



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:26 AM GMT

PDB ID : 2WSE  
Title : Improved Model of Plant Photosystem I  
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.  
Deposited on : 2009-09-05  
Resolution : 3.49 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

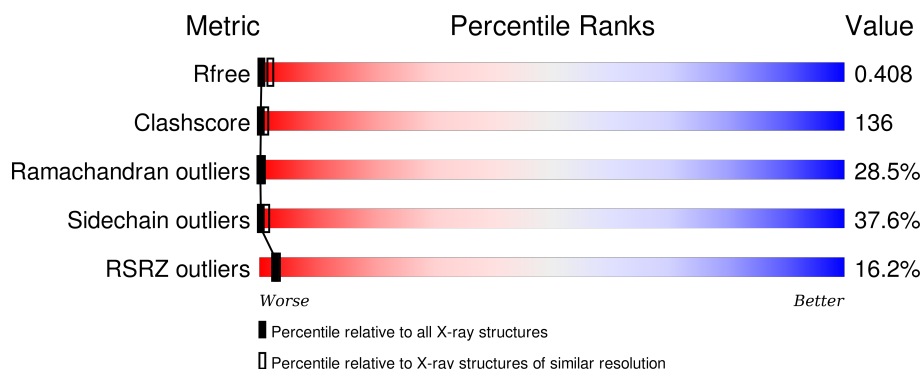
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	1	241	
2	2	269	
3	3	276	
4	4	251	
5	A	758	

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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	212	
9	E	143	
10	F	231	
11	G	167	
12	H	144	
13	I	40	
14	J	44	
15	K	131	
16	L	216	
17	N	170	
18	R	53	

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
19	CLA	1	1010	X	-	-	-
19	CLA	1	1014	X	-	X	-
19	CLA	1	1142	X	-	-	-
19	CLA	1	1145	X	-	X	-
19	CLA	1	1146	X	-	-	-
19	CLA	1	1148	X	-	X	-
19	CLA	1	1149	X	-	-	-
19	CLA	1	1187	X	-	-	-
19	CLA	1	1188	X	-	X	-
19	CLA	1	1189	X	-	-	-
19	CLA	1	1190	X	-	-	-
19	CLA	1	1191	X	-	-	-
19	CLA	1	1192	X	-	-	-
19	CLA	1	1193	X	-	-	-
19	CLA	1	1194	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	1195	X	-	-	-
19	CLA	1	1196	X	-	-	-
19	CLA	1	1197	X	-	-	-
19	CLA	1	1198	X	-	-	-
19	CLA	1	1241	X	-	-	-
19	CLA	1	1303	X	-	-	-
19	CLA	1	1307	X	-	-	-
19	CLA	1	1308	X	-	X	-
19	CLA	1	1309	X	-	-	-
19	CLA	1	1505	X	-	-	-
19	CLA	2	1212	X	-	-	-
19	CLA	2	1213	X	-	-	-
19	CLA	2	1214	X	-	-	-
19	CLA	2	1215	X	-	-	-
19	CLA	2	1216	X	-	-	-
19	CLA	2	1217	X	-	-	-
19	CLA	2	1218	X	-	-	-
19	CLA	2	1219	X	-	-	-
19	CLA	2	1220	X	-	-	-
19	CLA	2	1221	X	-	-	X
19	CLA	2	1222	X	-	-	-
19	CLA	2	1223	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	3	1212	X	-	X	-
19	CLA	3	1213	X	-	-	-
19	CLA	3	1214	X	-	-	-
19	CLA	3	1215	X	-	-	-
19	CLA	3	1216	X	-	-	X
19	CLA	3	1217	X	-	-	-
19	CLA	3	1218	X	-	-	-
19	CLA	3	1219	X	-	-	X
19	CLA	3	1220	X	-	-	-
19	CLA	3	1221	X	-	-	-
19	CLA	3	1222	X	-	-	-
19	CLA	3	1223	X	-	-	-
19	CLA	3	1224	X	-	X	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3008	X	-	-	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3015	X	-	-	-
19	CLA	4	1196	X	-	X	-
19	CLA	4	1197	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	1198	X	-	X	-
19	CLA	4	1199	X	-	-	-
19	CLA	4	1200	X	-	-	X
19	CLA	4	1201	X	-	-	-
19	CLA	4	1202	X	-	-	-
19	CLA	4	1203	X	-	-	X
19	CLA	4	1204	X	-	-	-
19	CLA	4	1205	X	-	-	-
19	CLA	4	1206	X	-	-	-
19	CLA	4	1207	X	-	-	-
19	CLA	4	1208	X	-	-	-
19	CLA	4	1209	X	-	-	-
19	CLA	4	1210	X	-	-	-
19	CLA	4	1211	X	-	-	-
19	CLA	4	4007	X	-	-	-
19	CLA	4	4014	X	-	-	-
19	CLA	A	1759	X	-	-	-
19	CLA	A	1760	X	-	X	-
19	CLA	A	1761	X	-	X	-
19	CLA	A	1762	X	-	X	-
19	CLA	A	1763	X	-	X	X
19	CLA	A	1764	X	-	X	-
19	CLA	A	1765	X	-	X	-
19	CLA	A	1766	X	-	-	X
19	CLA	A	1767	X	-	X	X
19	CLA	A	1768	X	-	-	-
19	CLA	A	1769	X	-	-	-
19	CLA	A	1770	X	-	X	X
19	CLA	A	1771	X	-	X	-
19	CLA	A	1772	X	-	X	X
19	CLA	A	1773	X	-	-	-
19	CLA	A	1774	X	-	X	X
19	CLA	A	1775	X	-	-	-
19	CLA	A	1776	X	-	X	X
19	CLA	A	1777	X	-	-	X
19	CLA	A	1778	X	-	-	-
19	CLA	A	1779	X	-	X	-
19	CLA	A	1780	X	-	-	X
19	CLA	A	1781	X	-	X	-
19	CLA	A	1782	X	-	X	-
19	CLA	A	1783	X	-	X	X
19	CLA	A	1784	X	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1785	X	-	-	-
19	CLA	A	1786	X	-	-	X
19	CLA	A	1787	X	-	X	-
19	CLA	A	1788	X	-	X	-
19	CLA	A	1789	X	-	-	-
19	CLA	A	1790	X	-	-	-
19	CLA	A	1791	X	-	-	-
19	CLA	A	1792	X	-	-	-
19	CLA	A	1793	X	-	-	-
19	CLA	A	1794	X	-	-	-
19	CLA	A	1795	X	-	-	-
19	CLA	A	1796	X	-	X	-
19	CLA	A	1797	X	-	X	-
19	CLA	A	1798	X	-	-	-
19	CLA	A	1799	X	-	X	-
19	CLA	A	1800	X	-	-	X
19	CLA	A	1810	X	-	-	-
19	CLA	A	1811	X	-	X	-
19	CLA	A	1812	X	-	X	-
19	CLA	B	1735	X	-	X	-
19	CLA	B	1736	X	-	-	-
19	CLA	B	1737	X	-	-	-
19	CLA	B	1738	X	-	-	-
19	CLA	B	1739	X	-	X	-
19	CLA	B	1740	X	-	X	-
19	CLA	B	1741	X	-	-	-
19	CLA	B	1742	X	-	-	-
19	CLA	B	1743	X	-	-	-
19	CLA	B	1744	X	-	X	-
19	CLA	B	1745	X	-	-	-
19	CLA	B	1746	X	-	-	-
19	CLA	B	1747	X	-	X	X
19	CLA	B	1748	X	-	X	-
19	CLA	B	1749	X	-	-	-
19	CLA	B	1750	X	-	-	-
19	CLA	B	1751	X	-	-	-
19	CLA	B	1752	X	-	X	-
19	CLA	B	1753	X	-	-	-
19	CLA	B	1754	X	-	X	-
19	CLA	B	1755	X	-	X	-
19	CLA	B	1756	X	-	X	-
19	CLA	B	1757	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1758	X	-	X	-
19	CLA	B	1759	X	-	X	-
19	CLA	B	1760	X	-	X	-
19	CLA	B	1761	X	-	-	-
19	CLA	B	1762	X	-	-	-
19	CLA	B	1763	X	-	X	-
19	CLA	B	1764	X	-	-	-
19	CLA	B	1765	X	-	X	-
19	CLA	B	1766	X	-	X	X
19	CLA	B	1767	X	-	-	-
19	CLA	B	1768	X	-	-	-
19	CLA	B	1769	X	-	X	-
19	CLA	B	1770	X	-	X	-
19	CLA	B	1771	X	-	X	X
19	CLA	B	1772	X	-	X	-
19	CLA	B	1773	X	-	-	X
19	CLA	B	1786	X	-	X	-
19	CLA	B	1787	X	-	X	-
19	CLA	B	1788	X	-	X	-
19	CLA	F	1155	X	-	-	-
19	CLA	F	1156	X	-	-	-
19	CLA	F	1157	X	-	-	-
19	CLA	G	1099	X	-	-	-
19	CLA	I	1031	X	-	-	-
19	CLA	J	1043	X	-	X	-
19	CLA	J	1044	X	-	X	-
19	CLA	K	1085	X	-	X	-
19	CLA	L	1166	X	-	-	-
19	CLA	L	1167	X	-	X	-
19	CLA	L	1168	X	-	-	-
19	CLA	R	1054	X	-	-	-
19	CLA	R	1055	X	-	-	-
20	LMU	A	1808	-	-	-	X
20	LMU	A	1809	-	-	-	X
20	LMU	A	7014	X	-	-	-
20	LMU	A	7016	-	-	X	-
20	LMU	A	7021	-	-	X	-
20	LMU	A	7023	-	-	X	-
20	LMU	A	7032	-	-	X	-
20	LMU	A	7037	-	-	X	-
20	LMU	A	7042	-	-	X	-
20	LMU	A	7047	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	LMU	A	7048	-	-	X	-
20	LMU	A	7050	-	-	X	-
20	LMU	B	1783	-	-	X	-
20	LMU	N	1086	-	-	X	-
20	LMU	R	1056	-	-	X	-
21	SUC	2	1225	X	-	X	-
21	SUC	3	1226	X	-	X	-
21	SUC	B	8051	X	-	-	-
21	SUC	B	8052	X	-	X	-
21	SUC	B	8053	X	-	X	-
21	SUC	B	8054	X	-	-	-
21	SUC	B	8055	X	-	X	-
21	SUC	B	8056	X	-	-	-
21	SUC	B	8059	X	-	X	-
21	SUC	B	8060	X	-	-	-
21	SUC	B	8061	X	-	-	-
21	SUC	B	8062	X	-	X	-
21	SUC	F	1158	X	-	-	-
22	BCR	3	1225	-	-	X	-
22	BCR	A	1802	-	-	X	X
22	BCR	A	1803	-	-	X	X
22	BCR	A	1804	-	-	X	-
22	BCR	A	1805	-	-	X	-
22	BCR	A	1806	-	-	X	X
22	BCR	A	1807	-	-	X	X
22	BCR	B	1776	-	-	-	X
22	BCR	B	1778	-	-	X	X
22	BCR	B	1779	-	-	X	X
22	BCR	B	1780	-	-	X	-
22	BCR	B	1781	-	-	X	X
22	BCR	B	1782	-	-	-	X
22	BCR	I	1032	-	-	X	X
22	BCR	L	1169	-	-	X	X
23	PQN	A	1801	X	-	-	X
23	PQN	B	1774	X	-	X	X
24	LMG	B	1784	-	-	X	X
25	SF4	B	1785	-	-	X	-
25	SF4	C	1082	-	-	X	-
25	SF4	C	1083	-	-	X	-



## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36461 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 AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	164	Total	C	N	O	S	0	0	0
			1255	817	206	228	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	CONFLICT	UNP Q9C5R7
1	-1	ARG	LYS	CONFLICT	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1380	902	229	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	INSERTION	UNP Q41038
2	.	-	GLY	DELETION	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	160	Total	C	N	O	S	0	0	0
			1233	811	200	217	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1322	864	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	.	-	ALA	DELETION	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	CONFLICT	UNP P12353
D	-50	PRO	GLN	CONFLICT	UNP P12353
D	-44	ARG	PRO	CONFLICT	UNP P12353
D	-34	GLU	ASP	CONFLICT	UNP P12353
D	-11	LEU	HIS	CONFLICT	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	CONFLICT	UNP P12353
D	12	THR	PRO	CONFLICT	UNP P12353
D	14	ALA	GLY	CONFLICT	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	ILE	LEU	CONFLICT	UNP P36886

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	161	Total	C	N	O	S	0	0	0
			1203	791	193	214	5			

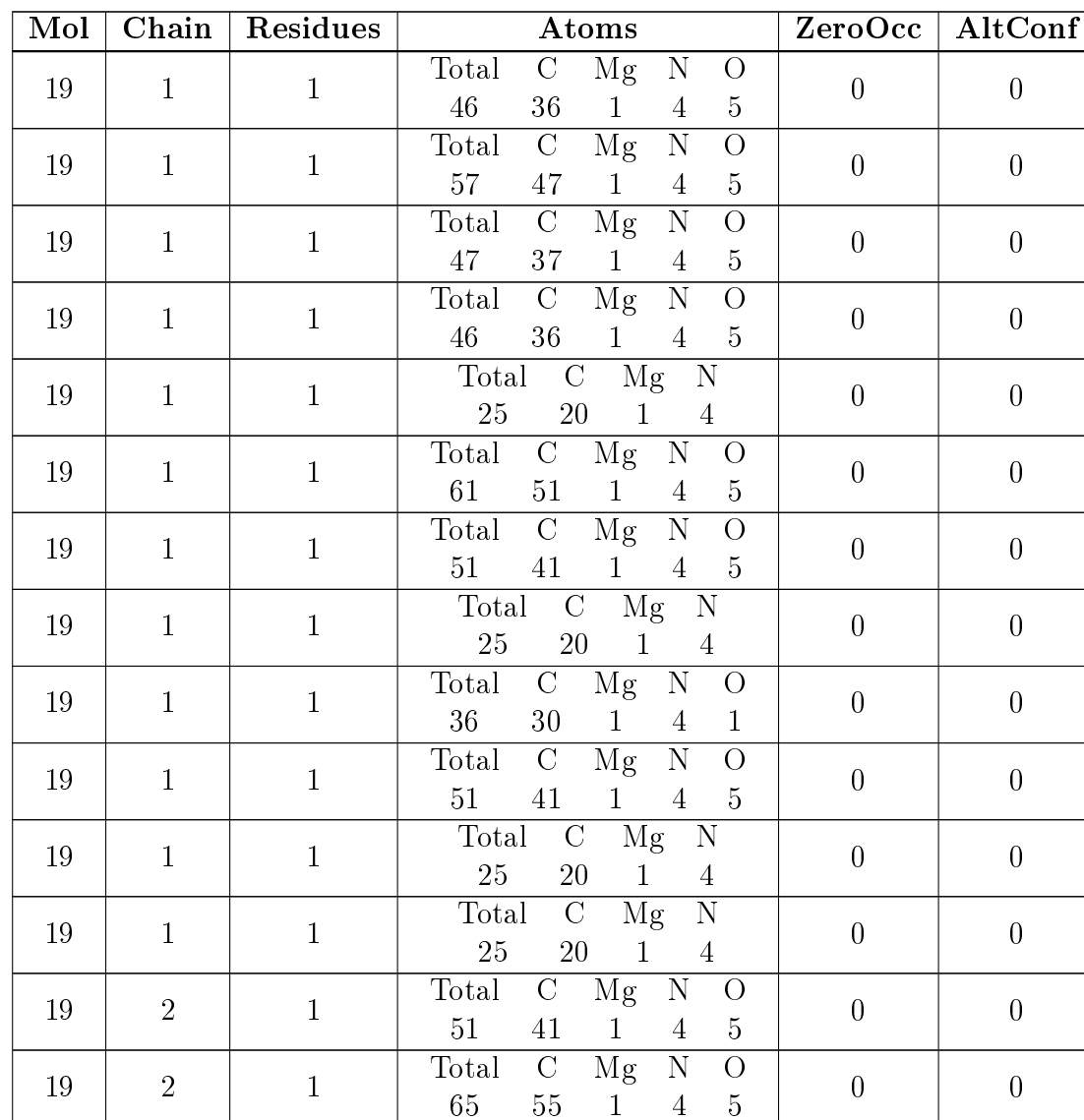
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 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
19	2	1	Total 25	C 20	Mg 1	N 4	0	0
19	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	2	1	Total 25	C 20	Mg 1	N 4	0	0
19	2	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	2	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	2	1	Total 25	C 20	Mg 1	N 4	0	0
19	2	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	2	1	Total 25	C 20	Mg 1	N 4	0	0
19	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	3	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 42	C 34	Mg 1	N 4 O 3	0	0
19	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	3	1	Total 25	C 20	Mg 1	N 4	0	0
19	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	4	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	4	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	4	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	4	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	4	1	Total 52	C 42	Mg 1	N 4 O 5	0	0
19	4	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	4	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	4	1	Total 25	C 20	Mg 1	N 4	0	0
19	4	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
19	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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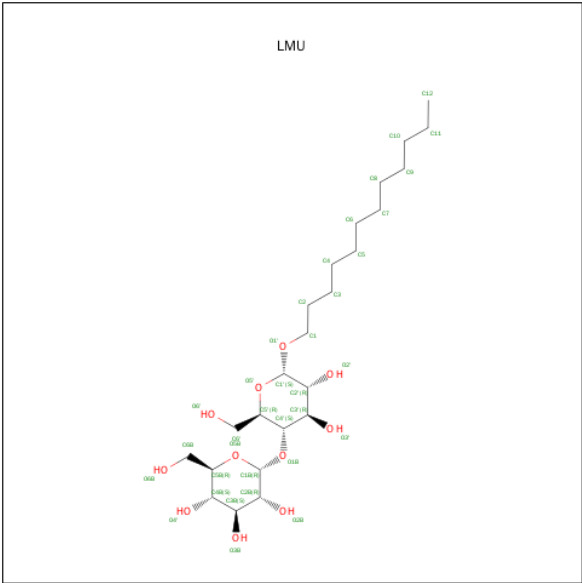
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	1	1	Total	C	Mg	N	0	0
			48	38	1	4		
19	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	1	1	Total	C	Mg	N	0	0
			55	45	1	4		
19	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	3	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	4	1	Total	C	Mg	N	0	0
			52	42	1	4		
19	4	1	Total	C	Mg	N	0	0
			47	37	1	4		

