S,5'R,6'S) BETA-CAROTENE-3,23-DIOL (three-letter code: ZEX) (formula: $C_{40}H_{56}O_2$).

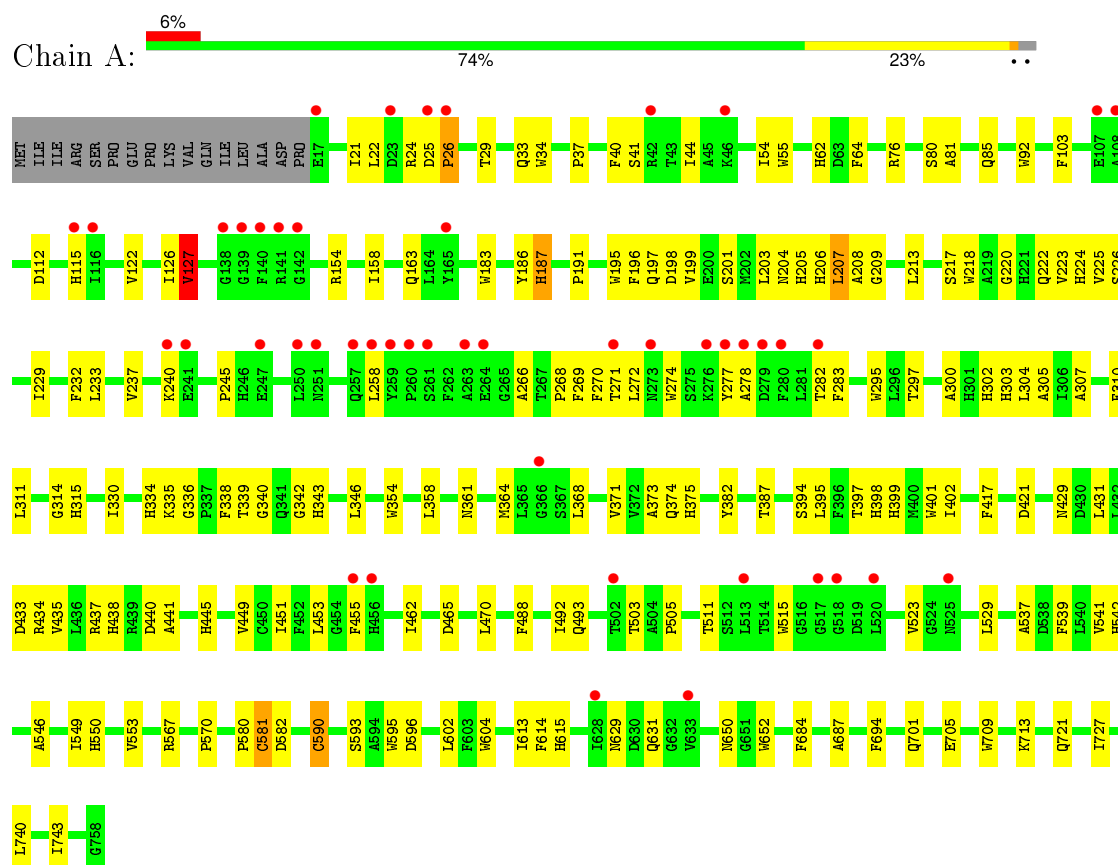


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	4	1	Total	C	O	0	0
			42	40	2		

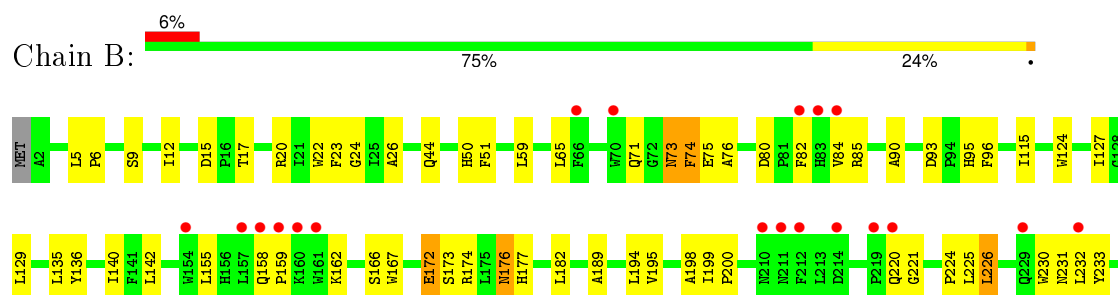
3 Residue-property plots

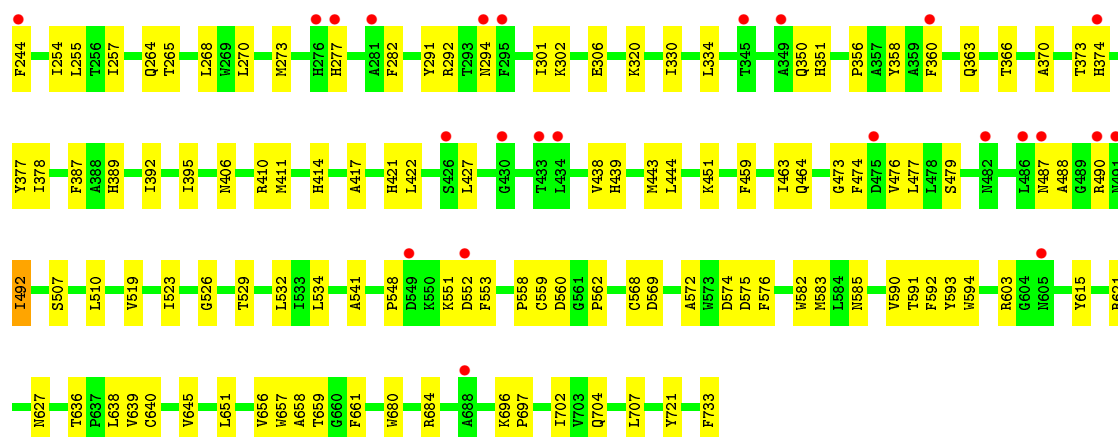
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

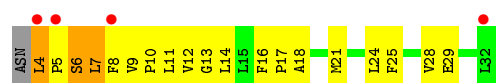


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





• Molecule 3: Photosystem I reaction center subunit VIII



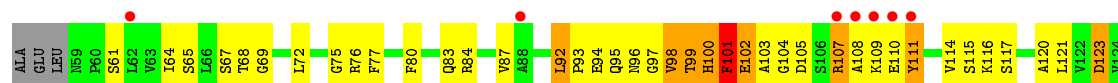
• Molecule 4: Photosystem I reaction center subunit IX



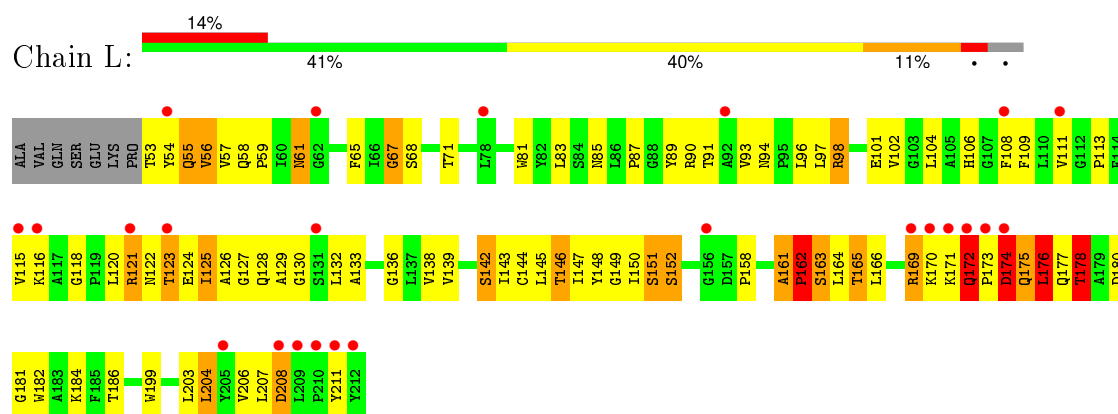
• Molecule 5: Photosystem I reaction center subunit III



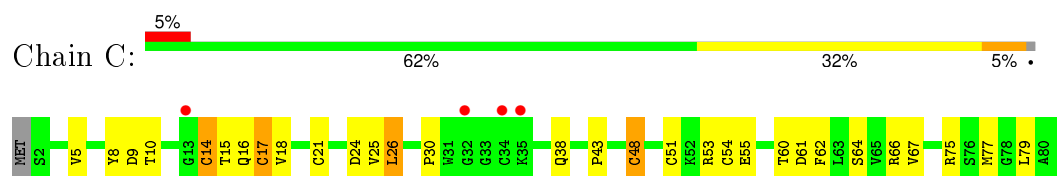
• Molecule 6: photosystem I reaction center



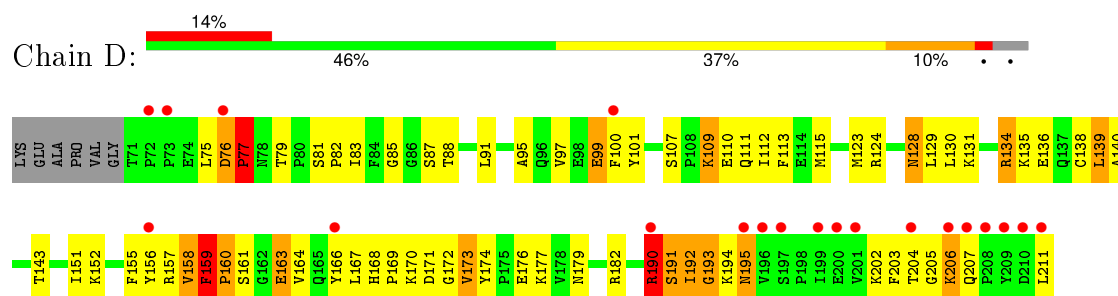
• Molecule 7: Putative uncharacterized protein



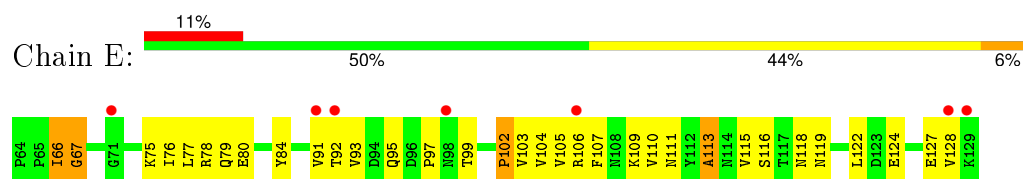
- Molecule 8: Photosystem I iron-sulfur center



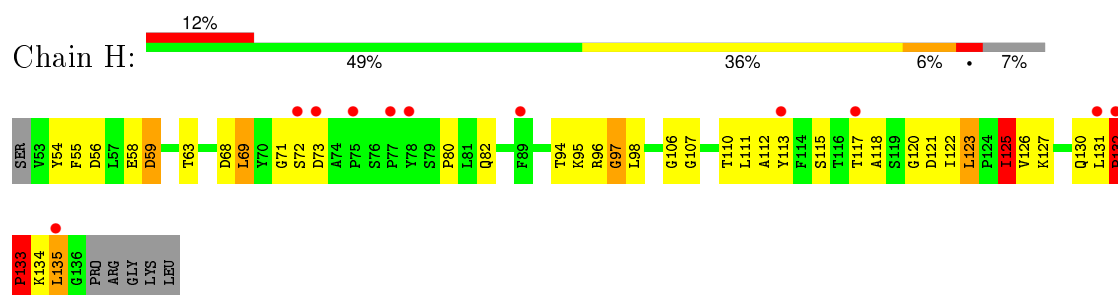
- Molecule 9: Photosystem I reaction center subunit II, chloroplastic



