



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:26 AM GMT

PDB ID : 2WSF
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-05
Resolution : 3.48 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

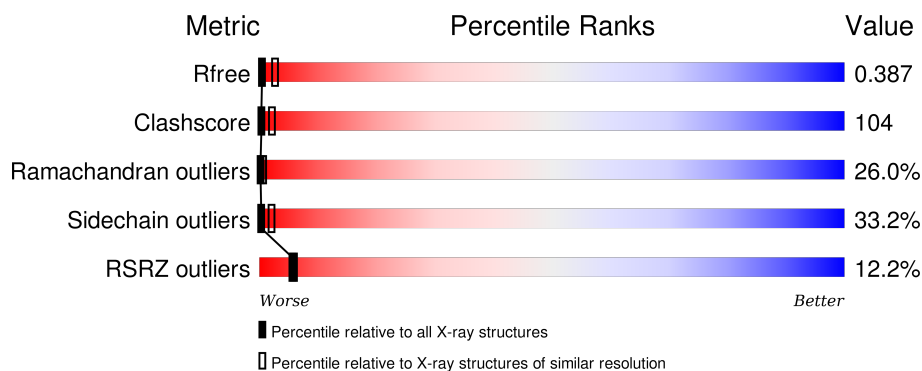
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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

Mol	Chain	Length	Quality of chain
1	1	241	<div> <div>17%</div> <div>27%</div> <div>29%</div> <div>10%</div> <div>32%</div> </div>
2	2	269	<div> <div>14%</div> <div>10%</div> <div>23%</div> <div>23%</div> <div>10%</div> <div>35%</div> </div>
3	3	276	<div> <div>11%</div> <div>15%</div> <div>21%</div> <div>13%</div> <div>5%</div> <div>45%</div> </div>
4	4	251	<div> <div>5%</div> <div>7%</div> <div>22%</div> <div>25%</div> <div>12%</div> <div>34%</div> </div>
5	A	758	<div> <div>7%</div> <div>10%</div> <div>50%</div> <div>30%</div> <div>7%</div> </div>

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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	1014	X	-	-	-
19	CLA	1	1142	X	-	-	-
19	CLA	1	1143	X	-	X	-
19	CLA	1	1145	X	-	-	-
19	CLA	1	1146	X	-	-	-
19	CLA	1	1148	X	-	-	-
19	CLA	1	1149	X	-	-	-
19	CLA	1	1187	X	-	-	-
19	CLA	1	1188	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	-	-	X
19	CLA	1	1198	X	-	-	-
19	CLA	1	1199	X	-	-	-
19	CLA	1	1200	X	-	-	-
19	CLA	1	1307	X	-	-	-
19	CLA	1	1308	X	-	-	-
19	CLA	1	1309	X	-	-	-
19	CLA	1	1505	X	-	-	-
19	CLA	2	1212	X	-	-	-
19	CLA	2	1213	X	-	X	-
19	CLA	2	1214	X	-	-	-
19	CLA	2	1215	X	-	-	-
19	CLA	2	1216	X	-	-	-
19	CLA	2	1217	X	-	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	2006	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	-	-	-
19	CLA	3	1217	X	-	-	-
19	CLA	3	1218	X	-	-	-
19	CLA	3	1219	X	-	-	-
19	CLA	3	1220	X	-	-	-
19	CLA	3	1221	X	-	-	-
19	CLA	3	1222	X	-	-	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3008	X	-	-	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3014	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	-	-	-
19	CLA	4	1199	X	-	X	-
19	CLA	4	1200	X	-	-	X
19	CLA	4	1201	X	-	-	-
19	CLA	4	1202	X	-	-	-
19	CLA	4	1203	X	-	-	-
19	CLA	4	1204	X	-	-	-
19	CLA	4	1205	X	-	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	-	-	-
19	CLA	A	1762	X	-	-	-
19	CLA	A	1763	X	-	X	-
19	CLA	A	1764	X	-	X	-
19	CLA	A	1765	X	-	X	-
19	CLA	A	1766	X	-	-	-
19	CLA	A	1767	X	-	X	-
19	CLA	A	1768	X	-	-	-
19	CLA	A	1769	X	-	X	-
19	CLA	A	1770	X	-	-	-
19	CLA	A	1771	X	-	-	-
19	CLA	A	1772	X	-	X	-
19	CLA	A	1773	X	-	-	-
19	CLA	A	1774	X	-	X	-
19	CLA	A	1775	X	-	-	-
19	CLA	A	1776	X	-	X	X
19	CLA	A	1777	X	-	-	-
19	CLA	A	1778	X	-	-	-
19	CLA	A	1779	X	-	-	-
19	CLA	A	1780	X	-	-	-
19	CLA	A	1781	X	-	X	-
19	CLA	A	1782	X	-	X	-
19	CLA	A	1783	X	-	X	-
19	CLA	A	1784	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1785	X	-	-	-
19	CLA	A	1786	X	-	-	-
19	CLA	A	1787	X	-	X	-
19	CLA	A	1788	X	-	X	-
19	CLA	A	1789	X	-	X	-
19	CLA	A	1790	X	-	-	-
19	CLA	A	1791	X	-	-	-
19	CLA	A	1792	X	-	-	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	-	-	-
19	CLA	A	1800	X	-	X	-
19	CLA	A	1801	X	-	-	X
19	CLA	A	1813	X	-	X	-
19	CLA	A	1814	X	-	X	-
19	CLA	A	1815	X	-	X	-
19	CLA	A	1816	X	-	-	-
19	CLA	A	1817	X	-	X	-
19	CLA	B	1735	X	-	X	-
19	CLA	B	1736	X	-	-	-
19	CLA	B	1737	X	-	X	-
19	CLA	B	1738	X	-	X	-
19	CLA	B	1739	X	-	-	-
19	CLA	B	1740	X	-	-	-
19	CLA	B	1741	X	-	-	-
19	CLA	B	1742	X	-	-	-
19	CLA	B	1743	X	-	X	-
19	CLA	B	1744	X	-	-	-
19	CLA	B	1745	X	-	-	-
19	CLA	B	1746	X	-	-	X
19	CLA	B	1747	X	-	-	-
19	CLA	B	1748	X	-	-	-
19	CLA	B	1749	X	-	-	-
19	CLA	B	1750	X	-	-	-
19	CLA	B	1751	X	-	-	-
19	CLA	B	1752	X	-	-	-
19	CLA	B	1753	X	-	X	-
19	CLA	B	1754	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1755	X	-	X	-
19	CLA	B	1756	X	-	X	-
19	CLA	B	1757	X	-	-	-
19	CLA	B	1758	X	-	X	-
19	CLA	B	1759	X	-	X	-
19	CLA	B	1760	X	-	-	-
19	CLA	B	1761	X	-	X	-
19	CLA	B	1762	X	-	X	-
19	CLA	B	1763	X	-	-	-
19	CLA	B	1764	X	-	X	-
19	CLA	B	1765	X	-	X	-
19	CLA	B	1766	X	-	-	-
19	CLA	B	1767	X	-	-	-
19	CLA	B	1768	X	-	X	-
19	CLA	B	1769	X	-	X	-
19	CLA	B	1770	X	-	-	-
19	CLA	B	1771	X	-	-	-
19	CLA	B	1772	X	-	-	-
19	CLA	B	1784	X	-	-	-
19	CLA	F	1155	X	-	-	-
19	CLA	F	1156	X	-	-	-
19	CLA	F	1157	X	-	-	-
19	CLA	G	1099	X	-	-	X
19	CLA	H	1079	X	-	X	-
19	CLA	H	1080	X	-	-	-
19	CLA	H	1081	X	-	-	-
19	CLA	I	1031	X	-	-	-
19	CLA	J	1043	X	-	-	-
19	CLA	L	1167	X	-	X	-
19	CLA	L	1168	X	-	-	-
19	CLA	R	1054	X	-	-	-
19	CLA	R	1055	X	-	-	-
20	LMU	2	1224	-	-	X	-
20	LMU	A	7008	-	-	X	-
20	LMU	A	7016	-	-	X	-
20	LMU	A	7042	-	-	X	-
21	SUC	2	1225	X	-	X	-
21	SUC	3	1223	X	-	-	-
21	SUC	B	8051	X	-	-	-
21	SUC	B	8052	X	-	-	-
21	SUC	B	8053	X	-	-	-
21	SUC	B	8054	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	SUC	B	8055	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	H	1082	X	-	X	-
22	PQN	A	1802	X	-	-	-
22	PQN	B	1773	X	-	X	-
23	BCR	A	1803	-	-	X	X
23	BCR	A	1804	-	-	X	X
23	BCR	A	1805	-	-	X	-
23	BCR	A	1806	-	-	X	-
23	BCR	A	1808	-	-	X	-
23	BCR	B	1774	-	-	-	X
23	BCR	B	1777	-	-	X	-
23	BCR	B	1778	-	-	X	-
23	BCR	B	1779	-	-	X	-
23	BCR	B	1780	-	-	X	-
23	BCR	I	1032	-	-	X	X
23	BCR	L	1169	-	-	X	X
25	SF4	B	1783	-	-	X	-
25	SF4	C	1082	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36033 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	165	Total	C	N	O	S	0	0	0
			1264	822	208	230	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
			1374	899	226	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	153	Total	C	N	O	S	0	0	0
			1186	781	193	207	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
			1319	861	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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	162	Total	C	N	O	S	0	0	0
			1215	800	194	216	5			

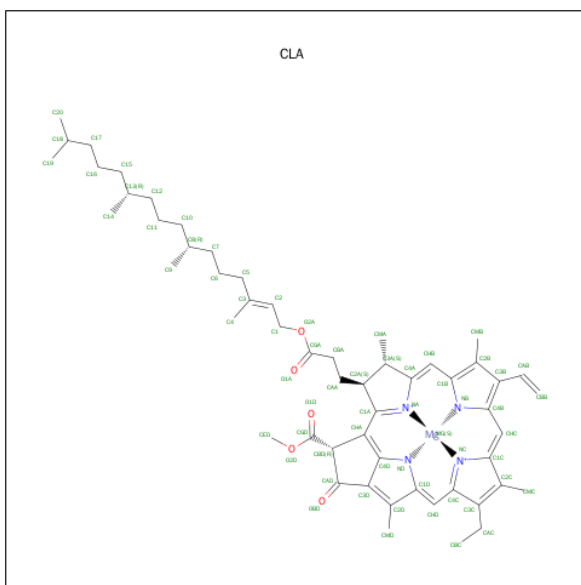
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	1	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
19	1	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	1	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
19	1	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
19	1	1	Total 25	C 20	Mg 1	N 4		0	0
19	1	1	Total 25	C 20	Mg 1	N 4		0	0
19	1	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
19	1	1	Total 25	C 20	Mg 1	N 4		0	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
19	1	1	Total 25	C 20	Mg 1	N 4		0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	3	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
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	3	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			46	36	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
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			56	46	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
			60	50	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
			50	40	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
			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
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	A	1	Total	C	Mg	N	O	0	0
			58	48	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
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			59	49	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
			60	50	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
			45	35	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
			47	37	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
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			59	49	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		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
			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		

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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
			54	44	1	4	5		
19	A	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
			45	35	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
			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
			25	20	1	4			
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
			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
			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
			53	43	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
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		

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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
			54	44	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
			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
			59	49	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
			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		

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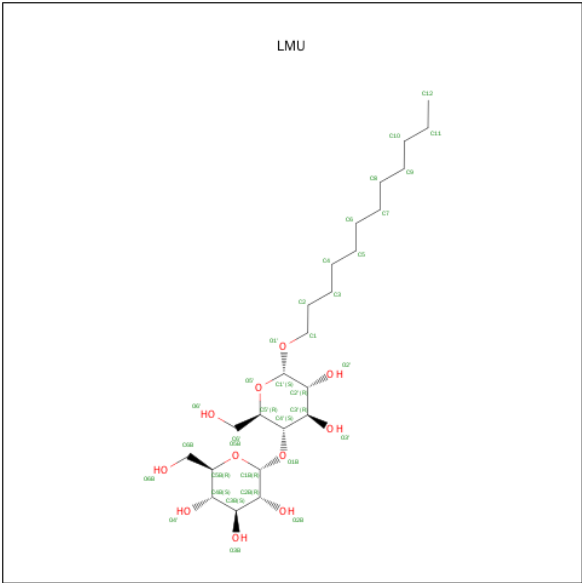
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			50	40	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	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
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	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
			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
			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		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
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	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	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	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

- Molecule 20 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	A	1	Total	C	O	0	0
			35	24	11		
20	B	1	Total	C	O	0	0
			25	14	11		
20	L	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
			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		
20	A	1	Total	C	O	0	0
			35	24	11		

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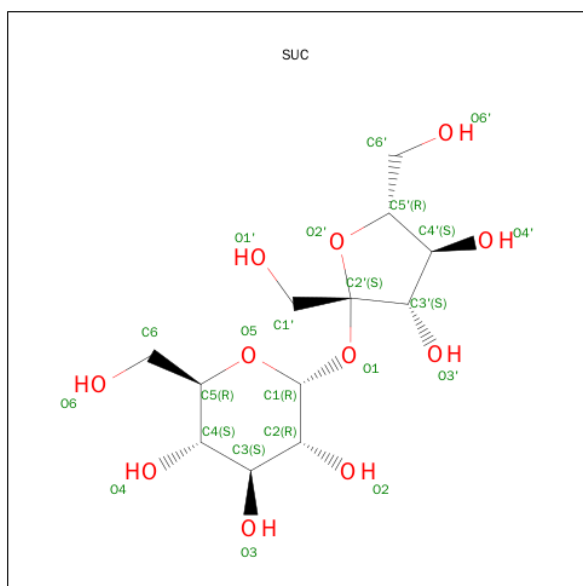
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 21 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



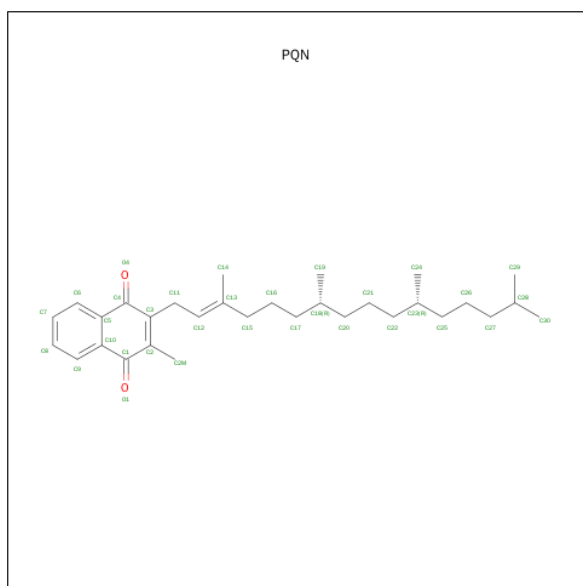
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			22	12	10		
21	3	1	Total	C	O	0	0
			23	12	11		
21	H	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			22	12	10		

