



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2WSC
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-04
Resolution : 3.30 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

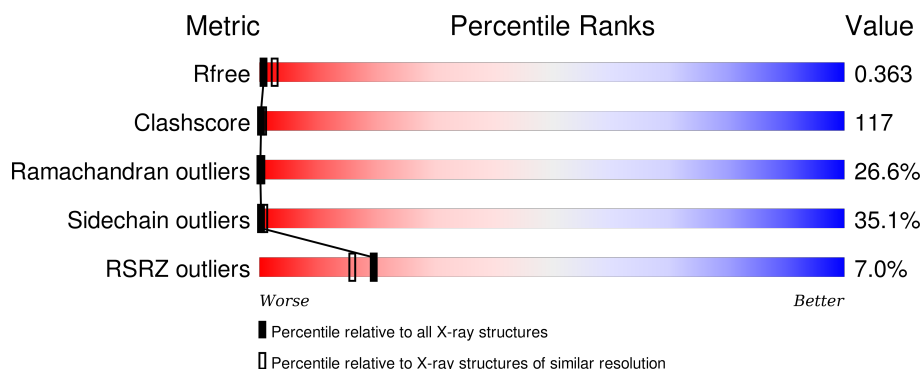
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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>10%</div> <div>30% 25% 11% 32%</div> </div>
2	2	269	<div> <div>6%</div> <div>24% 30% 10% 35%</div> </div>
3	3	276	<div> <div>8%</div> <div>16% 21% 16% 6% 41%</div> </div>
4	4	251	<div> <div>10%</div> <div>22% 27% 14% 34%</div> </div>
5	A	758	<div> <div>4%</div> <div>6% 48% 34% 9%</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	1187	X	-	-	-
19	CLA	1	1188	X	-	-	-
19	CLA	1	1189	X	-	-	-
19	CLA	1	1190	X	-	-	-
19	CLA	1	1191	X	-	-	X
19	CLA	1	1192	X	-	-	-
19	CLA	1	1193	X	-	-	-
19	CLA	1	1194	X	-	-	-
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	1201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	1212	X	-	-	-
19	CLA	2	1213	X	-	-	-
19	CLA	2	1214	X	-	-	-
19	CLA	2	1215	X	-	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	-	X	-
19	CLA	2	1221	X	-	-	-
19	CLA	2	1222	X	-	-	-
19	CLA	2	1223	X	-	-	-
19	CLA	2	1224	X	-	-	-
19	CLA	2	1227	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	3	1212	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	-	X	-
19	CLA	3	1219	X	-	-	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3002	X	-	-	-
19	CLA	3	3007	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	-	-	-
19	CLA	4	1198	X	-	X	-
19	CLA	4	1199	X	-	X	-
19	CLA	4	1200	X	-	-	X
19	CLA	4	1201	X	-	X	-
19	CLA	4	1202	X	-	-	X
19	CLA	4	1203	X	-	-	-
19	CLA	4	1204	X	-	-	-
19	CLA	4	1205	X	-	-	-
19	CLA	4	1206	X	-	-	-
19	CLA	4	1207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	1208	X	-	-	-
19	CLA	4	1209	X	-	-	-
19	CLA	4	4003	X	-	-	-
19	CLA	4	4007	X	-	-	-
19	CLA	4	4014	X	-	-	-
19	CLA	A	1759	X	-	-	-
19	CLA	A	1760	X	-	X	-
19	CLA	A	1761	X	-	X	-
19	CLA	A	1762	X	-	-	-
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	-	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	-
19	CLA	A	1777	X	-	-	X
19	CLA	A	1778	X	-	-	-
19	CLA	A	1779	X	-	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	-	-	-
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	-	-	-
19	CLA	A	1790	X	-	-	-
19	CLA	A	1791	X	-	X	-
19	CLA	A	1792	X	-	X	-
19	CLA	A	1793	X	-	X	X
19	CLA	A	1794	X	-	X	-
19	CLA	A	1795	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1796	X	-	X	-
19	CLA	A	1797	X	-	X	-
19	CLA	A	1798	X	-	X	-
19	CLA	A	1799	X	-	-	-
19	CLA	A	1800	X	-	X	-
19	CLA	A	1801	X	-	-	X
19	CLA	A	1811	X	-	-	-
19	CLA	A	1812	X	-	X	-
19	CLA	A	1813	X	-	X	-
19	CLA	A	1815	X	-	-	-
19	CLA	A	1816	X	-	X	-
19	CLA	A	1817	X	-	-	-
19	CLA	B	1735	X	-	X	-
19	CLA	B	1736	X	-	-	-
19	CLA	B	1737	X	-	X	-
19	CLA	B	1738	X	-	-	-
19	CLA	B	1739	X	-	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	X
19	CLA	B	1747	X	-	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	-
19	CLA	B	1755	X	-	X	X
19	CLA	B	1756	X	-	X	-
19	CLA	B	1757	X	-	X	-
19	CLA	B	1758	X	-	X	-
19	CLA	B	1759	X	-	X	-
19	CLA	B	1760	X	-	-	-
19	CLA	B	1761	X	-	-	-
19	CLA	B	1762	X	-	X	-
19	CLA	B	1763	X	-	-	-
19	CLA	B	1764	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1765	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	-	X	-
19	CLA	B	1771	X	-	X	-
19	CLA	B	1772	X	-	-	-
19	CLA	B	1785	X	-	X	-
19	CLA	B	1786	X	-	X	-
19	CLA	B	1787	X	-	X	-
19	CLA	F	1155	X	-	-	-
19	CLA	F	1156	X	-	-	-
19	CLA	F	1157	X	-	-	-
19	CLA	G	1099	X	-	-	-
19	CLA	H	1079	X	-	-	-
19	CLA	I	1031	X	-	-	-
19	CLA	I	1033	X	-	-	-
19	CLA	J	1043	X	-	X	-
19	CLA	J	1044	X	-	X	-
19	CLA	J	1045	X	-	X	-
19	CLA	J	1046	X	-	-	-
19	CLA	K	1085	X	-	X	-
19	CLA	K	1142	X	-	X	-
19	CLA	K	1146	X	-	-	-
19	CLA	K	3009	X	-	-	-
19	CLA	L	1166	X	-	-	-
19	CLA	L	1167	X	-	-	-
19	CLA	L	1168	X	-	-	-
19	CLA	L	1505	X	-	-	-
19	CLA	R	1054	X	-	-	-
19	CLA	R	1055	X	-	-	-
20	LMU	A	7016	-	-	X	-
20	LMU	A	7020	-	-	X	-
20	LMU	A	7021	-	-	X	-
20	LMU	A	7023	-	-	X	-
20	LMU	A	7032	-	-	X	-
20	LMU	A	7037	-	-	X	-
20	LMU	A	7042	-	-	X	-
20	LMU	R	1057	X	-	-	-
21	SUC	2	1226	X	-	X	-
21	SUC	3	1221	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	SUC	B	8051	X	-	-	-
21	SUC	B	8052	X	-	X	-
21	SUC	B	8053	X	-	-	-
21	SUC	B	8054	X	-	X	-
21	SUC	B	8055	X	-	X	-
21	SUC	B	8056	X	-	-	-
21	SUC	B	8059	X	-	X	-
21	SUC	B	8060	X	-	-	-
21	SUC	B	8061	X	-	-	-
21	SUC	B	8062	X	-	X	-
21	SUC	H	1080	X	-	-	-
22	BCR	3	1220	-	-	X	-
22	BCR	A	1803	-	-	X	X
22	BCR	A	1804	-	-	X	-
22	BCR	A	1805	-	-	X	-
22	BCR	A	1806	-	-	X	X
22	BCR	A	1807	-	-	X	-
22	BCR	A	1808	-	-	X	X
22	BCR	B	1775	-	-	-	X
22	BCR	B	1777	-	-	X	-
22	BCR	B	1778	-	-	X	-
22	BCR	B	1779	-	-	X	-
22	BCR	B	1780	-	-	X	-
22	BCR	B	1781	-	-	-	X
22	BCR	I	1032	-	-	X	X
22	BCR	L	1169	-	-	X	X
23	PQN	A	1802	X	-	-	-
23	PQN	B	1773	X	-	X	-
24	LMG	B	1783	-	-	X	-
25	SF4	B	1784	-	-	X	-
25	SF4	C	1082	-	-	X	-
25	SF4	C	1083	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36379 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	162	Total	C	N	O	S	0	0	0
			1254	826	203	220	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			

There is a discrepancy between the modelled and reference sequences:

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

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

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

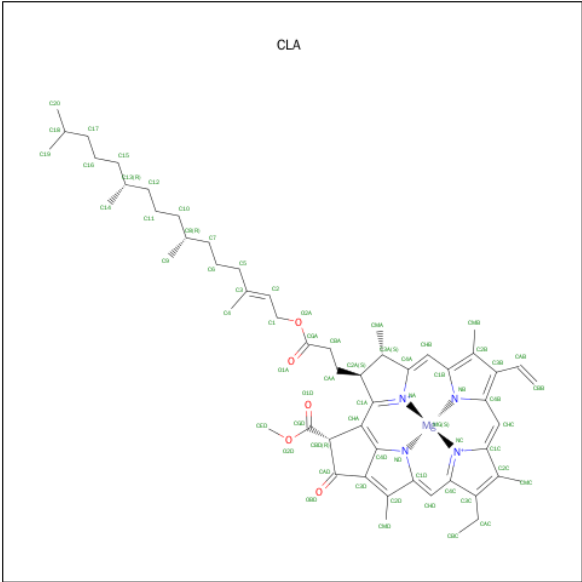
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

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

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

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	3	1	Total	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	O	0	0
			55	45	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
			50	40	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
			57	47	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		

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

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

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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
			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
			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
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
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		

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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
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	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		

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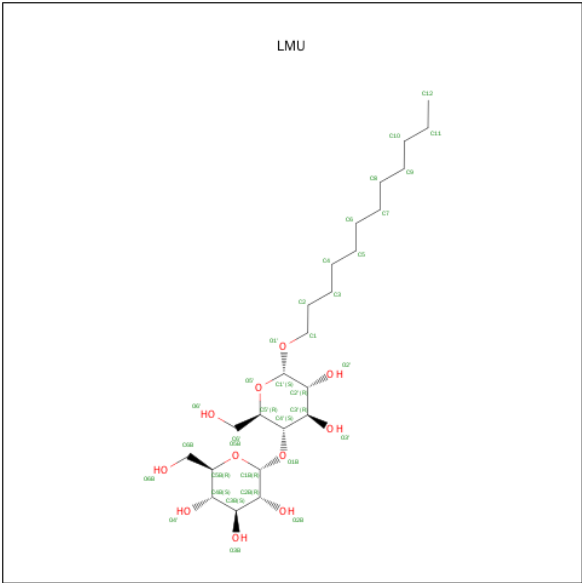
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	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
			46	36	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	J	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			42	34	1	4		
19	3	1	Total	C	Mg	N	0	0
			50	40	1	4		
19	K	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	3	1	Total	C	Mg	N	0	0
			65	55	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	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
			52	42	1	4		
19	4	1	Total	C	Mg	N	0	0
			47	37	1	4		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	1	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	4	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	B	1	Total	C	O	0	0
			25	14	11		
20	K	1	Total	C	O	0	0
			35	24	11		
20	L	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	2	1	Total	C	O	0	0
			35	24	11		
20	1	1	Total	C	O	0	0
			35	24	11		
20	3	1	Total	C	O	0	0
			35	24	11		
20	2	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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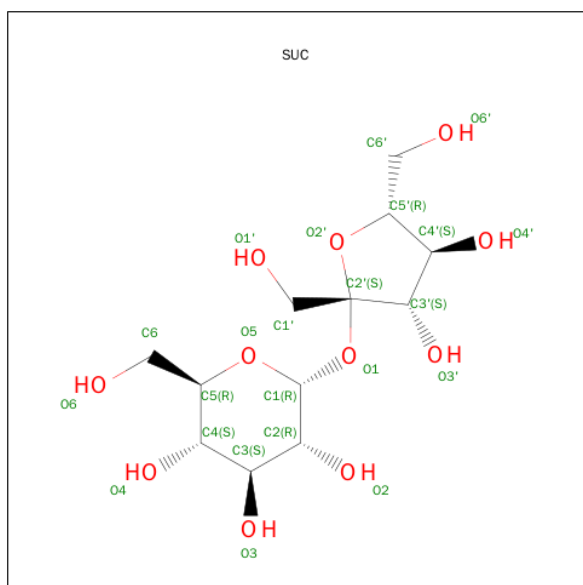
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

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



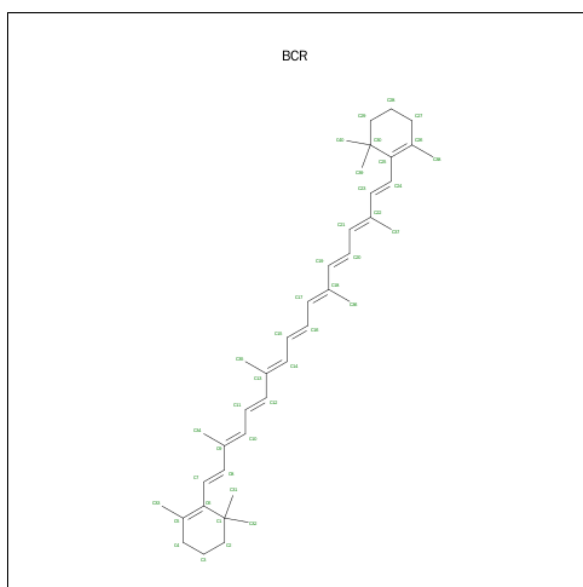
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			22	12	10		
21	3	1	Total	C	O	0	0
			23	12	11		
21	H	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total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

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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		

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



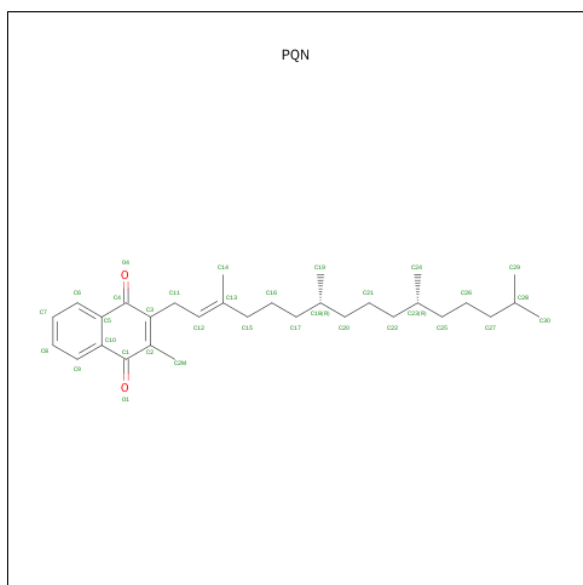
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	3	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		

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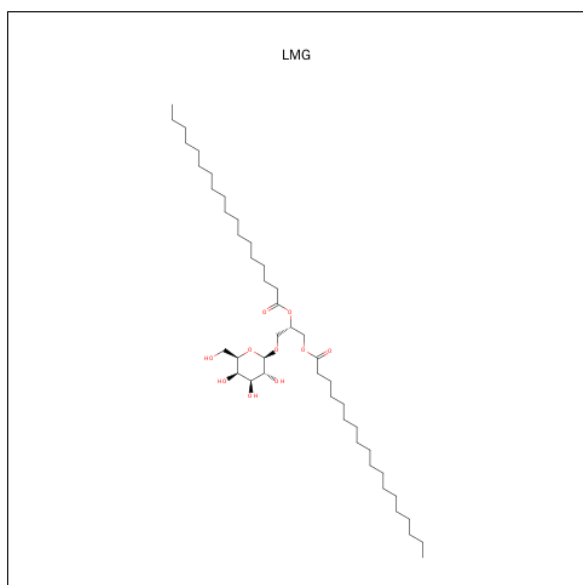
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total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