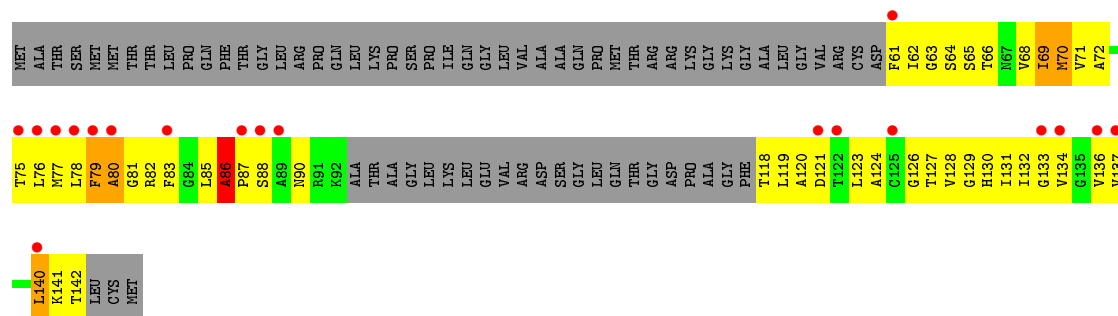
- Molecule 10: Photosystem I reaction center subunit IV A, chloroplastic



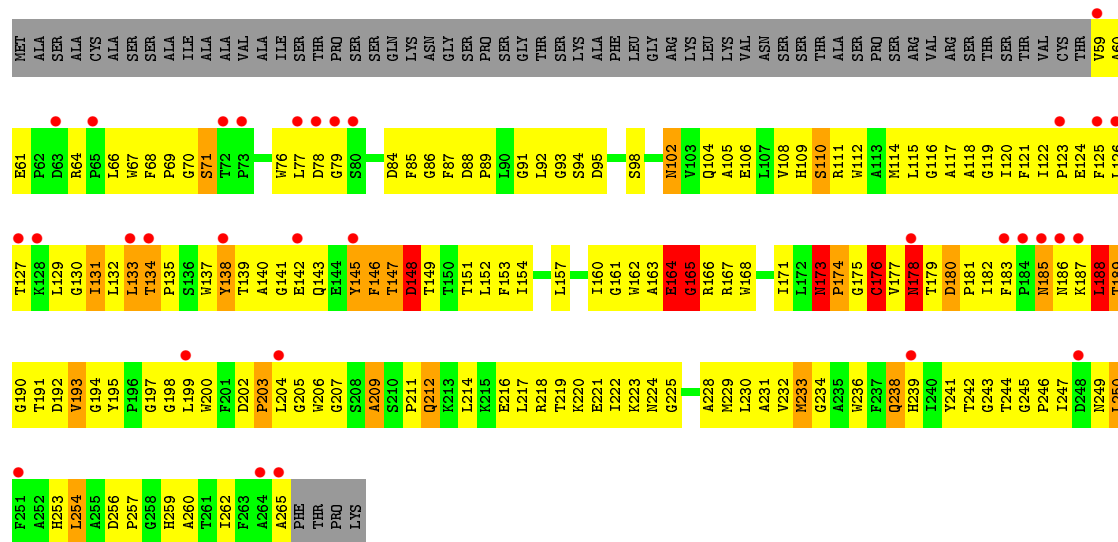
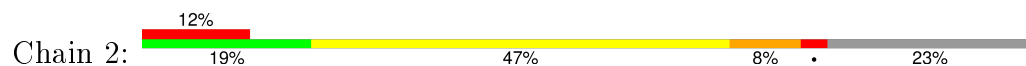
- Molecule 11: Photosystem I reaction center subunit VI



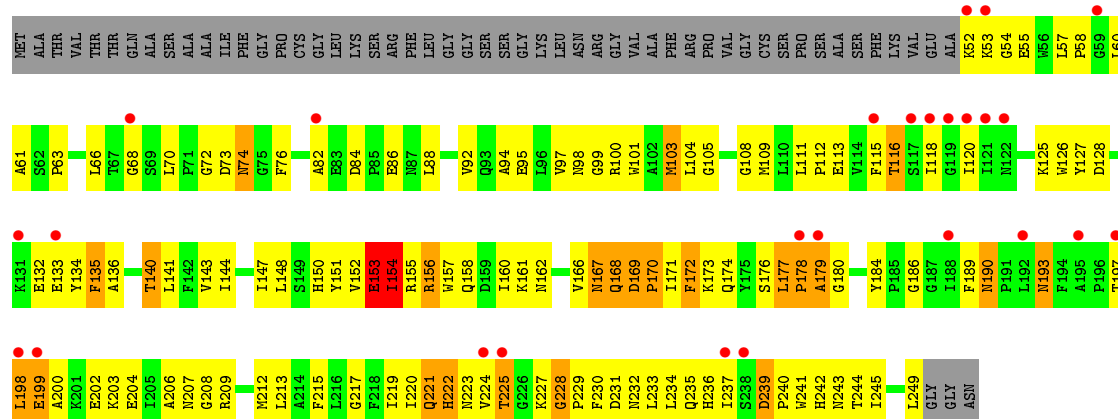
- Molecule 12: Photosystem I reaction center subunit X psak



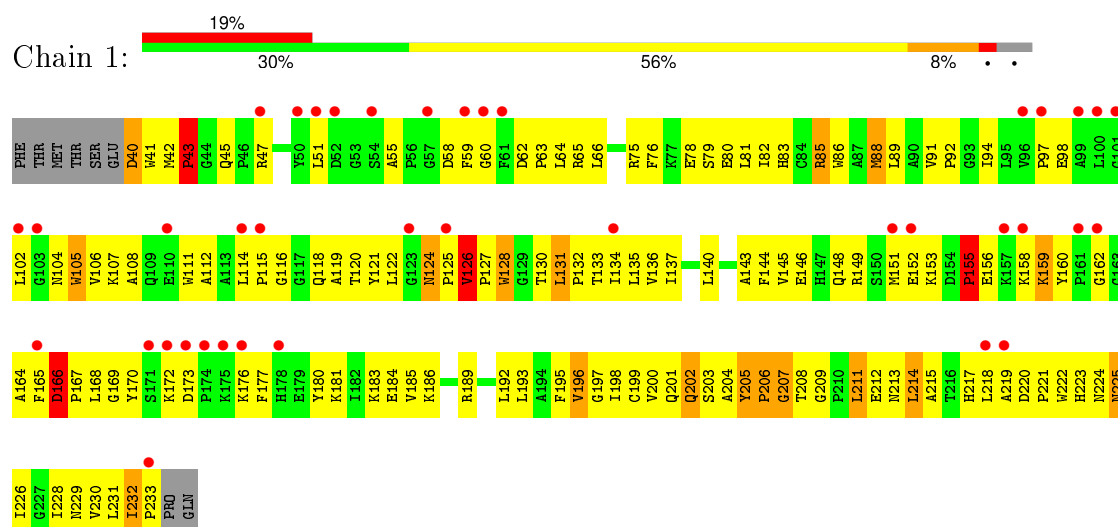
- Molecule 13: Type II chlorophyll a/b binding protein from photosystem I



- Molecule 14: Chlorophyll a-b binding protein P4, chloroplastic



- Molecule 15: Light-harvesting complex I chlorophyll A/B-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	189.00Å 201.90Å 213.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.80 39.89 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.65-2.80) 88.8 (39.89-2.79)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.268 0.280 , 0.292	Depositor DCC
R_{free} test set	3970 reflections (2.27%)	DCC
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 199903 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	35653	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, LUT, DGD, SF4, CHL, CLA, PQN, LMU, ZEX, CL0, CA, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/6049	0.40	0/8253
2	B	0.24	0/6067	0.40	0/8287
3	I	0.92	0/230	1.02	2/313 (0.6%)
4	J	0.76	0/330	0.90	2/452 (0.4%)
5	F	0.62	0/1214	0.64	0/1638
6	G	0.78	0/705	1.01	3/956 (0.3%)
7	L	0.76	0/1233	0.94	7/1690 (0.4%)
8	C	0.82	0/625	0.81	1/846 (0.1%)
9	D	1.00	0/1146	1.06	7/1550 (0.5%)
10	E	0.89	0/542	0.90	3/737 (0.4%)
11	H	0.62	0/662	0.85	4/902 (0.4%)
12	K	0.48	0/381	0.87	1/517 (0.2%)
13	2	0.94	2/1672 (0.1%)	1.09	11/2292 (0.5%)
14	4	0.93	2/1592 (0.1%)	0.99	10/2174 (0.5%)
15	1	0.86	0/1563	1.04	6/2132 (0.3%)
16	3	0.86	2/1666 (0.1%)	1.08	11/2265 (0.5%)
All	All	0.63	6/25677 (0.0%)	0.76	68/35004 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	1
7	L	0	1
13	2	0	1
14	4	0	1
16	3	0	1
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	153	GLU	C-O	-10.68	1.03	1.23
13	2	164	GLU	C-O	-10.38	1.03	1.23
16	3	205	GLY	C-N	7.70	1.48	1.34
16	3	205	GLY	C-O	-7.23	1.12	1.23
13	2	164	GLU	C-N	6.29	1.44	1.33

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	101	PHE	C-N-CA	11.02	149.25	121.70
6	G	100	HIS	N-CA-C	-10.25	83.33	111.00
13	2	165	GLY	N-CA-C	-9.45	89.48	113.10
11	H	120	GLY	N-CA-C	-8.68	91.41	113.10
16	3	206	PRO	CA-N-CD	-8.59	99.47	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	2	164	GLU	Mainchain
16	3	205	GLY	Mainchain
14	4	153	GLU	Mainchain
6	G	101	PHE	Peptide
7	L	98	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5852	0	5710	169	0
2	B	5856	0	5666	146	0
3	I	224	0	247	34	0
4	J	321	0	328	48	0
5	F	1187	0	1226	39	3
6	G	689	0	675	112	0
7	L	1197	0	1187	165	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	612	0	594	36	0
9	D	1116	0	1126	103	0
10	E	530	0	530	44	0
11	H	642	0	637	48	0
12	K	379	0	386	92	0
13	2	1613	0	1554	371	0
14	4	1544	0	1489	230	0
15	1	1513	0	1495	379	0
16	3	1619	0	1554	472	0
17	A	65	0	72	6	0
18	1	615	0	511	235	0
18	2	628	0	538	255	0
18	3	698	0	559	265	0
18	4	677	0	635	195	0
18	A	2583	0	2555	197	0
18	B	2519	0	2617	217	0
18	F	95	0	72	20	0
18	G	161	0	141	92	0
18	H	46	0	33	4	0
18	J	50	0	39	7	0
18	K	46	0	33	12	0
18	L	160	0	137	39	0
19	A	8	0	0	1	0
19	C	16	0	0	0	0
20	A	33	0	46	3	0
20	B	33	0	46	5	0
21	1	49	0	74	15	0
21	2	24	0	18	6	0
21	A	89	0	127	12	0
21	B	21	0	12	1	0
22	3	40	0	48	21	0
22	A	240	0	292	21	0
22	B	200	0	245	24	0
22	F	80	0	98	19	0
22	G	40	0	49	29	0
22	I	40	0	49	3	0
22	J	80	0	98	15	0
22	K	40	0	49	17	0
22	L	80	0	98	28	0
23	2	35	0	40	9	0
23	4	35	0	40	6	0
23	B	38	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	F	60	0	60	13	0
23	G	41	0	52	20	0
23	J	55	0	86	9	0
24	B	1	0	0	0	0
25	B	61	0	83	4	0
26	B	70	0	92	4	0
27	1	84	0	110	48	0
27	2	84	0	110	55	0
27	3	84	0	110	62	0
27	4	126	0	165	84	0
27	I	42	0	55	14	0
28	1	103	0	78	35	0
28	2	141	0	95	39	0
28	3	56	0	47	22	0
28	4	145	0	99	44	0
29	4	42	0	56	12	0
All	All	35653	0	35119	3560	3

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 50.