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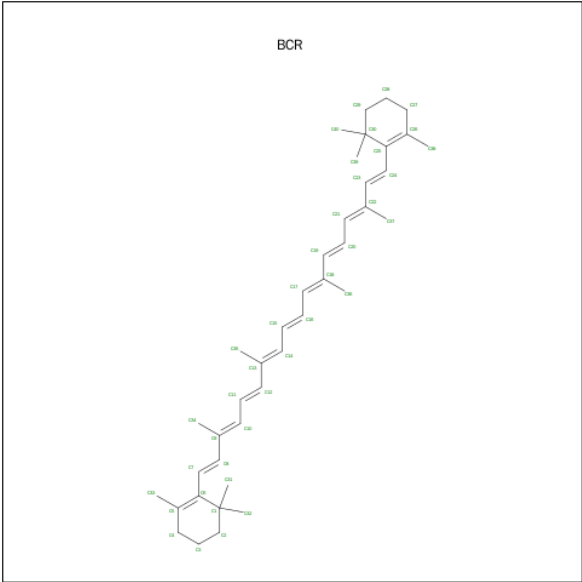
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



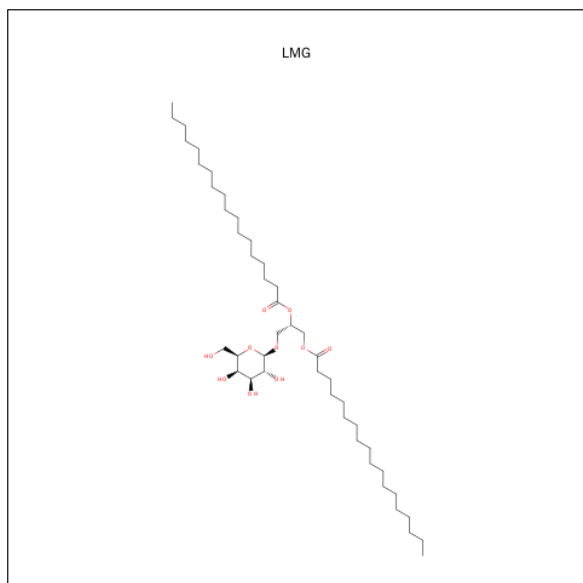
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 39 39	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	I	1	Total C 40 40	0	0
23	L	1	Total C 40 40	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_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		

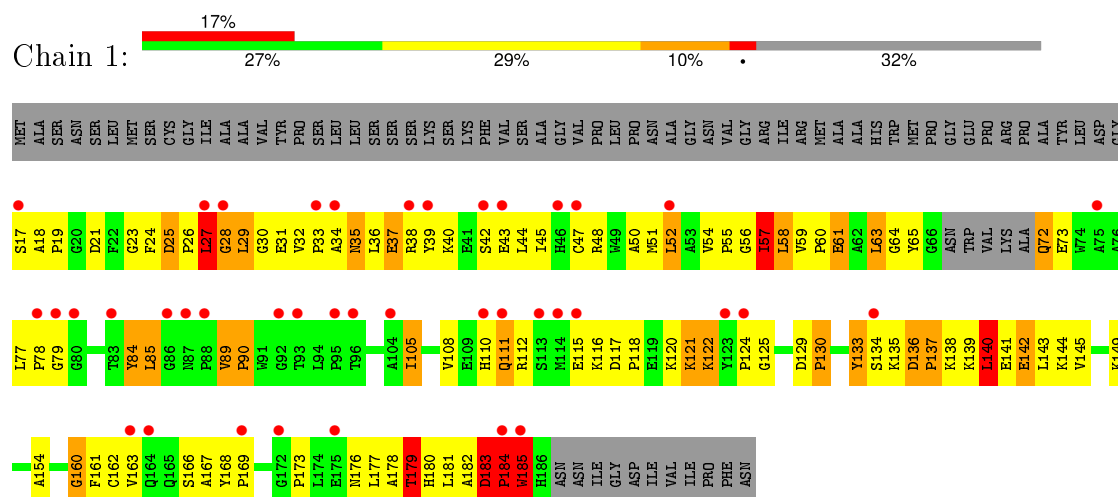
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

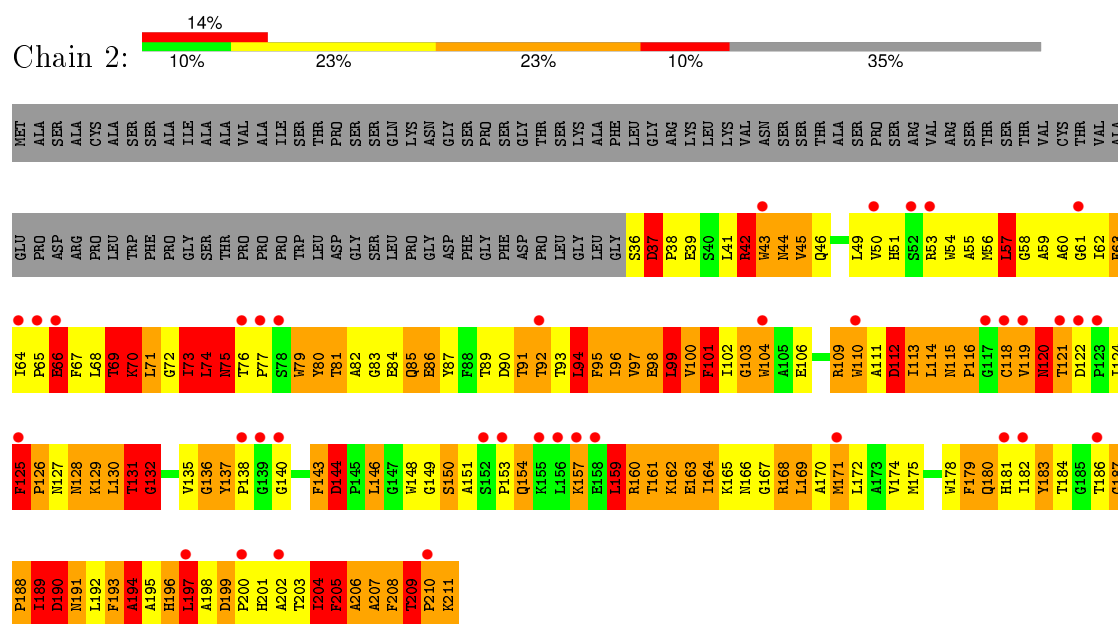
3 Residue-property plots

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.

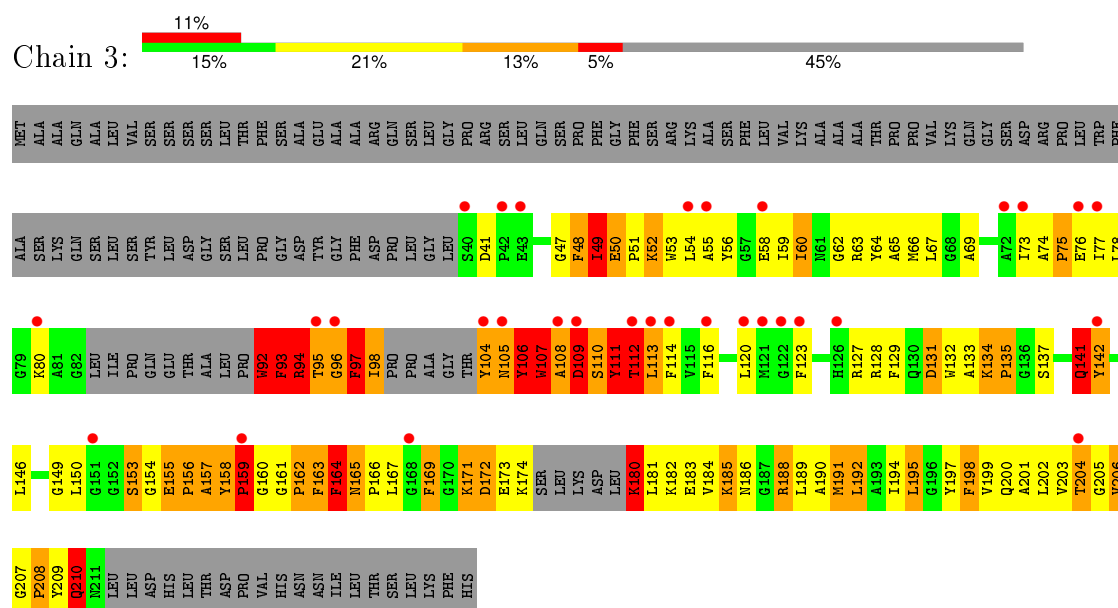
• Molecule 1: AT3G54890



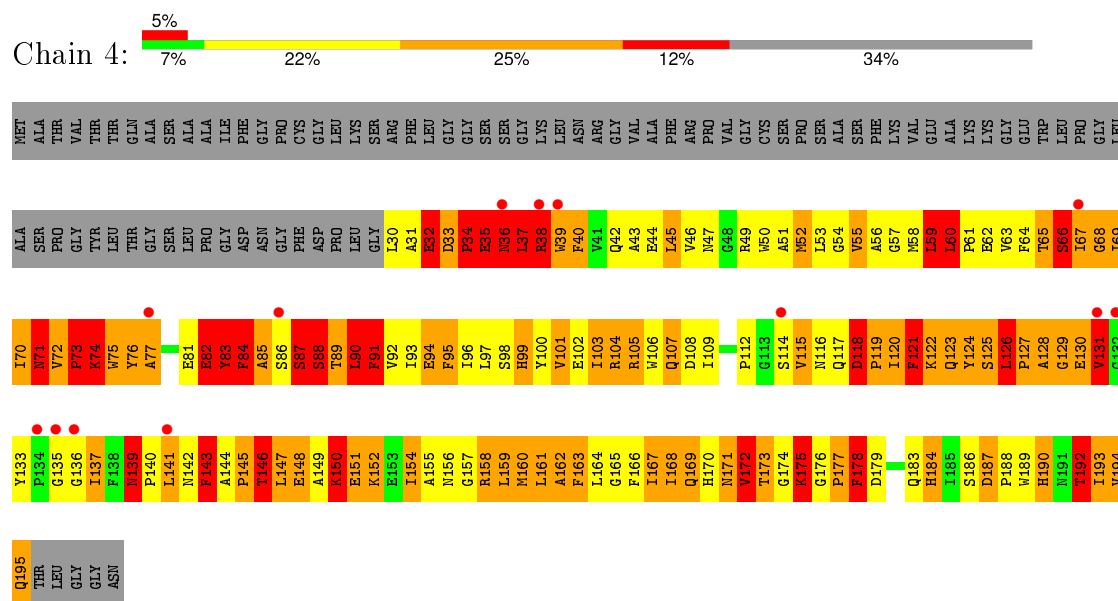
• Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I