- Molecule 20 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	1	1	Total	C	O	0	0
			35	24	11		
20	1	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	4	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	B	1	Total	C	O	0	0
			35	24	11		
20	K	1	Total	C	O	0	0
			35	24	11		
20	L	1	Total	C	O	0	0
			35	24	11		
20	N	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			34	23	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

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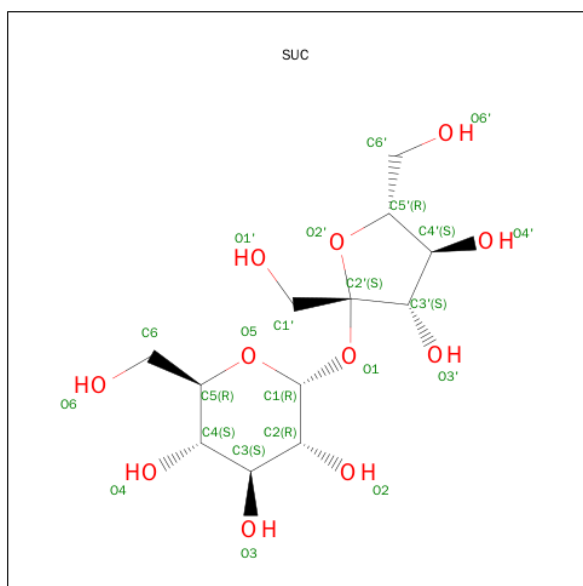
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 21 is SUGAR (SUCROSE) (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			22	12	10		
21	3	1	Total	C	O	0	0
			23	12	11		
21	F	1	Total	C	O	0	0
			23	12	11		

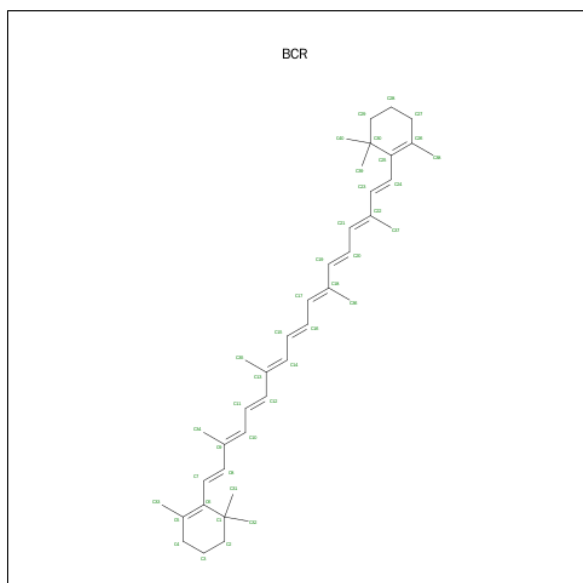
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		

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



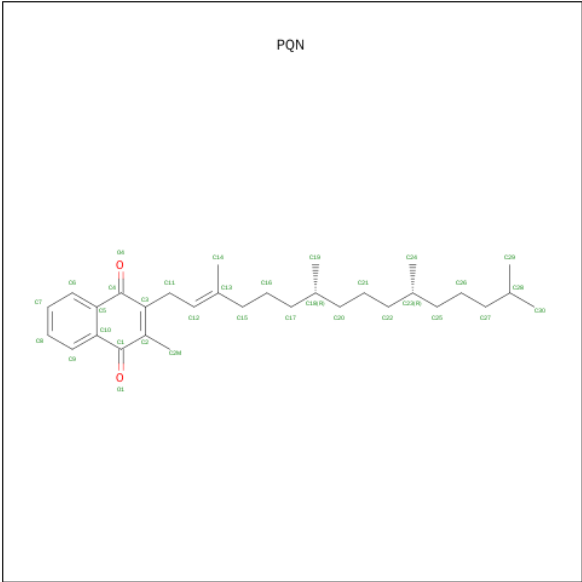
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	3	1	Total	C	0	0
			40	40		

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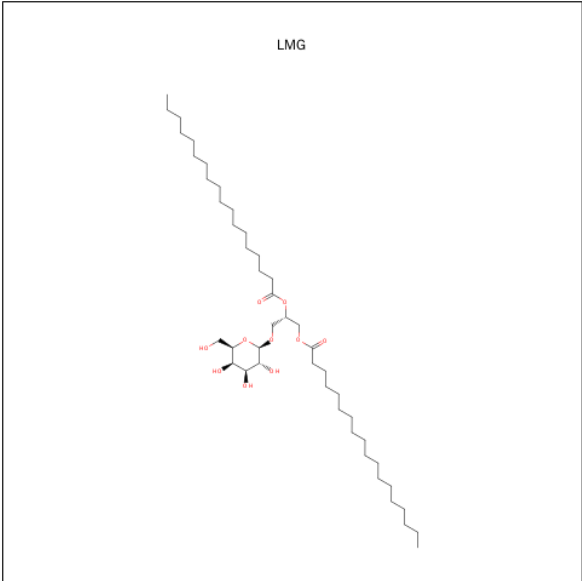
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total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

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



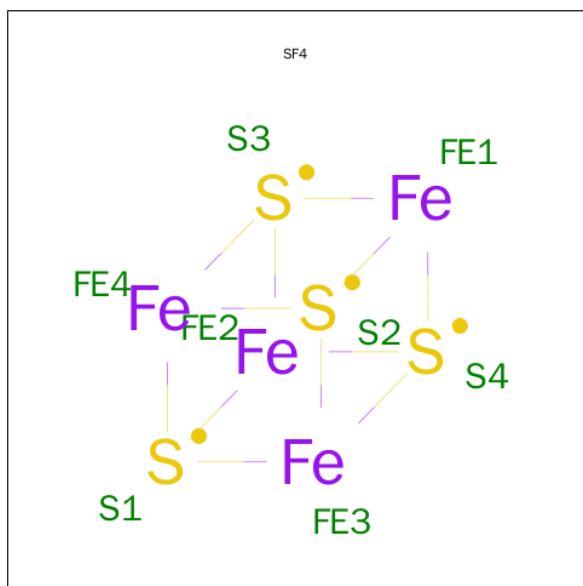
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			33	31	2		
23	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		

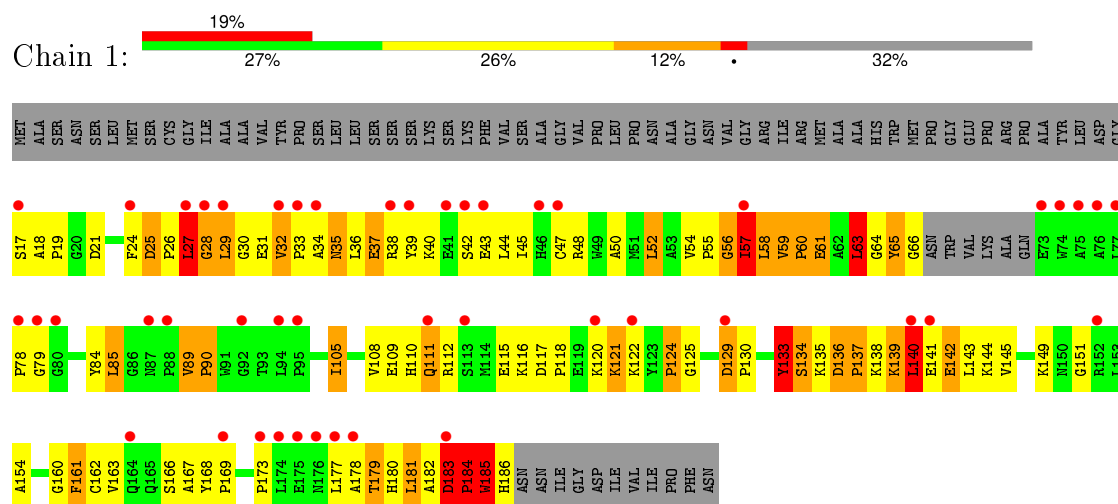
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			23	12	11		

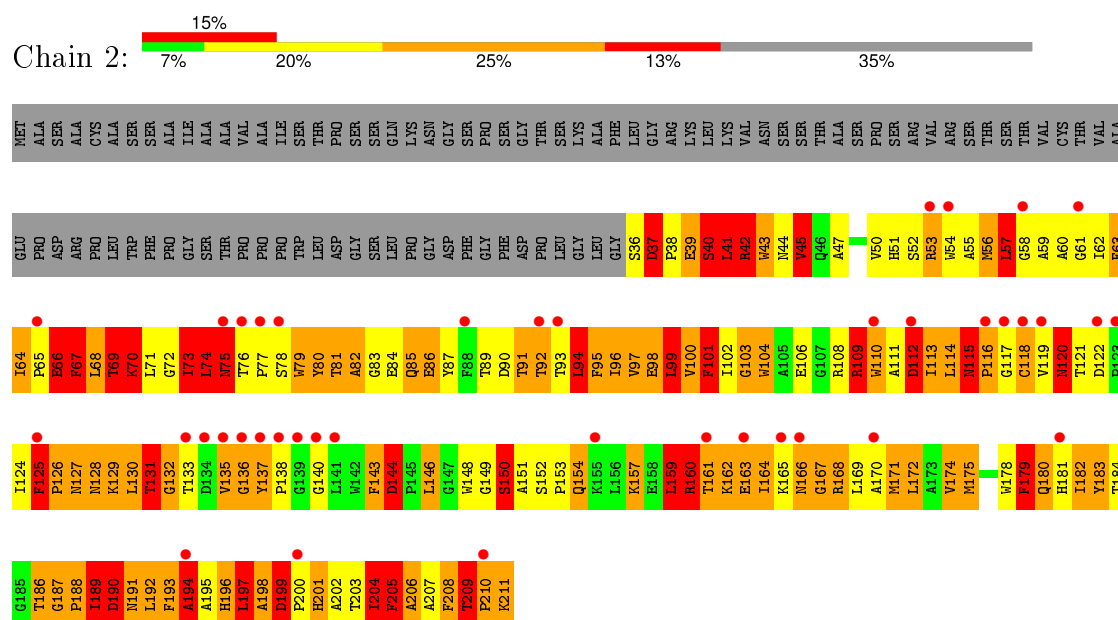
### 3 Residue-property plots

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.

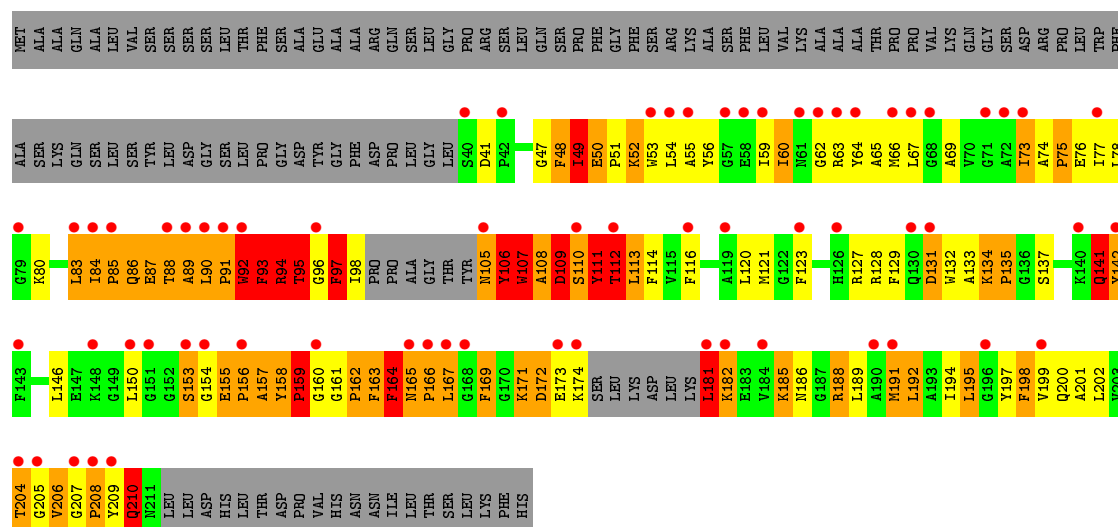
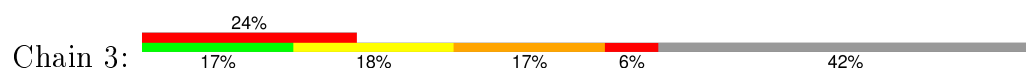
#### • Molecule 1: AT3G54890



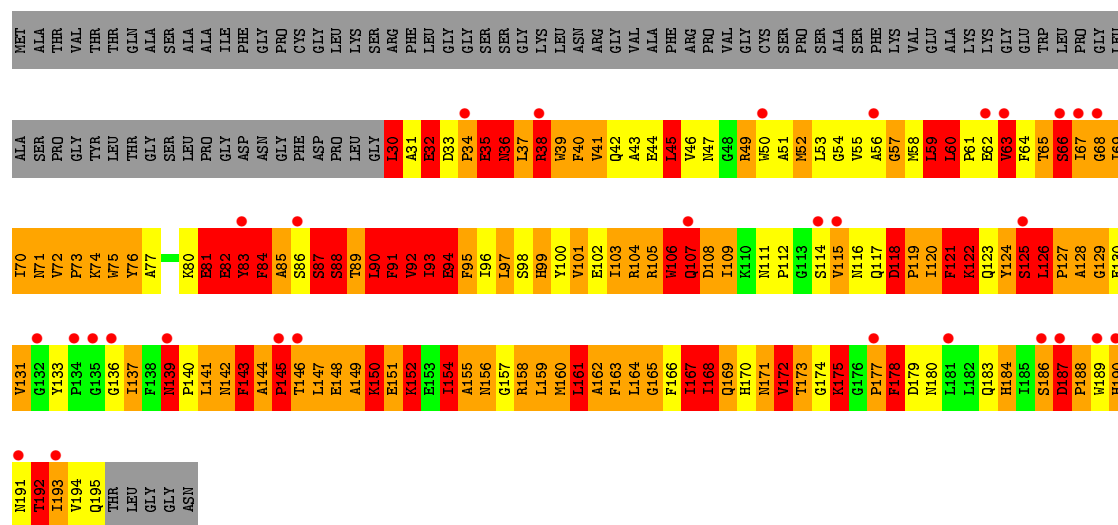
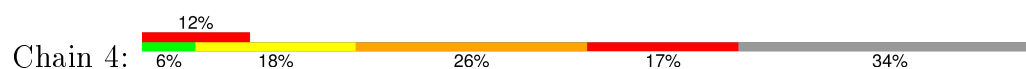
#### • Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I