The worst 5 of 3560 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)
16:3:138:GLN:HB2	16:3:145:ALA:HB2	1.25	1.18
18:3:3012:CLA:HBB1	18:3:3012:CLA:HMB1	1.18	1.17
16:3:268:VAL:HG21	18:3:3003:CLA:H43	1.17	1.16
18:3:3004:CLA:HBB1	18:3:3004:CLA:HMB1	1.25	1.15
16:3:111:LEU:HD22	18:3:3006:CLA:CBB	1.74	1.15

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:96:LYS:CD	7:L:170:LYS:NZ[3_555]	1.69	0.51
5:F:96:LYS:CE	7:L:170:LYS:NZ[3_555]	1.86	0.34
5:F:96:LYS:CG	7:L:170:LYS:NZ[3_555]	1.99	0.21

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/758 (98%)	691 (93%)	45 (6%)	4 (0%)	34	69
2	B	730/733 (100%)	695 (95%)	30 (4%)	5 (1%)	26	62
3	I	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	4	14
4	J	39/42 (93%)	34 (87%)	3 (8%)	2 (5%)	2	8
5	F	148/154 (96%)	138 (93%)	8 (5%)	2 (1%)	14	42
6	G	89/97 (92%)	76 (85%)	8 (9%)	5 (6%)	2	6
7	L	158/167 (95%)	133 (84%)	15 (10%)	10 (6%)	2	4
8	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
9	D	139/147 (95%)	116 (84%)	14 (10%)	9 (6%)	1	4
10	E	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	12	38
11	H	82/90 (91%)	65 (79%)	10 (12%)	7 (8%)	1	2
12	K	53/129 (41%)	49 (92%)	2 (4%)	2 (4%)	4	13
13	2	205/269 (76%)	184 (90%)	7 (3%)	14 (7%)	1	4
14	4	196/252 (78%)	174 (89%)	15 (8%)	7 (4%)	4	14
15	1	192/202 (95%)	168 (88%)	17 (9%)	7 (4%)	4	14
16	3	213/275 (78%)	189 (89%)	15 (7%)	9 (4%)	3	11
All	All	3153/3492 (90%)	2866 (91%)	202 (6%)	85 (3%)	6	21

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
3	I	6	SER
4	J	11	ALA
6	G	101	PHE
6	G	102	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/619 (97%)	595 (99%)	8 (1%)	76	94
2	B	599/600 (100%)	587 (98%)	12 (2%)	63	90
3	I	25/26 (96%)	23 (92%)	2 (8%)	15	40
4	J	33/35 (94%)	29 (88%)	4 (12%)	6	18
5	F	123/127 (97%)	115 (94%)	8 (6%)	21	52
6	G	71/76 (93%)	65 (92%)	6 (8%)	13	36
7	L	124/133 (93%)	107 (86%)	17 (14%)	4	13
8	C	69/70 (99%)	65 (94%)	4 (6%)	25	57
9	D	120/125 (96%)	110 (92%)	10 (8%)	14	38
10	E	59/59 (100%)	57 (97%)	2 (3%)	44	78
11	H	69/74 (93%)	63 (91%)	6 (9%)	13	35
12	K	38/99 (38%)	32 (84%)	6 (16%)	3	9
13	2	166/216 (77%)	148 (89%)	18 (11%)	8	23
14	4	161/202 (80%)	145 (90%)	16 (10%)	10	28
15	1	158/167 (95%)	141 (89%)	17 (11%)	8	23
16	3	159/213 (75%)	135 (85%)	24 (15%)	3	10
All	All	2577/2841 (91%)	2417 (94%)	160 (6%)	23	54