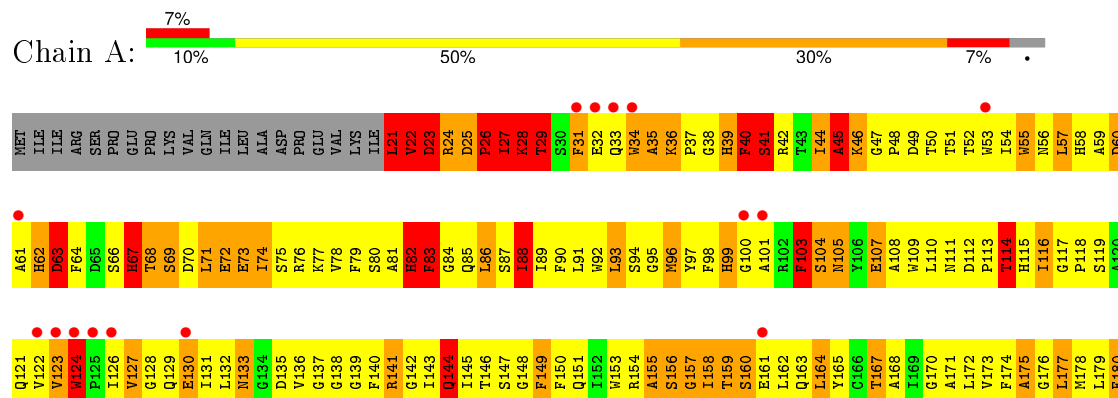
• Molecule 3: LHCA3

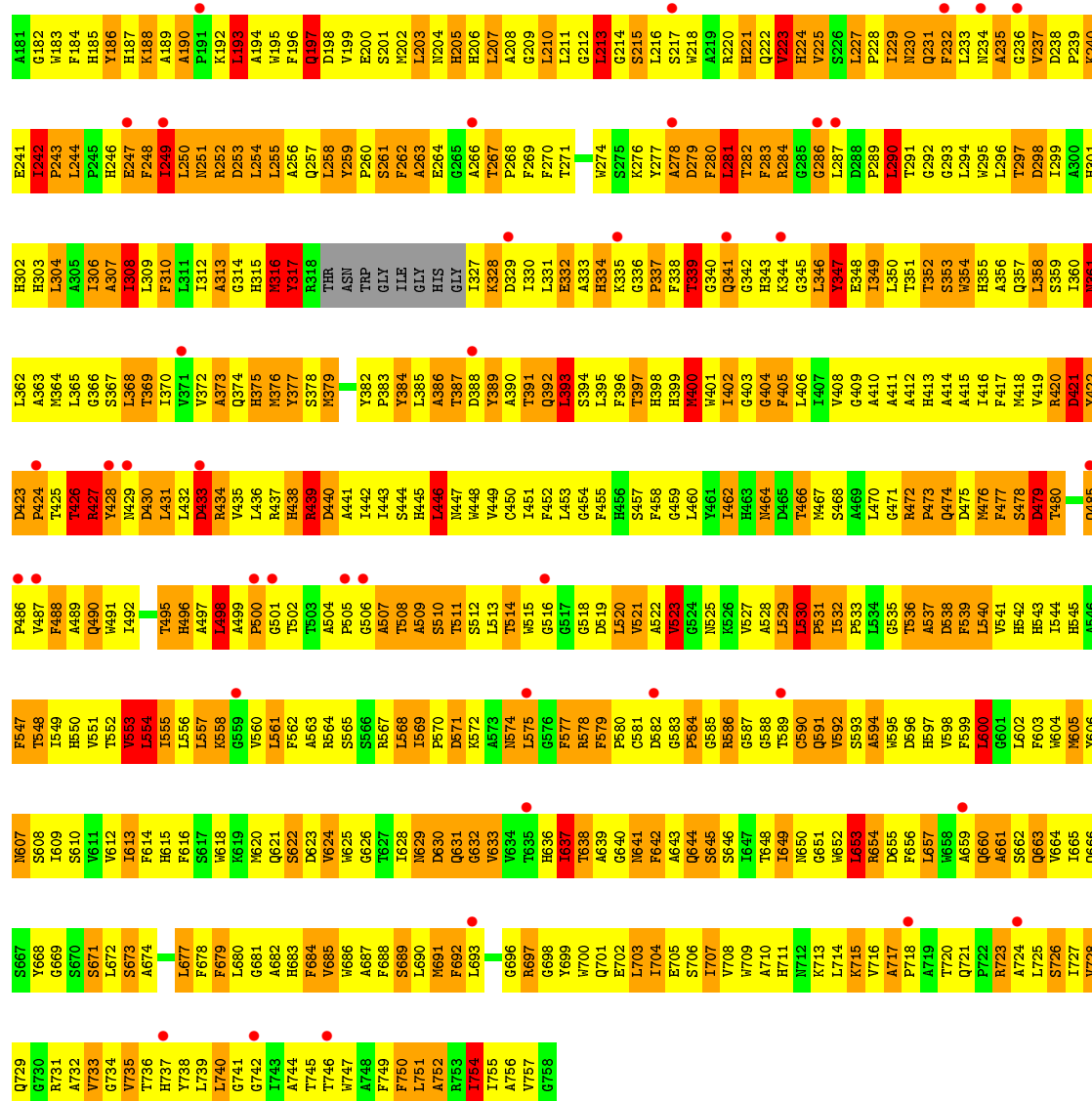


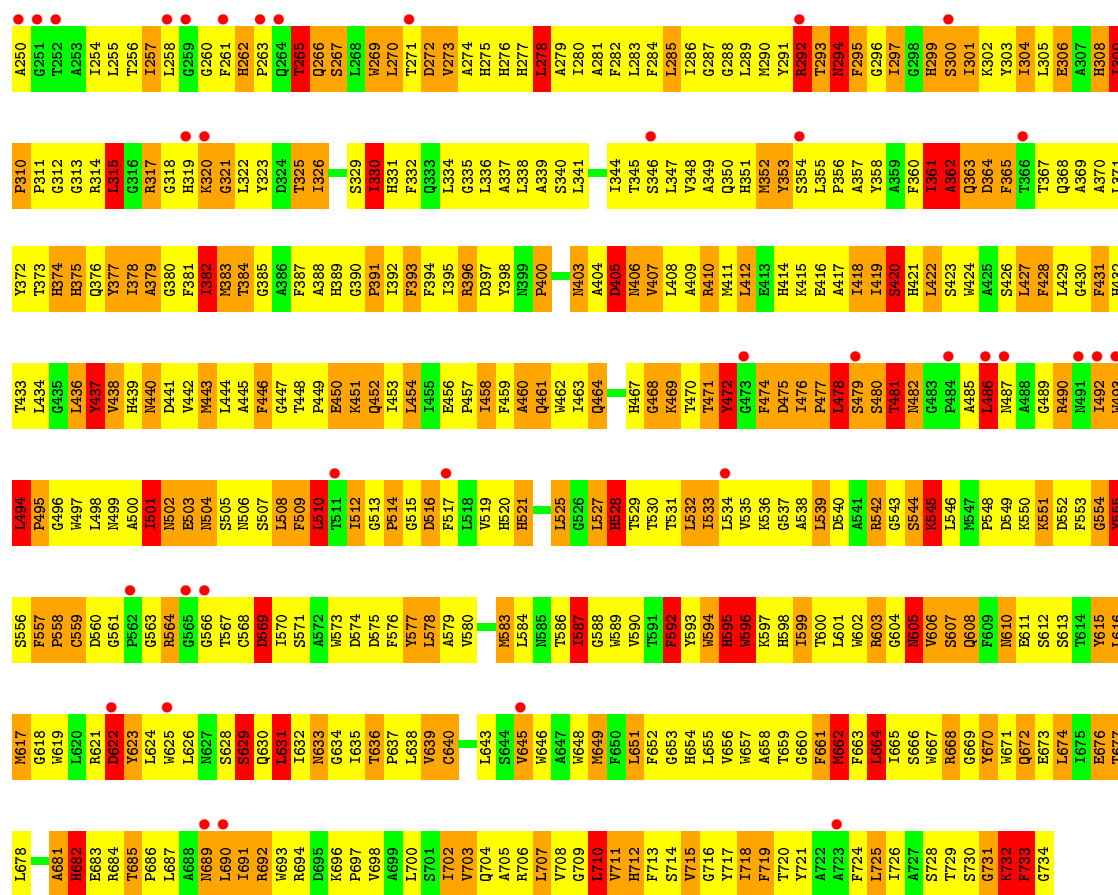
• Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC



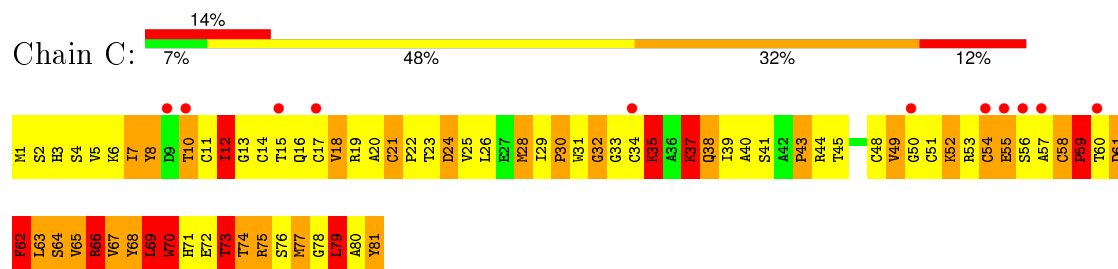
• Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



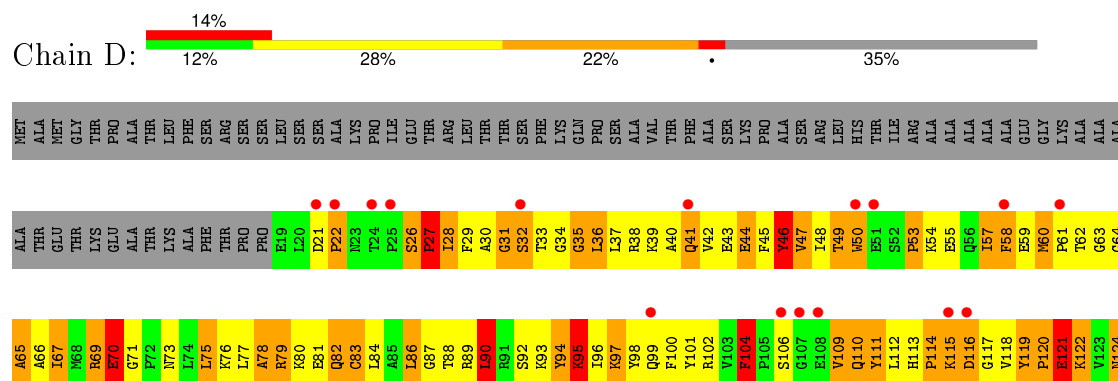


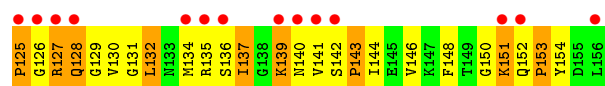


● Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

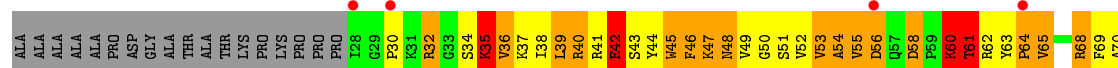
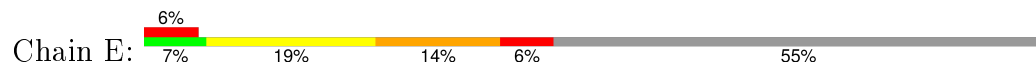


● Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC

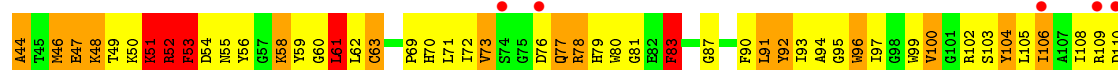
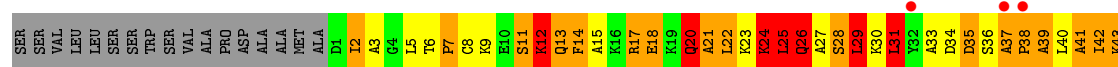




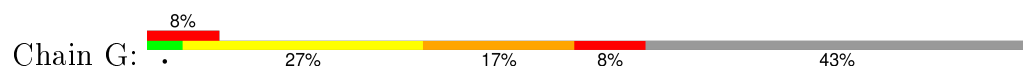
- Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC



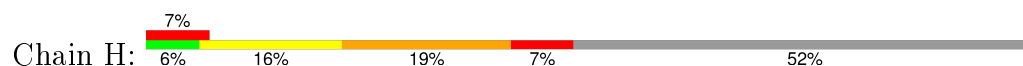
- Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

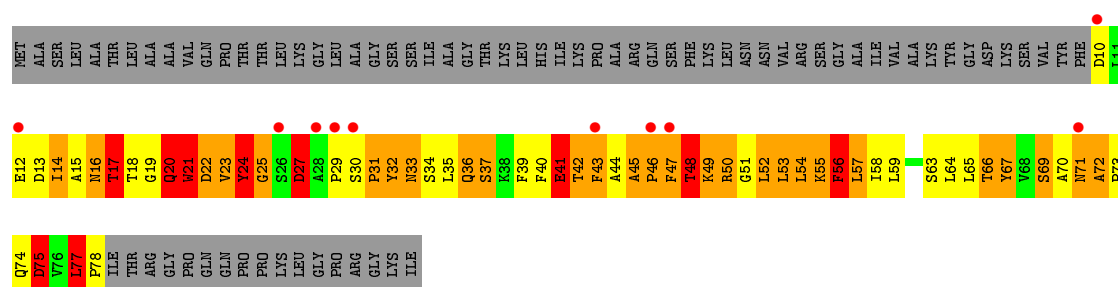


- Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

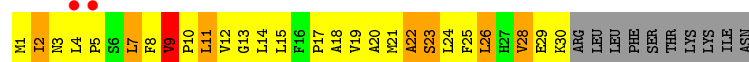


- Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC





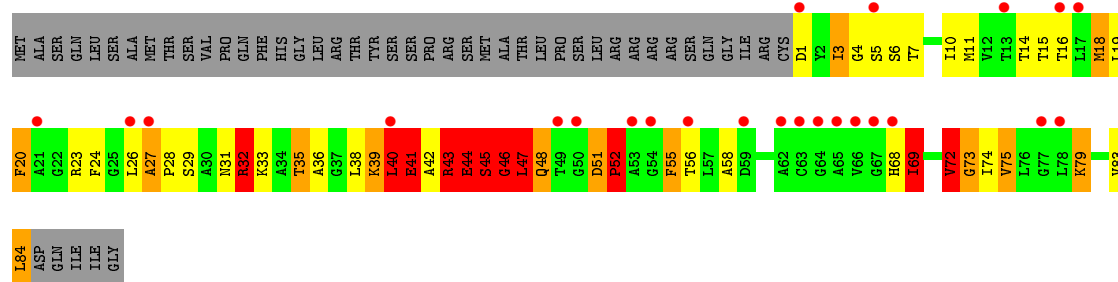
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



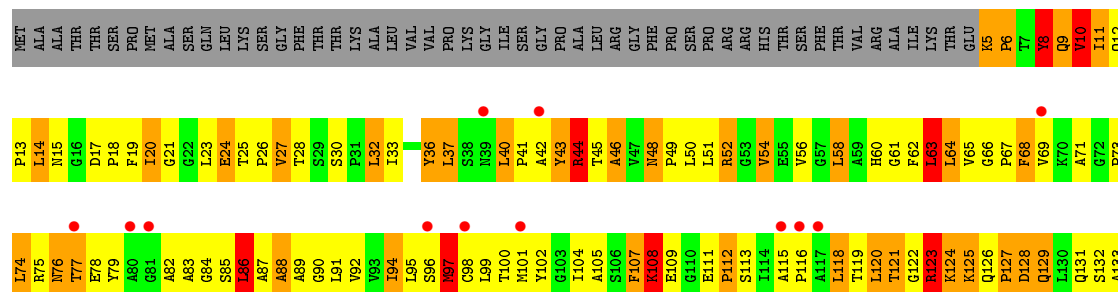
• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

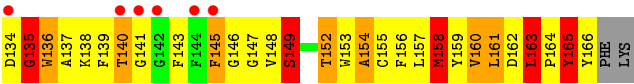


• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

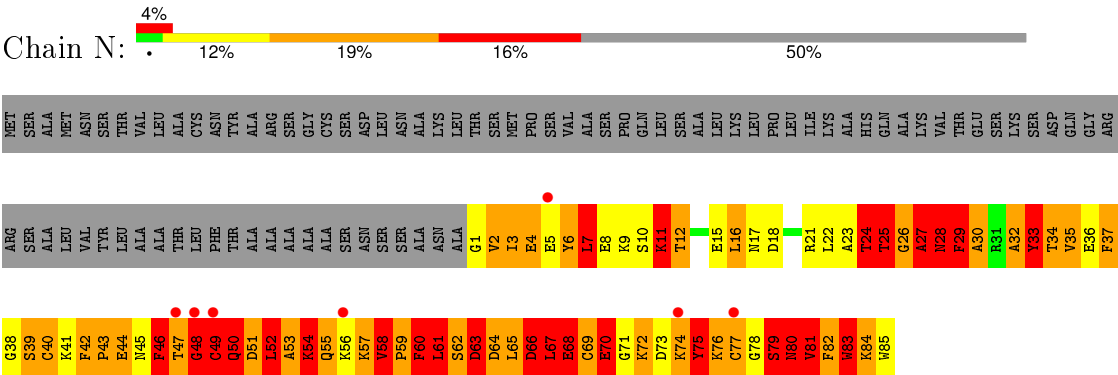


• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

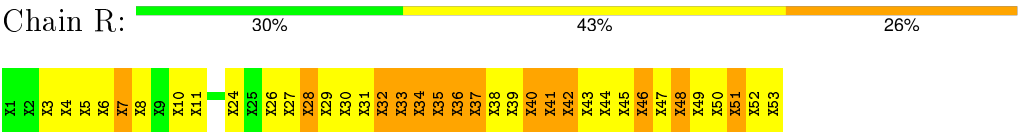




● Molecule 17: PHOTOSYSTEM I-N SUBUNIT



● 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, α , β , γ	120.20Å 190.20Å 130.30Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	50.00 – 3.48 49.46 – 3.47	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-3.48) 96.2 (49.46-3.47)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.391 , 0.425 0.383 , 0.387	Depositor DCC
R_{free} test set	1456 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 30.0	EDS
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 72533 reflections	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	36033	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	0.55	1/1303 (0.1%)	0.73	1/1774 (0.1%)
2	2	0.67	0/1420	1.10	7/1943 (0.4%)
3	3	0.60	0/1221	0.91	2/1642 (0.1%)
4	4	0.77	0/1359	1.12	10/1851 (0.5%)
5	A	0.61	1/5938 (0.0%)	0.88	9/8104 (0.1%)
6	B	0.58	0/6058	0.86	8/8278 (0.1%)
7	C	0.78	0/632	1.05	1/856 (0.1%)
8	D	0.71	0/1122	0.91	0/1514
9	E	0.70	0/530	0.95	1/718 (0.1%)
10	F	0.67	0/1250	0.88	0/1687
11	G	0.84	1/760 (0.1%)	1.20	7/1031 (0.7%)
12	H	0.70	0/543	1.02	0/741
13	I	0.62	0/235	0.80	0/320
14	J	0.65	0/349	0.91	0/475
15	K	0.65	1/599 (0.2%)	0.88	1/810 (0.1%)
16	L	0.69	1/1251 (0.1%)	0.94	2/1709 (0.1%)
17	N	0.89	0/699	1.22	5/936 (0.5%)
All	All	0.65	5/25269 (0.0%)	0.93	54/34389 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	17
3	3	0	17
4	4	0	20
5	A	0	20
6	B	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1
8	D	0	1
9	E	0	3
10	F	0	7
11	G	1	13
12	H	0	9
15	K	0	6
16	L	0	2
17	N	0	22
18	R	0	16
All	All	1	169