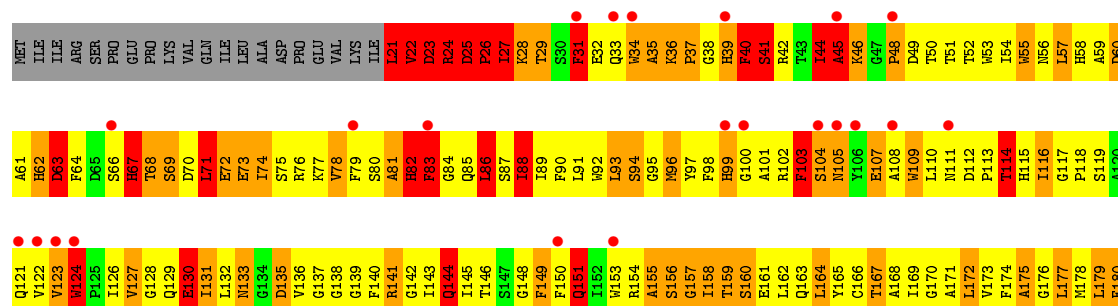
#### • Molecule 3: LHCA3



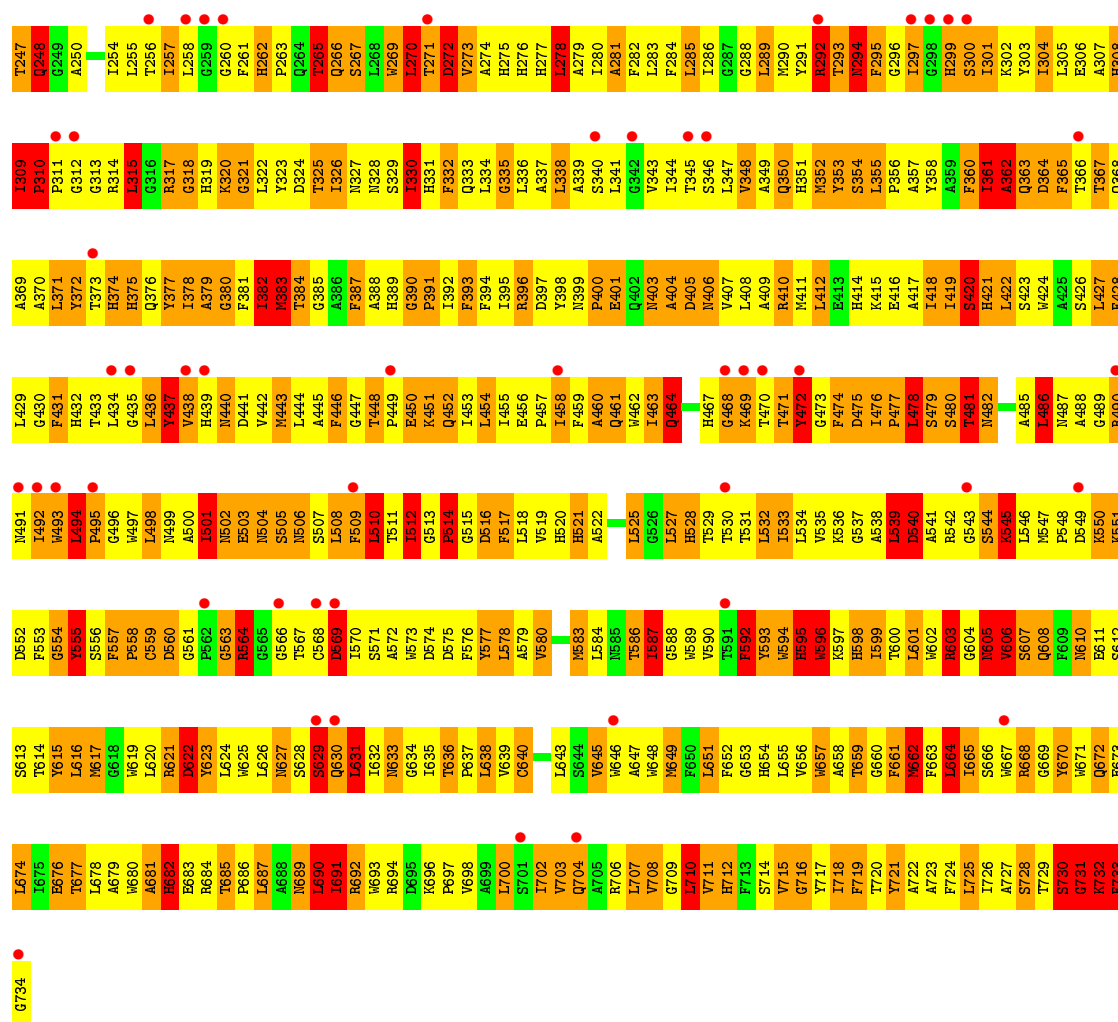
• Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC



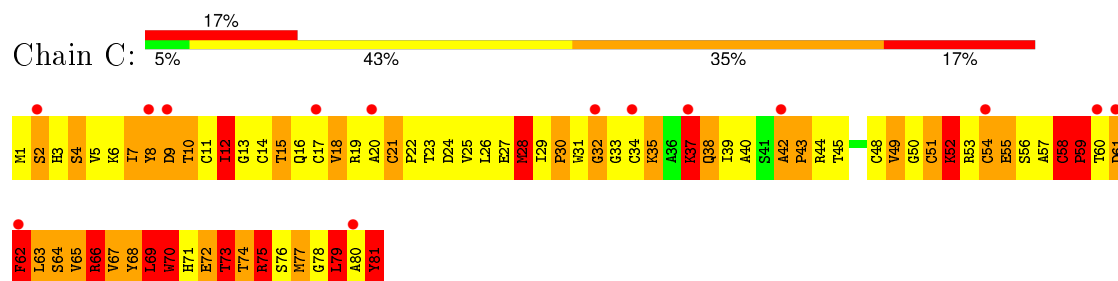
• Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



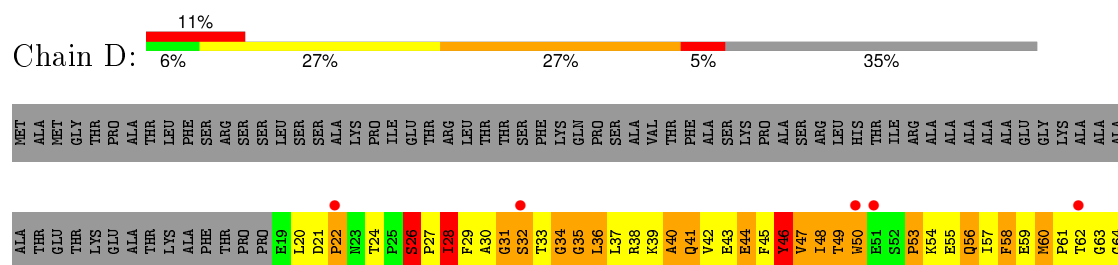




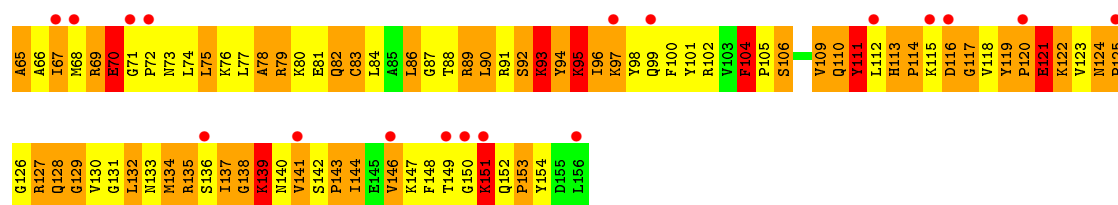
### • Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



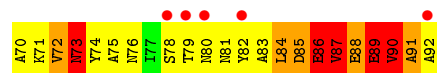
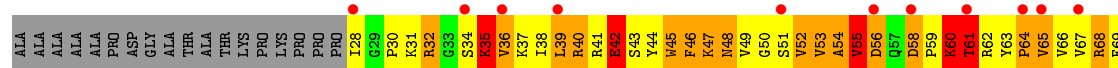
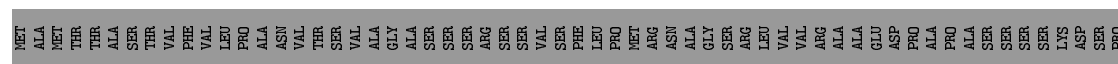
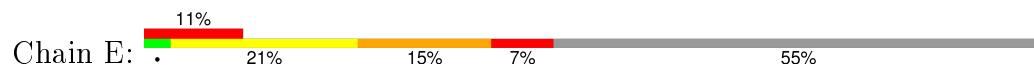
### • Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC



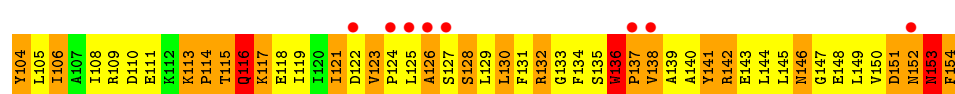
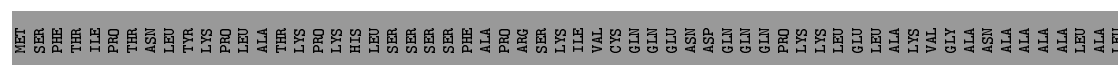




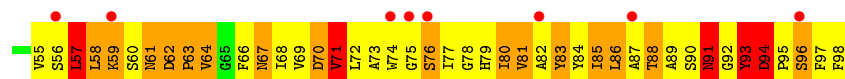
• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC



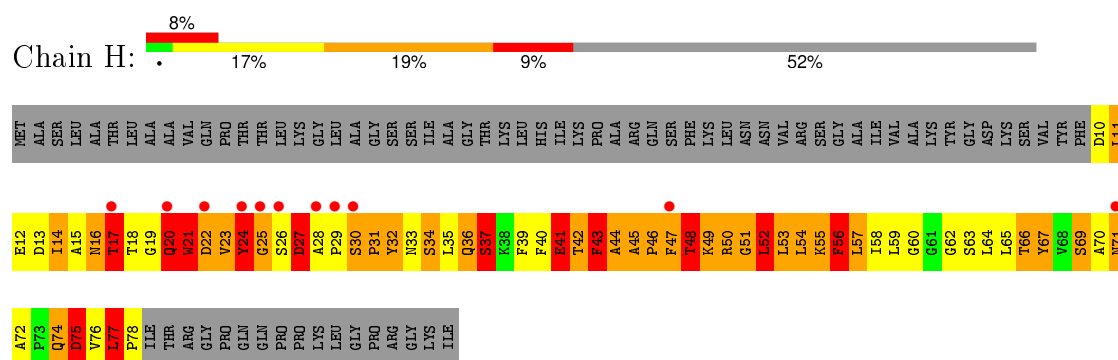
• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC



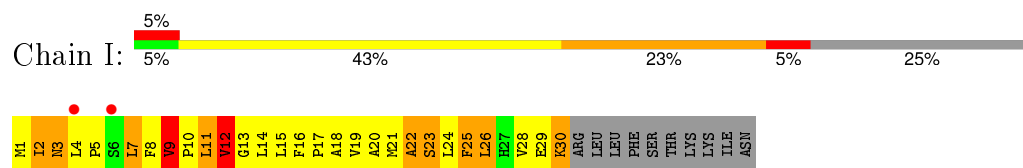
• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC



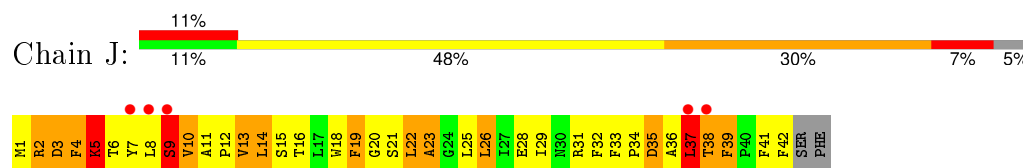
• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC



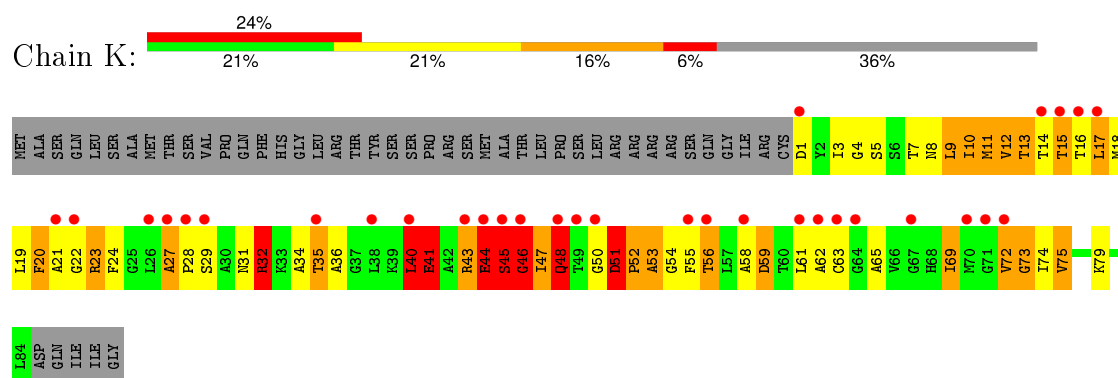
- Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



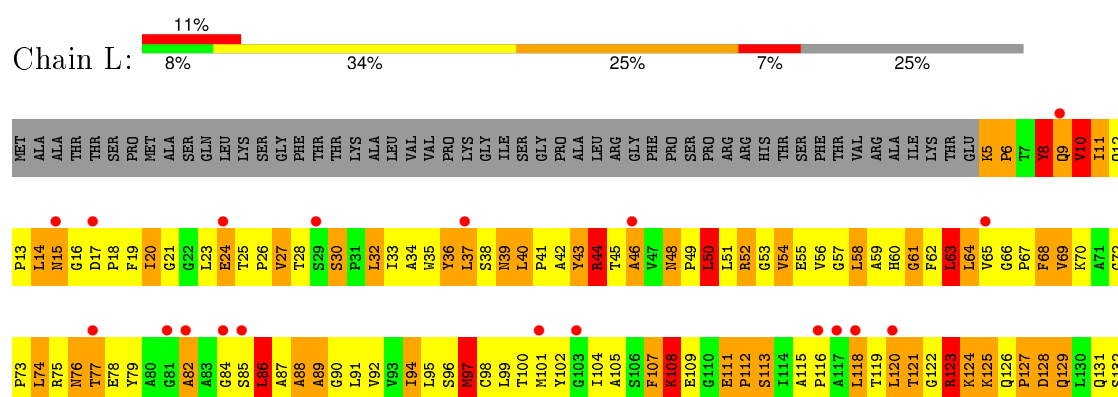
- Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

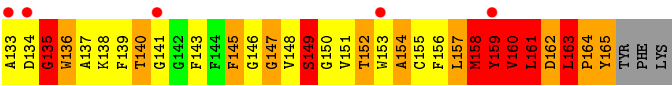


- Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

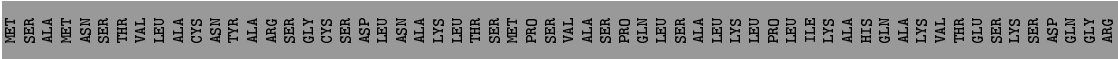
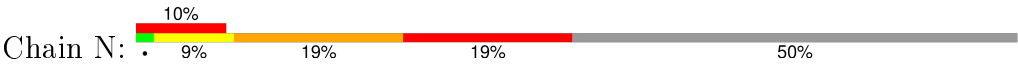


- Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC





• Molecule 17: PHOTOSYSTEM I-N SUBUNIT



• Molecule 18: PHOTOSYSTEM I-N SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.49 39.96 – 3.49	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-3.49) 90.6 (39.96-3.49)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.369 , 0.375 0.392 , 0.408	Depositor DCC
$R_{free}$ test set	1333 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	90.9	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 113.5	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 66880 reflections	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	36461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, 0.375 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: SUC, SF4, CLA, PQN, LMU, UNL, 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	1	0.62	0/1294	0.89	5/1762 (0.3%)
2	2	1.05	1/1426 (0.1%)	1.32	15/1950 (0.8%)
3	3	0.88	6/1270 (0.5%)	0.96	4/1714 (0.2%)
4	4	1.27	9/1362 (0.7%)	1.35	17/1855 (0.9%)
5	A	0.89	0/5938	1.06	15/8104 (0.2%)
6	B	0.89	2/6058 (0.0%)	1.03	13/8278 (0.2%)
7	C	1.42	7/632 (1.1%)	1.34	5/856 (0.6%)
8	D	1.00	0/1122	1.06	0/1514
9	E	1.10	0/530	1.17	2/718 (0.3%)
10	F	1.05	1/1250 (0.1%)	1.07	3/1687 (0.2%)
11	G	1.04	0/760	1.27	10/1031 (1.0%)
12	H	1.10	0/543	1.20	2/741 (0.3%)
13	I	0.89	0/235	0.98	0/320
14	J	0.93	0/349	1.09	1/475 (0.2%)
15	K	0.63	0/599	1.16	6/810 (0.7%)
16	L	1.02	0/1238	1.14	6/1691 (0.4%)
17	N	1.28	1/699 (0.1%)	1.32	7/936 (0.7%)
All	All	0.97	27/25305 (0.1%)	1.11	111/34442 (0.3%)

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
1	1	0	6
2	2	3	22
3	3	0	19
4	4	0	22
5	A	0	30
6	B	0	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	3
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	3
16	L	0	5
17	N	0	21
18	R	0	17
All	All	4	217

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.89	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
7	C	72	GLU	CD-OE1	-7.90	1.17	1.25
4	4	83	TYR	CE1-CZ	-7.46	1.28	1.38
3	3	93	PHE	CD2-CE2	7.39	1.54	1.39

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	57	ILE	N-CA-C	9.01	135.32	111.00
5	A	93	LEU	CA-CB-CG	8.09	133.90	115.30
6	B	732	LYS	N-CA-C	-8.08	89.19	111.00
16	L	160	VAL	CB-CA-C	-7.79	96.61	111.40
4	4	39	TRP	C-N-CA	-7.68	102.51	121.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	67	PHE	CA
2	2	101	PHE	CA
2	2	174	VAL	CA
11	G	21	PHE	CA

5 of 217 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	1	56	GLY	Peptide
1	1	57	ILE	Peptide
1	1	60	PRO	Peptide
1	1	63	LEU	Peptide

## 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	1	1255	0	1222	206	0
2	2	1380	0	1341	484	0
3	3	1233	0	1199	280	7
4	4	1322	0	1287	741	7
5	A	5745	0	5595	1663	0
6	B	5848	0	5653	1489	8
7	C	619	0	608	234	0
8	D	1095	0	1112	222	0
9	E	520	0	528	154	0
10	F	1221	0	1246	306	1
11	G	740	0	709	304	11
12	H	529	0	514	122	0
13	I	229	0	252	63	0
14	J	338	0	340	78	0
15	K	593	0	618	120	0
16	L	1203	0	1213	369	7
17	N	685	0	670	446	11
18	R	265	0	65	65	0
19	1	1065	0	708	316	1
19	2	557	0	397	100	0
19	3	663	0	432	131	0
19	4	775	0	534	179	0
19	A	2523	0	2349	1000	1
19	B	2420	0	2313	850	0
19	F	130	0	86	31	0
19	G	51	0	40	20	0
19	I	60	0	58	12	0
19	J	122	0	120	59	0
19	K	50	0	36	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	147	0	110	44	0
19	R	115	0	106	22	0
20	1	70	0	92	15	0
20	2	35	0	46	3	1
20	4	35	0	46	4	0
20	A	1468	0	1909	526	6
20	B	35	0	46	28	30
20	K	35	0	45	6	0
20	L	35	0	46	3	0
20	N	35	0	45	36	0
20	R	35	0	46	20	4
21	2	22	0	19	10	0
21	3	23	0	22	14	0
21	B	230	0	219	108	0
21	F	23	0	19	5	0
22	3	40	0	54	19	28
22	A	240	0	321	252	0
22	B	320	0	432	226	0
22	I	40	0	54	46	0
22	L	80	0	105	64	0
23	A	33	0	46	15	0
23	B	33	0	46	32	0
24	B	49	0	71	30	0
25	B	8	0	0	19	0
25	C	16	0	0	8	0
26	B	23	0	0	2	0
All	All	36461	0	35190	9731	62

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 136.

The worst 5 of 9731 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)
4:4:69:ILE:CD1	4:4:175:LYS:HG2	1.30	1.61
2:2:43:TRP:CH2	2:2:125:PHE:CE1	1.88	1.61
4:4:69:ILE:HD11	4:4:175:LYS:CG	1.24	1.61
2:2:43:TRP:CZ3	2:2:125:PHE:CD1	1.89	1.59
16:L:164:PRO:HD2	16:L:165:TYR:CE2	1.36	1.59

The worst 5 of 62 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)
22:3:1225:BCR:C28	20:B:1783:LMU:C5[2_556]	0.48	1.72
22:3:1225:BCR:C40	20:B:1783:LMU:C8[2_556]	0.57	1.63
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	0.69	1.51
3:3:181:LEU:CG	6:B:490:ARG:NH2[1_556]	0.72	1.48
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.72	1.48

## 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	1	160/241 (66%)	83 (52%)	47 (29%)	30 (19%)	0	2
2	2	174/269 (65%)	62 (36%)	48 (28%)	64 (37%)	0	0
3	3	154/276 (56%)	77 (50%)	42 (27%)	35 (23%)	0	1
4	4	164/251 (65%)	56 (34%)	47 (29%)	61 (37%)	0	0
5	A	726/758 (96%)	333 (46%)	198 (27%)	195 (27%)	0	0
6	B	731/734 (100%)	362 (50%)	186 (25%)	183 (25%)	0	1
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	49 (36%)	41 (30%)	46 (34%)	0	0
9	E	63/143 (44%)	28 (44%)	15 (24%)	20 (32%)	0	0
10	F	152/231 (66%)	69 (45%)	41 (27%)	42 (28%)	0	0
11	G	93/167 (56%)	37 (40%)	25 (27%)	31 (33%)	0	0
12	H	67/144 (46%)	28 (42%)	15 (22%)	24 (36%)	0	0
13	I	28/40 (70%)	10 (36%)	11 (39%)	7 (25%)	0	1
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	1
15	K	82/131 (63%)	54 (66%)	12 (15%)	16 (20%)	0	2
16	L	159/216 (74%)	65 (41%)	46 (29%)	48 (30%)	0	0
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3091/4108 (75%)	1377 (44%)	833 (27%)	881 (28%)	<b>0</b> <b>0</b>

5 of 881 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	90	PRO
1	1	130	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	126/190 (66%)	99 (79%)	27 (21%)	<b>1</b> <b>7</b>
2	2	141/216 (65%)	78 (55%)	63 (45%)	<b>0</b> <b>0</b>
3	3	118/215 (55%)	78 (66%)	40 (34%)	<b>0</b> <b>2</b>
4	4	139/201 (69%)	73 (52%)	66 (48%)	<b>0</b> <b>0</b>
5	A	592/618 (96%)	395 (67%)	197 (33%)	<b>0</b> <b>2</b>
6	B	598/600 (100%)	369 (62%)	229 (38%)	<b>0</b> <b>1</b>
7	C	70/70 (100%)	40 (57%)	30 (43%)	<b>0</b> <b>1</b>
8	D	118/173 (68%)	75 (64%)	43 (36%)	<b>0</b> <b>1</b>
9	E	56/114 (49%)	36 (64%)	20 (36%)	<b>0</b> <b>1</b>
10	F	127/190 (67%)	74 (58%)	53 (42%)	<b>0</b> <b>1</b>
11	G	79/144 (55%)	47 (60%)	32 (40%)	<b>0</b> <b>1</b>
12	H	57/115 (50%)	26 (46%)	31 (54%)	<b>0</b> <b>0</b>
13	I	26/36 (72%)	18 (69%)	8 (31%)	<b>0</b> <b>3</b>
14	J	36/39 (92%)	24 (67%)	12 (33%)	<b>0</b> <b>2</b>
15	K	61/102 (60%)	39 (64%)	22 (36%)	<b>0</b> <b>1</b>
16	L	124/169 (73%)	81 (65%)	43 (35%)	<b>0</b> <b>2</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	74/139 (53%)	33 (45%)	41 (55%)	0	0
All	All	2542/3331 (76%)	1585 (62%)	957 (38%)	0	1

5 of 957 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	136	TYR
6	B	481	THR
16	L	40	LEU
6	B	175	LEU
6	B	325	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	95	HIS
6	B	403	ASN
14	J	30	ASN
6	B	122	GLN
6	B	266	GLN