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	E	127	GLU
13	2	138	TYR
16	3	206	PRO
11	H	59	ASP
12	K	70	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
6	G	144	ASN
10	E	111	ASN
16	3	174	GLN
7	L	122	ASN
9	D	78	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 209 ligands modelled in this entry, 1 is monoatomic - leaving 208 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	CLA	1	1001	15	52,68,73	1.80	12 (23%)	55,107,113	2.25	12 (21%)
18	CLA	1	1002	-	38,54,73	2.21	13 (34%)	41,90,113	2.47	16 (39%)
18	CLA	1	1003	15	47,63,73	1.93	13 (27%)	49,101,113	2.45	19 (38%)
18	CLA	1	1004	15	57,73,73	1.74	13 (22%)	61,113,113	2.21	14 (22%)
18	CLA	1	1005	-	47,63,73	1.85	12 (25%)	49,101,113	2.42	15 (30%)
18	CLA	1	1006	-	42,58,73	2.00	14 (33%)	44,95,113	2.57	15 (34%)
18	CLA	1	1007	21	38,54,73	2.15	13 (34%)	41,90,113	2.52	13 (31%)
18	CLA	1	1008	-	38,54,73	2.17	12 (31%)	41,90,113	2.54	15 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CHL	1	1009	-	48,64,74	1.83	8 (16%)	46,102,114	1.36	5 (10%)
28	CHL	1	1010	15	39,55,74	1.93	7 (17%)	38,91,114	1.52	4 (10%)
18	CLA	1	1011	-	42,58,73	2.02	13 (30%)	44,95,113	2.50	15 (34%)
18	CLA	1	1012	15	42,58,73	2.01	13 (30%)	44,95,113	2.45	14 (31%)
18	CLA	1	1013	-	38,54,73	2.18	13 (34%)	41,90,113	2.56	13 (31%)
18	CLA	1	1014	15	38,54,73	2.23	13 (34%)	41,90,113	2.49	12 (29%)
27	LUT	1	1501	-	42,43,43	2.58	5 (11%)	49,60,60	1.94	12 (24%)
27	LUT	1	1502	-	42,43,43	2.53	6 (14%)	49,60,60	2.12	16 (32%)
21	LHG	1	1801	18	48,48,48	0.89	2 (4%)	49,54,54	1.21	3 (6%)
18	CLA	2	2001	13	52,68,73	1.79	14 (26%)	55,107,113	2.40	20 (36%)
18	CLA	2	2002	-	38,54,73	2.12	13 (34%)	41,90,113	2.39	14 (34%)
18	CLA	2	2003	-	47,63,73	1.92	13 (27%)	49,101,113	2.41	15 (30%)
18	CLA	2	2004	13	57,73,73	1.78	12 (21%)	61,113,113	2.20	13 (21%)
18	CLA	2	2005	-	47,63,73	1.99	12 (25%)	49,101,113	2.21	12 (24%)
18	CLA	2	2006	-	47,63,73	1.98	12 (25%)	49,101,113	2.35	14 (28%)
18	CLA	2	2007	-	52,68,73	1.88	12 (23%)	55,107,113	2.19	13 (23%)
18	CLA	2	2008	-	42,58,73	1.99	12 (28%)	44,95,113	2.73	18 (40%)
18	CLA	2	2009	13	42,58,73	2.01	13 (30%)	44,95,113	2.46	14 (31%)
28	CHL	2	2010	-	39,55,74	2.24	10 (25%)	38,91,114	1.66	6 (15%)
28	CHL	2	2011	-	40,56,74	2.26	11 (27%)	39,92,114	1.65	4 (10%)
18	CLA	2	2012	13	47,63,73	1.82	13 (27%)	49,101,113	2.38	15 (30%)
28	CHL	2	2013	-	35,54,74	1.87	5 (14%)	34,90,114	1.60	4 (11%)
18	CLA	2	2016	13	42,58,73	2.12	12 (28%)	44,95,113	2.99	17 (38%)
18	CLA	2	2019	-	20,35,73	2.80	9 (45%)	25,60,113	3.01	12 (48%)
27	LUT	2	2501	-	42,43,43	2.45	5 (11%)	49,60,60	2.07	15 (30%)
27	LUT	2	2502	-	42,43,43	2.53	5 (11%)	49,60,60	1.98	13 (26%)
21	LHG	2	2801	-	23,23,48	1.29	2 (8%)	24,29,54	1.17	3 (12%)
23	LMG	2	2802	-	35,35,55	1.06	2 (5%)	43,43,63	1.38	7 (16%)
18	CLA	3	3001	16	42,58,73	2.05	13 (30%)	44,95,113	2.33	11 (25%)
18	CLA	3	3002	-	38,54,73	2.14	12 (31%)	41,90,113	2.68	18 (43%)
18	CLA	3	3003	16	52,68,73	1.79	13 (25%)	55,107,113	2.37	13 (23%)
18	CLA	3	3004	16	52,68,73	1.81	13 (25%)	55,107,113	2.35	13 (23%)
18	CLA	3	3005	-	47,63,73	1.85	12 (25%)	49,101,113	2.56	14 (28%)
18	CLA	3	3006	-	42,58,73	2.01	13 (30%)	44,95,113	2.69	16 (36%)
18	CLA	3	3007	-	42,58,73	2.06	13 (30%)	44,95,113	2.48	17 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	3008	-	40,56,73	2.10	11 (27%)	42,92,113	2.93	18 (42%)
18	CLA	3	3010	-	52,68,73	1.79	13 (25%)	55,107,113	2.34	15 (27%)
28	CHL	3	3011	-	48,64,74	2.09	11 (22%)	46,102,114	1.48	4 (8%)
18	CLA	3	3012	16	42,58,73	2.03	13 (30%)	44,95,113	2.51	14 (31%)
18	CLA	3	3013	-	38,54,73	2.21	12 (31%)	41,90,113	2.26	11 (26%)
18	CLA	3	3017	-	38,54,73	2.17	13 (34%)	41,90,113	2.32	14 (34%)
18	CLA	3	3018	16	42,58,73	2.02	13 (30%)	44,95,113	2.55	17 (38%)
18	CLA	3	3019	-	20,35,73	3.01	11 (55%)	25,60,113	2.95	13 (52%)
27	LUT	3	3501	-	42,43,43	2.37	4 (9%)	49,60,60	2.20	16 (32%)
27	LUT	3	3502	-	42,43,43	2.44	4 (9%)	49,60,60	2.22	17 (34%)
22	BCR	3	3503	-	41,41,41	3.04	9 (21%)	56,56,56	6.32	32 (57%)
18	CLA	4	4001	14	52,68,73	1.77	13 (25%)	55,107,113	2.28	18 (32%)
18	CLA	4	4002	-	42,58,73	1.98	13 (30%)	44,95,113	2.64	16 (36%)
18	CLA	4	4003	14	57,73,73	1.75	13 (22%)	61,113,113	2.13	16 (26%)
18	CLA	4	4004	14	52,68,73	1.78	12 (23%)	55,107,113	2.28	13 (23%)
18	CLA	4	4005	14	52,68,73	1.73	12 (23%)	55,107,113	2.54	19 (34%)
18	CLA	4	4006	-	42,58,73	1.98	13 (30%)	44,95,113	2.41	17 (38%)
18	CLA	4	4007	-	52,68,73	1.78	13 (25%)	55,107,113	2.35	13 (23%)
18	CLA	4	4008	-	38,54,73	2.03	12 (31%)	41,90,113	2.76	15 (36%)
18	CLA	4	4009	14	42,58,73	1.93	13 (30%)	44,95,113	2.46	12 (27%)
28	CHL	4	4010	-	39,55,74	2.32	11 (28%)	38,91,114	1.84	8 (21%)
28	CHL	4	4011	-	43,59,74	2.11	11 (25%)	41,96,114	1.65	5 (12%)
18	CLA	4	4012	14	57,73,73	1.65	12 (21%)	61,113,113	2.14	14 (22%)
28	CHL	4	4013	-	39,55,74	2.27	10 (25%)	38,91,114	1.80	4 (10%)
18	CLA	4	4016	-	38,54,73	2.29	12 (31%)	41,90,113	2.37	16 (39%)
18	CLA	4	4017	-	57,73,73	1.70	12 (21%)	61,113,113	2.15	15 (24%)
27	LUT	4	4501	-	42,43,43	2.47	6 (14%)	49,60,60	2.13	14 (28%)
27	LUT	4	4502	-	42,43,43	2.41	5 (11%)	49,60,60	2.03	14 (28%)
27	LUT	4	4503	-	42,43,43	2.48	5 (11%)	49,60,60	2.27	11 (22%)
29	ZEX	4	4505	-	41,43,43	1.08	3 (7%)	51,60,60	2.04	17 (33%)
23	LMG	4	4801	-	35,35,55	1.01	2 (5%)	43,43,63	1.65	9 (20%)
17	CL0	A	1011	-	57,73,73	1.84	13 (22%)	61,113,113	2.16	12 (19%)
18	CLA	A	1013	-	57,73,73	1.87	12 (21%)	61,113,113	2.01	14 (22%)
18	CLA	A	1022	-	57,73,73	1.83	12 (21%)	61,113,113	2.19	14 (22%)
18	CLA	A	1101	-	57,73,73	1.86	12 (21%)	61,113,113	2.17	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1102	-	42,58,73	2.18	12 (28%)	44,95,113	2.40	14 (31%)
18	CLA	A	1103	-	57,73,73	1.84	12 (21%)	61,113,113	2.11	16 (26%)
18	CLA	A	1104	-	57,73,73	1.86	13 (22%)	61,113,113	2.06	12 (19%)
18	CLA	A	1105	-	43,59,73	2.15	13 (30%)	43,96,113	2.31	12 (27%)
18	CLA	A	1106	1	57,73,73	1.89	13 (22%)	61,113,113	2.21	14 (22%)
18	CLA	A	1107	1	57,73,73	1.87	12 (21%)	61,113,113	2.10	13 (21%)
18	CLA	A	1108	-	38,54,73	2.40	13 (34%)	41,90,113	2.40	13 (31%)
18	CLA	A	1109	-	57,73,73	1.85	12 (21%)	61,113,113	2.02	11 (18%)
18	CLA	A	1110	-	47,63,73	2.07	13 (27%)	49,101,113	2.24	13 (26%)
18	CLA	A	1111	-	52,68,73	1.93	12 (23%)	55,107,113	2.20	15 (27%)
18	CLA	A	1112	-	57,73,73	1.82	12 (21%)	61,113,113	2.20	13 (21%)
18	CLA	A	1113	-	38,54,73	2.35	12 (31%)	41,90,113	2.42	15 (36%)
18	CLA	A	1114	-	38,54,73	2.35	12 (31%)	41,90,113	2.48	11 (26%)
18	CLA	A	1115	-	38,54,73	2.37	13 (34%)	41,90,113	2.36	12 (29%)
18	CLA	A	1116	-	52,68,73	1.94	12 (23%)	55,107,113	2.24	14 (25%)
18	CLA	A	1117	-	57,73,73	1.86	12 (21%)	61,113,113	2.08	14 (22%)
18	CLA	A	1118	-	38,54,73	2.36	11 (28%)	41,90,113	2.53	13 (31%)
18	CLA	A	1119	-	57,73,73	1.83	12 (21%)	61,113,113	2.13	13 (21%)
18	CLA	A	1120	-	52,68,73	1.94	12 (23%)	55,107,113	2.18	14 (25%)
18	CLA	A	1121	-	47,63,73	2.05	13 (27%)	49,101,113	2.38	15 (30%)
18	CLA	A	1122	-	57,73,73	1.85	12 (21%)	61,113,113	2.10	13 (21%)
18	CLA	A	1123	-	57,73,73	1.88	13 (22%)	61,113,113	2.21	15 (24%)