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	165	TYR	CE2-CZ	-6.04	1.30	1.38
11	G	15	SER	CB-OG	5.83	1.49	1.42
1	1	185	TRP	CB-CG	-5.34	1.40	1.50
15	K	41	GLU	CG-CD	5.15	1.59	1.51
5	A	22	VAL	CA-CB	-5.05	1.44	1.54

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	180	LYS	C-N-CA	-10.34	95.85	121.70
11	G	46	ALA	N-CA-C	-10.20	83.47	111.00
6	B	731	GLY	N-CA-C	-7.75	93.73	113.10
11	G	16	LEU	CA-CB-CG	7.25	131.98	115.30
6	B	315	LEU	CA-CB-CG	7.00	131.41	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide
1	1	185	TRP	Peptide
1	1	72	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	2	42	ARG	Peptide
2	2	73	ILE	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	1264	0	1229	137	3
2	2	1374	0	1331	301	2
3	3	1186	0	1147	291	6
4	4	1319	0	1282	609	3
5	A	5745	0	5597	1350	0
6	B	5848	0	5655	1211	5
7	C	619	0	608	204	0
8	D	1095	0	1112	189	0
9	E	520	0	528	128	0
10	F	1221	0	1249	201	0
11	G	740	0	708	190	1
12	H	529	0	514	106	0
13	I	229	0	252	55	0
14	J	338	0	340	64	0
15	K	593	0	619	110	0
16	L	1215	0	1222	311	3
17	N	685	0	668	320	1
18	R	265	0	68	78	0
19	1	1072	0	710	174	1
19	2	596	0	409	136	0
19	3	604	0	376	84	0
19	4	759	0	514	177	0
19	A	2610	0	2341	814	0
19	B	2157	0	1981	654	0
19	F	130	0	86	17	0
19	G	51	0	40	4	0
19	H	163	0	140	43	0
19	I	60	0	58	12	0
19	J	61	0	60	14	0
19	L	97	0	72	36	0
19	R	122	0	123	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	2	35	0	46	29	0
20	4	35	0	46	1	0
20	A	1503	0	1967	302	18
20	B	25	0	23	1	0
20	L	35	0	46	1	0
20	R	35	0	46	9	1
21	2	22	0	19	10	0
21	3	23	0	22	6	0
21	B	229	0	217	35	17
21	H	23	0	22	14	0
22	A	33	0	46	7	0
22	B	33	0	46	28	0
23	A	279	0	375	178	0
23	B	280	0	378	155	0
23	I	40	0	54	38	0
23	L	40	0	54	36	0
24	B	49	0	71	17	0
25	B	8	0	0	17	0
25	C	16	0	0	5	0
26	B	23	0	0	1	0
All	All	36033	0	34517	7355	31

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 104.

The worst 5 of 7355 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)
4:4:160:MET:CE	19:4:1201:CLA:HBB2	1.18	1.65
4:4:69:ILE:HD11	4:4:175:LYS:CB	1.26	1.65
3:3:97:PHE:CD2	3:3:98:ILE:HG23	1.33	1.62
1:1:185:TRP:CH2	19:1:1199:CLA:H12	1.38	1.59
3:3:97:PHE:CE2	3:3:98:ILE:HD13	1.42	1.55

The worst 5 of 31 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)
20:A:7008:LMU:C5B	21:B:8062:SUC:O1[1_654]	0.08	2.12
3:3:180:LYS:CD	6:B:490:ARG:CZ[1_556]	0.31	1.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:180:LYS:NZ	6:B:490:ARG:CD[1_556]	0.56	1.64
20:A:7008:LMU:O4'	21:B:8062:SUC:O2[1_654]	1.01	1.19
3:3:180:LYS:CG	6:B:490:ARG:NE[1_556]	1.05	1.15

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	161/241 (67%)	84 (52%)	39 (24%)	38 (24%)	0	1
2	2	174/269 (65%)	67 (38%)	51 (29%)	56 (32%)	0	0
3	3	145/276 (52%)	76 (52%)	36 (25%)	33 (23%)	0	1
4	4	164/251 (65%)	57 (35%)	44 (27%)	63 (38%)	0	0
5	A	726/758 (96%)	366 (50%)	187 (26%)	173 (24%)	0	1
6	B	731/734 (100%)	379 (52%)	204 (28%)	148 (20%)	0	1
7	C	79/81 (98%)	23 (29%)	31 (39%)	25 (32%)	0	0
8	D	136/212 (64%)	47 (35%)	48 (35%)	41 (30%)	0	0
9	E	63/143 (44%)	30 (48%)	15 (24%)	18 (29%)	0	0
10	F	152/231 (66%)	71 (47%)	40 (26%)	41 (27%)	0	0
11	G	93/167 (56%)	38 (41%)	27 (29%)	28 (30%)	0	0
12	H	67/144 (46%)	30 (45%)	16 (24%)	21 (31%)	0	0
13	I	28/40 (70%)	11 (39%)	10 (36%)	7 (25%)	0	1
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	1
15	K	82/131 (63%)	50 (61%)	13 (16%)	19 (23%)	0	1
16	L	160/216 (74%)	72 (45%)	49 (31%)	39 (24%)	0	1
17	N	83/170 (49%)	21 (25%)	19 (23%)	43 (52%)	0	0
All	All	3084/4108 (75%)	1441 (47%)	840 (27%)	803 (26%)	0	0

5 of 803 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU
1	1	73	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	127/190 (67%)	100 (79%)	27 (21%)	1	7
2	2	140/216 (65%)	81 (58%)	59 (42%)	0	1
3	3	112/215 (52%)	76 (68%)	36 (32%)	0	2
4	4	138/201 (69%)	85 (62%)	53 (38%)	0	1
5	A	592/618 (96%)	410 (69%)	182 (31%)	0	3
6	B	598/600 (100%)	397 (66%)	201 (34%)	0	2
7	C	70/70 (100%)	41 (59%)	29 (41%)	0	1
8	D	118/173 (68%)	82 (70%)	36 (30%)	0	3
9	E	56/114 (49%)	38 (68%)	18 (32%)	0	2
10	F	127/190 (67%)	80 (63%)	47 (37%)	0	1
11	G	79/144 (55%)	53 (67%)	26 (33%)	0	2
12	H	57/115 (50%)	30 (53%)	27 (47%)	0	0
13	I	26/36 (72%)	22 (85%)	4 (15%)	3	20
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	3
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	3
16	L	125/169 (74%)	88 (70%)	37 (30%)	0	3
17	N	74/139 (53%)	43 (58%)	31 (42%)	0	1
All	All	2536/3331 (76%)	1694 (67%)	842 (33%)	0	2

5 of 842 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	121	TYR
6	B	438	VAL
16	L	14	LEU
6	B	142	LEU
6	B	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	67	HIS
6	B	333	GLN
15	K	80	ASN
6	B	71	GLN
6	B	193	HIS