### 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 262 ligands modelled in this entry, 1 is unknown - leaving 261 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
19	CLA	1	1010	-	16,32,73	1.80	3 (18%)	21,54,113	3.20	12 (57%)
19	CLA	1	1014	-	51,69,73	2.06	13 (25%)	56,108,113	4.77	27 (48%)
19	CLA	1	1142	-	32,53,73	2.51	11 (34%)	37,89,113	5.57	15 (40%)
19	CLA	1	1145	-	45,63,73	2.38	15 (33%)	49,101,113	5.77	23 (46%)
19	CLA	1	1146	-	40,58,73	2.50	15 (37%)	44,95,113	5.40	21 (47%)
19	CLA	1	1148	-	45,63,73	2.31	13 (28%)	49,101,113	4.74	19 (38%)
19	CLA	1	1149	-	36,54,73	2.67	13 (36%)	42,90,113	4.93	25 (59%)
19	CLA	1	1187	1	36,54,73	2.50	14 (38%)	41,90,113	5.55	26 (63%)
19	CLA	1	1188	19	47,65,73	2.12	14 (29%)	50,103,113	5.06	24 (48%)
19	CLA	1	1189	-	37,55,73	2.42	10 (27%)	42,91,113	5.12	18 (42%)
19	CLA	1	1190	-	36,54,73	2.53	11 (30%)	41,90,113	4.45	17 (41%)
19	CLA	1	1191	-	16,32,73	1.72	5 (31%)	21,54,113	4.20	14 (66%)
19	CLA	1	1192	19	51,69,73	2.12	10 (19%)	56,108,113	3.69	17 (30%)
19	CLA	1	1193	-	41,59,73	2.43	14 (34%)	44,96,113	4.89	21 (47%)
19	CLA	1	1194	-	16,32,73	2.05	7 (43%)	21,54,113	4.15	12 (57%)
19	CLA	1	1195	1	24,44,73	2.82	8 (33%)	28,78,113	4.34	11 (39%)
19	CLA	1	1196	-	41,59,73	2.95	18 (43%)	44,96,113	5.39	22 (50%)
19	CLA	1	1197	-	16,32,73	1.81	4 (25%)	21,54,113	3.36	12 (57%)
19	CLA	1	1198	-	16,32,73	1.78	4 (25%)	21,54,113	3.77	12 (57%)
20	LMU	1	1199	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
20	LMU	1	1200	-	36,36,36	0.80	0	47,47,47	2.18	16 (34%)
19	CLA	1	1241	-	45,63,73	2.25	10 (22%)	49,101,113	4.83	19 (38%)
19	CLA	1	1303	-	16,32,73	1.77	6 (37%)	21,54,113	2.91	10 (47%)
19	CLA	1	1307	-	16,32,73	1.94	7 (43%)	21,54,113	3.81	14 (66%)
19	CLA	1	1308	-	38,56,73	2.38	12 (31%)	42,92,113	5.25	16 (38%)
19	CLA	1	1309	-	16,32,73	1.80	5 (31%)	21,54,113	3.93	10 (47%)
19	CLA	1	1505	-	45,63,73	2.20	12 (26%)	49,101,113	4.68	20 (40%)
19	CLA	2	1212	-	41,59,73	2.29	11 (26%)	44,96,113	5.18	17 (38%)
19	CLA	2	1213	-	55,73,73	2.01	11 (20%)	61,113,113	3.68	20 (32%)
19	CLA	2	1214	-	16,32,73	1.92	7 (43%)	21,54,113	3.71	12 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	2	1215	-	40,58,73	2.27	11 (27%)	44,95,113	4.49	17 (38%)
19	CLA	2	1216	-	16,32,73	1.93	7 (43%)	21,54,113	3.57	12 (57%)
19	CLA	2	1217	2	55,73,73	2.14	11 (20%)	61,113,113	4.44	19 (31%)
19	CLA	2	1218	-	55,73,73	2.01	9 (16%)	61,113,113	4.08	21 (34%)
19	CLA	2	1219	-	16,32,73	1.70	3 (18%)	21,54,113	3.15	12 (57%)
19	CLA	2	1220	-	24,44,73	2.66	8 (33%)	28,78,113	5.04	16 (57%)
19	CLA	2	1221	-	16,32,73	1.73	3 (18%)	21,54,113	3.16	12 (57%)
19	CLA	2	1222	2	40,58,73	2.32	10 (25%)	44,95,113	4.34	18 (40%)
19	CLA	2	1223	-	40,58,73	2.38	10 (25%)	44,95,113	5.00	16 (36%)
20	LMU	2	1224	-	36,36,36	0.80	1 (2%)	47,47,47	0.94	2 (4%)
21	SUC	2	1225	-	23,23,24	1.10	2 (8%)	35,35,36	2.24	12 (34%)
19	CLA	2	2010	-	16,32,73	1.79	4 (25%)	21,54,113	2.85	8 (38%)
19	CLA	3	1212	3	40,58,73	2.41	13 (32%)	44,95,113	4.97	22 (50%)
19	CLA	3	1213	-	16,32,73	2.02	7 (43%)	21,54,113	3.33	12 (57%)
19	CLA	3	1214	-	24,44,73	2.73	8 (33%)	28,78,113	4.06	13 (46%)
19	CLA	3	1215	-	16,32,73	1.97	5 (31%)	21,54,113	3.29	12 (57%)
19	CLA	3	1216	-	16,32,73	1.83	5 (31%)	21,54,113	3.26	11 (52%)
19	CLA	3	1217	-	16,32,73	1.83	5 (31%)	21,54,113	3.27	12 (57%)
19	CLA	3	1218	-	32,50,73	2.43	9 (28%)	36,85,113	5.45	19 (52%)
19	CLA	3	1219	-	55,73,73	2.01	9 (16%)	61,113,113	4.19	19 (31%)
19	CLA	3	1220	-	16,32,73	1.63	3 (18%)	21,54,113	3.01	11 (52%)
19	CLA	3	1221	-	16,32,73	2.01	6 (37%)	21,54,113	3.60	12 (57%)
19	CLA	3	1222	3	55,73,73	2.22	16 (29%)	61,113,113	5.29	21 (34%)
19	CLA	3	1223	-	16,32,73	2.07	6 (37%)	21,54,113	4.68	14 (66%)
19	CLA	3	1224	-	55,73,73	2.23	13 (23%)	61,113,113	5.00	20 (32%)
22	BCR	3	1225	-	41,41,41	2.05	5 (12%)	56,56,56	5.88	21 (37%)
21	SUC	3	1226	-	24,24,24	0.90	0	36,36,36	2.21	8 (22%)
19	CLA	3	3001	-	16,32,73	1.94	4 (25%)	21,54,113	3.30	11 (52%)
19	CLA	3	3008	-	40,58,73	2.33	8 (20%)	44,95,113	4.42	18 (40%)
19	CLA	3	3011	-	55,73,73	1.87	10 (18%)	61,113,113	3.98	17 (27%)
19	CLA	3	3015	-	16,32,73	1.99	6 (37%)	21,54,113	3.77	11 (52%)
19	CLA	4	1196	4	45,63,73	2.23	12 (26%)	49,101,113	4.91	17 (34%)
19	CLA	4	1197	-	24,44,73	2.84	8 (33%)	28,78,113	4.76	16 (57%)
19	CLA	4	1198	-	55,73,73	2.30	16 (29%)	61,113,113	4.57	24 (39%)
19	CLA	4	1199	-	45,63,73	2.12	10 (22%)	49,101,113	4.29	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	4	1200	-	40,58,73	2.46	12 (30%)	44,95,113	6.11	23 (52%)
19	CLA	4	1201	4	42,60,73	2.74	20 (47%)	45,97,113	5.78	32 (71%)
19	CLA	4	1202	-	24,44,73	2.72	9 (37%)	28,78,113	4.49	13 (46%)
19	CLA	4	1203	-	16,32,73	2.46	7 (43%)	21,54,113	4.02	12 (57%)
19	CLA	4	1204	-	16,32,73	1.90	6 (37%)	21,54,113	3.13	10 (47%)
19	CLA	4	1205	-	45,63,73	2.26	9 (20%)	49,101,113	4.46	17 (34%)
19	CLA	4	1206	-	55,73,73	2.01	11 (20%)	61,113,113	4.46	20 (32%)
19	CLA	4	1207	-	16,32,73	1.74	4 (25%)	21,54,113	3.28	11 (52%)
19	CLA	4	1208	-	16,32,73	1.59	2 (12%)	21,54,113	3.30	13 (61%)
19	CLA	4	1209	4	24,44,73	2.67	8 (33%)	28,78,113	5.08	15 (53%)
19	CLA	4	1210	4	16,32,73	1.72	4 (25%)	21,54,113	2.62	11 (52%)
19	CLA	4	1211	-	36,54,73	2.68	15 (41%)	41,90,113	5.09	15 (36%)
20	LMU	4	1212	-	36,36,36	0.73	0	47,47,47	1.20	4 (8%)
19	CLA	4	4007	-	42,60,73	2.71	16 (38%)	45,97,113	5.28	21 (46%)
19	CLA	4	4014	20	37,55,73	2.34	11 (29%)	42,91,113	5.25	16 (38%)
19	CLA	A	1759	-	40,58,73	2.38	13 (32%)	44,95,113	5.05	19 (43%)
19	CLA	A	1760	19	45,63,73	2.33	12 (26%)	49,101,113	3.53	17 (34%)
19	CLA	A	1761	-	55,73,73	2.00	11 (20%)	61,113,113	3.97	19 (31%)
19	CLA	A	1762	-	45,63,73	2.19	10 (22%)	49,101,113	4.90	19 (38%)
19	CLA	A	1763	5,22	36,54,73	2.77	16 (44%)	41,90,113	6.33	20 (48%)
19	CLA	A	1764	5	55,73,73	2.11	13 (23%)	61,113,113	4.10	21 (34%)
19	CLA	A	1765	-	42,60,73	2.19	10 (23%)	45,97,113	4.47	19 (42%)
19	CLA	A	1766	-	32,53,73	2.52	9 (28%)	37,89,113	5.25	19 (51%)
19	CLA	A	1767	19,5	55,73,73	2.07	11 (20%)	61,113,113	3.99	22 (36%)
19	CLA	A	1768	5	44,62,73	2.17	11 (25%)	47,99,113	4.12	15 (31%)
19	CLA	A	1769	-	44,62,73	2.08	11 (25%)	47,99,113	4.06	20 (42%)
19	CLA	A	1770	-	32,53,73	2.63	9 (28%)	37,89,113	4.66	15 (40%)
19	CLA	A	1771	5	40,58,73	2.74	16 (40%)	44,95,113	5.73	29 (65%)
19	CLA	A	1772	5	44,62,73	2.38	13 (29%)	47,99,113	5.01	20 (42%)
19	CLA	A	1773	-	42,60,73	2.34	11 (26%)	45,97,113	5.00	16 (35%)
19	CLA	A	1774	-	55,73,73	1.99	11 (20%)	61,113,113	3.64	20 (32%)
19	CLA	A	1775	-	16,32,73	1.81	3 (18%)	21,54,113	2.78	8 (38%)
19	CLA	A	1776	-	55,73,73	1.94	9 (16%)	61,113,113	4.02	20 (32%)
19	CLA	A	1777	-	41,59,73	2.32	11 (26%)	44,96,113	4.90	17 (38%)
19	CLA	A	1778	5	32,50,73	2.48	10 (31%)	36,85,113	5.20	16 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	A	1779	-	45,63,73	2.22	11 (24%)	49,101,113	4.58	18 (36%)
19	CLA	A	1780	-	55,73,73	1.83	10 (18%)	61,113,113	3.61	19 (31%)
19	CLA	A	1781	-	55,73,73	1.93	11 (20%)	61,113,113	4.42	17 (27%)
19	CLA	A	1782	19	55,73,73	1.94	11 (20%)	61,113,113	4.42	17 (27%)
19	CLA	A	1783	-	55,73,73	2.00	10 (18%)	61,113,113	4.28	20 (32%)
19	CLA	A	1784	5	45,63,73	2.24	11 (24%)	49,101,113	4.54	16 (32%)
19	CLA	A	1785	-	55,73,73	1.97	12 (21%)	61,113,113	4.05	22 (36%)
19	CLA	A	1786	-	40,58,73	2.26	10 (25%)	44,95,113	5.05	21 (47%)
19	CLA	A	1787	5	55,73,73	2.02	10 (18%)	61,113,113	4.09	20 (32%)
19	CLA	A	1788	-	55,73,73	1.97	11 (20%)	61,113,113	4.30	18 (29%)
19	CLA	A	1789	-	45,63,73	2.14	11 (24%)	49,101,113	4.80	22 (44%)
19	CLA	A	1790	19,5	40,58,73	2.27	10 (25%)	44,95,113	4.51	16 (36%)
19	CLA	A	1791	19,5	32,53,73	2.41	10 (31%)	37,89,113	5.69	19 (51%)
19	CLA	A	1792	-	39,57,73	2.40	10 (25%)	43,93,113	4.88	17 (39%)
19	CLA	A	1793	-	55,73,73	2.06	12 (21%)	61,113,113	4.17	19 (31%)
19	CLA	A	1794	-	37,55,73	2.33	11 (29%)	42,91,113	4.27	14 (33%)
19	CLA	A	1795	-	37,55,73	2.51	12 (32%)	42,91,113	4.91	19 (45%)
19	CLA	A	1796	-	55,73,73	2.07	10 (18%)	61,113,113	4.36	20 (32%)
19	CLA	A	1797	19	55,73,73	2.26	14 (25%)	61,113,113	4.78	25 (40%)
19	CLA	A	1798	-	40,58,73	2.29	9 (22%)	44,95,113	5.02	17 (38%)
19	CLA	A	1799	-	55,73,73	1.98	12 (21%)	61,113,113	4.45	20 (32%)
19	CLA	A	1800	-	45,63,73	2.29	9 (20%)	49,101,113	4.20	18 (36%)
23	PQN	A	1801	-	34,34,34	1.54	3 (8%)	44,45,45	1.44	7 (15%)
22	BCR	A	1802	5	41,41,41	1.92	4 (9%)	56,56,56	5.89	19 (33%)
22	BCR	A	1803	-	41,41,41	2.02	3 (7%)	56,56,56	5.93	19 (33%)
22	BCR	A	1804	-	41,41,41	1.99	5 (12%)	56,56,56	5.92	22 (39%)
22	BCR	A	1805	-	41,41,41	2.07	4 (9%)	56,56,56	5.91	23 (41%)
22	BCR	A	1806	-	41,41,41	2.05	5 (12%)	56,56,56	5.93	23 (41%)
22	BCR	A	1807	19	41,41,41	1.92	4 (9%)	56,56,56	5.91	19 (33%)
20	LMU	A	1808	-	36,36,36	0.84	0	47,47,47	1.45	7 (14%)
20	LMU	A	1809	-	36,36,36	0.84	1 (2%)	47,47,47	1.76	11 (23%)
19	CLA	A	1810	-	55,73,73	2.09	13 (23%)	61,113,113	4.48	20 (32%)
19	CLA	A	1811	-	55,73,73	2.02	12 (21%)	61,113,113	4.19	19 (31%)
19	CLA	A	1812	-	55,73,73	2.14	11 (20%)	61,113,113	4.39	19 (31%)
20	LMU	A	7003	-	36,36,36	0.39	0	47,47,47	0.73	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMU	A	7004	-	36,36,36	0.37	0	47,47,47	0.71	1 (2%)
20	LMU	A	7005	-	36,36,36	0.70	0	47,47,47	1.94	12 (25%)
20	LMU	A	7006	-	36,36,36	0.38	0	47,47,47	0.73	1 (2%)
20	LMU	A	7009	20	35,35,36	0.29	0	46,46,47	0.73	1 (2%)
20	LMU	A	7010	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
20	LMU	A	7013	-	36,36,36	0.43	0	47,47,47	1.64	11 (23%)
20	LMU	A	7014	-	36,36,36	1.01	2 (5%)	47,47,47	2.53	15 (31%)
20	LMU	A	7015	-	36,36,36	0.82	1 (2%)	47,47,47	1.48	7 (14%)
20	LMU	A	7016	-	36,36,36	0.67	1 (2%)	47,47,47	1.98	12 (25%)
20	LMU	A	7017	-	36,36,36	0.68	2 (5%)	47,47,47	2.35	15 (31%)
20	LMU	A	7019	-	36,36,36	0.92	1 (2%)	47,47,47	1.43	7 (14%)
20	LMU	A	7020	-	36,36,36	0.42	0	47,47,47	1.81	12 (25%)
20	LMU	A	7021	-	36,36,36	0.77	0	47,47,47	2.09	14 (29%)
20	LMU	A	7022	-	36,36,36	0.75	0	47,47,47	2.23	17 (36%)
20	LMU	A	7023	-	36,36,36	0.77	1 (2%)	47,47,47	2.00	18 (38%)
20	LMU	A	7024	-	36,36,36	0.83	1 (2%)	47,47,47	1.72	11 (23%)
20	LMU	A	7025	-	36,36,36	0.86	1 (2%)	47,47,47	1.59	11 (23%)
20	LMU	A	7026	21	36,36,36	1.11	3 (8%)	47,47,47	3.17	22 (46%)
20	LMU	A	7027	-	36,36,36	1.03	1 (2%)	47,47,47	2.02	15 (31%)
20	LMU	A	7028	-	36,36,36	0.79	2 (5%)	47,47,47	1.92	17 (36%)
20	LMU	A	7030	-	36,36,36	0.97	1 (2%)	47,47,47	2.38	15 (31%)
20	LMU	A	7031	-	36,36,36	0.98	1 (2%)	47,47,47	1.38	5 (10%)
20	LMU	A	7032	-	36,36,36	1.03	4 (11%)	47,47,47	2.82	18 (38%)
20	LMU	A	7033	-	36,36,36	1.00	2 (5%)	47,47,47	2.27	14 (29%)
20	LMU	A	7034	19	36,36,36	0.72	1 (2%)	47,47,47	1.38	4 (8%)
20	LMU	A	7035	-	36,36,36	0.76	1 (2%)	47,47,47	1.65	9 (19%)
20	LMU	A	7036	-	35,35,36	1.28	4 (11%)	46,46,47	2.37	16 (34%)
20	LMU	A	7037	20	36,36,36	0.91	2 (5%)	47,47,47	3.13	25 (53%)
20	LMU	A	7038	-	36,36,36	0.66	0	47,47,47	2.47	17 (36%)
20	LMU	A	7039	-	36,36,36	0.99	2 (5%)	47,47,47	2.65	14 (29%)
20	LMU	A	7040	-	36,36,36	1.00	3 (8%)	47,47,47	2.54	13 (27%)
20	LMU	A	7041	-	36,36,36	0.66	1 (2%)	47,47,47	1.90	13 (27%)
20	LMU	A	7042	-	36,36,36	0.52	0	47,47,47	2.12	14 (29%)
20	LMU	A	7043	-	36,36,36	0.75	0	47,47,47	2.26	14 (29%)
20	LMU	A	7047	-	36,36,36	1.02	1 (2%)	47,47,47	1.49	4 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMU	A	7048	-	36,36,36	0.46	0	47,47,47	2.19	17 (36%)
20	LMU	A	7049	-	36,36,36	0.58	1 (2%)	47,47,47	1.42	8 (17%)
20	LMU	A	7050	-	36,36,36	1.01	3 (8%)	47,47,47	2.77	19 (40%)
20	LMU	A	7051	20	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
19	CLA	B	1735	-	55,73,73	2.14	12 (21%)	61,113,113	3.73	24 (39%)
19	CLA	B	1736	-	32,53,73	2.36	10 (31%)	37,89,113	4.51	15 (40%)
19	CLA	B	1737	-	50,68,73	2.08	10 (20%)	55,107,113	4.66	21 (38%)
19	CLA	B	1738	-	55,73,73	2.02	13 (23%)	61,113,113	4.34	28 (45%)
19	CLA	B	1739	-	55,73,73	2.15	11 (20%)	61,113,113	4.41	20 (32%)
19	CLA	B	1740	6	55,73,73	1.88	11 (20%)	61,113,113	4.47	17 (27%)
19	CLA	B	1741	-	50,68,73	2.06	11 (22%)	55,107,113	4.51	19 (34%)
19	CLA	B	1742	6	44,62,73	2.47	10 (22%)	49,100,113	3.24	20 (40%)
19	CLA	B	1743	6	45,63,73	2.07	12 (26%)	49,101,113	4.30	21 (42%)
19	CLA	B	1744	-	48,66,73	2.54	17 (35%)	52,104,113	4.99	22 (42%)
19	CLA	B	1745	-	55,73,73	2.07	11 (20%)	61,113,113	3.55	19 (31%)
19	CLA	B	1746	6	50,68,73	2.05	9 (18%)	55,107,113	4.17	18 (32%)
19	CLA	B	1747	-	36,54,73	2.46	10 (27%)	41,90,113	4.75	16 (39%)
19	CLA	B	1748	-	49,67,73	2.05	10 (20%)	53,105,113	3.75	18 (33%)
19	CLA	B	1749	-	50,68,73	1.98	11 (22%)	55,107,113	4.55	18 (32%)
19	CLA	B	1750	-	51,69,73	1.97	11 (21%)	56,108,113	4.50	19 (33%)
19	CLA	B	1751	-	40,58,73	2.25	12 (30%)	44,95,113	4.46	16 (36%)
19	CLA	B	1752	-	36,54,73	2.37	10 (27%)	41,90,113	4.97	15 (36%)
19	CLA	B	1753	6	45,63,73	2.26	9 (20%)	49,101,113	4.83	18 (36%)
19	CLA	B	1754	-	55,73,73	2.56	18 (32%)	61,113,113	4.63	19 (31%)
19	CLA	B	1755	-	44,62,73	2.30	12 (27%)	47,99,113	4.39	21 (44%)
19	CLA	B	1756	-	48,66,73	2.13	12 (25%)	52,104,113	4.76	16 (30%)
19	CLA	B	1757	6	55,73,73	1.94	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	B	1758	-	55,73,73	2.11	11 (20%)	61,113,113	4.39	20 (32%)
19	CLA	B	1759	-	55,73,73	2.04	12 (21%)	61,113,113	4.02	20 (32%)
19	CLA	B	1760	-	55,73,73	1.96	13 (23%)	61,113,113	4.21	18 (29%)
19	CLA	B	1761	-	40,58,73	2.40	8 (20%)	44,95,113	4.17	20 (45%)
19	CLA	B	1762	6	40,58,73	2.21	10 (25%)	44,95,113	4.93	18 (40%)
19	CLA	B	1763	6	55,73,73	2.07	13 (23%)	61,113,113	4.39	19 (31%)
19	CLA	B	1764	6	40,58,73	2.38	12 (30%)	44,95,113	4.75	21 (47%)
19	CLA	B	1765	19	32,53,73	2.69	11 (34%)	37,89,113	5.08	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	B	1766	19	32,53,73	2.51	10 (31%)	37,89,113	5.46	15 (40%)
19	CLA	B	1767	-	41,59,73	2.40	11 (26%)	44,96,113	4.81	17 (38%)
19	CLA	B	1768	-	50,68,73	2.01	11 (22%)	55,107,113	4.48	15 (27%)
19	CLA	B	1769	6	55,73,73	1.91	11 (20%)	61,113,113	3.92	17 (27%)
19	CLA	B	1770	-	37,55,73	2.29	10 (27%)	42,91,113	4.46	17 (40%)
19	CLA	B	1771	-	55,73,73	1.95	10 (18%)	61,113,113	4.10	22 (36%)
19	CLA	B	1772	-	55,73,73	1.93	12 (21%)	61,113,113	3.95	22 (36%)
19	CLA	B	1773	-	24,44,73	2.79	8 (33%)	28,78,113	4.92	16 (57%)
23	PQN	B	1774	-	34,34,34	1.47	2 (5%)	44,45,45	1.51	5 (11%)
22	BCR	B	1775	-	41,41,41	1.96	4 (9%)	56,56,56	5.89	20 (35%)
22	BCR	B	1776	-	41,41,41	2.10	5 (12%)	56,56,56	5.92	22 (39%)
22	BCR	B	1777	-	41,41,41	1.90	4 (9%)	56,56,56	5.03	24 (42%)
22	BCR	B	1778	-	41,41,41	2.15	5 (12%)	56,56,56	5.93	25 (44%)
22	BCR	B	1779	-	41,41,41	1.98	4 (9%)	56,56,56	5.88	18 (32%)
22	BCR	B	1780	-	41,41,41	2.99	14 (34%)	56,56,56	6.07	31 (55%)
22	BCR	B	1781	-	41,41,41	2.09	4 (9%)	56,56,56	5.92	20 (35%)
22	BCR	B	1782	-	41,41,41	2.81	17 (41%)	56,56,56	5.39	30 (53%)
20	LMU	B	1783	-	36,36,36	0.98	1 (2%)	47,47,47	2.43	16 (34%)
24	LMG	B	1784	-	49,49,55	0.93	2 (4%)	57,57,63	1.04	3 (5%)
25	SF4	B	1785	5,6	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	B	1786	-	55,73,73	1.97	11 (20%)	61,113,113	4.25	23 (37%)
19	CLA	B	1787	-	55,73,73	1.98	13 (23%)	61,113,113	4.12	23 (37%)
19	CLA	B	1788	-	55,73,73	2.01	11 (20%)	61,113,113	3.93	19 (31%)
21	SUC	B	8051	-	24,24,24	0.64	0	36,36,36	1.40	2 (5%)
21	SUC	B	8052	-	24,24,24	0.93	0	36,36,36	1.70	9 (25%)
21	SUC	B	8053	-	24,24,24	0.74	0	36,36,36	1.68	10 (27%)
21	SUC	B	8054	-	24,24,24	1.25	3 (12%)	36,36,36	1.76	9 (25%)
21	SUC	B	8055	-	24,24,24	0.96	0	36,36,36	1.27	3 (8%)
21	SUC	B	8056	-	24,24,24	1.11	1 (4%)	36,36,36	1.88	14 (38%)
21	SUC	B	8059	-	24,24,24	1.09	2 (8%)	36,36,36	2.11	12 (33%)
21	SUC	B	8060	-	24,24,24	1.10	0	36,36,36	1.86	7 (19%)
21	SUC	B	8061	-	24,24,24	0.94	1 (4%)	36,36,36	2.31	15 (41%)
21	SUC	B	8062	20	24,24,24	1.07	3 (12%)	36,36,36	2.80	16 (44%)
25	SF4	C	1082	7	0,12,12	0.00	-	0,24,24	0.00	-
25	SF4	C	1083	7	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
19	CLA	F	1155	-	24,44,73	2.73	8 (33%)	28,78,113	3.66	14 (50%)
19	CLA	F	1156	19	30,49,73	2.48	10 (33%)	34,84,113	5.81	17 (50%)
19	CLA	F	1157	19	43,61,73	2.60	15 (34%)	46,98,113	4.73	18 (39%)
21	SUC	F	1158	10	24,24,24	0.95	1 (4%)	36,36,36	1.59	9 (25%)
19	CLA	G	1099	-	41,59,73	2.46	14 (34%)	44,96,113	5.41	18 (40%)
19	CLA	I	1031	-	50,68,73	2.05	11 (22%)	55,107,113	4.89	16 (29%)
22	BCR	I	1032	-	41,41,41	2.80	9 (21%)	56,56,56	6.52	29 (51%)
19	CLA	J	1043	-	51,69,73	2.05	12 (23%)	56,108,113	4.61	17 (30%)
19	CLA	J	1044	-	51,69,73	2.05	12 (23%)	56,108,113	4.68	26 (46%)
19	CLA	K	1085	20	40,58,73	2.26	11 (27%)	44,95,113	5.18	18 (40%)
20	LMU	K	1086	19	36,36,36	0.77	1 (2%)	47,47,47	2.40	12 (25%)
19	CLA	L	1166	16	40,58,73	2.35	10 (25%)	44,95,113	5.08	16 (36%)
19	CLA	L	1167	22,16	37,55,73	2.36	10 (27%)	42,91,113	5.16	21 (50%)
19	CLA	L	1168	-	40,58,73	2.45	14 (35%)	44,95,113	5.64	17 (38%)
22	BCR	L	1169	-	41,41,41	2.53	10 (24%)	56,56,56	5.72	20 (35%)
22	BCR	L	1170	19	41,41,41	3.43	20 (48%)	56,56,56	6.42	27 (48%)
20	LMU	L	1171	-	36,36,36	0.85	1 (2%)	47,47,47	1.54	11 (23%)
20	LMU	N	1086	17	36,36,36	0.54	0	47,47,47	2.15	13 (27%)
19	CLA	R	1054	-	47,65,73	2.14	12 (25%)	50,103,113	4.89	18 (36%)
19	CLA	R	1055	-	48,66,73	2.49	15 (31%)	52,104,113	4.47	23 (44%)
20	LMU	R	1056	20	36,36,36	0.36	0	47,47,47	0.72	1 (2%)