18	CLA	A	1124	-	47,63,73	2.05	13 (27%)	49,101,113	2.39	14 (28%)
18	CLA	A	1125	-	52,68,73	1.90	12 (23%)	55,107,113	2.22	15 (27%)
18	CLA	A	1126	-	57,73,73	1.85	13 (22%)	61,113,113	2.14	17 (27%)
18	CLA	A	1127	-	57,73,73	1.87	12 (21%)	61,113,113	2.14	13 (21%)
18	CLA	A	1128	-	57,73,73	1.85	12 (21%)	61,113,113	2.26	14 (22%)
18	CLA	A	1129	-	42,58,73	2.16	12 (28%)	44,95,113	2.47	15 (34%)
18	CLA	A	1130	-	42,58,73	2.21	13 (30%)	44,95,113	2.43	13 (29%)
18	CLA	A	1131	-	57,73,73	1.86	12 (21%)	61,113,113	2.10	13 (21%)
18	CLA	A	1132	-	57,73,73	1.86	13 (22%)	61,113,113	2.22	13 (21%)
18	CLA	A	1133	-	47,63,73	2.04	13 (27%)	49,101,113	2.42	14 (28%)
18	CLA	A	1134	-	47,63,73	2.05	12 (25%)	49,101,113	2.36	14 (28%)
18	CLA	A	1135	-	43,59,73	2.13	12 (27%)	43,96,113	2.50	13 (30%)
18	CLA	A	1136	-	48,64,73	2.03	13 (27%)	49,102,113	2.33	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1137	-	47,63,73	2.06	13 (27%)	49,101,113	2.30	14 (28%)
18	CLA	A	1138	-	57,73,73	1.90	12 (21%)	61,113,113	1.99	15 (24%)
18	CLA	A	1139	-	57,73,73	1.86	13 (22%)	61,113,113	2.10	14 (22%)
18	CLA	A	1140	-	57,73,73	1.88	13 (22%)	61,113,113	2.01	14 (22%)
18	CLA	A	1151	21	42,58,73	2.22	13 (30%)	44,95,113	2.51	13 (29%)
18	CLA	A	1237	-	52,68,73	1.94	12 (23%)	55,107,113	2.22	15 (27%)
19	SF4	A	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
20	PQN	A	5001	-	34,34,34	1.42	2 (5%)	45,45,45	1.16	2 (4%)
21	LHG	A	5003	18	39,39,48	1.02	2 (5%)	40,45,54	1.21	4 (10%)
22	BCR	A	6002	-	41,41,41	2.82	7 (17%)	56,56,56	6.34	23 (41%)
22	BCR	A	6003	-	41,41,41	2.87	6 (14%)	56,56,56	6.37	20 (35%)
22	BCR	A	6007	-	41,41,41	2.84	7 (17%)	56,56,56	6.41	22 (39%)
22	BCR	A	6008	-	41,41,41	2.92	6 (14%)	56,56,56	6.46	26 (46%)
22	BCR	A	6011	-	41,41,41	2.97	6 (14%)	56,56,56	6.62	28 (50%)
22	BCR	A	6017	-	41,41,41	2.75	6 (14%)	56,56,56	7.01	28 (50%)
21	LHG	A	7001	-	48,48,48	0.94	2 (4%)	49,54,54	1.15	4 (8%)
18	CLA	B	1012	-	57,73,73	1.83	12 (21%)	61,113,113	2.25	17 (27%)
18	CLA	B	1021	-	57,73,73	1.87	11 (19%)	61,113,113	2.12	17 (27%)
18	CLA	B	1023	-	57,73,73	1.86	12 (21%)	61,113,113	2.08	17 (27%)
18	CLA	B	1201	-	42,58,73	2.17	13 (30%)	44,95,113	2.32	14 (31%)
18	CLA	B	1202	-	57,73,73	1.87	12 (21%)	61,113,113	2.11	14 (22%)
18	CLA	B	1203	2	57,73,73	1.82	12 (21%)	61,113,113	2.09	13 (21%)
18	CLA	B	1204	-	47,63,73	2.08	12 (25%)	49,101,113	2.22	12 (24%)
18	CLA	B	1205	-	57,73,73	1.84	12 (21%)	61,113,113	2.03	14 (22%)
18	CLA	B	1206	2	57,73,73	1.87	12 (21%)	61,113,113	2.21	15 (24%)
18	CLA	B	1207	-	57,73,73	1.86	13 (22%)	61,113,113	2.07	15 (24%)
18	CLA	B	1208	-	47,63,73	2.08	13 (27%)	49,101,113	2.31	13 (26%)
18	CLA	B	1209	-	38,54,73	2.40	12 (31%)	41,90,113	2.47	12 (29%)
18	CLA	B	1210	-	57,73,73	1.83	12 (21%)	61,113,113	2.07	13 (21%)
18	CLA	B	1211	-	57,73,73	1.85	12 (21%)	61,113,113	2.12	14 (22%)
18	CLA	B	1212	-	47,63,73	2.06	13 (27%)	49,101,113	2.36	14 (28%)
18	CLA	B	1213	-	52,68,73	1.96	11 (21%)	55,107,113	2.11	12 (21%)
18	CLA	B	1214	-	51,67,73	1.96	12 (23%)	53,105,113	2.27	15 (28%)
18	CLA	B	1215	-	52,68,73	1.97	13 (25%)	55,107,113	2.21	14 (25%)
18	CLA	B	1216	-	57,73,73	1.83	13 (22%)	61,113,113	2.16	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1217	-	38,54,73	2.36	13 (34%)	41,90,113	2.44	12 (29%)
18	CLA	B	1218	-	57,73,73	1.86	13 (22%)	61,113,113	2.23	13 (21%)
18	CLA	B	1219	-	52,68,73	1.96	13 (25%)	55,107,113	2.19	13 (23%)
18	CLA	B	1220	-	57,73,73	1.84	13 (22%)	61,113,113	2.03	16 (26%)
18	CLA	B	1221	-	57,73,73	1.85	12 (21%)	61,113,113	2.23	16 (26%)
18	CLA	B	1222	-	57,73,73	1.86	12 (21%)	61,113,113	2.12	15 (24%)
18	CLA	B	1223	-	57,73,73	1.81	11 (19%)	61,113,113	2.20	14 (22%)
18	CLA	B	1224	-	57,73,73	1.83	12 (21%)	61,113,113	2.20	16 (26%)
18	CLA	B	1225	-	57,73,73	1.88	12 (21%)	61,113,113	2.13	13 (21%)
18	CLA	B	1226	-	57,73,73	1.79	12 (21%)	61,113,113	2.20	14 (22%)
18	CLA	B	1227	-	57,73,73	1.85	13 (22%)	61,113,113	2.14	14 (22%)
18	CLA	B	1228	-	52,68,73	1.96	11 (21%)	55,107,113	2.10	14 (25%)
18	CLA	B	1229	-	57,73,73	1.87	12 (21%)	61,113,113	2.18	15 (24%)
18	CLA	B	1230	-	50,66,73	1.99	11 (22%)	52,104,113	2.46	15 (28%)
18	CLA	B	1231	-	52,68,73	1.97	13 (25%)	55,107,113	2.09	12 (21%)
18	CLA	B	1232	-	47,63,73	2.04	13 (27%)	49,101,113	2.23	12 (24%)
18	CLA	B	1234	-	52,68,73	1.98	13 (25%)	55,107,113	2.22	15 (27%)
18	CLA	B	1235	-	57,73,73	1.86	12 (21%)	61,113,113	2.15	14 (22%)
18	CLA	B	1236	-	47,63,73	2.05	12 (25%)	49,101,113	2.32	14 (28%)
18	CLA	B	1238	-	57,73,73	1.87	12 (21%)	61,113,113	2.13	12 (19%)
18	CLA	B	1239	-	57,73,73	1.86	13 (22%)	61,113,113	2.11	13 (21%)
18	CLA	B	1240	21	57,73,73	1.84	11 (19%)	61,113,113	2.14	15 (24%)
20	PQN	B	5002	-	34,34,34	1.49	2 (5%)	45,45,45	1.04	1 (2%)
21	LHG	B	5004	18	20,20,48	1.32	2 (10%)	21,26,54	1.56	3 (14%)
23	LMG	B	5005	-	38,38,55	1.05	2 (5%)	46,46,63	1.07	3 (6%)
22	BCR	B	6004	-	41,41,41	2.86	6 (14%)	56,56,56	6.58	29 (51%)
22	BCR	B	6005	-	41,41,41	2.79	6 (14%)	56,56,56	6.70	24 (42%)
22	BCR	B	6006	-	41,41,41	2.87	6 (14%)	56,56,56	6.74	27 (48%)
22	BCR	B	6009	-	41,41,41	2.89	6 (14%)	56,56,56	6.29	21 (37%)
22	BCR	B	6010	-	41,41,41	2.81	6 (14%)	56,56,56	6.45	23 (41%)
25	DGD	B	7101	-	62,62,67	0.89	1 (1%)	76,76,81	1.34	11 (14%)
26	LMU	B	8001	-	36,36,36	0.48	0	47,47,47	1.18	4 (8%)
26	LMU	B	8002	-	36,36,36	0.44	0	47,47,47	1.05	3 (6%)
19	SF4	C	3002	8	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	C	3003	8	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	F	1301	-	34,53,73	2.17	11 (32%)	37,89,113	2.35	9 (24%)
18	CLA	F	1302	5	42,58,73	2.10	12 (28%)	44,95,113	2.50	14 (31%)
23	LMG	F	5001	-	23,23,55	1.22	2 (8%)	31,31,63	1.69	6 (19%)
23	LMG	F	5002	-	37,37,55	1.04	2 (5%)	45,45,63	1.27	5 (11%)
22	BCR	F	6014	-	41,41,41	3.12	7 (17%)	56,56,56	6.58	23 (41%)
22	BCR	F	6016	-	41,41,41	3.15	9 (21%)	56,56,56	6.59	25 (44%)
18	CLA	G	1001	-	47,63,73	1.89	13 (27%)	49,101,113	2.64	16 (32%)
18	CLA	G	1002	-	38,54,73	2.21	12 (31%)	41,90,113	2.66	13 (31%)
18	CLA	G	1003	-	52,68,73	1.82	12 (23%)	55,107,113	2.24	15 (27%)
22	BCR	G	2011	-	41,41,41	3.13	7 (17%)	56,56,56	6.64	29 (51%)
23	LMG	G	2021	-	41,41,55	0.93	2 (4%)	49,49,63	1.17	5 (10%)
18	CLA	H	1000	11	38,54,73	2.35	12 (31%)	41,90,113	2.46	13 (31%)
27	LUT	I	6018	-	42,43,43	2.50	4 (9%)	49,60,60	2.13	17 (34%)
22	BCR	I	6020	-	41,41,41	2.85	7 (17%)	56,56,56	6.55	21 (37%)
18	CLA	J	1302	4	42,58,73	2.17	13 (30%)	44,95,113	2.57	16 (36%)
23	LMG	J	5001	-	55,55,55	0.86	2 (3%)	63,63,63	1.43	6 (9%)
22	BCR	J	6012	-	41,41,41	2.99	8 (19%)	56,56,56	6.47	29 (51%)
22	BCR	J	6013	-	41,41,41	2.97	8 (19%)	56,56,56	6.46	29 (51%)
18	CLA	K	1001	-	38,54,73	2.22	13 (34%)	41,90,113	2.63	14 (34%)
22	BCR	K	2011	-	41,41,41	2.79	6 (14%)	56,56,56	6.64	29 (51%)
18	CLA	L	1501	7	42,58,73	2.00	13 (30%)	44,95,113	2.58	18 (40%)
18	CLA	L	1502	-	52,68,73	1.84	13 (25%)	55,107,113	2.26	14 (25%)
18	CLA	L	1503	-	42,58,73	2.04	13 (30%)	44,95,113	2.50	15 (34%)
22	BCR	L	6019	-	41,41,41	3.01	8 (19%)	56,56,56	6.44	24 (42%)
22	BCR	L	6020	-	41,41,41	2.91	7 (17%)	56,56,56	6.44	29 (51%)