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 257 ligands modelled in this entry, 1 is unknown - leaving 256 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	1014	-	41,59,73	2.31	12 (29%)	44,96,113	4.39	16 (36%)
19	CLA	1	1142	-	36,54,73	2.39	11 (30%)	41,90,113	5.20	14 (34%)
19	CLA	1	1143	-	40,58,73	2.28	11 (27%)	44,95,113	4.93	18 (40%)
19	CLA	1	1145	-	45,63,73	2.24	10 (22%)	49,101,113	4.99	17 (34%)
19	CLA	1	1146	-	40,58,73	2.28	10 (25%)	44,95,113	4.80	20 (45%)
19	CLA	1	1148	-	45,63,73	2.16	11 (24%)	49,101,113	4.64	17 (34%)
19	CLA	1	1149	-	36,54,73	2.62	12 (33%)	42,90,113	4.67	22 (52%)
19	CLA	1	1187	1	36,54,73	2.33	11 (30%)	41,90,113	5.22	21 (51%)
19	CLA	1	1188	-	30,49,73	2.51	10 (33%)	34,84,113	5.23	15 (44%)
19	CLA	1	1189	-	37,55,73	2.45	13 (35%)	42,91,113	5.61	19 (45%)
19	CLA	1	1190	-	36,54,73	2.45	12 (33%)	41,90,113	5.30	20 (48%)
19	CLA	1	1191	-	24,44,73	2.89	8 (33%)	28,78,113	4.50	13 (46%)
19	CLA	1	1192	-	51,69,73	2.06	11 (21%)	56,108,113	4.02	18 (32%)
19	CLA	1	1193	-	41,59,73	2.40	13 (31%)	44,96,113	5.00	21 (47%)
19	CLA	1	1194	-	16,32,73	1.72	3 (18%)	21,54,113	3.12	12 (57%)
19	CLA	1	1195	-	16,32,73	1.71	3 (18%)	21,54,113	3.36	12 (57%)
19	CLA	1	1196	1	24,44,73	2.71	9 (37%)	28,78,113	4.50	12 (42%)
19	CLA	1	1197	-	41,59,73	2.52	14 (34%)	44,96,113	5.12	21 (47%)
19	CLA	1	1198	-	16,32,73	1.74	3 (18%)	21,54,113	3.14	11 (52%)
19	CLA	1	1199	-	41,59,73	2.49	15 (36%)	44,96,113	5.47	19 (43%)
19	CLA	1	1200	-	16,32,73	1.70	3 (18%)	21,54,113	3.38	11 (52%)
19	CLA	1	1307	-	16,32,73	1.72	3 (18%)	21,54,113	3.20	12 (57%)
19	CLA	1	1308	-	38,56,73	2.32	11 (28%)	42,92,113	4.93	16 (38%)
19	CLA	1	1309	-	16,32,73	1.76	3 (18%)	21,54,113	3.41	12 (57%)
19	CLA	1	1505	-	45,63,73	2.15	11 (24%)	49,101,113	4.63	19 (38%)
19	CLA	2	1212	-	41,59,73	2.35	11 (26%)	44,96,113	4.85	18 (40%)
19	CLA	2	1213	-	48,66,73	2.20	13 (27%)	52,104,113	4.66	20 (38%)
19	CLA	2	1214	-	16,32,73	1.74	6 (37%)	21,54,113	3.21	11 (52%)
19	CLA	2	1215	-	40,58,73	2.28	10 (25%)	44,95,113	4.49	16 (36%)
19	CLA	2	1216	-	16,32,73	1.68	3 (18%)	21,54,113	2.76	11 (52%)
19	CLA	2	1217	-	55,73,73	1.96	10 (18%)	61,113,113	4.09	19 (31%)
19	CLA	2	1218	-	16,32,73	1.77	6 (37%)	21,54,113	3.41	11 (52%)
19	CLA	2	1219	-	24,44,73	2.72	9 (37%)	28,78,113	4.86	13 (46%)
19	CLA	2	1220	-	16,32,73	1.64	3 (18%)	21,54,113	3.03	11 (52%)
19	CLA	2	1221	2	40,58,73	2.36	12 (30%)	44,95,113	5.00	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	1222	-	40,58,73	2.28	11 (27%)	44,95,113	4.98	19 (43%)
19	CLA	2	1223	-	51,69,73	2.02	11 (21%)	56,108,113	4.64	23 (41%)
20	LMU	2	1224	-	36,36,36	0.50	0	47,47,47	1.71	6 (12%)
21	SUC	2	1225	-	23,23,24	0.59	0	35,35,36	1.42	5 (14%)
19	CLA	2	2006	-	40,58,73	2.37	12 (30%)	44,95,113	4.87	17 (38%)
19	CLA	2	2010	-	16,32,73	1.63	3 (18%)	21,54,113	2.78	11 (52%)
19	CLA	3	1212	-	16,32,73	1.75	3 (18%)	21,54,113	3.02	11 (52%)
19	CLA	3	1213	-	24,44,73	2.80	7 (29%)	28,78,113	4.43	13 (46%)
19	CLA	3	1214	-	16,32,73	1.73	4 (25%)	21,54,113	3.19	11 (52%)
19	CLA	3	1215	-	16,32,73	1.75	3 (18%)	21,54,113	2.96	9 (42%)
19	CLA	3	1216	-	16,32,73	1.72	3 (18%)	21,54,113	3.17	12 (57%)
19	CLA	3	1217	-	32,50,73	2.49	10 (31%)	36,85,113	5.89	17 (47%)
19	CLA	3	1218	-	46,64,73	2.15	12 (26%)	50,102,113	4.62	19 (38%)
19	CLA	3	1219	-	16,32,73	1.67	3 (18%)	21,54,113	3.28	12 (57%)
19	CLA	3	1220	-	16,32,73	1.74	4 (25%)	21,54,113	3.49	11 (52%)
19	CLA	3	1221	-	55,73,73	1.96	11 (20%)	61,113,113	3.84	22 (36%)
19	CLA	3	1222	-	55,73,73	1.96	11 (20%)	61,113,113	4.25	18 (29%)
21	SUC	3	1223	-	24,24,24	0.51	0	36,36,36	1.45	5 (13%)
19	CLA	3	3001	-	16,32,73	1.79	3 (18%)	21,54,113	3.19	12 (57%)
19	CLA	3	3008	-	40,58,73	2.29	9 (22%)	44,95,113	4.66	17 (38%)
19	CLA	3	3011	-	55,73,73	1.93	13 (23%)	61,113,113	4.24	18 (29%)
19	CLA	3	3014	-	16,32,73	1.74	4 (25%)	21,54,113	3.42	12 (57%)
19	CLA	3	3015	-	16,32,73	1.69	3 (18%)	21,54,113	3.25	11 (52%)
19	CLA	4	1196	-	45,63,73	2.20	11 (24%)	49,101,113	4.64	19 (38%)
19	CLA	4	1197	-	24,44,73	2.83	9 (37%)	28,78,113	4.62	15 (53%)
19	CLA	4	1198	-	55,73,73	2.03	11 (20%)	61,113,113	4.23	20 (32%)
19	CLA	4	1199	-	45,63,73	2.14	10 (22%)	49,101,113	4.21	17 (34%)
19	CLA	4	1200	-	40,58,73	2.34	12 (30%)	44,95,113	5.16	18 (40%)
19	CLA	4	1201	-	42,60,73	2.34	11 (26%)	45,97,113	4.79	27 (60%)
19	CLA	4	1202	-	16,32,73	1.73	4 (25%)	21,54,113	3.14	11 (52%)
19	CLA	4	1203	-	16,32,73	1.74	5 (31%)	21,54,113	3.38	12 (57%)
19	CLA	4	1204	-	16,32,73	1.75	3 (18%)	21,54,113	3.12	11 (52%)
19	CLA	4	1205	-	40,58,73	2.32	12 (30%)	44,95,113	4.24	16 (36%)
19	CLA	4	1206	-	55,73,73	1.98	13 (23%)	61,113,113	4.37	19 (31%)
19	CLA	4	1207	-	16,32,73	1.72	4 (25%)	21,54,113	3.18	11 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	1208	-	16,32,73	1.68	3 (18%)	21,54,113	3.21	12 (57%)
19	CLA	4	1209	4	24,44,73	2.67	8 (33%)	28,78,113	4.88	16 (57%)
19	CLA	4	1210	4	16,32,73	1.78	4 (25%)	21,54,113	2.88	12 (57%)
19	CLA	4	1211	-	36,54,73	2.38	12 (33%)	41,90,113	4.74	15 (36%)
20	LMU	4	1212	-	36,36,36	0.71	1 (2%)	47,47,47	1.13	3 (6%)
19	CLA	4	4007	-	42,60,73	2.28	12 (28%)	45,97,113	5.06	20 (44%)
19	CLA	4	4014	-	37,55,73	2.34	12 (32%)	42,91,113	5.24	19 (45%)
19	CLA	A	1759	-	36,54,73	2.53	12 (33%)	41,90,113	5.17	15 (36%)
19	CLA	A	1760	19	45,63,73	2.27	11 (24%)	49,101,113	4.18	19 (38%)
19	CLA	A	1761	-	44,62,73	2.16	12 (27%)	47,99,113	3.98	17 (36%)
19	CLA	A	1762	-	46,64,73	2.10	10 (21%)	50,102,113	4.61	19 (38%)
19	CLA	A	1763	-	36,54,73	2.34	10 (27%)	41,90,113	5.26	18 (43%)
19	CLA	A	1764	5	50,68,73	2.11	12 (24%)	55,107,113	3.98	19 (34%)
19	CLA	A	1765	-	42,60,73	2.17	10 (23%)	45,97,113	4.48	19 (42%)
19	CLA	A	1766	-	32,53,73	2.49	10 (31%)	37,89,113	5.41	18 (48%)
19	CLA	A	1767	19,5	55,73,73	2.01	12 (21%)	61,113,113	3.80	19 (31%)
19	CLA	A	1768	5	44,62,73	2.13	10 (22%)	47,99,113	4.35	15 (31%)
19	CLA	A	1769	-	40,58,73	2.24	10 (25%)	44,95,113	4.67	18 (40%)
19	CLA	A	1770	-	16,32,73	1.80	6 (37%)	21,54,113	3.23	11 (52%)
19	CLA	A	1771	-	40,58,73	2.31	10 (25%)	44,95,113	4.83	19 (43%)
19	CLA	A	1772	-	44,62,73	2.18	12 (27%)	47,99,113	4.65	19 (40%)
19	CLA	A	1773	-	42,60,73	2.25	11 (26%)	45,97,113	4.99	15 (33%)
19	CLA	A	1774	-	50,68,73	2.20	13 (26%)	55,107,113	3.65	24 (43%)
19	CLA	A	1775	-	24,44,73	2.78	8 (33%)	28,78,113	4.53	14 (50%)
19	CLA	A	1776	-	48,66,73	2.11	10 (20%)	52,104,113	4.36	21 (40%)
19	CLA	A	1777	-	41,59,73	2.27	11 (26%)	44,96,113	4.74	17 (38%)
19	CLA	A	1778	5	32,50,73	2.44	10 (31%)	36,85,113	5.27	15 (41%)
19	CLA	A	1779	-	40,58,73	2.27	11 (27%)	44,95,113	4.48	17 (38%)
19	CLA	A	1780	-	48,66,73	2.03	11 (22%)	52,104,113	3.97	18 (34%)
19	CLA	A	1781	-	49,67,73	2.05	11 (22%)	53,105,113	4.42	18 (33%)
19	CLA	A	1782	-	55,73,73	1.90	11 (20%)	61,113,113	3.61	16 (26%)
19	CLA	A	1783	-	55,73,73	1.94	11 (20%)	61,113,113	4.36	16 (26%)
19	CLA	A	1784	5	45,63,73	2.17	11 (24%)	49,101,113	4.57	18 (36%)
19	CLA	A	1785	-	55,73,73	1.97	12 (21%)	61,113,113	3.85	19 (31%)
19	CLA	A	1786	-	40,58,73	2.31	12 (30%)	44,95,113	5.08	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1787	5	50,68,73	2.09	10 (20%)	55,107,113	4.20	19 (34%)
19	CLA	A	1788	-	55,73,73	1.94	11 (20%)	61,113,113	4.25	15 (24%)
19	CLA	A	1789	5	55,73,73	1.96	12 (21%)	61,113,113	4.61	25 (40%)
19	CLA	A	1790	5	40,58,73	2.25	10 (25%)	44,95,113	4.80	18 (40%)
19	CLA	A	1791	19,5	32,53,73	2.40	10 (31%)	37,89,113	5.47	18 (48%)
19	CLA	A	1792	-	36,54,73	2.41	10 (27%)	41,90,113	5.08	17 (41%)
19	CLA	A	1793	-	55,73,73	2.04	11 (20%)	61,113,113	4.24	19 (31%)
19	CLA	A	1794	-	37,55,73	2.40	11 (29%)	42,91,113	4.61	15 (35%)
19	CLA	A	1795	-	41,59,73	2.30	11 (26%)	44,96,113	4.92	18 (40%)
19	CLA	A	1796	-	55,73,73	1.98	10 (18%)	61,113,113	4.03	21 (34%)
19	CLA	A	1797	19	49,67,73	2.31	14 (28%)	53,105,113	4.16	21 (39%)
19	CLA	A	1798	-	45,63,73	2.15	11 (24%)	49,101,113	4.81	17 (34%)
19	CLA	A	1799	-	16,32,73	1.80	3 (18%)	21,54,113	3.39	12 (57%)
19	CLA	A	1800	-	55,73,73	1.92	11 (20%)	61,113,113	4.31	19 (31%)
19	CLA	A	1801	-	45,63,73	2.25	10 (22%)	49,101,113	4.42	20 (40%)
22	PQN	A	1802	-	34,34,34	1.49	2 (5%)	44,45,45	1.14	3 (6%)
23	BCR	A	1803	-	41,41,41	1.95	3 (7%)	56,56,56	5.47	20 (35%)
23	BCR	A	1804	-	41,41,41	2.01	3 (7%)	56,56,56	5.56	21 (37%)
23	BCR	A	1805	-	41,41,41	2.00	4 (9%)	56,56,56	5.70	26 (46%)
23	BCR	A	1806	-	41,41,41	1.92	3 (7%)	56,56,56	5.52	17 (30%)
23	BCR	A	1807	-	40,40,41	1.65	3 (7%)	50,53,56	4.35	19 (38%)
23	BCR	A	1808	-	41,41,41	2.51	6 (14%)	56,56,56	6.05	21 (37%)
23	BCR	A	1809	-	41,41,41	1.96	3 (7%)	56,56,56	5.69	21 (37%)
20	LMU	A	1810	-	36,36,36	0.68	0	47,47,47	1.33	7 (14%)
20	LMU	A	1811	-	36,36,36	0.66	1 (2%)	47,47,47	1.49	7 (14%)
20	LMU	A	1812	-	36,36,36	0.47	0	47,47,47	0.88	4 (8%)
19	CLA	A	1813	-	55,73,73	1.95	12 (21%)	61,113,113	4.36	19 (31%)
19	CLA	A	1814	-	55,73,73	1.99	12 (21%)	61,113,113	4.26	19 (31%)
19	CLA	A	1815	-	55,73,73	2.03	11 (20%)	61,113,113	4.18	17 (27%)
19	CLA	A	1816	-	44,62,73	2.18	11 (25%)	47,99,113	4.82	21 (44%)
19	CLA	A	1817	-	55,73,73	1.97	10 (18%)	61,113,113	4.17	17 (27%)
20	LMU	A	7001	-	36,36,36	0.66	0	47,47,47	1.65	9 (19%)
20	LMU	A	7003	-	36,36,36	0.48	0	47,47,47	0.75	1 (2%)
20	LMU	A	7004	-	36,36,36	0.45	0	47,47,47	1.45	6 (12%)
20	LMU	A	7005	-	36,36,36	0.43	0	47,47,47	1.17	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	A	7006	-	36,36,36	0.55	0	47,47,47	0.70	0
20	LMU	A	7008	21	36,36,36	1.08	3 (8%)	47,47,47	2.20	11 (23%)
20	LMU	A	7009	20	35,35,36	0.78	2 (5%)	46,46,47	1.85	11 (23%)
20	LMU	A	7010	-	36,36,36	0.54	0	47,47,47	0.89	2 (4%)
20	LMU	A	7011	-	36,36,36	0.46	0	47,47,47	1.55	6 (12%)
20	LMU	A	7013	20	36,36,36	0.56	0	47,47,47	1.01	2 (4%)
20	LMU	A	7014	-	36,36,36	0.84	1 (2%)	47,47,47	2.13	12 (25%)
20	LMU	A	7015	-	36,36,36	0.68	1 (2%)	47,47,47	1.35	4 (8%)
20	LMU	A	7016	-	36,36,36	0.49	0	47,47,47	1.50	6 (12%)
20	LMU	A	7017	-	36,36,36	0.63	0	47,47,47	1.90	14 (29%)
20	LMU	A	7019	-	36,36,36	0.75	1 (2%)	47,47,47	1.33	8 (17%)
20	LMU	A	7020	-	36,36,36	0.56	0	47,47,47	1.56	9 (19%)
20	LMU	A	7021	-	36,36,36	0.69	0	47,47,47	1.52	6 (12%)
20	LMU	A	7022	-	36,36,36	0.56	0	47,47,47	1.33	5 (10%)
20	LMU	A	7023	-	36,36,36	0.50	0	47,47,47	1.36	7 (14%)
20	LMU	A	7024	-	36,36,36	0.73	1 (2%)	47,47,47	1.46	8 (17%)
20	LMU	A	7025	-	36,36,36	0.51	0	47,47,47	1.26	6 (12%)
20	LMU	A	7026	-	36,36,36	0.84	1 (2%)	47,47,47	2.15	14 (29%)
20	LMU	A	7027	-	36,36,36	0.80	1 (2%)	47,47,47	1.63	11 (23%)
20	LMU	A	7028	-	36,36,36	0.50	0	47,47,47	1.05	3 (6%)
20	LMU	A	7030	-	36,36,36	0.59	0	47,47,47	1.67	8 (17%)
20	LMU	A	7031	-	36,36,36	0.45	0	47,47,47	1.29	4 (8%)
20	LMU	A	7032	-	36,36,36	0.71	1 (2%)	47,47,47	1.70	8 (17%)
20	LMU	A	7033	-	36,36,36	0.68	0	47,47,47	1.67	9 (19%)
20	LMU	A	7034	-	36,36,36	0.45	0	47,47,47	1.51	8 (17%)
20	LMU	A	7035	-	36,36,36	0.64	0	47,47,47	1.44	9 (19%)
20	LMU	A	7036	-	35,35,36	0.58	1 (2%)	46,46,47	1.37	5 (10%)
20	LMU	A	7037	-	36,36,36	0.60	0	47,47,47	1.90	13 (27%)
20	LMU	A	7038	-	36,36,36	0.69	0	47,47,47	1.77	11 (23%)
20	LMU	A	7039	-	36,36,36	0.60	0	47,47,47	1.64	8 (17%)
20	LMU	A	7040	-	36,36,36	0.66	1 (2%)	47,47,47	1.71	12 (25%)
20	LMU	A	7041	-	36,36,36	0.37	0	47,47,47	1.05	3 (6%)
20	LMU	A	7042	-	36,36,36	0.51	0	47,47,47	1.32	7 (14%)
20	LMU	A	7043	-	36,36,36	0.59	1 (2%)	47,47,47	1.61	11 (23%)
20	LMU	A	7047	-	36,36,36	0.80	1 (2%)	47,47,47	1.24	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	A	7049	20	36,36,36	0.49	0	47,47,47	0.97	2 (4%)
19	CLA	B	1735	-	55,73,73	2.01	11 (20%)	61,113,113	3.94	18 (29%)
19	CLA	B	1736	-	32,53,73	2.46	11 (34%)	37,89,113	4.93	14 (37%)
19	CLA	B	1737	-	51,69,73	1.98	12 (23%)	56,108,113	4.12	19 (33%)
19	CLA	B	1738	-	55,73,73	1.98	12 (21%)	61,113,113	4.25	22 (36%)
19	CLA	B	1739	-	50,68,73	2.11	11 (22%)	55,107,113	4.42	19 (34%)
19	CLA	B	1740	6	16,32,73	1.82	4 (25%)	21,54,113	2.96	11 (52%)
19	CLA	B	1741	6	44,62,73	2.39	11 (25%)	49,100,113	3.97	18 (36%)
19	CLA	B	1742	6	45,63,73	2.08	10 (22%)	49,101,113	4.52	18 (36%)
19	CLA	B	1743	-	55,73,73	1.97	10 (18%)	61,113,113	4.03	16 (26%)
19	CLA	B	1744	-	50,68,73	2.11	11 (22%)	55,107,113	4.06	16 (29%)
19	CLA	B	1745	6	50,68,73	2.03	10 (20%)	55,107,113	4.01	18 (32%)
19	CLA	B	1746	-	36,54,73	2.37	10 (27%)	41,90,113	4.54	16 (39%)
19	CLA	B	1747	-	43,61,73	2.21	11 (25%)	46,98,113	4.54	17 (36%)
19	CLA	B	1748	-	30,49,73	2.53	12 (40%)	34,84,113	6.00	17 (50%)
19	CLA	B	1749	-	51,69,73	1.96	11 (21%)	56,108,113	4.54	19 (33%)
19	CLA	B	1750	-	40,58,73	2.26	11 (27%)	44,95,113	4.93	15 (34%)
19	CLA	B	1751	-	36,54,73	2.37	11 (30%)	41,90,113	5.24	13 (31%)
19	CLA	B	1752	6	45,63,73	2.19	10 (22%)	49,101,113	4.69	18 (36%)
19	CLA	B	1753	-	55,73,73	2.08	14 (25%)	61,113,113	4.33	19 (31%)
19	CLA	B	1754	-	44,62,73	2.26	12 (27%)	47,99,113	4.56	19 (40%)
19	CLA	B	1755	-	48,66,73	2.09	11 (22%)	52,104,113	4.53	18 (34%)
19	CLA	B	1756	6	55,73,73	1.92	11 (20%)	61,113,113	4.21	19 (31%)
19	CLA	B	1757	-	55,73,73	1.99	11 (20%)	61,113,113	4.25	19 (31%)
19	CLA	B	1758	-	55,73,73	1.97	12 (21%)	61,113,113	3.89	20 (32%)
19	CLA	B	1759	-	55,73,73	1.96	12 (21%)	61,113,113	3.82	18 (29%)
19	CLA	B	1760	-	40,58,73	2.29	10 (25%)	44,95,113	4.66	17 (38%)
19	CLA	B	1761	10,6	40,58,73	2.35	14 (35%)	44,95,113	5.17	17 (38%)
19	CLA	B	1762	6	49,67,73	2.14	12 (24%)	53,105,113	4.33	18 (33%)
19	CLA	B	1763	6	40,58,73	2.28	12 (30%)	44,95,113	4.72	18 (40%)
19	CLA	B	1764	19	32,53,73	2.47	10 (31%)	37,89,113	5.33	13 (35%)
19	CLA	B	1765	19	32,53,73	2.47	10 (31%)	37,89,113	4.95	15 (40%)
19	CLA	B	1766	-	41,59,73	2.22	11 (26%)	44,96,113	4.97	20 (45%)
19	CLA	B	1767	-	50,68,73	2.04	11 (22%)	55,107,113	4.30	14 (25%)
19	CLA	B	1768	6	55,73,73	1.90	11 (20%)	61,113,113	3.75	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1769	-	37,55,73	2.53	14 (37%)	42,91,113	5.43	18 (42%)
19	CLA	B	1770	-	55,73,73	1.94	11 (20%)	61,113,113	3.74	18 (29%)
19	CLA	B	1771	-	55,73,73	1.90	12 (21%)	61,113,113	3.69	18 (29%)
19	CLA	B	1772	-	24,44,73	2.77	8 (33%)	28,78,113	4.80	15 (53%)
22	PQN	B	1773	-	34,34,34	1.44	2 (5%)	44,45,45	1.28	6 (13%)
23	BCR	B	1774	-	41,41,41	1.86	3 (7%)	56,56,56	5.72	17 (30%)
23	BCR	B	1775	-	41,41,41	1.85	3 (7%)	56,56,56	5.19	24 (42%)
23	BCR	B	1776	-	41,41,41	1.75	3 (7%)	56,56,56	4.77	19 (33%)
23	BCR	B	1777	-	41,41,41	1.97	4 (9%)	56,56,56	5.55	20 (35%)
23	BCR	B	1778	-	41,41,41	2.00	3 (7%)	56,56,56	5.46	18 (32%)
23	BCR	B	1779	-	41,41,41	2.15	5 (12%)	56,56,56	5.72	23 (41%)
23	BCR	B	1780	-	41,41,41	1.94	3 (7%)	56,56,56	5.43	16 (28%)
24	LMG	B	1781	-	49,49,55	0.95	2 (4%)	57,57,63	1.08	2 (3%)
20	LMU	B	1782	-	26,26,36	0.75	1 (3%)	37,37,47	1.36	6 (16%)
25	SF4	B	1783	5,6	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	B	1784	-	55,73,73	1.93	11 (20%)	61,113,113	4.00	19 (31%)
21	SUC	B	8051	-	24,24,24	0.44	0	36,36,36	1.22	2 (5%)
21	SUC	B	8052	-	24,24,24	0.34	0	36,36,36	0.95	0
21	SUC	B	8053	-	23,23,24	0.62	0	35,35,36	1.41	6 (17%)
21	SUC	B	8054	-	24,24,24	0.57	0	36,36,36	0.99	2 (5%)
21	SUC	B	8055	-	24,24,24	0.45	0	36,36,36	1.25	4 (11%)
21	SUC	B	8056	-	24,24,24	0.49	0	36,36,36	1.20	6 (16%)
21	SUC	B	8059	-	24,24,24	0.51	0	36,36,36	1.22	2 (5%)
21	SUC	B	8060	-	24,24,24	0.48	0	36,36,36	0.98	2 (5%)
21	SUC	B	8061	-	24,24,24	0.51	0	36,36,36	1.63	9 (25%)
21	SUC	B	8062	20	24,24,24	1.05	2 (8%)	36,36,36	2.09	11 (30%)
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	-
19	CLA	F	1155	-	24,44,73	2.59	8 (33%)	28,78,113	3.93	14 (50%)
19	CLA	F	1156	19	30,49,73	2.49	10 (33%)	34,84,113	5.48	16 (47%)
19	CLA	F	1157	19	43,61,73	2.51	17 (39%)	46,98,113	4.53	20 (43%)
19	CLA	G	1099	-	41,59,73	2.30	12 (29%)	44,96,113	4.33	17 (38%)
19	CLA	H	1079	-	48,66,73	2.15	12 (25%)	52,104,113	4.20	21 (40%)
19	CLA	H	1080	-	45,63,73	2.16	10 (22%)	49,101,113	4.72	18 (36%)
19	CLA	H	1081	16	40,58,73	2.29	10 (25%)	44,95,113	4.94	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	SUC	H	1082	-	24,24,24	0.43	0	36,36,36	0.90	1 (2%)
19	CLA	I	1031	-	50,68,73	2.04	11 (22%)	55,107,113	4.58	16 (29%)
23	BCR	I	1032	-	41,41,41	2.12	5 (12%)	56,56,56	6.12	27 (48%)
19	CLA	J	1043	-	51,69,73	2.00	11 (21%)	56,108,113	4.34	15 (26%)
19	CLA	L	1167	-	37,55,73	2.40	11 (29%)	42,91,113	5.14	17 (40%)
19	CLA	L	1168	-	40,58,73	2.36	12 (30%)	44,95,113	5.35	18 (40%)
23	BCR	L	1169	-	41,41,41	1.99	4 (9%)	56,56,56	5.63	16 (28%)
20	LMU	L	1170	-	36,36,36	0.69	1 (2%)	47,47,47	1.33	5 (10%)
19	CLA	R	1054	-	47,65,73	2.14	11 (23%)	50,103,113	4.77	20 (40%)
19	CLA	R	1055	-	55,73,73	2.01	10 (18%)	61,113,113	4.16	20 (32%)
20	LMU	R	1056	20	36,36,36	0.48	0	47,47,47	0.88	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	1014	-	4/4/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1142	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1143	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	1	1145	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1146	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	1	1148	-	4/4/18/25	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
19	CLA	1	1188	-	3/3/15/25	0/8/106/135	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	0/15/113/135	0/0/9/9
19	CLA	1	1191	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1192	-	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	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1196	1	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1197	-	4/4/17/25	1/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1198	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1199	-	5/5/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1200	-	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	-	4/4/18/25	0/29/127/135	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	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	1218	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1219	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	2	1220	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1221	2	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1222	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1223	-	4/4/19/25	0/33/131/135	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	2006	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	2	2010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1212	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1213	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	1214	-	3/3/7/25	0/0/66/135	0/0/8/9
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	-	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	3	1218	-	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	3	1219	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1220	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1221	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1222	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	3	1223	-	1/1/9/9	0/12/51/51	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3014	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3015	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1196	-	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	-	4/4/17/25	0/22/120/135	0/0/9/9
19	CLA	4	1202	-	3/3/7/25	0/0/66/135	0/0/8/9
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	-	3/3/17/25	1/19/117/135	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
19	CLA	4	4007	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4014	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1759	-	3/3/16/25	0/15/113/135	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	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1762	-	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	A	1763	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	1764	5	4/4/19/25	0/31/129/135	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1769	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1770	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	A	1771	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1772	-	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	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	A	1775	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	A	1776	-	4/4/18/25	0/29/127/135	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	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1780	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	A	1781	-	4/4/18/25	1/30/128/135	0/0/9/9
19	CLA	A	1782	-	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	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	A	1788	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1789	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1790	5	3/3/17/25	0/19/117/135	0/0/9/9
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	0/15/113/135	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	-	3/3/17/25	0/21/119/135	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	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	A	1798	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	A	1799	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	A	1800	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1801	-	4/4/18/25	0/25/123/135	0/0/9/9
22	PQN	A	1802	-	1/1/8/9	0/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A	1803	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1804	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1805	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1806	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1807	-	-	0/29/60/63	0/2/2/2
23	BCR	A	1808	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1809	-	-	1/29/63/63	0/2/2/2
20	LMU	A	1810	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1811	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1812	-	-	0/21/61/61	0/2/2/2
19	CLA	A	1813	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1814	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1815	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1816	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1817	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	A	7001	-	-	0/21/61/61	0/2/2/2
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	7008	21	-	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	7011	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7013	20	-	0/21/61/61	0/2/2/2
20	LMU	A	7014	-	-	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
20	LMU	A	7025	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7026	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7027	-	-	1/21/61/61	0/2/2/2
20	LMU	A	7028	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7030	-	-	1/21/61/61	0/2/2/2
20	LMU	A	7031	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMU	A	7032	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7033	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7034	-	-	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	-	-	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	7049	20	-	0/21/61/61	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	0/33/131/135	0/0/9/9
19	CLA	B	1738	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1739	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1740	6	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	B	1741	6	4/4/18/25	0/25/121/135	0/0/9/9
19	CLA	B	1742	6	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1743	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1744	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1745	6	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1746	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1747	-	3/3/17/25	0/23/121/135	0/0/9/9
19	CLA	B	1748	-	3/3/15/25	0/8/106/135	0/0/9/9
19	CLA	B	1749	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	B	1750	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1751	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1752	6	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1753	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1754	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	B	1755	-	4/4/18/25	1/29/127/135	0/0/9/9
19	CLA	B	1756	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1757	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	B	1761	10,6	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1762	6	4/4/18/25	0/30/128/135	0/0/9/9
19	CLA	B	1763	6	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1764	19	3/3/16/25	0/11/111/135	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	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	B	1767	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1768	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1769	-	3/3/16/25	1/16/114/135	0/0/9/9
19	CLA	B	1770	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1771	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1772	-	3/3/14/25	0/0/96/135	0/0/9/9
22	PQN	B	1773	-	1/1/8/9	0/23/43/43	0/2/2/2
23	BCR	B	1774	-	-	2/29/63/63	0/2/2/2
23	BCR	B	1775	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1776	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1777	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1778	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1779	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1780	-	-	2/29/63/63	0/2/2/2
24	LMG	B	1781	-	-	0/44/64/70	0/1/1/1
20	LMU	B	1782	-	-	0/11/51/61	0/2/2/2
25	SF4	B	1783	5,6	-	0/0/48/48	0/6/5/5
19	CLA	B	1784	-	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	0/10/49/51	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SF4	C	1083	7	-	0/0/48/48	0/6/5/5
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
19	CLA	G	1099	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	H	1079	-	4/4/18/25	0/29/127/135	0/0/9/9
19	CLA	H	1080	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	H	1081	16	3/3/17/25	0/19/117/135	0/0/9/9
21	SUC	H	1082	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	I	1031	-	4/4/19/25	0/31/129/135	0/0/9/9
23	BCR	I	1032	-	-	0/29/63/63	0/2/2/2
19	CLA	J	1043	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	L	1167	-	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
23	BCR	L	1169	-	-	0/29/63/63	0/2/2/2
20	LMU	L	1170	-	-	0/21/61/61	0/2/2/2
19	CLA	R	1054	-	4/4/18/25	0/28/126/135	0/0/9/9
19	CLA	R	1055	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	R	1056	20	-	0/21/61/61	0/2/2/2