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

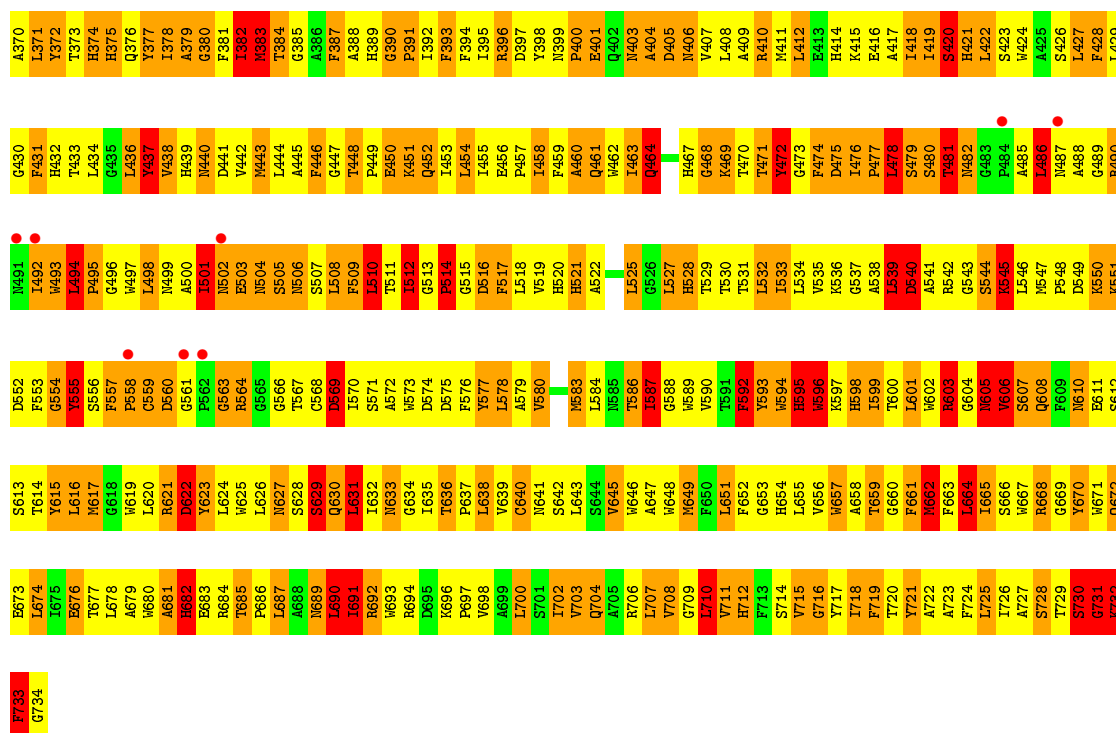


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		

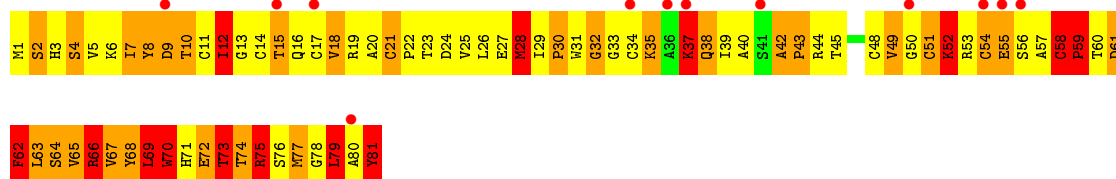
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

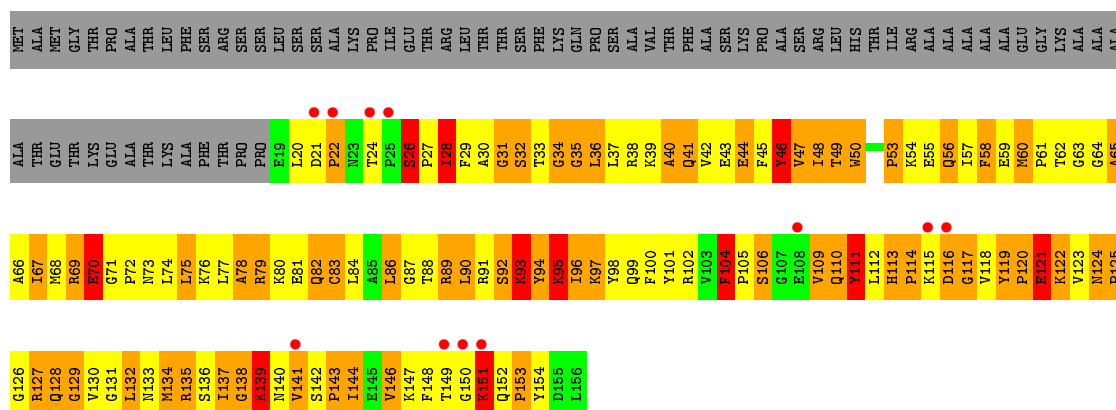




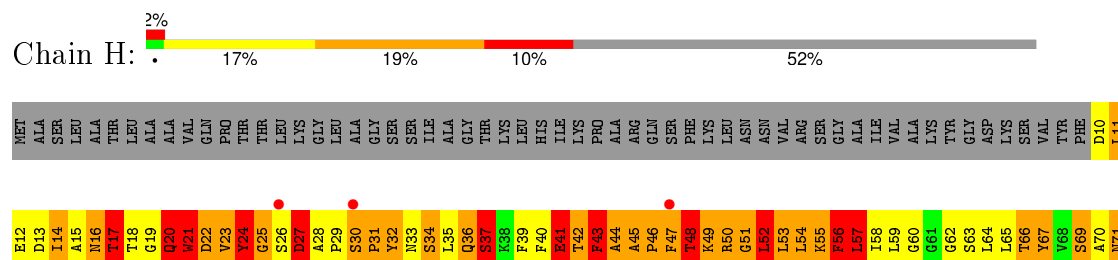
• Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

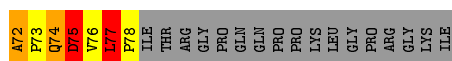


• Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC

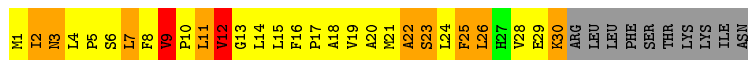


• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC





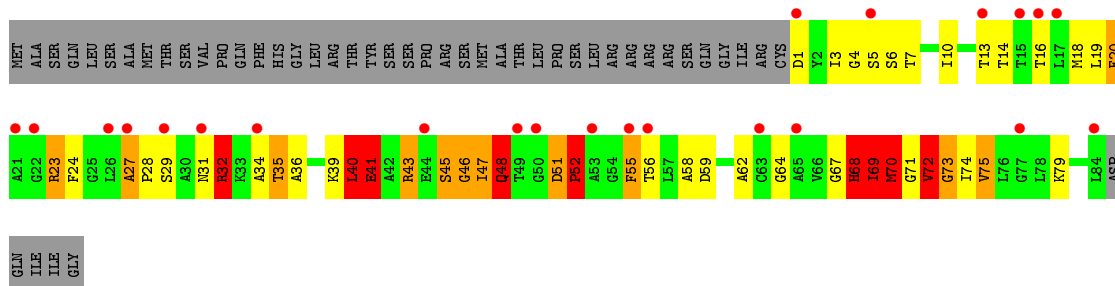
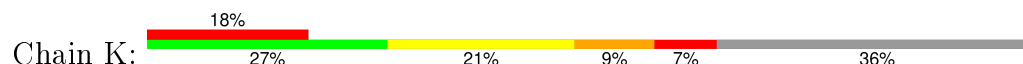
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



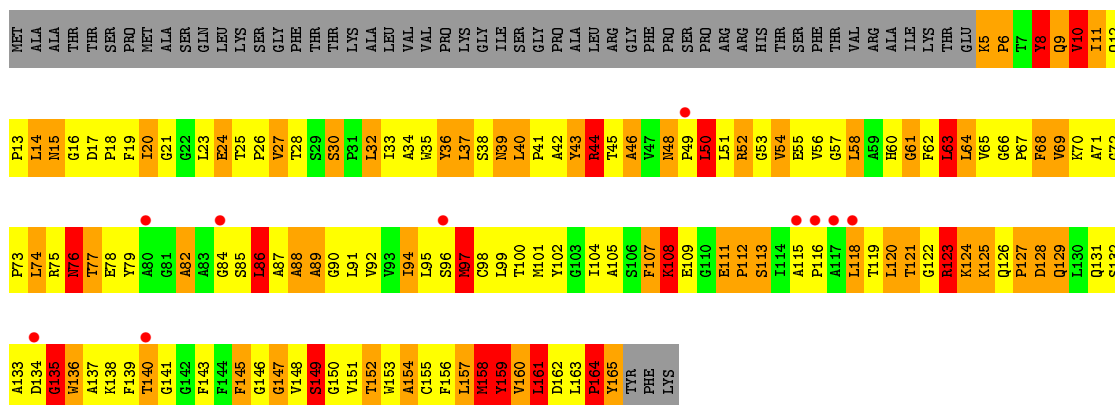
• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX



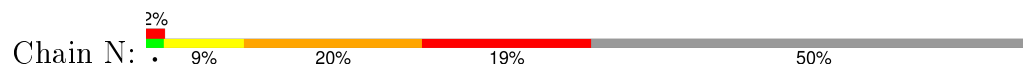
• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

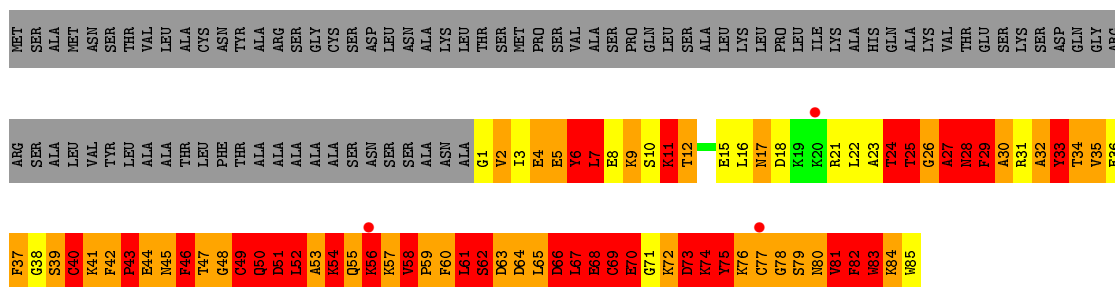


• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

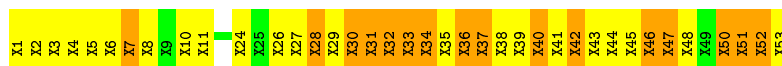
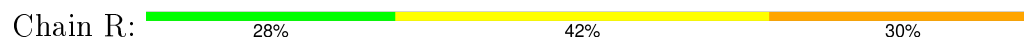