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
18	CLA	1	1001	15	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	1	1002	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	1	1003	15	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	1	1004	15	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	1005	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	1	1006	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	1	1007	21	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	1	1008	-	3/3/16/25	0/15/113/135	0/0/9/9
28	CHL	1	1009	-	-	0/27/125/137	0/0/9/9
28	CHL	1	1010	15	-	0/17/115/137	0/0/9/9
18	CLA	1	1011	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	1	1012	15	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	1	1013	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	1	1014	15	3/3/16/25	0/15/113/135	0/0/9/9
27	LUT	1	1501	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	1	1502	-	1/1/12/27	0/29/67/67	0/2/2/2
21	LHG	1	1801	18	-	2/53/53/53	0/0/0/0
18	CLA	2	2001	13	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	2	2002	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	2	2003	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	2	2004	13	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	2	2005	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	2	2006	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	2	2007	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	2	2008	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	2	2009	13	3/3/17/25	0/19/117/135	0/0/9/9
28	CHL	2	2010	-	-	0/17/115/137	0/0/9/9
28	CHL	2	2011	-	-	0/18/116/137	0/0/9/9
18	CLA	2	2012	13	3/3/18/25	0/25/123/135	0/0/9/9
28	CHL	2	2013	-	-	0/13/113/137	0/0/9/9
18	CLA	2	2016	13	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	2	2019	-	3/3/8/25	0/0/75/135	0/0/9/9
27	LUT	2	2501	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	2	2502	-	1/1/12/27	0/29/67/67	0/2/2/2
21	LHG	2	2801	-	-	0/28/28/53	0/0/0/0
23	LMG	2	2802	-	-	0/30/50/70	0/1/1/1
18	CLA	3	3001	16	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3002	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	3	3003	16	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	3	3004	16	3/3/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	3005	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	3	3006	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3007	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3008	-	3/3/16/25	0/17/115/135	0/0/9/9
18	CLA	3	3010	-	3/3/19/25	0/31/129/135	0/0/9/9
28	CHL	3	3011	-	-	0/27/125/137	0/0/9/9
18	CLA	3	3012	16	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3013	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	3	3017	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	3	3018	16	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	3	3019	-	3/3/8/25	0/0/75/135	0/0/9/9
27	LUT	3	3501	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	3	3502	-	1/1/12/27	1/29/67/67	0/2/2/2
22	BCR	3	3503	-	-	0/29/63/63	0/2/2/2
18	CLA	4	4001	14	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	4	4002	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	4	4003	14	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	4	4004	14	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	4	4005	14	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	4	4006	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	4	4007	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	4	4008	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	4	4009	14	3/3/17/25	0/19/117/135	0/0/9/9
28	CHL	4	4010	-	-	0/17/115/137	0/0/9/9
28	CHL	4	4011	-	-	0/21/119/137	0/0/9/9
18	CLA	4	4012	14	3/3/20/25	0/37/135/135	0/0/9/9
28	CHL	4	4013	-	-	0/17/115/137	0/0/9/9
18	CLA	4	4016	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	4	4017	-	3/3/20/25	0/37/135/135	0/0/9/9
27	LUT	4	4501	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	4	4502	-	1/1/12/27	0/29/67/67	0/2/2/2
27	LUT	4	4503	-	1/1/12/27	0/29/67/67	0/2/2/2
29	ZEX	4	4505	-	-	0/29/67/67	0/2/2/2
23	LMG	4	4801	-	-	1/30/50/70	0/1/1/1
17	CL0	A	1011	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1013	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1022	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1102	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	A	1103	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1104	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1105	-	3/3/17/25	0/21/119/135	0/0/9/9
18	CLA	A	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1107	1	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1108	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1109	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1110	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1111	-	2/2/19/25	0/31/129/135	0/0/9/9
18	CLA	A	1112	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1113	-	2/2/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1114	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1115	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1116	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	A	1117	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1118	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	A	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1120	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	A	1121	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1122	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1125	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	A	1126	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1129	-	2/2/17/25	0/19/117/135	0/0/9/9
18	CLA	A	1130	-	2/2/17/25	0/19/117/135	0/0/9/9
18	CLA	A	1131	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1133	-	2/2/18/25	0/25/123/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1134	-	2/2/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1135	-	2/2/17/25	0/21/119/135	0/0/9/9
18	CLA	A	1136	-	3/3/18/25	0/27/125/135	0/0/9/9
18	CLA	A	1137	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	A	1138	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1139	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	A	1151	21	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	A	1237	-	3/3/19/25	0/31/129/135	0/0/9/9
19	SF4	A	3001	1,2	-	0/0/48/48	0/6/5/5
20	PQN	A	5001	-	-	0/23/43/43	0/2/2/2
21	LHG	A	5003	18	-	0/44/44/53	0/0/0/0
22	BCR	A	6002	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6003	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6007	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6008	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6011	-	-	0/29/63/63	0/2/2/2
22	BCR	A	6017	-	-	0/29/63/63	0/2/2/2
21	LHG	A	7001	-	-	0/53/53/53	0/0/0/0
18	CLA	B	1012	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1023	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1201	-	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	B	1202	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1203	2	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1204	-	2/2/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1205	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1206	2	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1207	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1208	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1209	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	B	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1211	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1212	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1213	-	2/2/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1214	-	3/3/18/25	0/30/128/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1215	-	2/2/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1217	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	B	1218	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1219	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1220	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1221	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1222	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1223	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1224	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1227	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1228	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1229	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1230	-	3/3/18/25	0/29/127/135	0/0/9/9
18	CLA	B	1231	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1232	-	3/3/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1234	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	B	1235	-	2/2/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1236	-	2/2/18/25	0/25/123/135	0/0/9/9
18	CLA	B	1238	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1239	-	3/3/20/25	0/37/135/135	0/0/9/9
18	CLA	B	1240	21	2/2/20/25	0/37/135/135	0/0/9/9
20	PQN	B	5002	-	-	0/23/43/43	0/2/2/2
21	LHG	B	5004	18	-	0/23/23/53	0/0/0/0
23	LMG	B	5005	-	-	0/33/53/70	0/1/1/1
22	BCR	B	6004	-	-	0/29/63/63	0/2/2/2
22	BCR	B	6005	-	-	0/29/63/63	0/2/2/2
22	BCR	B	6006	-	-	0/29/63/63	0/2/2/2
22	BCR	B	6009	-	-	0/29/63/63	0/2/2/2
22	BCR	B	6010	-	-	0/29/63/63	0/2/2/2
25	DGD	B	7101	-	-	0/50/90/95	0/2/2/2
26	LMU	B	8001	-	-	0/21/61/61	0/2/2/2
26	LMU	B	8002	-	-	0/21/61/61	0/2/2/2
19	SF4	C	3002	8	-	0/0/48/48	0/6/5/5
19	SF4	C	3003	8	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	1301	-	3/3/16/25	0/11/111/135	0/0/9/9
18	CLA	F	1302	5	3/3/17/25	0/19/117/135	0/0/9/9
23	LMG	F	5001	-	-	0/16/36/70	0/1/1/1
23	LMG	F	5002	-	-	0/32/52/70	0/1/1/1
22	BCR	F	6014	-	-	0/29/63/63	0/2/2/2
22	BCR	F	6016	-	-	0/29/63/63	0/2/2/2
18	CLA	G	1001	-	3/3/18/25	1/25/123/135	0/0/9/9
18	CLA	G	1002	-	3/3/16/25	0/15/113/135	0/0/9/9
18	CLA	G	1003	-	3/3/19/25	0/31/129/135	0/0/9/9
22	BCR	G	2011	-	-	0/29/63/63	0/2/2/2
23	LMG	G	2021	-	-	0/36/56/70	0/1/1/1
18	CLA	H	1000	11	3/3/16/25	0/15/113/135	0/0/9/9
27	LUT	I	6018	-	1/1/12/27	0/29/67/67	0/2/2/2
22	BCR	I	6020	-	-	0/29/63/63	0/2/2/2
18	CLA	J	1302	4	3/3/17/25	0/19/117/135	0/0/9/9
23	LMG	J	5001	-	-	0/50/70/70	0/1/1/1
22	BCR	J	6012	-	-	0/29/63/63	0/2/2/2
22	BCR	J	6013	-	-	0/29/63/63	0/2/2/2
18	CLA	K	1001	-	3/3/16/25	0/15/113/135	0/0/9/9
22	BCR	K	2011	-	-	0/29/63/63	0/2/2/2
18	CLA	L	1501	7	3/3/17/25	0/19/117/135	0/0/9/9
18	CLA	L	1502	-	3/3/19/25	0/31/129/135	0/0/9/9
18	CLA	L	1503	-	3/3/17/25	0/19/117/135	0/0/9/9
22	BCR	L	6019	-	-	0/29/63/63	0/2/2/2
22	BCR	L	6020	-	-	0/29/63/63	0/2/2/2