The worst 5 of 1783 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1808	BCR	C21-C22	-9.92	1.22	1.35
23	A	1808	BCR	C20-C21	-9.28	1.14	1.43
19	1	1191	CLA	CAB-C3B	-8.99	1.33	1.51
19	B	1741	CLA	CAB-C3B	-8.90	1.33	1.51
19	4	1197	CLA	CAB-C3B	-8.65	1.34	1.51

The worst 5 of 3617 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1189	CLA	OBD-CAD-CBD	-17.99	98.80	125.94
19	1	1199	CLA	OBD-CAD-CBD	-17.48	99.56	125.94
19	A	1789	CLA	OBD-CAD-CBD	-17.41	99.66	125.94
19	B	1748	CLA	OBD-CAD-CBD	-17.02	100.26	125.94
19	A	1763	CLA	OBD-CAD-CBD	-16.60	100.89	125.94

5 of 617 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	1194	CLA	NC
19	1	1194	CLA	ND
19	1	1194	CLA	NA
19	1	1308	CLA	NC
19	1	1308	CLA	ND

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	1774	BCR	C20-C21-C22-C37
23	B	1774	BCR	C20-C21-C22-C23
23	B	1780	BCR	C20-C21-C22-C23
23	B	1780	BCR	C20-C21-C22-C37
23	A	1809	BCR	C21-C20-C19-C18

There are no ring outliers.