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	CLA	1	1010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1014	-	4/4/19/25	1/33/131/135	0/0/9/9
19	CLA	1	1142	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	1	1145	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	1	1146	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	1	1148	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1149	-	5/5/16/25	0/16/112/135	0/0/9/9
19	CLA	1	1187	1	3/3/16/25	0/15/113/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1188	19	4/4/18/25	1/28/126/135	0/0/9/9
19	CLA	1	1189	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	1190	-	3/3/16/25	1/15/113/135	0/0/9/9
19	CLA	1	1191	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1192	19	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1193	-	4/4/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1194	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1195	1	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1196	-	4/4/17/25	1/21/119/135	0/0/9/9
19	CLA	1	1197	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1198	-	3/3/7/25	0/0/66/135	0/0/8/9
20	LMU	1	1199	-	-	0/21/61/61	0/2/2/2
20	LMU	1	1200	-	-	0/21/61/61	0/2/2/2
19	CLA	1	1241	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1303	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1307	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1308	-	3/3/16/25	0/17/115/135	0/0/9/9
19	CLA	1	1309	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1505	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	2	1212	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	2	1213	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	1214	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1215	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1216	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1217	2	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	2	1218	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	1219	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1220	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	2	1221	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1222	2	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1223	-	3/3/17/25	0/19/117/135	0/0/9/9
20	LMU	2	1224	-	-	0/21/61/61	0/2/2/2
21	SUC	2	1225	-	1/1/9/9	0/10/49/51	0/2/2/2
19	CLA	2	2010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1212	3	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	1213	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1214	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	1215	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1216	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1217	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1218	-	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	3	1219	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1220	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1221	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1222	3	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1223	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1224	-	4/4/20/25	1/37/135/135	0/0/9/9
22	BCR	3	1225	-	-	1/29/63/63	0/2/2/2
21	SUC	3	1226	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	3	3001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3008	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	3	3011	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3015	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1196	4	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1197	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1198	-	5/5/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1199	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1200	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	4	1201	4	4/4/17/25	0/22/120/135	0/0/9/9
19	CLA	4	1202	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1203	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1204	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1205	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1206	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1207	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1208	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1209	4	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1210	4	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
20	LMU	4	1212	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	4007	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4014	20	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1759	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1760	19	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1761	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1762	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1763	5,22	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	1764	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1765	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	1766	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1767	19,5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1768	5	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1769	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1770	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1771	5	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1772	5	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1773	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	1774	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1775	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	A	1776	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1777	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1778	5	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	A	1779	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1780	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1781	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1782	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1783	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1784	5	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1785	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1786	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1787	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1788	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1789	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1790	19,5	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1791	19,5	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1792	-	3/3/16/25	0/18/116/135	0/0/9/9
19	CLA	A	1793	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1794	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1795	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1796	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1797	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1798	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1799	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1800	-	4/4/18/25	0/25/123/135	0/0/9/9
23	PQN	A	1801	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	A	1802	5	-	1/29/63/63	0/2/2/2
22	BCR	A	1803	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1804	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1805	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1806	-	-	1/29/63/63	0/2/2/2
22	BCR	A	1807	19	-	0/29/63/63	0/2/2/2
20	LMU	A	1808	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1809	-	-	1/21/61/61	0/2/2/2
19	CLA	A	1810	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1811	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1812	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	A	7003	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7004	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7005	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7006	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7009	20	-	0/20/60/61	0/2/2/2
20	LMU	A	7010	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7013	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7014	-	1/1/10/10	0/21/61/61	0/2/2/2
20	LMU	A	7015	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7016	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7017	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7019	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7020	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7021	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7022	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7023	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7024	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMU	A	7025	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7026	21	-	0/21/61/61	0/2/2/2
20	LMU	A	7027	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7028	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7030	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7031	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7032	-	-	1/21/61/61	0/2/2/2
20	LMU	A	7033	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7034	19	-	0/21/61/61	0/2/2/2
20	LMU	A	7035	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7036	-	-	0/20/60/61	0/2/2/2
20	LMU	A	7037	20	-	0/21/61/61	0/2/2/2
20	LMU	A	7038	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7039	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7040	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7041	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7042	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7043	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7047	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7048	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7049	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7050	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7051	20	-	1/21/61/61	0/2/2/2
19	CLA	B	1735	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1736	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1737	-	4/4/19/25	1/31/129/135	0/0/9/9
19	CLA	B	1738	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1739	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1740	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1741	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1742	6	4/4/18/25	0/25/121/135	0/0/9/9
19	CLA	B	1743	6	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1744	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	B	1745	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1746	6	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1747	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1748	-	4/4/18/25	0/30/128/135	0/0/9/9
19	CLA	B	1749	-	4/4/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1750	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	B	1751	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1752	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1753	6	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1754	-	3/3/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1755	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	B	1756	-	4/4/18/25	1/29/127/135	0/0/9/9
19	CLA	B	1757	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1758	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1759	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1760	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1761	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	B	1762	6	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1763	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1764	6	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1765	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1766	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1767	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	B	1768	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1769	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1770	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	B	1771	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1772	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1773	-	3/3/14/25	0/0/96/135	0/0/9/9
23	PQN	B	1774	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	B	1775	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1776	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1777	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1778	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1779	-	-	1/29/63/63	0/2/2/2
22	BCR	B	1780	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1781	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1782	-	-	0/29/63/63	0/2/2/2
20	LMU	B	1783	-	-	0/21/61/61	0/2/2/2
24	LMG	B	1784	-	-	0/44/64/70	0/1/1/1
25	SF4	B	1785	5,6	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1786	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1787	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1788	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	B	8051	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8052	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8053	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8054	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8055	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8056	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8059	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8060	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8061	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8062	20	1/1/9/9	0/12/51/51	0/2/2/2
25	SF4	C	1082	7	-	0/0/48/48	0/6/5/5
25	SF4	C	1083	7	-	0/0/48/48	1/6/5/5
19	CLA	F	1155	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	F	1156	19	3/3/15/25	0/8/106/135	0/0/9/9
19	CLA	F	1157	19	6/6/17/25	1/23/121/135	0/0/9/9
21	SUC	F	1158	10	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	G	1099	-	3/3/17/25	1/21/119/135	0/0/9/9
19	CLA	I	1031	-	4/4/19/25	0/31/129/135	0/0/9/9
22	BCR	I	1032	-	-	1/29/63/63	0/2/2/2
19	CLA	J	1043	-	4/4/19/25	1/33/131/135	0/0/9/9
19	CLA	J	1044	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	K	1085	20	3/3/17/25	0/19/117/135	0/0/9/9
20	LMU	K	1086	19	-	0/21/61/61	0/2/2/2
19	CLA	L	1166	16	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	L	1167	22,16	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	L	1168	-	4/4/17/25	0/19/117/135	0/0/9/9
22	BCR	L	1169	-	-	2/29/63/63	0/2/2/2
22	BCR	L	1170	19	-	0/29/63/63	0/2/2/2
20	LMU	L	1171	-	-	0/21/61/61	0/2/2/2
20	LMU	N	1086	17	-	0/21/61/61	0/2/2/2
19	CLA	R	1054	-	4/4/18/25	1/28/126/135	0/0/9/9
19	CLA	R	1055	-	4/4/18/25	0/29/127/135	0/0/9/9
20	LMU	R	1056	20	-	0/21/61/61	0/2/2/2

The worst 5 of 1984 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1170	BCR	C21-C22	-11.56	1.20	1.35
22	B	1782	BCR	C21-C22	-10.75	1.21	1.35
22	B	1780	BCR	C21-C22	-10.23	1.22	1.35
22	L	1170	BCR	C20-C21	-10.19	1.12	1.43
22	I	1032	BCR	C21-C22	-9.52	1.23	1.35

The worst 5 of 4178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1763	CLA	OBD-CAD-CBD	-22.01	92.73	125.94
19	1	1145	CLA	OBD-CAD-CBD	-21.73	93.14	125.94
19	3	1222	CLA	OBD-CAD-CBD	-21.06	94.17	125.94
19	4	1200	CLA	OBD-CAD-CBD	-20.75	94.63	125.94
19	3	1224	CLA	OBD-CAD-CBD	-17.75	99.15	125.94

5 of 623 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	B	1755	CLA	NC
19	B	1755	CLA	ND
19	B	1755	CLA	NA
19	R	1055	CLA	C8
19	R	1055	CLA	NC

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	3	1225	BCR	C21-C20-C19-C18
22	I	1032	BCR	C20-C21-C22-C23
22	L	1169	BCR	C20-C21-C22-C37
22	A	1806	BCR	C21-C20-C19-C18
22	L	1169	BCR	C20-C21-C22-C23

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	C	1083	SF4	FE1-FE3-S2-S4

239 monomers are involved in 3843 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1014	CLA	52	0
19	1	1142	CLA	19	1