The worst 5 of 2131 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	2011	BCR	C11-C10	-9.27	1.16	1.43
22	F	6016	BCR	C11-C10	-9.02	1.17	1.43
22	F	6014	BCR	C11-C10	-8.85	1.17	1.43
22	A	6011	BCR	C11-C10	-8.79	1.17	1.43
22	A	6008	BCR	C11-C10	-8.72	1.18	1.43

The worst 5 of 2912 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	4013	CHL	C3C-C4C-NC	-8.29	105.27	110.05
22	A	6017	BCR	C15-C14-C13	-7.65	116.11	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	2011	CHL	C3C-C4C-NC	-7.47	105.74	110.05
28	4	4011	CHL	C3C-C4C-NC	-7.44	105.76	110.05
18	2	2019	CLA	C3B-C2B-C1B	-7.35	99.86	106.29

5 of 425 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1132	CLA	NC
18	A	1132	CLA	ND
18	A	1132	CLA	NA
18	B	1220	CLA	NC
18	B	1220	CLA	NA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	4	4801	LMG	C7-O1-C1-O6
27	3	3502	LUT	C28-C27-C26-C21
18	G	1001	CLA	CED-O2D-CGD-CBD
21	1	1801	LHG	C5-O7-C7-O9
21	1	1801	LHG	C5-O7-C7-C8

There are no ring outliers.

205 monomers are involved in 1953 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	1001	CLA	48	0
18	1	1002	CLA	21	0
18	1	1003	CLA	32	0
18	1	1004	CLA	26	0
18	1	1005	CLA	15	0
18	1	1006	CLA	11	0
18	1	1007	CLA	10	0
18	1	1008	CLA	34	0
28	1	1009	CHL	27	0
28	1	1010	CHL	8	0
18	1	1011	CLA	18	0
18	1	1012	CLA	16	0
18	1	1013	CLA	16	0
18	1	1014	CLA	14	0
27	1	1501	LUT	31	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	1502	LUT	17	0
21	1	1801	LHG	15	0
18	2	2001	CLA	33	0
18	2	2002	CLA	38	0
18	2	2003	CLA	30	0
18	2	2004	CLA	23	0
18	2	2005	CLA	24	0
18	2	2006	CLA	22	0
18	2	2007	CLA	26	0
18	2	2008	CLA	16	0
18	2	2009	CLA	15	0
28	2	2010	CHL	18	0
28	2	2011	CHL	6	0
18	2	2012	CLA	24	0
28	2	2013	CHL	18	0
18	2	2016	CLA	36	0
27	2	2501	LUT	23	0
27	2	2502	LUT	32	0
21	2	2801	LHG	6	0
23	2	2802	LMG	9	0
18	3	3001	CLA	24	0
18	3	3002	CLA	10	0
18	3	3003	CLA	51	0
18	3	3004	CLA	20	0
18	3	3005	CLA	18	0
18	3	3006	CLA	36	0
18	3	3007	CLA	8	0
18	3	3008	CLA	19	0
18	3	3010	CLA	34	0
28	3	3011	CHL	22	0
18	3	3012	CLA	32	0
18	3	3013	CLA	23	0
18	3	3017	CLA	11	0
18	3	3018	CLA	19	0
18	3	3019	CLA	1	0
27	3	3501	LUT	38	0
27	3	3502	LUT	24	0
22	3	3503	BCR	21	0
18	4	4001	CLA	25	0
18	4	4002	CLA	11	0
18	4	4003	CLA	13	0
18	4	4004	CLA	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	4005	CLA	16	0
18	4	4006	CLA	21	0
18	4	4007	CLA	20	0
18	4	4008	CLA	15	0
18	4	4009	CLA	9	0
28	4	4010	CHL	8	0
28	4	4011	CHL	20	0
18	4	4012	CLA	28	0
28	4	4013	CHL	19	0
18	4	4016	CLA	24	0
18	4	4017	CLA	11	0
27	4	4501	LUT	21	0
27	4	4502	LUT	31	0
27	4	4503	LUT	32	0
29	4	4505	ZEX	12	0
23	4	4801	LMG	6	0
17	A	1011	CL0	6	0
18	A	1013	CLA	8	0
18	A	1022	CLA	7	0
18	A	1101	CLA	6	0
18	A	1102	CLA	4	0
18	A	1103	CLA	6	0
18	A	1104	CLA	4	0
18	A	1105	CLA	3	0
18	A	1106	CLA	9	0
18	A	1107	CLA	3	0
18	A	1108	CLA	3	0
18	A	1109	CLA	8	0
18	A	1110	CLA	10	0
18	A	1111	CLA	8	0
18	A	1112	CLA	13	0
18	A	1113	CLA	2	0
18	A	1114	CLA	3	0
18	A	1115	CLA	3	0
18	A	1116	CLA	7	0
18	A	1117	CLA	4	0
18	A	1118	CLA	3	0
18	A	1119	CLA	7	0
18	A	1120	CLA	3	0
18	A	1121	CLA	4	0
18	A	1122	CLA	6	0
18	A	1123	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1124	CLA	4	0
18	A	1125	CLA	3	0
18	A	1126	CLA	10	0
18	A	1127	CLA	6	0
18	A	1128	CLA	11	0
18	A	1129	CLA	1	0
18	A	1130	CLA	4	0
18	A	1131	CLA	3	0
18	A	1132	CLA	7	0
18	A	1133	CLA	3	0
18	A	1134	CLA	2	0
18	A	1135	CLA	4	0
18	A	1136	CLA	7	0
18	A	1137	CLA	3	0
18	A	1138	CLA	4	0
18	A	1139	CLA	5	0
18	A	1140	CLA	5	0
18	A	1151	CLA	4	0
18	A	1237	CLA	5	0
19	A	3001	SF4	1	0
20	A	5001	PQN	3	0
21	A	5003	LHG	5	0
22	A	6002	BCR	4	0
22	A	6003	BCR	2	0
22	A	6007	BCR	3	0
22	A	6008	BCR	2	0
22	A	6011	BCR	5	0
22	A	6017	BCR	5	0
21	A	7001	LHG	7	0
18	B	1012	CLA	6	0
18	B	1021	CLA	9	0
18	B	1023	CLA	5	0
18	B	1201	CLA	2	0
18	B	1202	CLA	7	0
18	B	1203	CLA	3	0
18	B	1204	CLA	10	0
18	B	1205	CLA	8	0
18	B	1206	CLA	6	0
18	B	1207	CLA	12	0
18	B	1208	CLA	7	0
18	B	1209	CLA	3	0
18	B	1210	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1211	CLA	7	0
18	B	1212	CLA	5	0
18	B	1213	CLA	6	0
18	B	1214	CLA	3	0
18	B	1215	CLA	4	0
18	B	1216	CLA	7	0
18	B	1217	CLA	1	0
18	B	1218	CLA	11	0
18	B	1219	CLA	2	0
18	B	1220	CLA	11	0
18	B	1221	CLA	14	0
18	B	1222	CLA	8	0
18	B	1223	CLA	4	0
18	B	1224	CLA	7	0
18	B	1225	CLA	4	0
18	B	1226	CLA	7	0
18	B	1227	CLA	8	0
18	B	1228	CLA	1	0
18	B	1229	CLA	6	0
18	B	1230	CLA	8	0
18	B	1231	CLA	3	0
18	B	1232	CLA	3	0
18	B	1234	CLA	8	0
18	B	1235	CLA	5	0
18	B	1236	CLA	5	0
18	B	1238	CLA	9	0
18	B	1239	CLA	5	0
18	B	1240	CLA	10	0
20	B	5002	PQN	5	0
21	B	5004	LHG	1	0
23	B	5005	LMG	3	0
22	B	6004	BCR	10	0
22	B	6005	BCR	2	0
22	B	6006	BCR	5	0
22	B	6009	BCR	6	0
22	B	6010	BCR	1	0
25	B	7101	DGD	4	0
26	B	8001	LMU	1	0
26	B	8002	LMU	3	0
18	F	1301	CLA	6	0
18	F	1302	CLA	14	0
23	F	5001	LMG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	F	5002	LMG	6	0
22	F	6014	BCR	8	0
22	F	6016	BCR	11	0
18	G	1001	CLA	36	0
18	G	1002	CLA	26	0
18	G	1003	CLA	30	0
22	G	2011	BCR	29	0
23	G	2021	LMG	20	0
18	H	1000	CLA	4	0
27	I	6018	LUT	14	0
22	I	6020	BCR	3	0
18	J	1302	CLA	7	0
23	J	5001	LMG	9	0
22	J	6012	BCR	7	0
22	J	6013	BCR	8	0
18	K	1001	CLA	12	0
22	K	2011	BCR	17	0
18	L	1501	CLA	15	0
18	L	1502	CLA	13	0
18	L	1503	CLA	11	0
22	L	6019	BCR	22	0
22	L	6020	BCR	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	742/758 (97%)	0.36	47 (6%) 23 14	56, 92, 150, 244	0
2	B	732/733 (99%)	0.30	43 (5%) 26 16	61, 89, 126, 157	0
3	I	29/30 (96%)	0.53	4 (13%) 4 2	89, 114, 148, 153	0
4	J	41/42 (97%)	0.17	3 (7%) 18 10	70, 80, 116, 164	0
5	F	150/154 (97%)	0.08	6 (4%) 42 30	66, 90, 122, 157	0
6	G	91/97 (93%)	0.49	11 (12%) 6 3	98, 129, 174, 184	0
7	L	160/167 (95%)	0.68	24 (15%) 3 2	86, 123, 172, 197	0
8	C	80/81 (98%)	0.10	4 (5%) 32 21	66, 81, 96, 106	0
9	D	141/147 (95%)	0.56	20 (14%) 4 2	77, 97, 120, 139	0
10	E	66/66 (100%)	0.35	7 (10%) 8 4	65, 91, 136, 183	0
11	H	84/90 (93%)	0.33	11 (13%) 5 2	103, 138, 178, 234	0
12	K	57/129 (44%)	1.58	19 (33%) 0 0	147, 215, 286, 324	0
13	2	207/269 (76%)	0.61	32 (15%) 3 1	85, 130, 180, 270	0
14	4	198/252 (78%)	0.60	26 (13%) 5 2	84, 121, 193, 274	0
15	1	194/202 (96%)	0.86	39 (20%) 1 1	95, 147, 225, 289	0
16	3	215/275 (78%)	0.73	31 (14%) 3 2	111, 179, 317, 368	0
All	All	3187/3492 (91%)	0.46	327 (10%) 9 4	56, 106, 205, 368	0