• Molecule 17: PHOTOSYSTEM I-N SUBUNIT





- 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	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 49.14 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 98.5 (49.14-3.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.363 , 0.366 0.358 , 0.363	Depositor DCC
R_{free} test set	4345 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 81.2	EDS
Estimated twinning fraction	0.032 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 93389 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	36379	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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	0.48	0/1303	0.72	3/1774 (0.2%)
2	2	0.45	0/1420	0.71	0/1943
3	3	0.87	6/1292 (0.5%)	0.96	3/1743 (0.2%)
4	4	0.49	0/1359	0.75	2/1851 (0.1%)
5	A	0.95	3/5938 (0.1%)	1.04	11/8104 (0.1%)
6	B	0.95	2/6058 (0.0%)	1.02	14/8278 (0.2%)
7	C	1.43	7/632 (1.1%)	1.33	4/856 (0.5%)
8	D	1.10	0/1122	1.05	0/1514
9	E	1.15	0/530	1.17	2/718 (0.3%)
10	F	1.10	1/1250 (0.1%)	1.07	2/1687 (0.1%)
11	G	1.07	0/760	1.28	9/1031 (0.9%)
12	H	1.16	0/543	1.19	3/741 (0.4%)
13	I	1.00	0/235	0.97	0/320
14	J	1.02	0/349	1.09	1/475 (0.2%)
15	K	0.55	0/599	0.83	1/810 (0.1%)
16	L	1.08	0/1238	1.10	5/1691 (0.3%)
17	N	1.23	1/699 (0.1%)	1.33	7/936 (0.7%)
All	All	0.94	20/25327 (0.1%)	1.02	67/34472 (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	1
3	3	0	19
5	A	0	28
6	B	0	20
7	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	2
16	L	0	3
17	N	0	21
18	R	0	17
All	All	1	166

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.88	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
6	B	640	CYS	CB-SG	7.67	1.95	1.82
7	C	72	GLU	CD-OE1	-7.43	1.17	1.25
3	3	93	PHE	CD2-CE2	7.38	1.54	1.39

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	732	LYS	N-CA-C	-8.11	89.10	111.00
5	A	93	LEU	CA-CB-CG	8.06	133.84	115.30
5	A	530	LEU	CA-CB-CG	7.27	132.02	115.30
6	B	486	LEU	CA-CB-CG	7.27	132.01	115.30
6	B	315	LEU	CA-CB-CG	7.21	131.88	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

5 of 166 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	182	ALA	Peptide
1	1	183	ASP	Peptide
1	1	184	PRO	Peptide
2	2	120	ASN	Peptide
3	3	49	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	1230	91	1
2	2	1374	0	1329	142	0
3	3	1254	0	1221	331	1
4	4	1319	0	1283	201	10
5	A	5745	0	5595	1659	0
6	B	5848	0	5655	1447	1
7	C	619	0	608	236	0
8	D	1095	0	1112	226	0
9	E	520	0	528	150	0
10	F	1221	0	1246	289	0
11	G	740	0	709	296	7
12	H	529	0	514	120	0
13	I	229	0	252	58	0
14	J	338	0	340	80	0
15	K	593	0	619	65	1
16	L	1203	0	1213	326	10
17	N	685	0	671	447	7
18	R	265	0	67	77	0
19	1	644	0	429	113	1
19	2	658	0	480	160	0
19	3	548	0	326	115	0
19	4	699	0	454	157	0
19	A	2777	0	2599	1119	1
19	B	2372	0	2285	808	0
19	F	130	0	86	27	0
19	G	51	0	40	6	0
19	H	65	0	71	19	0
19	I	115	0	106	26	0
19	J	202	0	169	98	0
19	K	210	0	177	44	1
19	L	202	0	158	40	0
19	R	122	0	123	17	0
20	1	70	0	92	15	0
20	2	105	0	138	15	1
20	3	35	0	46	3	0
20	4	35	0	46	0	0
20	A	1153	0	1505	396	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	25	0	23	1	0
20	K	35	0	45	6	0
20	L	35	0	46	3	0
20	R	70	0	91	24	0
21	2	22	0	19	10	0
21	3	23	0	22	14	0
21	B	230	0	218	85	0
21	H	23	0	20	5	0
22	3	40	0	54	21	0
22	A	240	0	323	250	0
22	B	320	0	432	225	0
22	I	40	0	54	47	0
22	L	80	0	105	61	0
23	A	33	0	46	12	0
23	B	33	0	46	33	0
24	B	49	0	71	30	0
25	B	8	0	0	18	0
25	C	16	0	0	9	0
26	B	23	0	0	2	0
All	All	36379	0	35137	8375	21

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 117.

The worst 5 of 8375 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:SD	19:4:1201:CLA:HBB1	1.28	1.66
19:A:1776:CLA:H92	22:A:1805:BCR:C37	1.17	1.58
6:B:25:ILE:HG21	22:L:1169:BCR:C29	1.11	1.58
5:A:51:THR:HG21	19:A:1795:CLA:CBB	1.24	1.57
20:A:7036:LMU:C2	20:A:7036:LMU:H82	1.34	1.57

The worst 5 of 21 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)
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.92	1.28
11:G:31:MET:CE	17:N:85:TRP:CE2[2_546]	1.19	1.01
11:G:31:MET:SD	17:N:85:TRP:CE2[2_546]	1.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	1.50	0.70
11:G:31:MET:SD	17:N:85:TRP:CD2[2_546]	1.65	0.55

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%)	83 (52%)	43 (27%)	35 (22%)	0	0
2	2	174/269 (65%)	88 (51%)	56 (32%)	30 (17%)	0	1
3	3	156/276 (56%)	78 (50%)	43 (28%)	35 (22%)	0	0
4	4	164/251 (65%)	79 (48%)	47 (29%)	38 (23%)	0	0
5	A	726/758 (96%)	334 (46%)	200 (28%)	192 (26%)	0	0
6	B	731/734 (100%)	361 (49%)	189 (26%)	181 (25%)	0	0
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	48 (35%)	42 (31%)	46 (34%)	0	0
9	E	63/143 (44%)	29 (46%)	14 (22%)	20 (32%)	0	0
10	F	152/231 (66%)	67 (44%)	44 (29%)	41 (27%)	0	0
11	G	93/167 (56%)	35 (38%)	28 (30%)	30 (32%)	0	0
12	H	67/144 (46%)	28 (42%)	15 (22%)	24 (36%)	0	0
13	I	28/40 (70%)	10 (36%)	11 (39%)	7 (25%)	0	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	49 (60%)	15 (18%)	18 (22%)	0	0
16	L	159/216 (74%)	66 (42%)	47 (30%)	46 (29%)	0	0
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0
All	All	3094/4108 (75%)	1419 (46%)	853 (28%)	822 (27%)	0	0

5 of 822 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	29	LEU
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU

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%)	102 (80%)	25 (20%)	1	7
2	2	140/216 (65%)	107 (76%)	33 (24%)	1	3
3	3	120/215 (56%)	82 (68%)	38 (32%)	0	1
4	4	138/201 (69%)	103 (75%)	35 (25%)	1	2
5	A	592/618 (96%)	392 (66%)	200 (34%)	0	1
6	B	598/600 (100%)	367 (61%)	231 (39%)	0	0
7	C	70/70 (100%)	40 (57%)	30 (43%)	0	0
8	D	118/173 (68%)	75 (64%)	43 (36%)	0	1
9	E	56/114 (49%)	37 (66%)	19 (34%)	0	1
10	F	127/190 (67%)	73 (58%)	54 (42%)	0	0
11	G	79/144 (55%)	46 (58%)	33 (42%)	0	0
12	H	57/115 (50%)	26 (46%)	31 (54%)	0	0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0	1
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	1
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	1
16	L	124/169 (73%)	81 (65%)	43 (35%)	0	1
17	N	74/139 (53%)	33 (45%)	41 (55%)	0	0
All	All	2543/3331 (76%)	1650 (65%)	893 (35%)	0	1