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1145	CLA	31	0
19	1	1146	CLA	11	0
19	1	1148	CLA	35	0
19	1	1149	CLA	9	0
19	1	1187	CLA	13	0
19	1	1188	CLA	40	0
19	1	1189	CLA	13	0
19	1	1190	CLA	5	0
19	1	1192	CLA	16	0
19	1	1193	CLA	6	1
19	1	1195	CLA	11	0
19	1	1196	CLA	9	0
19	1	1197	CLA	5	0
20	1	1199	LMU	7	0
20	1	1200	LMU	8	0
19	1	1241	CLA	15	0
19	1	1308	CLA	27	0
19	1	1505	CLA	3	0
19	2	1212	CLA	17	0
19	2	1213	CLA	13	0
19	2	1214	CLA	5	0
19	2	1215	CLA	13	0
19	2	1217	CLA	18	0
19	2	1218	CLA	9	0
19	2	1220	CLA	1	0
19	2	1222	CLA	18	0
19	2	1223	CLA	10	0
20	2	1224	LMU	3	1
21	2	1225	SUC	10	0
19	3	1212	CLA	27	0
19	3	1214	CLA	14	0
19	3	1215	CLA	1	0
19	3	1216	CLA	3	0
19	3	1217	CLA	16	0
19	3	1218	CLA	2	0
19	3	1219	CLA	3	0
19	3	1220	CLA	5	0
19	3	1221	CLA	7	0
19	3	1222	CLA	20	0
19	3	1224	CLA	25	0
22	3	1225	BCR	19	28
21	3	1226	SUC	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	3008	CLA	3	0
19	3	3011	CLA	17	0
19	4	1196	CLA	26	0
19	4	1197	CLA	6	0
19	4	1198	CLA	24	0
19	4	1199	CLA	20	0
19	4	1200	CLA	9	0
19	4	1201	CLA	15	0
19	4	1203	CLA	1	0
19	4	1204	CLA	3	0
19	4	1205	CLA	17	0
19	4	1206	CLA	6	0
19	4	1207	CLA	4	0
19	4	1208	CLA	5	0
19	4	1209	CLA	5	0
19	4	1210	CLA	3	0
19	4	1211	CLA	6	0
20	4	1212	LMU	4	0
19	4	4007	CLA	19	0
19	4	4014	CLA	11	0
19	A	1759	CLA	14	0
19	A	1760	CLA	28	0
19	A	1761	CLA	28	0
19	A	1762	CLA	21	0
19	A	1763	CLA	27	0
19	A	1764	CLA	26	0
19	A	1765	CLA	26	0
19	A	1766	CLA	4	0
19	A	1767	CLA	22	0
19	A	1768	CLA	4	0
19	A	1769	CLA	20	0
19	A	1770	CLA	35	0
19	A	1771	CLA	44	0
19	A	1772	CLA	35	0
19	A	1773	CLA	12	0
19	A	1774	CLA	29	0
19	A	1776	CLA	45	0
19	A	1777	CLA	17	0
19	A	1778	CLA	10	0
19	A	1779	CLA	34	0
19	A	1780	CLA	18	0
19	A	1781	CLA	86	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1782	CLA	79	0
19	A	1783	CLA	63	0
19	A	1784	CLA	21	0
19	A	1785	CLA	17	0
19	A	1786	CLA	11	0
19	A	1787	CLA	26	0
19	A	1788	CLA	38	0
19	A	1789	CLA	16	0
19	A	1790	CLA	16	0
19	A	1791	CLA	18	1
19	A	1792	CLA	10	0
19	A	1793	CLA	19	0
19	A	1794	CLA	19	0
19	A	1795	CLA	18	0
19	A	1796	CLA	42	0
19	A	1797	CLA	42	0
19	A	1798	CLA	8	0
19	A	1799	CLA	30	0
19	A	1800	CLA	17	0
23	A	1801	PQN	15	0
22	A	1802	BCR	45	0
22	A	1803	BCR	24	0
22	A	1804	BCR	45	0
22	A	1805	BCR	37	0
22	A	1806	BCR	63	0
22	A	1807	BCR	40	0
20	A	1808	LMU	3	0
20	A	1809	LMU	4	0
19	A	1810	CLA	20	0
19	A	1811	CLA	36	0
19	A	1812	CLA	27	0
20	A	7003	LMU	4	0
20	A	7004	LMU	10	0
20	A	7005	LMU	8	0
20	A	7006	LMU	12	0
20	A	7009	LMU	9	4
20	A	7010	LMU	8	0
20	A	7013	LMU	8	0
20	A	7014	LMU	6	0
20	A	7016	LMU	42	0
20	A	7017	LMU	3	0
20	A	7019	LMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	7020	LMU	20	0
20	A	7021	LMU	25	0
20	A	7022	LMU	11	0
20	A	7023	LMU	27	0
20	A	7025	LMU	2	0
20	A	7026	LMU	20	0
20	A	7027	LMU	6	0
20	A	7028	LMU	4	0
20	A	7030	LMU	12	0
20	A	7031	LMU	4	0
20	A	7032	LMU	29	0
20	A	7033	LMU	20	0
20	A	7034	LMU	1	0
20	A	7036	LMU	19	0
20	A	7037	LMU	30	0
20	A	7038	LMU	13	0
20	A	7039	LMU	19	0
20	A	7040	LMU	4	0
20	A	7041	LMU	8	0
20	A	7042	LMU	35	0
20	A	7043	LMU	11	0
20	A	7047	LMU	0	2
20	A	7048	LMU	47	0
20	A	7050	LMU	38	0
20	A	7051	LMU	12	0
19	B	1735	CLA	28	0
19	B	1736	CLA	9	0
19	B	1737	CLA	19	0
19	B	1738	CLA	20	0
19	B	1739	CLA	23	0
19	B	1740	CLA	21	0
19	B	1741	CLA	17	0
19	B	1742	CLA	6	0
19	B	1743	CLA	17	0
19	B	1744	CLA	29	0
19	B	1745	CLA	20	0
19	B	1746	CLA	13	0
19	B	1747	CLA	24	0
19	B	1748	CLA	24	0
19	B	1749	CLA	15	0
19	B	1750	CLA	19	0
19	B	1751	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1752	CLA	21	0
19	B	1753	CLA	15	0
19	B	1754	CLA	39	0
19	B	1755	CLA	25	0
19	B	1756	CLA	62	0
19	B	1757	CLA	50	0
19	B	1758	CLA	25	0
19	B	1759	CLA	33	0
19	B	1760	CLA	32	0
19	B	1761	CLA	11	0
19	B	1762	CLA	13	0
19	B	1763	CLA	29	0
19	B	1764	CLA	16	0
19	B	1765	CLA	22	0
19	B	1766	CLA	23	0
19	B	1767	CLA	4	0
19	B	1768	CLA	16	0
19	B	1769	CLA	44	0
19	B	1770	CLA	25	0
19	B	1771	CLA	28	0
19	B	1772	CLA	26	0
19	B	1773	CLA	2	0
23	B	1774	PQN	32	0
22	B	1775	BCR	10	0
22	B	1776	BCR	17	0
22	B	1777	BCR	20	0
22	B	1778	BCR	32	0
22	B	1779	BCR	31	0
22	B	1780	BCR	45	0
22	B	1781	BCR	52	0
22	B	1782	BCR	19	0
20	B	1783	LMU	28	30
24	B	1784	LMG	30	0
25	B	1785	SF4	19	0
19	B	1786	CLA	22	0
19	B	1787	CLA	41	0
19	B	1788	CLA	51	0
21	B	8052	SUC	15	0
21	B	8053	SUC	10	0
21	B	8054	SUC	8	0
21	B	8055	SUC	22	0
21	B	8056	SUC	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	8059	SUC	19	0
21	B	8060	SUC	7	0
21	B	8061	SUC	2	0
21	B	8062	SUC	20	0
25	C	1082	SF4	4	0
25	C	1083	SF4	4	0
19	F	1155	CLA	1	0
19	F	1156	CLA	15	0
19	F	1157	CLA	15	0
21	F	1158	SUC	5	0
19	G	1099	CLA	20	0
19	I	1031	CLA	12	0
22	I	1032	BCR	46	0
19	J	1043	CLA	28	0
19	J	1044	CLA	35	0
19	K	1085	CLA	25	0
20	K	1086	LMU	6	0
19	L	1166	CLA	9	0
19	L	1167	CLA	22	0
19	L	1168	CLA	13	0
22	L	1169	BCR	51	0
22	L	1170	BCR	13	0
20	L	1171	LMU	3	0
20	N	1086	LMU	36	0
19	R	1054	CLA	10	0
19	R	1055	CLA	12	0
20	R	1056	LMU	20	4

## 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, 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	1	164/241 (68%)	1.47	46 (28%) 1 1	32, 62, 71, 73	0
2	2	176/269 (65%)	1.17	40 (22%) 1 1	20, 20, 20, 20	0
3	3	160/276 (57%)	2.01	66 (41%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	0.96	30 (18%) 2 2	20, 20, 20, 20	0
5	A	730/758 (96%)	0.95	92 (12%) 5 6	20, 20, 20, 20	0
6	B	733/734 (99%)	0.83	62 (8%) 13 12	20, 20, 20, 20	0
7	C	81/81 (100%)	1.23	14 (17%) 2 2	20, 20, 20, 20	0
8	D	138/212 (65%)	1.09	23 (16%) 2 2	20, 20, 20, 20	0
9	E	65/143 (45%)	1.23	16 (24%) 1 1	20, 20, 20, 20	0
10	F	154/231 (66%)	0.62	15 (9%) 10 9	20, 20, 20, 20	0
11	G	95/167 (56%)	0.68	12 (12%) 5 6	20, 20, 20, 20	0
12	H	69/144 (47%)	0.87	11 (15%) 3 3	20, 20, 20, 20	0
13	I	30/40 (75%)	0.37	2 (6%) 21 16	20, 20, 20, 20	0
14	J	42/44 (95%)	0.64	5 (11%) 6 6	20, 20, 20, 20	0
15	K	84/131 (64%)	2.01	32 (38%) 0 0	20, 20, 20, 20	0
16	L	161/216 (74%)	0.78	24 (14%) 3 3	20, 20, 20, 20	0
17	N	85/170 (50%)	1.10	17 (20%) 1 2	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3133/4161 (75%)	1.02	507 (16%) 3 3	20, 20, 65, 112	0

The worst 5 of 507 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	61	ASN	12.5
1	1	75	ALA	10.1
4	4	67	ILE	9.7

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Mol	Chain	Res	Type	RSRZ
5	A	635	THR	9.1
6	B	491	ASN	8.8