236 monomers are involved in 2765 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1014	CLA	1	0
19	1	1142	CLA	16	1
19	1	1143	CLA	27	0
19	1	1145	CLA	15	0
19	1	1146	CLA	9	0
19	1	1148	CLA	10	0
19	1	1149	CLA	9	0
19	1	1187	CLA	13	0
19	1	1188	CLA	1	0
19	1	1189	CLA	8	0
19	1	1190	CLA	15	0
19	1	1191	CLA	6	0
19	1	1192	CLA	9	0
19	1	1193	CLA	6	1
19	1	1194	CLA	3	0
19	1	1195	CLA	1	0
19	1	1196	CLA	8	0
19	1	1197	CLA	7	0
19	1	1198	CLA	2	0
19	1	1199	CLA	16	0
19	1	1308	CLA	12	0
19	1	1505	CLA	2	0
19	2	1212	CLA	13	0
19	2	1213	CLA	25	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	1214	CLA	2	0
19	2	1215	CLA	16	0
19	2	1217	CLA	22	0
19	2	1218	CLA	1	0
19	2	1219	CLA	1	0
19	2	1221	CLA	21	0
19	2	1222	CLA	6	0
19	2	1223	CLA	19	0
20	2	1224	LMU	29	0
21	2	1225	SUC	10	0
19	2	2006	CLA	17	0
19	3	1213	CLA	4	0
19	3	1214	CLA	2	0
19	3	1215	CLA	3	0
19	3	1216	CLA	7	0
19	3	1217	CLA	14	0
19	3	1218	CLA	17	0
19	3	1219	CLA	2	0
19	3	1220	CLA	1	0
19	3	1221	CLA	17	0
19	3	1222	CLA	10	0
21	3	1223	SUC	6	0
19	3	3008	CLA	1	0
19	3	3011	CLA	13	0
19	4	1196	CLA	34	0
19	4	1197	CLA	3	0
19	4	1198	CLA	18	0
19	4	1199	CLA	21	0
19	4	1200	CLA	5	0
19	4	1201	CLA	18	0
19	4	1205	CLA	25	0
19	4	1206	CLA	11	0
19	4	1207	CLA	3	0
19	4	1208	CLA	4	0
19	4	1209	CLA	4	0
19	4	1210	CLA	10	0
19	4	1211	CLA	5	0
20	4	1212	LMU	1	0
19	4	4007	CLA	3	0
19	4	4014	CLA	14	0
19	A	1759	CLA	20	0
19	A	1760	CLA	36	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1761	CLA	16	0
19	A	1762	CLA	13	0
19	A	1763	CLA	33	0
19	A	1764	CLA	21	0
19	A	1765	CLA	32	0
19	A	1766	CLA	4	0
19	A	1767	CLA	22	0
19	A	1768	CLA	4	0
19	A	1769	CLA	21	0
19	A	1770	CLA	14	0
19	A	1771	CLA	4	0
19	A	1772	CLA	21	0
19	A	1773	CLA	8	0
19	A	1774	CLA	46	0
19	A	1776	CLA	33	0
19	A	1777	CLA	8	0
19	A	1778	CLA	8	0
19	A	1779	CLA	20	0
19	A	1780	CLA	10	0
19	A	1781	CLA	43	0
19	A	1782	CLA	51	0
19	A	1783	CLA	49	0
19	A	1784	CLA	19	0
19	A	1785	CLA	18	0
19	A	1786	CLA	7	0
19	A	1787	CLA	23	0
19	A	1788	CLA	31	0
19	A	1789	CLA	37	0
19	A	1790	CLA	19	0
19	A	1791	CLA	13	0
19	A	1792	CLA	7	0
19	A	1793	CLA	15	0
19	A	1794	CLA	6	0
19	A	1795	CLA	17	0
19	A	1796	CLA	33	0
19	A	1797	CLA	27	0
19	A	1798	CLA	6	0
19	A	1799	CLA	1	0
19	A	1800	CLA	29	0
19	A	1801	CLA	13	0
22	A	1802	PQN	7	0
23	A	1803	BCR	32	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1804	BCR	23	0
23	A	1805	BCR	48	0
23	A	1806	BCR	36	0
23	A	1807	BCR	9	0
23	A	1808	BCR	24	0
23	A	1809	BCR	9	0
20	A	1810	LMU	5	0
20	A	1811	LMU	4	0
20	A	1812	LMU	4	0
19	A	1813	CLA	21	0
19	A	1814	CLA	30	0
19	A	1815	CLA	26	0
19	A	1816	CLA	17	0
19	A	1817	CLA	44	0
20	A	7001	LMU	13	0
20	A	7003	LMU	2	0
20	A	7004	LMU	3	0
20	A	7005	LMU	14	0
20	A	7006	LMU	6	0
20	A	7008	LMU	4	17
20	A	7009	LMU	8	1
20	A	7010	LMU	5	0
20	A	7011	LMU	3	0
20	A	7013	LMU	20	0
20	A	7014	LMU	3	0
20	A	7016	LMU	21	0
20	A	7017	LMU	1	0
20	A	7019	LMU	2	0
20	A	7020	LMU	8	0
20	A	7021	LMU	9	0
20	A	7022	LMU	5	0
20	A	7023	LMU	15	0
20	A	7025	LMU	9	0
20	A	7026	LMU	6	0
20	A	7027	LMU	5	0
20	A	7030	LMU	9	0
20	A	7031	LMU	5	0
20	A	7032	LMU	18	0
20	A	7033	LMU	9	0
20	A	7034	LMU	13	0
20	A	7036	LMU	8	0
20	A	7037	LMU	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	7038	LMU	7	0
20	A	7039	LMU	7	0
20	A	7040	LMU	3	0
20	A	7041	LMU	8	0
20	A	7042	LMU	21	0
20	A	7043	LMU	9	0
20	A	7049	LMU	16	0
19	B	1735	CLA	25	0
19	B	1736	CLA	9	0
19	B	1737	CLA	31	0
19	B	1738	CLA	22	0
19	B	1739	CLA	18	0
19	B	1740	CLA	4	0
19	B	1741	CLA	9	0
19	B	1742	CLA	8	0
19	B	1743	CLA	30	0
19	B	1744	CLA	17	0
19	B	1745	CLA	8	0
19	B	1746	CLA	19	0
19	B	1747	CLA	17	0
19	B	1748	CLA	7	0
19	B	1749	CLA	17	0
19	B	1750	CLA	7	0
19	B	1751	CLA	16	0
19	B	1752	CLA	15	0
19	B	1753	CLA	30	0
19	B	1754	CLA	24	0
19	B	1755	CLA	39	0
19	B	1756	CLA	36	0
19	B	1757	CLA	13	0
19	B	1758	CLA	25	0
19	B	1759	CLA	24	0
19	B	1760	CLA	11	0
19	B	1761	CLA	29	0
19	B	1762	CLA	24	0
19	B	1763	CLA	18	0
19	B	1764	CLA	23	0
19	B	1765	CLA	30	0
19	B	1766	CLA	9	0
19	B	1767	CLA	12	0
19	B	1768	CLA	42	0
19	B	1769	CLA	47	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1770	CLA	18	0
19	B	1771	CLA	17	0
19	B	1772	CLA	2	0
22	B	1773	PQN	28	0
23	B	1774	BCR	5	0
23	B	1775	BCR	8	0
23	B	1776	BCR	18	0
23	B	1777	BCR	32	0
23	B	1778	BCR	26	0
23	B	1779	BCR	34	0
23	B	1780	BCR	32	0
24	B	1781	LMG	17	0
20	B	1782	LMU	1	0
25	B	1783	SF4	17	0
19	B	1784	CLA	18	0
21	B	8052	SUC	6	0
21	B	8053	SUC	3	0
21	B	8054	SUC	2	0
21	B	8055	SUC	4	0
21	B	8056	SUC	4	0
21	B	8059	SUC	11	0
21	B	8060	SUC	3	0
21	B	8061	SUC	1	0
21	B	8062	SUC	1	17
25	C	1082	SF4	4	0
25	C	1083	SF4	1	0
19	F	1155	CLA	1	0
19	F	1156	CLA	5	0
19	F	1157	CLA	13	0
19	G	1099	CLA	4	0
19	H	1079	CLA	27	0
19	H	1080	CLA	13	0
19	H	1081	CLA	3	0
21	H	1082	SUC	14	0
19	I	1031	CLA	12	0
23	I	1032	BCR	38	0
19	J	1043	CLA	14	0
19	L	1167	CLA	27	0
19	L	1168	CLA	9	0
23	L	1169	BCR	36	0
20	L	1170	LMU	1	0
19	R	1054	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	R	1055	CLA	4	0
20	R	1056	LMU	9	1

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	165/241 (68%)	1.37	40 (24%) 1 1	21, 24, 25, 25	0
2	2	176/269 (65%)	0.93	38 (21%) 1 1	21, 23, 24, 25	0
3	3	153/276 (55%)	1.18	31 (20%) 1 1	49, 78, 110, 112	0
4	4	166/251 (66%)	0.56	13 (7%) 16 13	21, 23, 24, 25	0
5	A	730/758 (96%)	0.66	56 (7%) 16 14	20, 22, 23, 25	0
6	B	733/734 (99%)	0.71	64 (8%) 13 12	20, 22, 24, 25	0
7	C	81/81 (100%)	0.87	11 (13%) 4 4	21, 22, 23, 23	0
8	D	138/212 (65%)	0.99	30 (21%) 1 1	21, 23, 24, 25	0
9	E	65/143 (45%)	0.69	9 (13%) 4 4	21, 22, 24, 24	0
10	F	154/231 (66%)	0.65	12 (7%) 16 13	21, 22, 23, 24	0
11	G	95/167 (56%)	0.99	13 (13%) 4 4	21, 23, 24, 25	0
12	H	69/144 (47%)	0.92	10 (14%) 3 3	21, 23, 24, 25	0
13	I	30/40 (75%)	0.43	2 (6%) 21 17	21, 22, 23, 23	0
14	J	42/44 (95%)	0.54	3 (7%) 19 16	21, 23, 23, 24	0
15	K	84/131 (64%)	1.54	24 (28%) 1 1	21, 24, 24, 26	0
16	L	162/216 (75%)	0.63	18 (11%) 7 7	20, 23, 24, 25	0
17	N	85/170 (50%)	0.68	7 (8%) 14 12	22, 23, 24, 25	0
18	R	0/53	-	-	-	-
All	All	3128/4161 (75%)	0.80	381 (12%) 5 6	20, 23, 25, 112	0

The worst 5 of 381 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	10.6
3	3	40	SER	8.5
1	1	92	GLY	7.9

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Mol	Chain	Res	Type	RSRZ
1	1	87	ASN	7.5
15	K	64	GLY	6.9