5 of 893 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	246	THR
6	B	551	LYS
16	L	63	LEU
6	B	285	LEU
6	B	419	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 256 ligands modelled in this entry, 1 is unknown - leaving 255 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	1187	1	36,54,73	2.53	13 (36%)	41,90,113	5.54	26 (63%)
19	CLA	1	1188	-	37,55,73	2.36	9 (24%)	42,91,113	4.62	20 (47%)
19	CLA	1	1189	-	37,55,73	2.43	10 (27%)	42,91,113	5.15	18 (42%)
19	CLA	1	1190	-	36,54,73	2.54	11 (30%)	41,90,113	4.44	17 (41%)
19	CLA	1	1191	-	24,44,73	2.97	8 (33%)	28,78,113	4.64	13 (46%)
19	CLA	1	1192	-	51,69,73	2.16	10 (19%)	56,108,113	3.72	17 (30%)
19	CLA	1	1193	19	41,59,73	2.46	13 (31%)	44,96,113	4.89	21 (47%)
19	CLA	1	1194	-	16,32,73	1.82	4 (25%)	21,54,113	3.21	12 (57%)
19	CLA	1	1195	-	24,44,73	3.25	12 (50%)	28,78,113	5.60	14 (50%)
19	CLA	1	1196	1	24,44,73	2.83	8 (33%)	28,78,113	4.37	11 (39%)
19	CLA	1	1197	19	41,59,73	2.87	18 (43%)	44,96,113	5.37	22 (50%)
19	CLA	1	1198	19	51,69,73	2.06	11 (21%)	56,108,113	4.58	20 (35%)
19	CLA	1	1199	-	16,32,73	1.83	4 (25%)	21,54,113	3.32	12 (57%)
19	CLA	1	1200	-	41,59,73	2.45	13 (31%)	44,96,113	6.51	24 (54%)
19	CLA	1	1201	-	16,32,73	1.77	3 (18%)	21,54,113	3.78	11 (52%)
20	LMU	1	1202	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
20	LMU	1	7004	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
19	CLA	2	1212	-	41,59,73	2.25	10 (24%)	44,96,113	5.18	17 (38%)
19	CLA	2	1213	-	46,64,73	2.20	10 (21%)	50,102,113	4.06	21 (42%)
19	CLA	2	1214	-	16,32,73	1.67	4 (25%)	21,54,113	3.24	11 (52%)
19	CLA	2	1215	-	40,58,73	2.27	11 (27%)	44,95,113	4.50	17 (38%)
19	CLA	2	1216	-	16,32,73	1.90	7 (43%)	21,54,113	3.52	12 (57%)
19	CLA	2	1217	-	55,73,73	2.08	10 (18%)	61,113,113	4.26	16 (26%)
19	CLA	2	1218	19	55,73,73	2.03	9 (16%)	61,113,113	4.09	21 (34%)
19	CLA	2	1219	-	16,32,73	1.69	3 (18%)	21,54,113	3.16	12 (57%)
19	CLA	2	1220	19	46,64,73	2.20	12 (26%)	50,102,113	5.06	18 (36%)
19	CLA	2	1221	-	16,32,73	1.79	3 (18%)	21,54,113	3.22	12 (57%)
19	CLA	2	1222	2	40,58,73	2.39	9 (22%)	44,95,113	4.32	19 (43%)
19	CLA	2	1223	-	40,58,73	2.38	10 (25%)	44,95,113	5.01	16 (36%)
19	CLA	2	1224	-	55,73,73	2.02	11 (20%)	61,113,113	4.45	21 (34%)
20	LMU	2	1225	-	36,36,36	0.87	1 (2%)	47,47,47	0.95	2 (4%)
21	SUC	2	1226	-	23,23,24	1.02	1 (4%)	35,35,36	2.23	13 (37%)
19	CLA	2	1227	-	16,32,73	1.88	7 (43%)	21,54,113	3.52	11 (52%)
19	CLA	2	2010	-	16,32,73	1.85	4 (25%)	21,54,113	2.79	8 (38%)
20	LMU	2	7003	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	2	7006	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
19	CLA	3	1212	-	24,44,73	2.77	8 (33%)	28,78,113	4.11	14 (50%)
19	CLA	3	1213	-	16,32,73	1.89	6 (37%)	21,54,113	3.35	12 (57%)
19	CLA	3	1214	-	16,32,73	1.89	5 (31%)	21,54,113	3.27	12 (57%)
19	CLA	3	1215	-	16,32,73	1.87	5 (31%)	21,54,113	3.29	12 (57%)
19	CLA	3	1216	-	16,32,73	1.65	3 (18%)	21,54,113	3.03	11 (52%)
19	CLA	3	1217	-	16,32,73	1.99	5 (31%)	21,54,113	3.52	12 (57%)
19	CLA	3	1218	-	55,73,73	2.19	14 (25%)	61,113,113	4.96	19 (31%)
19	CLA	3	1219	-	55,73,73	1.94	11 (20%)	61,113,113	4.40	17 (27%)
22	BCR	3	1220	-	41,41,41	2.05	5 (12%)	56,56,56	5.89	21 (37%)
21	SUC	3	1221	-	24,24,24	0.78	0	36,36,36	2.21	9 (25%)
19	CLA	3	3001	-	16,32,73	1.91	4 (25%)	21,54,113	3.29	11 (52%)
19	CLA	3	3002	-	16,32,73	1.80	4 (25%)	21,54,113	2.97	11 (52%)
19	CLA	3	3007	-	32,50,73	2.39	8 (25%)	36,85,113	5.45	17 (47%)
19	CLA	3	3008	-	40,58,73	2.26	12 (30%)	44,95,113	5.36	19 (43%)
19	CLA	3	3011	-	55,73,73	1.90	10 (18%)	61,113,113	4.01	18 (29%)
19	CLA	3	3014	-	16,32,73	1.77	4 (25%)	21,54,113	3.61	12 (57%)
19	CLA	3	3015	-	16,32,73	1.80	4 (25%)	21,54,113	2.96	10 (47%)
20	LMU	3	7005	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
19	CLA	4	1196	-	45,63,73	2.16	11 (24%)	49,101,113	4.90	17 (34%)
19	CLA	4	1197	-	24,44,73	2.95	8 (33%)	28,78,113	4.83	15 (53%)
19	CLA	4	1198	-	55,73,73	2.22	15 (27%)	61,113,113	4.54	25 (40%)
19	CLA	4	1199	-	45,63,73	2.17	9 (20%)	49,101,113	4.29	17 (34%)
19	CLA	4	1200	-	40,58,73	2.42	10 (25%)	44,95,113	4.74	18 (40%)
19	CLA	4	1201	-	42,60,73	2.62	19 (45%)	45,97,113	5.77	31 (68%)
19	CLA	4	1202	-	16,32,73	1.81	4 (25%)	21,54,113	3.32	12 (57%)
19	CLA	4	1203	-	16,32,73	1.92	4 (25%)	21,54,113	3.12	11 (52%)
19	CLA	4	1204	-	45,63,73	2.31	9 (20%)	49,101,113	4.47	17 (34%)
19	CLA	4	1205	-	16,32,73	1.77	4 (25%)	21,54,113	3.22	12 (57%)
19	CLA	4	1206	-	16,32,73	1.65	2 (12%)	21,54,113	3.29	13 (61%)
19	CLA	4	1207	-	24,44,73	2.72	7 (29%)	28,78,113	5.16	17 (60%)
19	CLA	4	1208	4	16,32,73	1.73	4 (25%)	21,54,113	2.62	11 (52%)
19	CLA	4	1209	-	36,54,73	2.58	13 (36%)	41,90,113	5.08	15 (36%)
20	LMU	4	1210	-	36,36,36	0.84	1 (2%)	47,47,47	1.24	4 (8%)
19	CLA	4	4003	-	16,32,73	1.73	4 (25%)	21,54,113	2.83	11 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	4007	-	42,60,73	2.36	10 (23%)	45,97,113	4.88	19 (42%)
19	CLA	4	4014	20	37,55,73	2.38	11 (29%)	42,91,113	5.25	16 (38%)
19	CLA	A	1759	-	40,58,73	2.29	10 (25%)	44,95,113	5.02	20 (45%)
19	CLA	A	1760	-	45,63,73	2.31	11 (24%)	49,101,113	3.52	18 (36%)
19	CLA	A	1761	-	55,73,73	2.04	11 (20%)	61,113,113	3.99	19 (31%)
19	CLA	A	1762	-	47,65,73	2.18	10 (21%)	50,103,113	4.84	19 (38%)
19	CLA	A	1763	-	36,54,73	2.34	9 (25%)	41,90,113	5.56	19 (46%)
19	CLA	A	1764	5	55,73,73	2.04	13 (23%)	61,113,113	4.10	21 (34%)
19	CLA	A	1765	-	45,63,73	2.12	9 (20%)	49,101,113	4.31	19 (38%)
19	CLA	A	1766	-	32,53,73	2.53	9 (28%)	37,89,113	5.25	18 (48%)
19	CLA	A	1767	5	55,73,73	2.09	11 (20%)	61,113,113	3.99	22 (36%)
19	CLA	A	1768	5	44,62,73	2.19	11 (25%)	47,99,113	4.10	15 (31%)