The worst 5 of 327 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	1	103	GLY	12.8
16	3	145	ALA	11.1
15	1	172	LYS	9.6
2	B	82	PHE	8.3
9	D	206	LYS	7.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	LUT	3	3501	42/42	0.68	0.63	5.74	202,209,216,218	0
29	ZEX	4	4505	42/42	0.89	0.25	4.93	85,96,107,114	0
22	BCR	B	6005	40/40	0.72	0.41	3.92	87,103,182,184	0
27	LUT	2	2502	42/42	0.85	0.36	3.79	102,115,124,131	0
22	BCR	J	6012	40/40	0.83	0.31	3.70	67,80,89,91	0
22	BCR	A	6007	40/40	0.86	0.30	3.29	77,90,147,151	0
22	BCR	L	6019	40/40	0.81	0.40	3.19	88,105,132,135	0
18	CLA	A	1117	65/65	0.93	0.36	3.16	85,98,110,114	0
22	BCR	A	6003	40/40	0.85	0.34	2.97	79,94,139,140	0
27	LUT	3	3502	42/42	0.74	0.34	2.89	133,142,164,166	0
27	LUT	4	4503	42/42	0.84	0.37	2.71	110,135,158,160	0
22	BCR	J	6013	40/40	0.75	0.34	2.66	74,94,112,116	0
18	CLA	3	3008	48/65	0.84	0.46	2.45	180,199,214,217	0
18	CLA	B	1222	65/65	0.86	0.30	2.37	58,74,103,110	0
28	CHL	3	3011	56/66	0.80	0.34	2.35	144,156,197,200	0
22	BCR	B	6004	40/40	0.77	0.36	2.30	105,112,138,144	0
18	CLA	A	1140	65/65	0.90	0.28	2.27	58,66,78,106	0
18	CLA	2	2012	55/65	0.90	0.29	2.22	86,104,149,153	0
22	BCR	B	6009	40/40	0.85	0.28	2.19	63,78,94,95	0
18	CLA	J	1302	50/65	0.84	0.35	2.13	137,152,189,196	0
22	BCR	L	6020	40/40	0.89	0.37	2.05	98,131,157,164	0
18	CLA	2	2005	55/65	0.91	0.25	1.98	93,103,129,135	0
18	CLA	A	1106	65/65	0.90	0.28	1.96	59,74,90,106	0
22	BCR	B	6010	40/40	0.85	0.28	1.93	64,73,96,100	0
21	LHG	A	7001	49/49	0.91	0.23	1.91	56,72,84,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CLA	B	1227	65/65	0.89	0.23	1.90	60,74,99,105	0
22	BCR	A	6002	40/40	0.91	0.28	1.89	82,115,168,169	0
27	LUT	2	2501	42/42	0.70	0.36	1.88	121,137,141,143	0
18	CLA	B	1220	65/65	0.92	0.23	1.88	61,76,114,118	0
18	CLA	A	1127	65/65	0.92	0.33	1.87	69,83,95,99	0
18	CLA	3	3001	50/65	0.87	0.31	1.80	147,169,201,206	0
22	BCR	A	6011	40/40	0.92	0.36	1.75	61,73,88,96	0
18	CLA	A	1122	65/65	0.92	0.23	1.73	76,96,122,139	0
22	BCR	A	6008	40/40	0.83	0.31	1.69	76,97,137,139	0
18	CLA	B	1234	60/65	0.85	0.29	1.62	64,77,106,108	0
27	LUT	1	1501	42/42	0.79	0.31	1.58	115,142,189,197	0
18	CLA	2	2001	60/65	0.89	0.29	1.54	114,134,167,169	0
22	BCR	G	2011	40/40	0.68	0.28	1.50	112,132,172,174	0
18	CLA	A	1126	65/65	0.92	0.28	1.48	65,79,87,97	0
25	DGD	B	7101	61/66	0.87	0.24	1.47	62,79,104,113	0
18	CLA	A	1104	65/65	0.89	0.28	1.44	55,73,81,85	0
18	CLA	A	1110	55/65	0.87	0.27	1.41	97,114,138,143	0
18	CLA	B	1210	65/65	0.92	0.28	1.30	81,94,107,113	0
18	CLA	A	1107	65/65	0.86	0.29	1.30	60,77,94,105	0
22	BCR	B	6006	40/40	0.78	0.35	1.28	94,115,164,164	0
18	CLA	3	3003	60/65	0.80	0.25	1.27	137,170,188,190	0
18	CLA	3	3010	60/65	0.82	0.29	1.26	122,158,181,196	0
18	CLA	A	1123	65/65	0.87	0.31	1.25	70,88,93,96	0
21	LHG	A	5003	40/49	0.92	0.21	1.23	101,117,132,134	0
18	CLA	A	1135	51/65	0.91	0.28	1.18	72,92,114,117	0
18	CLA	H	1000	46/65	0.85	0.31	1.18	119,150,170,176	0
22	BCR	K	2011	40/40	0.79	0.37	1.18	125,136,144,147	0
20	PQN	B	5002	33/33	0.94	0.23	1.13	54,72,91,93	0
18	CLA	B	1214	59/65	0.85	0.30	1.12	71,91,100,108	0
18	CLA	1	1013	46/65	0.77	0.34	1.12	127,154,181,185	0
18	CLA	B	1216	65/65	0.90	0.25	1.11	73,86,105,108	0
20	PQN	A	5001	33/33	0.92	0.23	1.10	53,63,76,85	0
18	CLA	A	1237	60/65	0.94	0.29	1.07	75,94,113,116	0
27	LUT	1	1502	42/42	0.85	0.26	1.02	85,116,128,129	0
18	CLA	A	1129	50/65	0.92	0.24	1.01	71,93,115,126	0
23	LMG	B	5005	38/55	0.60	0.31	1.00	76,120,141,143	0
18	CLA	A	1022	65/65	0.90	0.24	0.99	58,76,88,99	0
18	CLA	A	1013	65/65	0.93	0.32	0.97	49,62,74,90	0
18	CLA	1	1003	55/65	0.91	0.19	0.96	100,122,134,142	0
18	CLA	4	4016	46/65	0.79	0.30	0.96	126,166,177,183	0
18	CLA	A	1116	60/65	0.91	0.25	0.95	89,119,137,142	0
18	CLA	A	1139	65/65	0.91	0.25	0.93	56,70,98,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	CL0	A	1011	65/65	0.94	0.24	0.93	52,70,82,84	0
28	CHL	2	2011	48/66	0.88	0.24	0.92	108,124,129,136	0
22	BCR	F	6016	40/40	0.90	0.21	0.90	66,75,91,94	0
18	CLA	B	1226	65/65	0.93	0.23	0.89	65,76,97,103	0
22	BCR	F	6014	40/40	0.87	0.27	0.86	54,64,73,74	0
18	CLA	B	1224	65/65	0.92	0.30	0.85	65,83,100,107	0
18	CLA	B	1239	65/65	0.92	0.24	0.84	69,82,111,116	0
18	CLA	B	1207	65/65	0.92	0.23	0.80	78,102,122,129	0
18	CLA	A	1138	65/65	0.92	0.26	0.79	55,65,75,82	0
18	CLA	A	1130	50/65	0.90	0.23	0.79	83,100,123,127	0
18	CLA	K	1001	46/65	0.79	0.35	0.78	147,173,200,209	0
18	CLA	3	3013	46/65	0.86	0.19	0.77	127,157,166,176	0
18	CLA	B	1215	60/65	0.93	0.30	0.73	82,91,102,109	0
18	CLA	B	1225	65/65	0.92	0.30	0.73	66,81,98,105	0
18	CLA	B	1205	65/65	0.94	0.26	0.73	90,103,116,152	0
18	CLA	B	1240	65/65	0.93	0.19	0.69	66,84,103,108	0
18	CLA	A	1132	65/65	0.92	0.28	0.69	79,94,120,129	0
18	CLA	3	3002	46/65	0.89	0.24	0.68	173,188,195,222	0
23	LMG	G	2021	41/55	0.75	0.28	0.68	138,156,175,176	0
18	CLA	B	1229	65/65	0.91	0.26	0.65	60,72,82,84	0
22	BCR	3	3503	40/40	0.76	0.31	0.63	119,136,175,177	0
27	LUT	4	4502	42/42	0.86	0.26	0.63	88,106,117,121	0
18	CLA	A	1112	65/65	0.86	0.25	0.62	101,118,138,140	0
18	CLA	A	1108	46/65	0.91	0.29	0.61	85,101,121,126	0
18	CLA	B	1012	65/65	0.91	0.27	0.61	51,69,85,92	0
18	CLA	3	3004	60/65	0.81	0.26	0.59	125,139,154,155	0
18	CLA	A	1133	55/65	0.91	0.23	0.58	83,109,120,126	0
18	CLA	A	1111	60/65	0.90	0.24	0.58	75,91,112,118	0
18	CLA	2	2007	60/65	0.83	0.30	0.57	116,142,189,195	0
18	CLA	3	3005	55/65	0.87	0.25	0.56	107,131,144,157	0
18	CLA	B	1218	65/65	0.89	0.25	0.56	86,100,155,160	0
28	CHL	4	4010	47/66	0.83	0.28	0.54	105,125,180,187	0
18	CLA	A	1109	65/65	0.88	0.22	0.53	71,85,94,101	0
18	CLA	3	3012	50/65	0.85	0.22	0.51	117,135,142,144	0
18	CLA	F	1301	45/65	0.89	0.23	0.48	61,73,86,101	0
18	CLA	B	1206	65/65	0.94	0.21	0.47	86,104,112,127	0
21	LHG	1	1801	49/49	0.87	0.26	0.47	94,113,164,170	0
22	BCR	I	6020	40/40	0.92	0.25	0.44	85,97,110,111	0
27	LUT	4	4501	42/42	0.82	0.25	0.44	107,121,142,149	0
18	CLA	L	1502	60/65	0.89	0.23	0.43	86,116,125,130	0
18	CLA	A	1103	65/65	0.89	0.25	0.42	66,83,104,107	0
18	CLA	B	1238	65/65	0.93	0.22	0.42	70,85,96,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CLA	3	3007	50/65	0.81	0.23	0.41	175,193,239,246	0
18	CLA	B	1221	65/65	0.94	0.24	0.41	66,78,115,122	0
18	CLA	A	1119	65/65	0.92	0.23	0.40	78,95,107,115	0
18	CLA	A	1118	46/65	0.89	0.22	0.38	99,108,127,131	0
18	CLA	B	1217	46/65	0.92	0.27	0.34	96,109,124,127	0
18	CLA	B	1201	50/65	0.94	0.18	0.34	80,93,131,134	0
28	CHL	4	4011	51/66	0.91	0.23	0.32	117,131,149,154	0
22	BCR	A	6017	40/40	0.92	0.25	0.31	71,86,105,122	0
18	CLA	4	4001	60/65	0.84	0.28	0.28	113,129,158,160	0
23	LMG	4	4801	35/55	0.87	0.25	0.28	104,117,128,132	0
18	CLA	A	1131	65/65	0.93	0.30	0.28	79,93,103,112	0
18	CLA	4	4005	60/65	0.91	0.21	0.26	84,97,106,120	0
18	CLA	4	4007	60/65	0.85	0.29	0.25	110,130,179,183	0
18	CLA	A	1134	55/65	0.86	0.27	0.25	112,124,168,172	0
18	CLA	A	1151	50/65	0.86	0.24	0.24	99,113,187,189	0
18	CLA	1	1008	46/65	0.80	0.25	0.24	112,129,142,150	0
18	CLA	B	1023	65/65	0.88	0.24	0.23	57,70,94,105	0
18	CLA	A	1105	51/65	0.88	0.25	0.23	66,88,97,100	0
18	CLA	2	2016	50/65	0.66	0.30	0.22	114,164,207,211	0
18	CLA	2	2008	50/65	0.91	0.20	0.21	109,138,148,156	0
23	LMG	F	5001	23/55	0.87	0.27	0.21	86,94,106,109	0
18	CLA	B	1021	65/65	0.91	0.25	0.20	61,72,80,83	0
18	CLA	B	1202	65/65	0.95	0.22	0.20	71,82,91,104	0
18	CLA	B	1228	60/65	0.87	0.26	0.17	63,73,111,114	0
18	CLA	L	1501	50/65	0.86	0.22	0.17	106,129,153,159	0
18	CLA	1	1014	46/65	0.88	0.17	0.16	83,110,123,143	0
18	CLA	B	1213	60/65	0.86	0.23	0.14	85,105,118,126	0
18	CLA	B	1231	60/65	0.86	0.23	0.13	65,81,101,104	0
18	CLA	B	1211	65/65	0.91	0.23	0.11	93,107,131,136	0
18	CLA	4	4004	60/65	0.87	0.25	0.11	76,99,112,118	0
18	CLA	B	1235	65/65	0.92	0.22	0.10	54,68,78,92	0
18	CLA	A	1101	65/65	0.90	0.23	0.10	58,72,90,113	0
18	CLA	2	2004	65/65	0.91	0.22	0.10	84,105,117,125	0
23	LMG	J	5001	55/55	0.85	0.22	0.09	62,96,110,122	0
18	CLA	A	1102	50/65	0.92	0.20	0.08	58,69,95,104	0
18	CLA	1	1007	46/65	0.91	0.19	0.08	112,131,162,181	0
18	CLA	B	1212	55/65	0.84	0.26	0.08	109,129,146,154	0
18	CLA	4	4012	65/65	0.92	0.21	0.07	92,104,117,120	0
28	CHL	1	1009	56/66	0.87	0.25	0.05	92,105,113,130	0
18	CLA	4	4003	65/65	0.90	0.23	0.05	84,106,135,143	0
18	CLA	4	4008	46/65	0.85	0.25	0.02	93,112,129,137	0
18	CLA	3	3018	50/65	0.81	0.31	0.01	173,190,207,213	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CLA	A	1128	65/65	0.92	0.21	-0.06	56,66,74,85	0
18	CLA	3	3006	50/65	0.81	0.26	-0.06	125,157,167,170	0
18	CLA	1	1011	50/65	0.85	0.28	-0.07	126,153,175,185	0
28	CHL	2	2010	47/66	0.84	0.25	-0.08	111,134,142,143	0
18	CLA	4	4009	50/65	0.93	0.20	-0.09	85,94,116,131	0
18	CLA	B	1219	60/65	0.92	0.20	-0.09	82,97,134,135	0
18	CLA	L	1503	50/65	0.83	0.38	-0.10	106,114,143,149	0
28	CHL	2	2013	46/66	0.90	0.22	-0.11	110,125,130,135	0
21	LHG	B	5004	21/49	0.92	0.16	-0.13	86,102,116,119	0
18	CLA	A	1125	60/65	0.92	0.22	-0.14	79,94,102,114	0
18	CLA	A	1124	55/65	0.92	0.23	-0.15	59,77,104,116	0
18	CLA	2	2006	55/65	0.86	0.23	-0.17	105,132,173,174	0
18	CLA	G	1002	46/65	0.94	0.19	-0.19	142,160,173,181	0
18	CLA	G	1001	55/65	0.88	0.17	-0.19	119,145,181,184	0
18	CLA	2	2003	55/65	0.89	0.16	-0.20	103,127,135,158	0
18	CLA	A	1114	46/65	0.89	0.29	-0.20	107,117,124,136	0
18	CLA	G	1003	60/65	0.84	0.24	-0.21	97,121,149,153	0
18	CLA	1	1004	65/65	0.89	0.23	-0.26	98,114,122,125	0
18	CLA	B	1203	65/65	0.96	0.22	-0.26	68,82,97,104	0
18	CLA	B	1230	58/65	0.91	0.20	-0.26	58,74,83,86	0
18	CLA	4	4006	50/65	0.80	0.24	-0.28	110,127,148,156	0
18	CLA	B	1236	55/65	0.91	0.24	-0.31	56,69,117,124	0
18	CLA	B	1208	55/65	0.91	0.19	-0.31	82,114,133,137	0
18	CLA	1	1006	50/65	0.83	0.24	-0.35	125,138,144,148	0
18	CLA	A	1113	46/65	0.85	0.27	-0.36	119,135,172,187	0
18	CLA	A	1115	46/65	0.88	0.24	-0.39	107,141,170,178	0
18	CLA	A	1120	60/65	0.90	0.18	-0.40	95,118,178,182	0
18	CLA	B	1223	65/65	0.91	0.22	-0.42	59,78,90,96	0
26	LMU	B	8002	35/35	0.84	0.23	-0.44	162,173,189,191	0
18	CLA	1	1012	50/65	0.94	0.16	-0.56	103,125,130,132	0
18	CLA	A	1121	55/65	0.92	0.17	-0.56	104,123,209,211	0
28	CHL	1	1010	47/66	0.86	0.17	-0.58	125,137,152,155	0
18	CLA	B	1232	55/65	0.90	0.22	-0.61	80,97,118,122	0
21	LHG	2	2801	24/49	0.81	0.25	-0.62	109,123,148,152	0
28	CHL	4	4013	47/66	0.91	0.20	-0.62	98,118,130,134	0
18	CLA	1	1001	60/65	0.84	0.20	-0.63	122,151,165,171	0
18	CLA	2	2009	50/65	0.90	0.18	-0.63	100,117,138,139	0
18	CLA	A	1137	55/65	0.93	0.22	-0.66	71,85,125,126	0
18	CLA	B	1204	55/65	0.91	0.20	-0.70	80,103,118,124	0
18	CLA	B	1209	46/65	0.93	0.22	-0.71	100,109,118,145	0
18	CLA	A	1136	56/65	0.92	0.17	-0.91	84,98,115,119	0
18	CLA	F	1302	50/65	0.94	0.16	-1.13	67,84,114,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	SF4	C	3002	8/8	0.95	0.12	-1.47	73,103,107,107	0
19	SF4	C	3003	8/8	0.97	0.07	-2.30	89,106,119,126	0
19	SF4	A	3001	8/8	0.97	0.10	-2.79	69,95,97,99	0
24	CA	B	6000	1/1	0.89	0.06	-4.01	100,100,100,100	0
18	CLA	3	3019	27/65	0.29	0.59	-	158,174,188,189	1
23	LMG	2	2802	35/55	0.81	0.41	-	108,127,149,152	0
18	CLA	4	4002	50/65	0.81	0.24	-	107,141,171,211	0
18	CLA	2	2002	46/65	0.81	0.21	-	137,154,171,183	0
18	CLA	3	3017	46/65	0.88	0.24	-	101,119,134,145	0
18	CLA	4	4017	65/65	0.89	0.27	-	93,103,120,121	0
18	CLA	1	1002	46/65	0.88	0.19	-	120,155,171,194	0
18	CLA	1	1005	55/65	0.87	0.20	-	84,113,122,124	0
23	LMG	F	5002	37/55	0.85	0.39	-	84,107,120,126	0
18	CLA	2	2019	27/65	0.78	0.18	-	148,159,174,174	1
27	LUT	I	6018	42/42	0.87	0.28	-	101,109,116,121	0
26	LMU	B	8001	35/35	0.79	0.28	-	104,158,168,172	0

6.5 Other polymers

There are no such residues in this entry.