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
19	CLA	1	1197	51/65	0.59	0.53	4.78	2,42,60,60	0
19	CLA	4	1200	50/65	0.74	0.42	3.59	2,21,60,60	0
23	BCR	A	1803	40/40	0.63	0.44	2.48	2,45,60,60	0
19	CLA	A	1801	55/65	0.64	0.44	2.44	2,44,60,60	0
19	CLA	A	1776	58/65	0.81	0.36	2.11	2,20,60,60	0
23	BCR	I	1032	40/40	0.67	0.42	2.08	2,38,60,60	0
23	BCR	L	1169	40/40	0.72	0.48	2.03	2,18,60,60	0
23	BCR	A	1804	40/40	0.72	0.40	2.03	2,34,60,60	0
19	CLA	A	1792	46/65	0.80	0.41	1.97	2,20,60,60	0
23	BCR	B	1774	40/40	0.70	0.48	1.84	2,33,60,60	0
19	CLA	A	1780	58/65	0.78	0.36	1.83	2,18,60,60	0
23	BCR	A	1806	40/40	0.78	0.35	1.67	2,31,60,60	0
19	CLA	A	1775	36/65	0.66	0.40	1.63	2,51,60,60	0
23	BCR	A	1807	39/40	0.83	0.32	1.43	2,8,60,60	0
19	CLA	4	1199	55/65	0.68	0.39	1.21	4,39,60,60	0
19	CLA	4	1203	25/65	0.69	0.29	1.19	2,29,60,60	0
19	CLA	B	1746	46/65	0.64	0.42	0.96	2,28,60,60	0
20	LMU	A	7047	35/35	0.63	0.33	0.93	2,40,60,60	0
24	LMG	B	1781	49/55	0.77	0.35	0.93	2,20,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	A	1773	52/65	0.79	0.36	0.90	2,33,60,60	0
23	BCR	B	1775	40/40	0.84	0.30	0.84	2,5,60,60	0
19	CLA	G	1099	51/65	0.70	0.42	0.69	2,44,60,60	0
19	CLA	A	1782	65/65	0.81	0.33	0.68	2,16,60,60	0
19	CLA	A	1766	45/65	0.78	0.35	0.66	2,38,60,60	0
19	CLA	A	1774	60/65	0.84	0.33	0.64	2,11,52,60	0
19	CLA	A	1786	50/65	0.83	0.29	0.60	2,32,60,60	0
19	CLA	2	1222	50/65	0.75	0.31	0.58	2,25,60,60	0
19	CLA	H	1079	58/65	0.82	0.33	0.57	2,15,60,60	0
20	LMU	L	1170	35/35	0.75	0.29	0.56	2,22,60,60	0
23	BCR	B	1777	40/40	0.82	0.33	0.53	2,11,60,60	0
19	CLA	4	1196	55/65	0.74	0.36	0.52	2,33,60,60	0
19	CLA	4	1197	36/65	0.78	0.36	0.51	2,26,60,60	0
21	SUC	2	1225	22/23	0.74	0.28	0.51	2,35,60,60	0
23	BCR	A	1805	40/40	0.82	0.33	0.49	2,5,44,60	0
19	CLA	B	1749	61/65	0.82	0.30	0.45	2,16,60,60	0
23	BCR	B	1776	40/40	0.72	0.39	0.41	2,21,60,60	0
19	CLA	A	1764	60/65	0.90	0.30	0.40	2,10,60,60	0
19	CLA	A	1800	65/65	0.83	0.31	0.38	2,22,60,60	0
19	CLA	B	1771	65/65	0.86	0.32	0.34	2,2,55,60	0
23	BCR	B	1778	40/40	0.88	0.28	0.32	2,2,60,60	0
19	CLA	A	1787	60/65	0.82	0.28	0.29	2,18,60,60	0
19	CLA	B	1767	60/65	0.83	0.32	0.27	2,2,60,60	0
19	CLA	1	1192	61/65	0.72	0.31	0.26	2,35,60,60	0
23	BCR	B	1780	40/40	0.81	0.33	0.25	2,10,60,60	0
19	CLA	B	1762	59/65	0.85	0.28	0.22	2,6,60,60	0
19	CLA	4	1209	36/65	0.86	0.24	0.21	2,21,60,60	0
19	CLA	A	1777	51/65	0.74	0.30	0.19	2,44,60,60	0
19	CLA	B	1754	54/65	0.84	0.31	0.19	2,15,60,60	0
19	CLA	A	1781	59/65	0.82	0.29	0.15	2,25,60,60	0
19	CLA	B	1772	36/65	0.80	0.33	0.15	2,52,60,60	0
19	CLA	A	1790	50/65	0.84	0.27	0.14	2,18,56,60	0
19	CLA	A	1762	56/65	0.85	0.30	0.14	2,2,54,60	0
19	CLA	B	1736	45/65	0.84	0.27	0.13	2,14,56,60	0
19	CLA	3	1212	25/65	0.69	0.43	0.12	15,54,60,60	0
19	CLA	B	1784	65/65	0.88	0.28	0.12	2,2,55,60	0
19	CLA	B	1764	45/65	0.83	0.28	0.12	2,16,60,60	0
19	CLA	L	1167	47/65	0.84	0.26	0.08	2,13,45,60	0
19	CLA	B	1735	65/65	0.83	0.28	0.08	2,11,60,60	0
19	CLA	I	1031	60/65	0.84	0.30	0.08	2,18,60,60	0
19	CLA	B	1750	50/65	0.84	0.29	0.07	2,37,60,60	0
19	CLA	A	1760	55/65	0.83	0.31	0.07	2,11,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	B	1770	65/65	0.85	0.29	0.07	2,11,60,60	0
19	CLA	A	1783	65/65	0.88	0.29	0.06	2,2,50,60	0
19	CLA	B	1742	55/65	0.79	0.29	0.05	2,28,60,60	0
19	CLA	B	1744	60/65	0.78	0.35	0.04	2,19,60,60	0
19	CLA	2	1215	50/65	0.73	0.30	0.04	2,48,60,60	0
19	CLA	A	1767	65/65	0.76	0.39	0.04	2,15,60,60	0
19	CLA	H	1081	50/65	0.79	0.31	0.02	2,27,60,60	0
19	CLA	B	1745	60/65	0.71	0.35	0.00	2,40,60,60	0
19	CLA	A	1784	55/65	0.86	0.29	-0.01	2,12,60,60	0
19	CLA	A	1761	54/65	0.81	0.28	-0.01	2,10,60,60	0
19	CLA	A	1814	65/65	0.88	0.28	-0.01	2,4,48,60	0
19	CLA	B	1751	46/65	0.78	0.33	-0.02	2,34,60,60	0
19	CLA	B	1763	50/65	0.85	0.28	-0.06	2,11,53,60	0
19	CLA	A	1785	65/65	0.85	0.29	-0.09	2,12,60,60	0
19	CLA	L	1168	50/65	0.82	0.26	-0.10	2,18,60,60	0
19	CLA	A	1769	50/65	0.84	0.28	-0.11	2,29,60,60	0
19	CLA	A	1817	65/65	0.85	0.31	-0.14	2,14,56,60	0
19	CLA	B	1741	54/65	0.82	0.25	-0.14	2,17,60,60	0
19	CLA	B	1747	53/65	0.85	0.28	-0.20	2,14,60,60	0
19	CLA	1	1191	36/65	0.73	0.29	-0.20	2,52,60,60	0
22	PQN	A	1802	33/33	0.83	0.33	-0.20	2,4,59,60	0
19	CLA	F	1156	41/65	0.67	0.33	-0.24	2,41,60,60	0
23	BCR	A	1808	40/40	0.90	0.24	-0.25	2,4,50,60	0
19	CLA	A	1815	65/65	0.86	0.29	-0.28	2,2,60,60	0
19	CLA	B	1739	60/65	0.89	0.27	-0.29	2,2,60,60	0
19	CLA	A	1796	65/65	0.84	0.31	-0.29	2,8,60,60	0
19	CLA	2	1221	50/65	0.77	0.31	-0.33	2,18,60,60	0
19	CLA	B	1752	55/65	0.84	0.29	-0.34	2,30,60,60	0
19	CLA	A	1778	42/65	0.77	0.28	-0.35	2,46,60,60	0
19	CLA	B	1738	65/65	0.90	0.26	-0.36	2,2,53,60	0
19	CLA	B	1758	65/65	0.87	0.26	-0.36	2,11,46,60	0
19	CLA	B	1765	45/65	0.62	0.37	-0.36	12,37,60,60	0
19	CLA	A	1788	65/65	0.88	0.25	-0.37	2,9,59,60	0
19	CLA	B	1748	41/65	0.90	0.27	-0.38	2,5,40,60	0
19	CLA	B	1760	50/65	0.89	0.28	-0.39	2,12,60,60	0
19	CLA	B	1756	65/65	0.82	0.32	-0.42	2,15,60,60	0
19	CLA	A	1779	50/65	0.89	0.23	-0.42	2,7,60,60	0
19	CLA	B	1755	58/65	0.85	0.31	-0.42	2,13,60,60	0
19	CLA	B	1737	61/65	0.89	0.27	-0.45	2,9,48,60	0
20	LMU	A	1811	35/35	0.77	0.26	-0.47	2,27,60,60	0
19	CLA	A	1795	51/65	0.86	0.28	-0.49	2,12,60,60	0
20	LMU	A	1810	35/35	0.69	0.24	-0.51	2,26,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	A	1772	54/65	0.83	0.28	-0.51	2,31,60,60	0
19	CLA	B	1761	50/65	0.86	0.24	-0.51	2,7,51,60	0
19	CLA	F	1155	36/65	0.88	0.24	-0.51	2,17,60,60	0
19	CLA	A	1763	46/65	0.82	0.29	-0.52	2,20,60,60	0
19	CLA	B	1740	25/65	0.86	0.28	-0.53	2,2,60,60	0
19	CLA	A	1759	46/65	0.86	0.31	-0.54	2,14,49,60	0
19	CLA	A	1793	65/65	0.84	0.29	-0.55	2,6,60,60	0
19	CLA	B	1768	65/65	0.88	0.24	-0.56	2,7,60,60	0
19	CLA	A	1816	54/65	0.92	0.27	-0.57	2,6,45,60	0
19	CLA	1	1196	36/65	0.76	0.31	-0.61	2,35,60,60	0
19	CLA	A	1765	52/65	0.90	0.24	-0.67	2,10,60,60	0
19	CLA	A	1794	47/65	0.89	0.24	-0.68	2,8,50,60	0
19	CLA	A	1789	65/65	0.88	0.25	-0.68	2,14,60,60	0
19	CLA	B	1743	65/65	0.90	0.25	-0.69	2,13,60,60	0
19	CLA	B	1753	65/65	0.85	0.26	-0.69	2,17,60,60	0
19	CLA	A	1813	65/65	0.90	0.27	-0.70	2,2,48,60	0
19	CLA	B	1757	65/65	0.89	0.27	-0.71	2,10,56,60	0
19	CLA	3	1218	56/65	0.77	0.32	-0.71	2,36,60,60	0
19	CLA	4	1205	50/65	0.80	0.24	-0.75	2,20,60,60	0
19	CLA	1	1195	25/65	0.83	0.31	-0.78	11,37,60,60	0
19	CLA	B	1759	65/65	0.90	0.25	-0.83	2,6,53,60	0
19	CLA	A	1771	50/65	0.82	0.27	-0.84	2,21,60,60	0
19	CLA	1	1198	25/65	0.79	0.26	-0.91	2,42,60,60	0
22	PQN	B	1773	33/33	0.86	0.28	-0.92	2,2,46,51	0
19	CLA	4	1208	25/65	0.88	0.18	-0.92	2,2,26,32	0
19	CLA	1	1190	46/65	0.80	0.28	-0.96	2,35,60,60	0
19	CLA	B	1769	47/65	0.89	0.24	-0.96	2,5,55,60	0
23	BCR	B	1779	40/40	0.89	0.22	-0.97	2,6,60,60	0
19	CLA	1	1189	47/65	0.75	0.27	-1.03	2,17,60,60	0
19	CLA	3	1216	25/65	0.76	0.26	-1.04	2,56,60,60	0
19	CLA	3	1221	65/65	0.70	0.32	-1.14	2,26,60,60	0
25	SF4	C	1083	8/8	0.96	0.08	-2.02	12,19,20,24	0
25	SF4	C	1082	8/8	0.97	0.08	-2.30	18,22,26,32	0
25	SF4	B	1783	8/8	0.98	0.06	-2.71	23,24,24,25	0
19	CLA	4	1211	46/65	0.76	0.31	-	2,45,60,60	0
19	CLA	A	1770	25/65	0.80	0.28	-	2,31,60,60	0
20	LMU	A	7009	34/35	0.80	0.24	-	2,22,60,60	0
20	LMU	A	7037	35/35	0.68	0.29	-	2,30,60,60	0
21	SUC	B	8056	23/23	0.75	0.20	-	2,31,56,60	0
20	LMU	A	7033	35/35	0.81	0.20	-	2,46,60,60	0
20	LMU	A	7010	35/35	0.53	0.51	-	2,39,60,60	0
20	LMU	A	7038	35/35	0.58	0.32	-	2,34,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	1	1308	48/65	0.76	0.29	-	2,34,60,60	0
19	CLA	2	1218	25/65	0.86	0.19	-	2,12,60,60	0
19	CLA	2	1219	36/65	0.77	0.28	-	2,34,60,60	0
19	CLA	R	1054	57/65	0.72	0.29	-	2,38,60,60	0
19	CLA	3	3008	50/65	0.62	0.42	-	2,56,60,60	0
19	CLA	J	1043	61/65	0.78	0.24	-	2,19,60,60	0
20	LMU	A	7043	35/35	0.69	0.27	-	2,41,60,60	0
19	CLA	3	3015	25/65	0.74	0.30	-	2,42,60,60	0
20	LMU	A	7011	35/35	0.80	0.23	-	2,12,50,57	0
20	LMU	A	7030	35/35	0.77	0.23	-	2,16,60,60	0
19	CLA	1	1145	55/65	0.67	0.46	-	2,47,60,60	0
19	CLA	1	1014	51/65	0.62	0.43	-	2,51,60,60	0
20	LMU	4	1212	35/35	0.76	0.40	-	2,37,60,60	0
19	CLA	1	1188	41/65	0.86	0.22	-	2,41,60,60	0
19	CLA	2	1216	25/65	0.78	0.23	-	2,57,60,60	0
20	LMU	A	7036	34/35	0.79	0.23	-	2,23,60,60	0
21	SUC	B	8054	23/23	0.66	0.30	-	2,30,60,60	0
19	CLA	4	1202	25/65	0.68	0.37	-	2,39,60,60	0
19	CLA	A	1798	55/65	0.67	0.36	-	2,44,60,60	0
20	LMU	A	7001	35/35	0.75	0.25	-	2,37,60,60	0
19	CLA	2	1217	65/65	0.77	0.25	-	2,24,60,60	0
19	CLA	2	2006	50/65	0.77	0.41	-	2,33,60,60	0
20	LMU	A	7034	35/35	0.76	0.29	-	2,21,55,60	0
20	LMU	B	1782	25/35	0.81	0.21	-	2,36,60,60	0
19	CLA	4	1210	25/65	0.76	0.29	-	2,35,60,60	0
19	CLA	3	1219	25/65	0.79	0.26	-	2,37,60,60	0
20	LMU	2	1224	35/35	0.68	0.27	-	2,21,60,60	0
19	CLA	1	1505	55/65	0.56	0.41	-	2,49,60,60	0
19	CLA	1	1307	25/65	0.73	0.49	-	2,48,60,60	0
19	CLA	1	1193	51/65	0.71	0.32	-	2,36,60,60	0
19	CLA	1	1194	25/65	0.73	0.27	-	2,31,60,60	0
19	CLA	1	1148	55/65	0.72	0.46	-	2,46,60,60	0
19	CLA	1	1309	25/65	0.62	0.56	-	2,42,60,60	0
19	CLA	H	1080	55/65	0.67	0.35	-	2,33,60,60	0
20	LMU	A	7005	35/35	0.80	0.20	-	2,28,59,60	0
23	BCR	A	1809	40/40	0.59	0.41	-	2,32,60,60	0
21	SUC	B	8051	23/23	0.77	0.35	-	2,44,60,60	0
20	LMU	A	7013	35/35	0.69	0.23	-	2,44,60,60	0
20	LMU	A	7042	35/35	0.70	0.26	-	2,38,60,60	0
20	LMU	A	7022	35/35	0.67	0.23	-	2,36,60,60	0
19	CLA	2	1212	51/65	0.77	0.23	-	2,33,60,60	0
19	CLA	1	1199	51/65	0.76	0.38	-	2,39,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	LMU	A	7028	35/35	0.75	0.24	-	2,23,60,60	0
20	LMU	A	7040	35/35	0.69	0.30	-	2,37,60,60	0
19	CLA	1	1149	46/65	0.72	0.38	-	2,43,60,60	0
20	LMU	A	7026	35/35	0.61	0.34	-	2,15,60,60	0
21	SUC	B	8060	23/23	0.76	0.24	-	6,40,60,60	0
19	CLA	3	3011	65/65	0.79	0.31	-	2,33,60,60	0
19	CLA	A	1797	59/65	0.79	0.29	-	2,30,60,60	0
19	CLA	1	1146	50/65	0.65	0.32	-	2,60,60,60	0
21	SUC	B	8059	23/23	0.83	0.24	-	2,29,60,60	0
20	LMU	A	7021	35/35	0.72	0.37	-	2,35,60,60	0
20	LMU	A	7019	35/35	0.56	0.28	-	2,43,60,60	0
19	CLA	3	1222	65/65	0.66	0.42	-	2,46,60,60	0
20	LMU	A	7016	35/35	0.55	0.40	-	2,45,60,60	0
21	SUC	H	1082	23/23	0.73	0.28	-	3,33,60,60	0
20	LMU	A	7008	35/35	0.83	0.24	-	2,34,60,60	0
19	CLA	3	1213	36/65	0.70	0.26	-	2,53,60,60	0
19	CLA	2	1213	58/65	0.83	0.23	-	2,22,60,60	0
20	LMU	A	7006	35/35	0.79	0.20	-	2,25,60,60	0
19	CLA	A	1791	45/65	0.74	0.27	-	2,37,60,60	0
20	LMU	A	7015	35/35	0.73	0.38	-	2,35,60,60	0
19	CLA	3	1220	25/65	0.68	0.26	-	2,47,60,60	0
19	CLA	1	1143	50/65	0.75	0.33	-	2,28,60,60	0
20	LMU	A	7014	35/35	0.70	0.33	-	2,45,60,60	0
19	CLA	4	1207	25/65	0.84	0.26	-	2,15,60,60	0
19	CLA	4	1206	65/65	0.82	0.27	-	2,15,60,60	0
19	CLA	3	1215	25/65	0.64	0.31	-	17,42,60,60	0
19	CLA	F	1157	53/65	0.84	0.28	-	2,22,60,60	0
19	CLA	4	4007	52/65	0.61	0.44	-	2,34,60,60	0
21	SUC	B	8061	23/23	0.67	0.32	-	2,52,60,60	0
20	LMU	A	7031	35/35	0.60	0.39	-	2,40,60,60	0
21	SUC	3	1223	23/23	0.81	0.27	-	2,27,60,60	0
19	CLA	2	1214	25/65	0.72	0.48	-	2,27,60,60	0
20	LMU	A	7025	35/35	0.71	0.24	-	2,27,60,60	0
26	UNL	B	8057	23/-	0.80	0.22	-	2,31,60,60	0
21	SUC	B	8062	23/23	0.81	0.27	-	2,34,60,60	0
20	LMU	A	7004	35/35	0.83	0.25	-	2,11,50,60	0
19	CLA	4	1204	25/65	0.78	0.40	-	2,40,60,60	0
19	CLA	4	1201	52/65	0.82	0.26	-	2,26,60,60	0
19	CLA	2	2010	25/65	0.79	0.28	-	2,36,60,60	0
20	LMU	A	7027	35/35	0.75	0.25	-	2,29,60,60	0
19	CLA	3	1217	42/65	0.75	0.27	-	2,53,60,60	0
19	CLA	R	1055	65/65	0.70	0.34	-	2,35,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	1	1187	46/65	0.69	0.25	-	2,56,60,60	0
19	CLA	1	1142	46/65	0.71	0.25	-	2,51,60,60	0
19	CLA	A	1768	54/65	0.83	0.24	-	2,28,60,60	0
20	LMU	A	1812	35/35	0.65	0.29	-	2,45,60,60	0
20	LMU	R	1056	35/35	0.81	0.24	-	2,21,60,60	0
19	CLA	A	1799	25/65	0.71	0.30	-	2,43,60,60	0
20	LMU	A	7024	35/35	0.70	0.29	-	2,35,60,60	0
20	LMU	A	7003	35/35	0.72	0.31	-	2,44,60,60	0
20	LMU	A	7020	35/35	0.77	0.22	-	2,38,60,60	0
19	CLA	3	1214	25/65	0.82	0.19	-	2,28,60,60	0
19	CLA	3	3014	25/65	0.75	0.50	-	2,47,60,60	0
19	CLA	2	1223	61/65	0.70	0.25	-	2,34,60,60	0
20	LMU	A	7023	35/35	0.70	0.27	-	2,32,60,60	0
19	CLA	1	1200	25/65	0.80	0.28	-	5,42,60,60	0
19	CLA	3	3001	25/65	0.69	0.44	-	2,30,60,60	0
21	SUC	B	8053	22/23	0.66	0.44	-	6,52,60,60	0
19	CLA	4	4014	47/65	0.75	0.29	-	2,37,60,60	0
20	LMU	A	7049	35/35	0.58	0.30	-	2,51,60,60	0
21	SUC	B	8055	23/23	0.77	0.25	-	2,41,60,60	0
20	LMU	A	7041	35/35	0.68	0.24	-	2,38,60,60	0
19	CLA	2	1220	25/65	0.81	0.42	-	2,34,60,60	0
20	LMU	A	7035	35/35	0.82	0.23	-	2,29,60,60	0
19	CLA	4	1198	65/65	0.64	0.36	-	2,32,60,60	0
20	LMU	A	7039	35/35	0.73	0.26	-	2,33,60,60	0
19	CLA	B	1766	51/65	0.66	0.38	-	2,45,60,60	0
20	LMU	A	7032	35/35	0.85	0.21	-	2,31,60,60	0
21	SUC	B	8052	23/23	0.63	0.36	-	9,40,60,60	0
20	LMU	A	7017	35/35	0.61	0.22	-	2,31,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.