19	CLA	A	1769	-	44,62,73	2.05	10 (22%)	47,99,113	4.02	20 (42%)
19	CLA	A	1770	-	32,53,73	2.59	9 (28%)	37,89,113	4.65	15 (40%)
19	CLA	A	1771	5	40,58,73	2.42	10 (25%)	44,95,113	4.68	19 (43%)
19	CLA	A	1772	5	55,73,73	1.97	12 (21%)	61,113,113	4.31	22 (36%)
19	CLA	A	1773	-	42,60,73	2.34	10 (23%)	45,97,113	4.99	16 (35%)
19	CLA	A	1774	-	55,73,73	1.98	11 (20%)	61,113,113	3.64	20 (32%)
19	CLA	A	1775	-	24,44,73	2.82	8 (33%)	28,78,113	4.58	13 (46%)
19	CLA	A	1776	-	55,73,73	2.00	9 (16%)	61,113,113	4.01	20 (32%)
19	CLA	A	1777	-	41,59,73	2.32	10 (24%)	44,96,113	4.91	17 (38%)
19	CLA	A	1778	5	32,50,73	2.54	10 (31%)	36,85,113	5.20	17 (47%)
19	CLA	A	1779	-	45,63,73	2.23	11 (24%)	49,101,113	4.57	19 (38%)
19	CLA	A	1780	-	55,73,73	1.87	9 (16%)	61,113,113	3.62	19 (31%)
19	CLA	A	1781	-	55,73,73	1.95	11 (20%)	61,113,113	4.40	17 (27%)
19	CLA	A	1782	19	55,73,73	1.94	10 (18%)	61,113,113	4.41	17 (27%)
19	CLA	A	1783	-	55,73,73	2.02	10 (18%)	61,113,113	4.31	20 (32%)
19	CLA	A	1784	5	45,63,73	2.26	11 (24%)	49,101,113	4.57	16 (32%)
19	CLA	A	1785	-	55,73,73	2.02	11 (20%)	61,113,113	4.04	22 (36%)
19	CLA	A	1786	-	40,58,73	2.30	10 (25%)	44,95,113	5.05	22 (50%)
19	CLA	A	1787	5	55,73,73	2.07	9 (16%)	61,113,113	4.08	20 (32%)
19	CLA	A	1788	-	55,73,73	2.01	11 (20%)	61,113,113	4.29	18 (29%)
19	CLA	A	1789	-	55,73,73	2.02	11 (20%)	61,113,113	4.30	22 (36%)
19	CLA	A	1790	19,5	40,58,73	2.25	9 (22%)	44,95,113	4.52	16 (36%)
19	CLA	A	1791	5	32,53,73	2.42	10 (31%)	37,89,113	5.57	15 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1792	-	41,59,73	2.26	11 (26%)	44,96,113	5.17	17 (38%)
19	CLA	A	1793	-	55,73,73	1.95	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	A	1794	-	37,55,73	2.37	11 (29%)	42,91,113	5.26	16 (38%)
19	CLA	A	1795	-	41,59,73	2.26	11 (26%)	44,96,113	5.18	17 (38%)
19	CLA	A	1796	-	55,73,73	1.95	11 (20%)	61,113,113	4.40	17 (27%)
19	CLA	A	1797	-	55,73,73	1.95	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	A	1798	-	45,63,73	2.25	10 (22%)	49,101,113	4.67	18 (36%)
19	CLA	A	1799	-	40,58,73	2.31	9 (22%)	44,95,113	5.03	17 (38%)
19	CLA	A	1800	-	55,73,73	1.99	11 (20%)	61,113,113	4.46	20 (32%)
19	CLA	A	1801	-	45,63,73	2.36	9 (20%)	49,101,113	4.21	19 (38%)
23	PQN	A	1802	-	34,34,34	1.57	3 (8%)	44,45,45	1.41	5 (11%)
22	BCR	A	1803	5	41,41,41	1.93	3 (7%)	56,56,56	5.90	19 (33%)
22	BCR	A	1804	-	41,41,41	1.92	3 (7%)	56,56,56	5.90	19 (33%)
22	BCR	A	1805	-	41,41,41	1.93	3 (7%)	56,56,56	5.91	19 (33%)
22	BCR	A	1806	-	41,41,41	1.93	3 (7%)	56,56,56	5.91	19 (33%)
22	BCR	A	1807	-	41,41,41	1.93	3 (7%)	56,56,56	5.90	19 (33%)
22	BCR	A	1808	-	41,41,41	1.92	3 (7%)	56,56,56	5.91	19 (33%)
20	LMU	A	1809	-	36,36,36	0.92	0	47,47,47	1.42	8 (17%)
20	LMU	A	1810	-	36,36,36	0.92	1 (2%)	47,47,47	1.73	11 (23%)
19	CLA	A	1811	-	55,73,73	2.03	12 (21%)	61,113,113	4.48	20 (32%)
19	CLA	A	1812	-	55,73,73	2.05	13 (23%)	61,113,113	4.20	19 (31%)
19	CLA	A	1813	-	55,73,73	2.14	12 (21%)	61,113,113	4.39	19 (31%)
19	CLA	A	1815	-	45,63,73	2.28	11 (24%)	49,101,113	5.11	19 (38%)
19	CLA	A	1816	-	45,63,73	2.32	13 (28%)	49,101,113	4.74	20 (40%)
19	CLA	A	1817	-	36,54,73	2.73	13 (36%)	42,90,113	4.93	26 (61%)
20	LMU	A	7009	-	35,35,36	0.40	0	46,46,47	0.71	1 (2%)
20	LMU	A	7010	-	36,36,36	0.40	0	47,47,47	0.71	1 (2%)
20	LMU	A	7013	-	36,36,36	0.44	0	47,47,47	1.65	11 (23%)
20	LMU	A	7015	-	36,36,36	0.91	1 (2%)	47,47,47	1.45	7 (14%)
20	LMU	A	7016	-	36,36,36	0.61	1 (2%)	47,47,47	1.97	12 (25%)
20	LMU	A	7017	-	36,36,36	0.69	2 (5%)	47,47,47	2.36	15 (31%)
20	LMU	A	7019	-	36,36,36	1.00	1 (2%)	47,47,47	1.43	6 (12%)
20	LMU	A	7020	-	36,36,36	0.40	0	47,47,47	1.82	12 (25%)
20	LMU	A	7021	-	36,36,36	0.75	0	47,47,47	2.11	14 (29%)
20	LMU	A	7022	-	36,36,36	0.69	0	47,47,47	2.23	17 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	A	7023	-	36,36,36	0.67	1 (2%)	47,47,47	2.01	18 (38%)
20	LMU	A	7024	-	36,36,36	0.94	2 (5%)	47,47,47	1.71	11 (23%)
20	LMU	A	7025	-	36,36,36	0.94	1 (2%)	47,47,47	1.61	11 (23%)
20	LMU	A	7026	21	36,36,36	1.20	3 (8%)	47,47,47	3.16	23 (48%)
20	LMU	A	7027	-	36,36,36	1.09	1 (2%)	47,47,47	2.00	15 (31%)
20	LMU	A	7028	-	36,36,36	0.72	2 (5%)	47,47,47	1.92	17 (36%)
20	LMU	A	7030	-	36,36,36	0.90	1 (2%)	47,47,47	2.33	16 (34%)
20	LMU	A	7031	-	36,36,36	1.06	1 (2%)	47,47,47	1.37	6 (12%)
20	LMU	A	7032	-	36,36,36	0.97	3 (8%)	47,47,47	2.83	18 (38%)
20	LMU	A	7033	-	36,36,36	1.00	2 (5%)	47,47,47	2.29	14 (29%)
20	LMU	A	7034	19	36,36,36	0.83	1 (2%)	47,47,47	1.35	4 (8%)
20	LMU	A	7035	-	36,36,36	0.81	1 (2%)	47,47,47	1.63	8 (17%)
20	LMU	A	7036	-	35,35,36	1.20	4 (11%)	46,46,47	2.34	15 (32%)
20	LMU	A	7037	-	36,36,36	0.88	2 (5%)	47,47,47	3.15	22 (46%)
20	LMU	A	7038	-	36,36,36	0.65	0	47,47,47	2.43	17 (36%)
20	LMU	A	7039	-	36,36,36	0.96	2 (5%)	47,47,47	2.64	13 (27%)
20	LMU	A	7040	-	36,36,36	0.95	3 (8%)	47,47,47	2.52	14 (29%)
20	LMU	A	7041	-	36,36,36	0.61	0	47,47,47	1.90	13 (27%)
20	LMU	A	7042	-	36,36,36	0.47	0	47,47,47	2.13	16 (34%)
20	LMU	A	7043	21	36,36,36	0.74	0	47,47,47	2.29	18 (38%)
20	LMU	A	7047	-	36,36,36	1.09	1 (2%)	47,47,47	1.46	4 (8%)
19	CLA	B	1735	-	55,73,73	1.95	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	B	1736	-	32,53,73	2.41	8 (25%)	37,89,113	4.51	15 (40%)
19	CLA	B	1737	-	55,73,73	1.96	10 (18%)	61,113,113	4.42	23 (37%)
19	CLA	B	1738	-	55,73,73	2.04	12 (21%)	61,113,113	4.35	29 (47%)
19	CLA	B	1739	-	55,73,73	2.11	11 (20%)	61,113,113	4.41	20 (32%)
19	CLA	B	1740	6	55,73,73	1.89	11 (20%)	61,113,113	4.47	17 (27%)
19	CLA	B	1741	6	44,62,73	2.49	10 (22%)	49,100,113	3.25	20 (40%)
19	CLA	B	1742	6	45,63,73	2.11	11 (24%)	49,101,113	4.28	20 (40%)