## 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(Å <sup>2</sup> )	Q<0.9
22	BCR	A	1807	40/40	0.59	0.46	3.43	20,20,20,20	0
22	BCR	B	1776	40/40	0.80	0.37	3.41	20,20,20,20	0
22	BCR	A	1802	40/40	0.58	0.46	3.23	20,20,20,20	0
19	CLA	A	1770	45/65	0.61	0.52	3.14	20,20,20,20	0
19	CLA	4	1203	25/65	0.73	0.34	2.89	20,20,20,20	0
22	BCR	I	1032	40/40	0.69	0.47	2.83	20,20,20,20	0
22	BCR	B	1779	40/40	0.74	0.46	2.17	20,20,20,20	0
19	CLA	A	1772	54/65	0.71	0.39	2.14	20,20,20,20	0
19	CLA	B	1771	65/65	0.68	0.46	2.14	20,20,20,20	0
22	BCR	B	1782	40/40	0.81	0.38	2.06	20,20,20,20	0
19	CLA	3	1219	65/65	0.70	0.49	2.06	20,20,20,20	0
19	CLA	A	1800	55/65	0.69	0.42	2.04	20,20,20,20	0
19	CLA	B	1747	46/65	0.65	0.50	1.98	20,20,20,20	0
19	CLA	A	1786	50/65	0.72	0.41	1.96	20,20,20,20	0
22	BCR	A	1803	40/40	0.69	0.41	1.86	20,20,20,20	0
22	BCR	L	1169	40/40	0.70	0.46	1.83	20,20,20,20	0
19	CLA	4	1199	55/65	0.69	0.35	1.81	20,20,20,20	0
22	BCR	B	1781	40/40	0.69	0.46	1.79	20,20,20,20	0
19	CLA	B	1772	65/65	0.86	0.40	1.70	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	PQN	A	1801	33/33	0.73	0.47	1.68	20,20,20,20	0
19	CLA	A	1780	65/65	0.71	0.41	1.65	20,20,20,20	0
24	LMG	B	1784	49/55	0.71	0.42	1.54	20,20,20,20	0
19	CLA	A	1785	65/65	0.74	0.39	1.44	20,20,20,20	0
19	CLA	2	1223	50/65	0.75	0.31	1.41	20,20,20,20	0
19	CLA	A	1773	52/65	0.75	0.37	1.25	20,20,20,20	0
20	LMU	A	7047	35/35	0.59	0.54	1.20	20,20,20,20	0
19	CLA	A	1776	65/65	0.74	0.40	1.20	20,20,20,20	0
19	CLA	A	1762	55/65	0.74	0.39	1.13	20,20,20,20	0
21	SUC	2	1225	22/23	0.64	0.35	1.07	20,20,20,20	0
19	CLA	B	1786	65/65	0.76	0.40	1.04	20,20,20,20	0
19	CLA	A	1777	51/65	0.70	0.48	1.03	20,20,20,20	0
22	BCR	B	1778	40/40	0.77	0.40	1.01	20,20,20,20	0
19	CLA	A	1766	45/65	0.64	0.58	1.00	20,20,20,20	0
19	CLA	A	1793	65/65	0.78	0.35	0.98	20,20,20,20	0
22	BCR	B	1775	40/40	0.80	0.39	0.98	20,20,20,20	0
19	CLA	B	1741	60/65	0.74	0.35	0.97	20,20,20,20	0
23	PQN	B	1774	33/33	0.74	0.42	0.96	20,20,20,20	0
19	CLA	A	1794	47/65	0.80	0.35	0.96	20,20,20,20	0
19	CLA	B	1740	65/65	0.79	0.37	0.95	20,20,20,20	0
22	BCR	A	1806	40/40	0.73	0.47	0.92	20,20,20,20	0
19	CLA	A	1799	65/65	0.80	0.38	0.90	20,20,20,20	0
19	CLA	A	1783	65/65	0.75	0.45	0.88	20,20,20,20	0
22	BCR	B	1777	40/40	0.73	0.39	0.86	20,20,20,20	0
19	CLA	A	1761	65/65	0.74	0.38	0.83	20,20,20,20	0
19	CLA	B	1750	61/65	0.79	0.34	0.80	20,20,20,20	0
19	CLA	A	1774	65/65	0.70	0.43	0.75	20,20,20,20	0
19	CLA	B	1760	65/65	0.82	0.36	0.72	20,20,20,20	0
19	CLA	A	1788	65/65	0.81	0.35	0.69	20,20,20,20	0
19	CLA	B	1787	65/65	0.82	0.33	0.65	20,20,20,20	0
19	CLA	B	1746	60/65	0.72	0.36	0.63	20,20,20,20	0
19	CLA	4	1200	50/65	0.65	0.41	0.63	20,20,20,20	0
22	BCR	A	1804	40/40	0.70	0.37	0.63	20,20,20,20	0
19	CLA	A	1795	47/65	0.81	0.33	0.62	20,20,20,20	0
19	CLA	B	1758	65/65	0.85	0.36	0.61	20,20,20,20	0
19	CLA	A	1759	50/65	0.83	0.31	0.60	20,20,20,20	0
22	BCR	L	1170	40/40	0.79	0.36	0.60	20,20,20,20	0
19	CLA	A	1769	54/65	0.74	0.39	0.60	20,20,20,20	0
19	CLA	B	1788	65/65	0.79	0.35	0.59	20,20,20,20	0
19	CLA	B	1773	36/65	0.69	0.46	0.57	20,20,20,20	0
19	CLA	A	1787	65/65	0.78	0.36	0.56	20,20,20,20	0
19	CLA	L	1166	50/65	0.76	0.35	0.56	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	2	1214	25/65	0.71	0.36	0.55	20,20,20,20	0
19	CLA	A	1812	65/65	0.78	0.37	0.52	20,20,20,20	0
19	CLA	B	1745	65/65	0.79	0.34	0.50	20,20,20,20	0
19	CLA	B	1763	65/65	0.81	0.33	0.46	20,20,20,20	0
19	CLA	A	1796	65/65	0.81	0.34	0.45	20,20,20,20	0
19	CLA	1	1241	55/65	0.56	0.39	0.44	20,20,20,20	0
19	CLA	A	1767	65/65	0.70	0.43	0.44	20,20,20,20	0
19	CLA	2	1217	65/65	0.70	0.38	0.42	20,20,20,20	0
19	CLA	B	1762	50/65	0.79	0.36	0.41	20,20,20,20	0
19	CLA	B	1737	60/65	0.81	0.34	0.41	20,20,20,20	0
19	CLA	B	1752	46/65	0.73	0.39	0.40	20,20,20,20	0
19	CLA	B	1735	65/65	0.75	0.40	0.39	20,20,20,20	0
19	CLA	F	1155	36/65	0.77	0.35	0.38	20,20,20,20	0
19	CLA	B	1761	50/65	0.84	0.30	0.38	20,20,20,20	0
19	CLA	B	1751	50/65	0.82	0.35	0.36	20,20,20,20	0
19	CLA	A	1789	55/65	0.84	0.32	0.33	20,20,20,20	0
19	CLA	3	1222	65/65	0.63	0.38	0.33	20,20,20,20	0
19	CLA	B	1748	59/65	0.79	0.37	0.33	20,20,20,20	0
19	CLA	B	1738	65/65	0.83	0.35	0.33	20,20,20,20	0
19	CLA	1	1192	61/65	0.77	0.33	0.32	20,20,20,20	0
20	LMU	A	1809	35/35	0.65	0.41	0.31	20,20,20,20	0
19	CLA	A	1790	50/65	0.76	0.36	0.30	20,20,20,20	0
19	CLA	A	1811	65/65	0.77	0.37	0.30	20,20,20,20	0
19	CLA	4	1205	55/65	0.69	0.37	0.30	20,20,20,20	0
19	CLA	B	1736	45/65	0.80	0.34	0.26	20,20,20,20	0
19	CLA	B	1765	45/65	0.78	0.32	0.26	20,20,20,20	0
19	CLA	A	1781	65/65	0.77	0.36	0.24	20,20,20,20	0
19	CLA	A	1810	65/65	0.82	0.36	0.23	20,20,20,20	0
19	CLA	4	1196	55/65	0.65	0.35	0.23	20,20,20,20	0
19	CLA	A	1760	55/65	0.76	0.33	0.22	20,20,20,20	0
19	CLA	I	1031	60/65	0.84	0.28	0.22	20,20,20,20	0
20	LMU	L	1171	35/35	0.66	0.33	0.22	20,20,20,20	0
19	CLA	A	1784	55/65	0.80	0.40	0.19	20,20,20,20	0
19	CLA	B	1759	65/65	0.86	0.32	0.19	20,20,20,20	0
19	CLA	B	1764	50/65	0.75	0.39	0.19	20,20,20,20	0
19	CLA	B	1742	54/65	0.81	0.29	0.17	20,20,20,20	0
19	CLA	L	1167	47/65	0.83	0.30	0.16	20,20,20,20	0
19	CLA	B	1756	58/65	0.78	0.36	0.15	20,20,20,20	0
19	CLA	3	1213	25/65	0.76	0.36	0.14	20,20,20,20	0
19	CLA	B	1749	60/65	0.87	0.32	0.14	20,20,20,20	0
19	CLA	A	1764	65/65	0.87	0.34	0.12	20,20,20,20	0
19	CLA	B	1743	55/65	0.81	0.29	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CLA	A	1763	46/65	0.79	0.47	0.10	20,20,20,20	0
19	CLA	A	1779	55/65	0.79	0.34	0.02	20,20,20,20	0
19	CLA	3	1214	36/65	0.76	0.34	0.00	20,20,20,20	0
19	CLA	B	1766	45/65	0.57	0.44	-0.01	20,20,20,20	0
19	CLA	B	1739	65/65	0.88	0.33	-0.01	20,20,20,20	0
19	CLA	2	1222	50/65	0.81	0.27	-0.06	20,20,20,20	0
22	BCR	A	1805	40/40	0.83	0.32	-0.06	20,20,20,20	0
19	CLA	4	1209	36/65	0.81	0.29	-0.06	20,20,20,20	0
19	CLA	2	1215	50/65	0.73	0.34	-0.10	20,20,20,20	0
19	CLA	A	1778	42/65	0.72	0.37	-0.11	20,20,20,20	0
19	CLA	B	1768	60/65	0.80	0.34	-0.12	20,20,20,20	0
19	CLA	A	1782	65/65	0.79	0.35	-0.14	20,20,20,20	0
19	CLA	F	1156	41/65	0.73	0.30	-0.17	20,20,20,20	0
19	CLA	B	1744	58/65	0.84	0.28	-0.18	20,20,20,20	0
19	CLA	L	1168	50/65	0.74	0.31	-0.19	20,20,20,20	0
19	CLA	B	1755	54/65	0.83	0.32	-0.19	20,20,20,20	0
19	CLA	3	1217	25/65	0.65	0.38	-0.22	20,20,20,20	0
19	CLA	2	1221	25/65	0.70	0.41	-0.26	20,20,20,20	0
19	CLA	B	1757	65/65	0.73	0.38	-0.29	20,20,20,20	0
20	LMU	A	1808	35/35	0.60	0.46	-0.30	20,20,20,20	0
19	CLA	B	1753	55/65	0.84	0.30	-0.31	20,20,20,20	0
22	BCR	B	1780	40/40	0.77	0.32	-0.33	20,20,20,20	0
19	CLA	A	1765	52/65	0.80	0.34	-0.34	20,20,20,20	0
19	CLA	4	1201	52/65	0.79	0.26	-0.37	20,20,20,20	0
19	CLA	B	1769	65/65	0.88	0.28	-0.40	20,20,20,20	0
19	CLA	3	1212	50/65	0.67	0.34	-0.47	20,20,20,20	0
19	CLA	A	1792	49/65	0.84	0.29	-0.47	20,20,20,20	0
19	CLA	B	1770	47/65	0.86	0.30	-0.50	20,20,20,20	0
19	CLA	G	1099	51/65	0.75	0.31	-0.51	20,20,20,20	0
19	CLA	1	1194	25/65	0.81	0.34	-0.57	20,20,20,20	0
19	CLA	1	1197	25/65	0.66	0.36	-0.62	20,20,20,20	0
19	CLA	B	1754	65/65	0.82	0.28	-0.65	20,20,20,20	0
19	CLA	A	1771	50/65	0.79	0.31	-0.75	20,20,20,20	0
19	CLA	3	1216	25/65	0.55	0.41	-0.79	20,20,20,20	0
19	CLA	4	1197	36/65	0.86	0.33	-0.83	20,20,20,20	0
19	CLA	1	1195	36/65	0.85	0.27	-0.85	20,20,20,20	0
19	CLA	1	1189	47/65	0.75	0.27	-0.97	20,20,20,20	0
19	CLA	4	1208	25/65	0.86	0.29	-1.12	20,20,20,20	0
19	CLA	1	1190	46/65	0.80	0.27	-1.15	20,20,20,20	0
25	SF4	C	1082	8/8	0.86	0.17	-2.16	20,20,20,20	0
25	SF4	C	1083	8/8	0.91	0.14	-2.21	20,20,20,20	0
25	SF4	B	1785	8/8	0.94	0.14	-2.48	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	LMU	N	1086	35/35	0.69	0.33	-	2,39,60,60	0
20	LMU	A	7014	35/35	0.61	0.33	-	20,20,20,20	0
19	CLA	4	1198	65/65	0.70	0.30	-	20,20,20,20	0
20	LMU	A	7040	35/35	0.74	0.24	-	20,20,20,20	0
19	CLA	1	1196	51/65	0.66	0.40	-	20,20,20,20	0
20	LMU	R	1056	35/35	0.64	0.32	-	20,20,20,20	0
19	CLA	1	1010	25/65	0.79	0.20	-	20,20,20,20	0
19	CLA	3	3015	25/65	0.67	0.31	-	20,20,20,20	0
22	BCR	3	1225	40/40	0.64	0.37	-	20,20,20,20	0
20	LMU	A	7026	35/35	0.67	0.38	-	20,20,20,20	0
26	UNL	B	8057	23/-	0.78	0.24	-	20,20,20,20	0
19	CLA	3	1220	25/65	0.62	0.44	-	20,20,20,20	0
19	CLA	B	1767	51/65	0.55	0.47	-	20,20,20,20	0
19	CLA	4	1210	25/65	0.90	0.21	-	20,20,20,20	0
20	LMU	A	7006	35/35	0.68	0.31	-	20,20,20,20	0
20	LMU	A	7035	35/35	0.72	0.29	-	20,20,20,20	0
20	LMU	A	7041	35/35	0.66	0.43	-	20,20,20,20	0
21	SUC	B	8061	23/23	0.64	0.29	-	20,20,20,20	0
19	CLA	2	1213	65/65	0.70	0.35	-	20,20,20,20	0
20	LMU	A	7031	35/35	0.74	0.24	-	20,20,20,20	0
20	LMU	A	7009	34/35	0.66	0.41	-	20,20,20,20	0
19	CLA	3	3008	50/65	0.63	0.38	-	20,20,20,20	0
20	LMU	A	7021	35/35	0.67	0.29	-	20,20,20,20	0
21	SUC	B	8054	23/23	0.68	0.30	-	20,20,20,20	0
20	LMU	2	1224	35/35	0.63	0.40	-	20,20,20,20	0
20	LMU	A	7024	35/35	0.67	0.26	-	20,20,20,20	0
19	CLA	4	4014	47/65	0.69	0.29	-	20,20,20,20	0
19	CLA	1	1145	55/65	0.72	0.39	-	20,20,20,20	0
19	CLA	A	1791	45/65	0.70	0.40	-	20,20,20,20	0
20	LMU	A	7036	34/35	0.72	0.27	-	20,20,20,20	0
19	CLA	1	1142	45/65	0.60	0.37	-	20,20,20,20	0
19	CLA	J	1043	61/65	0.69	0.29	-	20,20,20,20	0
19	CLA	3	1218	42/65	0.63	0.37	-	20,20,20,20	0
20	LMU	A	7048	35/35	0.66	0.36	-	2,38,60,60	0
19	CLA	2	1218	65/65	0.60	0.43	-	20,20,20,20	0
20	LMU	A	7022	35/35	0.68	0.36	-	20,20,20,20	0
19	CLA	1	1308	48/65	0.82	0.24	-	20,20,20,20	0
19	CLA	3	3011	65/65	0.71	0.32	-	20,20,20,20	0
19	CLA	1	1307	25/65	0.61	0.68	-	20,20,20,20	0
19	CLA	3	3001	25/65	0.78	0.37	-	20,20,20,20	0
20	LMU	A	7020	35/35	0.48	0.49	-	20,20,20,20	0
20	LMU	A	7027	35/35	0.69	0.26	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	LMU	K	1086	35/35	0.66	0.39	-	20,20,20,20	0
21	SUC	B	8051	23/23	0.63	0.47	-	20,20,20,20	0
19	CLA	4	1204	25/65	0.79	0.27	-	20,20,20,20	0
19	CLA	A	1768	54/65	0.76	0.33	-	20,20,20,20	0
20	LMU	A	7043	35/35	0.64	0.33	-	20,20,20,20	0
21	SUC	3	1226	23/23	0.52	0.71	-	20,20,20,20	0
19	CLA	1	1191	25/65	0.72	0.31	-	20,20,20,20	0
19	CLA	R	1055	58/65	0.69	0.34	-	20,20,20,20	0
19	CLA	F	1157	53/65	0.70	0.34	-	20,20,20,20	0
21	SUC	F	1158	23/23	0.76	0.25	-	20,20,20,20	0
20	LMU	A	7032	35/35	0.80	0.33	-	20,20,20,20	0
21	SUC	B	8062	23/23	0.72	0.30	-	20,20,20,20	0
20	LMU	A	7017	35/35	0.56	0.51	-	20,20,20,20	0
21	SUC	B	8060	23/23	0.77	0.23	-	20,20,20,20	0
21	SUC	B	8056	23/23	0.62	0.38	-	20,20,20,20	0
20	LMU	A	7037	35/35	0.81	0.23	-	20,20,20,20	0
20	LMU	A	7042	35/35	0.78	0.27	-	20,20,20,20	0
19	CLA	3	1224	65/65	0.62	0.56	-	20,20,20,20	0
19	CLA	1	1014	61/65	0.68	0.29	-	2,35,60,60	0
21	SUC	B	8055	23/23	0.79	0.29	-	2,29,60,60	0
19	CLA	2	1219	25/65	0.79	0.31	-	20,20,20,20	0
20	LMU	A	7003	35/35	0.63	0.33	-	20,20,20,20	0
19	CLA	A	1797	65/65	0.55	0.47	-	20,20,20,20	0
20	LMU	A	7015	35/35	0.73	0.27	-	20,20,20,20	0
19	CLA	2	1216	25/65	0.64	0.36	-	20,20,20,20	0
19	CLA	1	1149	46/65	0.74	0.24	-	20,20,20,20	0
20	LMU	B	1783	35/35	0.77	0.28	-	2,35,60,60	0
19	CLA	A	1775	25/65	0.72	0.30	-	20,20,20,20	0
20	LMU	4	1212	35/35	0.62	0.32	-	20,20,20,20	0
19	CLA	K	1085	50/65	0.67	0.59	-	20,20,20,20	0
20	LMU	A	7050	35/35	0.60	0.37	-	2,41,60,60	0
19	CLA	4	1211	46/65	0.78	0.26	-	20,20,20,20	0
19	CLA	J	1044	61/65	0.57	0.36	-	20,20,20,20	0
20	LMU	A	7023	35/35	0.79	0.30	-	20,20,20,20	0
19	CLA	3	1223	25/65	0.74	0.26	-	20,20,20,20	0
20	LMU	A	7005	35/35	0.72	0.27	-	20,20,20,20	0
20	LMU	A	7010	35/35	0.55	0.51	-	20,20,20,20	0
20	LMU	A	7051	35/35	0.63	0.31	-	2,30,60,60	0
19	CLA	3	1215	25/65	0.74	0.34	-	20,20,20,20	0
20	LMU	A	7019	35/35	0.72	0.22	-	20,20,20,20	0
21	SUC	B	8059	23/23	0.71	0.38	-	20,20,20,20	0
21	SUC	B	8052	23/23	0.68	0.50	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	LMU	A	7030	35/35	0.60	0.32	-	20,20,20,20	0
20	LMU	A	7034	35/35	0.68	0.26	-	20,20,20,20	0
20	LMU	A	7013	35/35	0.46	0.44	-	20,20,20,20	0
20	LMU	A	7025	35/35	0.51	0.39	-	20,20,20,20	0
19	CLA	3	1221	25/65	0.45	0.43	-	20,20,20,20	0
19	CLA	1	1148	55/65	0.65	0.40	-	20,20,20,20	0
19	CLA	4	4007	52/65	0.68	0.32	-	20,20,20,20	0
19	CLA	1	1198	25/65	0.80	0.45	-	20,20,20,20	0
20	LMU	A	7016	35/35	0.74	0.28	-	20,20,20,20	0
19	CLA	1	1188	57/65	0.80	0.22	-	2,38,60,60	0
19	CLA	1	1146	50/65	0.60	0.50	-	20,20,20,20	0
19	CLA	4	1206	65/65	0.76	0.30	-	20,20,20,20	0
19	CLA	R	1054	57/65	0.67	0.50	-	20,20,20,20	0
19	CLA	4	1207	25/65	0.80	0.27	-	20,20,20,20	0
21	SUC	B	8053	23/23	0.77	0.20	-	2,41,60,60	0
19	CLA	2	1212	51/65	0.60	0.37	-	20,20,20,20	0
20	LMU	A	7038	35/35	0.56	0.49	-	20,20,20,20	0
19	CLA	1	1309	25/65	0.60	0.45	-	20,20,20,20	0
19	CLA	2	2010	25/65	0.77	0.33	-	20,20,20,20	0
20	LMU	A	7033	35/35	0.70	0.31	-	20,20,20,20	0
19	CLA	2	1220	36/65	0.57	0.49	-	20,20,20,20	0
20	LMU	1	1200	35/35	0.65	0.35	-	2,45,60,60	0
20	LMU	A	7004	35/35	0.65	0.48	-	20,20,20,20	0
20	LMU	A	7049	35/35	0.64	0.30	-	2,51,60,60	0
20	LMU	A	7028	35/35	0.75	0.24	-	20,20,20,20	0
20	LMU	A	7039	35/35	0.77	0.24	-	20,20,20,20	0
20	LMU	1	1199	35/35	0.58	0.36	-	20,20,20,20	0
19	CLA	1	1187	46/65	0.68	0.31	-	20,20,20,20	0
19	CLA	1	1193	51/65	0.75	0.33	-	20,20,20,20	0
19	CLA	4	1202	36/65	0.64	0.40	-	20,20,20,20	0
19	CLA	A	1798	50/65	0.62	0.34	-	20,20,20,20	0
19	CLA	1	1303	25/65	0.73	0.36	-	20,20,20,20	0
19	CLA	1	1505	55/65	0.60	0.50	-	20,20,20,20	0

## 6.5 Other polymers

There are no such residues in this entry.