19	CLA	B	1743	-	55,73,73	2.05	10 (18%)	61,113,113	4.10	19 (31%)
19	CLA	B	1744	-	55,73,73	2.11	10 (18%)	61,113,113	3.54	19 (31%)
19	CLA	B	1745	6	50,68,73	2.06	10 (20%)	55,107,113	4.16	19 (34%)
19	CLA	B	1746	-	36,54,73	2.47	10 (27%)	41,90,113	4.74	16 (39%)
19	CLA	B	1747	-	49,67,73	2.14	10 (20%)	53,105,113	3.75	17 (32%)
19	CLA	B	1748	-	50,68,73	1.99	11 (22%)	55,107,113	4.56	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1749	-	51,69,73	1.97	10 (19%)	56,108,113	4.50	19 (33%)
19	CLA	B	1750	-	40,58,73	2.29	11 (27%)	44,95,113	4.47	16 (36%)
19	CLA	B	1751	-	36,54,73	2.43	10 (27%)	41,90,113	5.00	16 (39%)
19	CLA	B	1752	6	45,63,73	2.31	9 (20%)	49,101,113	4.81	18 (36%)
19	CLA	B	1753	-	55,73,73	2.44	18 (32%)	61,113,113	4.63	19 (31%)
19	CLA	B	1754	-	44,62,73	2.30	12 (27%)	47,99,113	4.42	21 (44%)
19	CLA	B	1755	-	48,66,73	2.08	11 (22%)	52,104,113	4.77	17 (32%)
19	CLA	B	1756	-	55,73,73	1.96	11 (20%)	61,113,113	4.41	17 (27%)
19	CLA	B	1757	-	55,73,73	2.09	12 (21%)	61,113,113	4.41	20 (32%)
19	CLA	B	1758	-	55,73,73	2.02	12 (21%)	61,113,113	4.03	20 (32%)
19	CLA	B	1759	-	55,73,73	1.97	11 (20%)	61,113,113	4.22	20 (32%)
19	CLA	B	1760	-	40,58,73	2.41	8 (20%)	44,95,113	4.18	19 (43%)
19	CLA	B	1761	6	40,58,73	2.30	9 (22%)	44,95,113	4.92	19 (43%)
19	CLA	B	1762	6	55,73,73	2.10	13 (23%)	61,113,113	4.38	20 (32%)
19	CLA	B	1763	6	40,58,73	2.43	12 (30%)	44,95,113	4.76	19 (43%)
19	CLA	B	1764	19	32,53,73	2.68	9 (28%)	37,89,113	5.07	14 (37%)
19	CLA	B	1765	19	32,53,73	2.51	10 (31%)	37,89,113	5.46	14 (37%)
19	CLA	B	1766	-	41,59,73	2.40	9 (21%)	44,96,113	4.83	17 (38%)
19	CLA	B	1767	-	50,68,73	2.06	11 (22%)	55,107,113	4.48	15 (27%)
19	CLA	B	1768	6	55,73,73	1.93	10 (18%)	61,113,113	3.92	18 (29%)
19	CLA	B	1769	-	37,55,73	2.30	10 (27%)	42,91,113	4.44	17 (40%)
19	CLA	B	1770	-	55,73,73	1.96	10 (18%)	61,113,113	4.10	22 (36%)
19	CLA	B	1771	-	55,73,73	1.92	9 (16%)	61,113,113	3.95	25 (40%)
19	CLA	B	1772	-	24,44,73	2.83	8 (33%)	28,78,113	4.86	16 (57%)
23	PQN	B	1773	-	34,34,34	1.46	2 (5%)	44,45,45	1.50	6 (13%)
22	BCR	B	1774	-	41,41,41	1.94	4 (9%)	56,56,56	5.90	20 (35%)
22	BCR	B	1775	-	41,41,41	1.93	4 (9%)	56,56,56	5.89	19 (33%)
22	BCR	B	1776	-	41,41,41	1.85	5 (12%)	56,56,56	5.03	24 (42%)
22	BCR	B	1777	-	41,41,41	1.94	3 (7%)	56,56,56	5.90	22 (39%)
22	BCR	B	1778	-	41,41,41	1.93	3 (7%)	56,56,56	5.90	19 (33%)
22	BCR	B	1779	-	41,41,41	2.75	13 (31%)	56,56,56	6.07	31 (55%)
22	BCR	B	1780	-	41,41,41	1.92	3 (7%)	56,56,56	5.91	19 (33%)
22	BCR	B	1781	-	41,41,41	2.66	16 (39%)	56,56,56	5.39	30 (53%)
20	LMU	B	1782	-	26,26,36	1.01	1 (3%)	37,37,47	1.53	7 (18%)
24	LMG	B	1783	-	49,49,55	0.92	2 (4%)	57,57,63	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	SF4	B	1784	5,6	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	B	1785	-	55,73,73	1.97	11 (20%)	61,113,113	4.24	23 (37%)
19	CLA	B	1786	-	55,73,73	2.01	11 (20%)	61,113,113	4.11	23 (37%)
19	CLA	B	1787	-	55,73,73	2.08	10 (18%)	61,113,113	3.92	19 (31%)
21	SUC	B	8051	-	24,24,24	0.71	0	36,36,36	1.40	3 (8%)
21	SUC	B	8052	-	24,24,24	0.82	0	36,36,36	1.70	9 (25%)
21	SUC	B	8053	20	24,24,24	0.43	0	36,36,36	0.90	1 (2%)
21	SUC	B	8054	-	24,24,24	1.15	2 (8%)	36,36,36	1.78	10 (27%)
21	SUC	B	8055	-	24,24,24	0.81	1 (4%)	36,36,36	1.79	8 (22%)
21	SUC	B	8056	-	24,24,24	0.98	1 (4%)	36,36,36	1.86	13 (36%)
21	SUC	B	8059	-	24,24,24	0.96	1 (4%)	36,36,36	2.12	12 (33%)
21	SUC	B	8060	-	24,24,24	0.99	0	36,36,36	1.88	7 (19%)
21	SUC	B	8061	-	24,24,24	0.88	0	36,36,36	2.36	17 (47%)
21	SUC	B	8062	20	24,24,24	0.99	1 (4%)	36,36,36	2.80	16 (44%)
25	SF4	C	1082	7	0,12,12	0.00	-	0,24,24	0.00	-
25	SF4	C	1083	7	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	F	1155	-	24,44,73	2.73	8 (33%)	28,78,113	3.64	14 (50%)
19	CLA	F	1156	19	30,49,73	2.49	10 (33%)	34,84,113	5.82	15 (44%)
19	CLA	F	1157	19	43,61,73	2.57	15 (34%)	46,98,113	4.72	18 (39%)
19	CLA	G	1099	-	41,59,73	2.37	9 (21%)	44,96,113	4.61	20 (45%)
19	CLA	H	1079	-	55,73,73	2.02	12 (21%)	61,113,113	4.27	19 (31%)
21	SUC	H	1080	12	24,24,24	0.85	0	36,36,36	1.56	8 (22%)
19	CLA	I	1031	-	50,68,73	2.08	11 (22%)	55,107,113	4.88	16 (29%)
22	BCR	I	1032	-	41,41,41	2.65	8 (19%)	56,56,56	6.50	29 (51%)
19	CLA	I	1033	-	45,63,73	2.27	9 (20%)	49,101,113	4.82	19 (38%)
19	CLA	J	1043	-	51,69,73	2.01	11 (21%)	56,108,113	4.59	17 (30%)
19	CLA	J	1044	19	51,69,73	2.05	13 (25%)	56,108,113	4.69	25 (44%)
19	CLA	J	1045	19	45,63,73	2.27	13 (28%)	49,101,113	4.77	21 (42%)
19	CLA	J	1046	-	16,32,73	1.73	6 (37%)	21,54,113	2.96	11 (52%)
19	CLA	K	1085	20	40,58,73	2.28	11 (27%)	44,95,113	5.18	18 (40%)
20	LMU	K	1086	19	36,36,36	0.74	0	47,47,47	2.41	12 (25%)
19	CLA	K	1142	19	32,53,73	2.41	9 (28%)	37,89,113	5.57	15 (40%)
19	CLA	K	1146	-	40,58,73	2.45	13 (32%)	44,95,113	5.40	22 (50%)
19	CLA	K	3009	-	55,73,73	2.02	10 (18%)	61,113,113	4.20	19 (31%)
19	CLA	L	1166	16	40,58,73	2.35	9 (22%)	44,95,113	5.08	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	L	1167	22,16	37,55,73	2.38	10 (27%)	42,91,113	5.18	21 (50%)
19	CLA	L	1168	-	40,58,73	2.52	13 (32%)	44,95,113	5.64	17 (38%)
22	BCR	L	1169	-	41,41,41	2.45	8 (19%)	56,56,56	5.73	20 (35%)
22	BCR	L	1170	19	41,41,41	3.26	19 (46%)	56,56,56	6.41	27 (48%)
20	LMU	L	1171	-	36,36,36	0.97	3 (8%)	47,47,47	1.52	9 (19%)
19	CLA	L	1505	-	45,63,73	2.23	10 (22%)	49,101,113	4.67	19 (38%)
19	CLA	R	1054	-	47,65,73	2.20	12 (25%)	50,103,113	4.89	18 (36%)
19	CLA	R	1055	-	55,73,73	2.17	11 (20%)	61,113,113	3.96	21 (34%)
20	LMU	R	1056	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
20	LMU	R	1057	-	36,36,36	1.14	2 (5%)	47,47,47	2.53	15 (31%)

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	1187	1	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1188	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	1189	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	1190	-	3/3/16/25	1/15/113/135	0/0/9/9
19	CLA	1	1191	-	3/3/14/25	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	19	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	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1196	1	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1197	19	4/4/17/25	1/21/119/135	0/0/9/9
19	CLA	1	1198	19	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1199	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1200	-	5/5/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1201	-	3/3/7/25	0/0/66/135	0/0/8/9
20	LMU	1	1202	-	-	0/21/61/61	0/2/2/2
20	LMU	1	7004	-	-	0/21/61/61	0/2/2/2
19	CLA	2	1212	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	2	1213	-	4/4/18/25	0/27/125/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	1219	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1220	19	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	2	1221	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	1222	2	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1223	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	1224	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	2	1225	-	-	0/21/61/61	0/2/2/2
21	SUC	2	1226	-	1/1/9/9	0/10/49/51	0/2/2/2
19	CLA	2	1227	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2010	-	3/3/7/25	0/0/66/135	0/0/8/9
20	LMU	2	7003	-	-	0/21/61/61	0/2/2/2
20	LMU	2	7006	-	-	0/21/61/61	0/2/2/2
19	CLA	3	1212	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	1213	-	3/3/7/25	0/0/66/135	0/0/8/9
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	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	1218	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1219	-	4/4/20/25	0/37/135/135	0/0/9/9
22	BCR	3	1220	-	-	1/29/63/63	0/2/2/2
21	SUC	3	1221	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	3	3001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3002	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3007	-	3/3/15/25	0/10/108/135	0/0/9/9
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
20	LMU	3	7005	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1205	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1206	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1207	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1208	4	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	1209	-	3/3/16/25	0/15/113/135	0/0/9/9
20	LMU	4	1210	-	-	0/21/61/61	0/2/2/2
19	CLA	4	4003	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4007	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4014	20	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1759	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1760	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1761	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1762	-	4/4/18/25	0/28/126/135	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	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1765	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1766	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1767	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1768	5	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1769	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1770	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1771	5	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1772	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1773	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	1774	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1775	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	A	1776	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1777	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1778	5	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	A	1779	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1780	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1781	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1782	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1783	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1784	5	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1785	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1786	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1787	5	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1788	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1789	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1790	19,5	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1791	5	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1792	-	3/3/17/25	0/21/119/135	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	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1798	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	A	1799	-	3/3/17/25	0/19/117/135	0/0/9/9
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
23	PQN	A	1802	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	A	1803	5	-	3/29/63/63	0/2/2/2
22	BCR	A	1804	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1805	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1806	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1807	-	-	0/29/63/63	0/2/2/2
22	BCR	A	1808	-	-	1/29/63/63	0/2/2/2
20	LMU	A	1809	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1810	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1811	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1812	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1813	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1815	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1816	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1817	-	5/5/16/25	0/16/112/135	0/0/9/9
20	LMU	A	7009	-	-	0/20/60/61	0/2/2/2
20	LMU	A	7010	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7013	-	-	0/21/61/61	0/2/2/2
20	LMU	A	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	21	-	0/21/61/61	0/2/2/2
20	LMU	A	7027	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7028	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7030	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7031	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7032	-	-	1/21/61/61	0/2/2/2
20	LMU	A	7033	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7034	19	-	0/21/61/61	0/2/2/2
20	LMU	A	7035	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7036	-	-	0/20/60/61	0/2/2/2
20	LMU	A	7037	-	-	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	21	-	0/21/61/61	0/2/2/2
20	LMU	A	7047	-	-	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	-	4/4/20/25	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1738	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1739	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1740	6	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1741	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	-	4/4/20/25	0/37/135/135	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	-	4/4/18/25	0/30/128/135	0/0/9/9
19	CLA	B	1748	-	4/4/19/25	0/31/129/135	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	-	3/3/20/25	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	-	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
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	6	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1762	6	4/4/20/25	0/37/135/135	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	0/16/114/135	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1772	-	3/3/14/25	0/0/96/135	0/0/9/9
23	PQN	B	1773	-	1/1/8/9	0/23/43/43	0/2/2/2
22	BCR	B	1774	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1775	-	-	1/29/63/63	0/2/2/2
22	BCR	B	1776	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1777	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1778	-	-	1/29/63/63	0/2/2/2
22	BCR	B	1779	-	-	0/29/63/63	0/2/2/2
22	BCR	B	1780	-	-	1/29/63/63	0/2/2/2
22	BCR	B	1781	-	-	0/29/63/63	0/2/2/2
20	LMU	B	1782	-	-	0/11/51/61	0/2/2/2
24	LMG	B	1783	-	-	0/44/64/70	0/1/1/1
25	SF4	B	1784	5,6	-	0/0/48/48	0/6/5/5
19	CLA	B	1785	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1786	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1787	-	4/4/20/25	0/37/135/135	0/0/9/9
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	20	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8054	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8055	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8056	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8059	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8060	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8061	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8062	20	1/1/9/9	0/12/51/51	0/2/2/2
25	SF4	C	1082	7	-	0/0/48/48	0/6/5/5
25	SF4	C	1083	7	-	0/0/48/48	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	-	4/4/20/25	0/37/135/135	0/0/9/9
21	SUC	H	1080	12	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
22	BCR	I	1032	-	-	1/29/63/63	0/2/2/2
19	CLA	I	1033	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	J	1043	-	4/4/19/25	1/33/131/135	0/0/9/9
19	CLA	J	1044	19	4/4/19/25	0/33/131/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	J	1045	19	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	J	1046	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	K	1085	20	3/3/17/25	0/19/117/135	0/0/9/9
20	LMU	K	1086	19	-	0/21/61/61	0/2/2/2
19	CLA	K	1142	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	K	1146	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	K	3009	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	L	1166	16	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	L	1167	22,16	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	L	1168	-	4/4/17/25	0/19/117/135	0/0/9/9
22	BCR	L	1169	-	-	2/29/63/63	0/2/2/2
22	BCR	L	1170	19	-	0/29/63/63	0/2/2/2
20	LMU	L	1171	-	-	0/21/61/61	0/2/2/2
19	CLA	L	1505	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	R	1054	-	4/4/18/25	1/28/126/135	0/0/9/9
19	CLA	R	1055	-	4/4/20/25	0/37/135/135	0/0/9/9
20	LMU	R	1056	-	-	0/21/61/61	0/2/2/2
20	LMU	R	1057	-	1/1/10/10	0/21/61/61	0/2/2/2

The worst 5 of 1854 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1170	BCR	C21-C22	-11.05	1.21	1.35
19	1	1195	CLA	CAB-C3B	-10.42	1.30	1.51
22	B	1781	BCR	C21-C22	-10.01	1.22	1.35
22	L	1170	BCR	C20-C21	-9.97	1.12	1.43
22	B	1779	BCR	C21-C22	-9.41	1.23	1.35

The worst 5 of 4035 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1200	CLA	OBD-CAD-CBD	-24.06	89.63	125.94
19	A	1763	CLA	OBD-CAD-CBD	-18.56	97.94	125.94
19	B	1748	CLA	OBD-CAD-CBD	-17.07	100.19	125.94
19	4	1201	CLA	OBD-CAD-CBD	-16.53	100.99	125.94
19	2	1224	CLA	OBD-CAD-CBD	-16.52	101.01	125.94

5 of 630 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1760	CLA	C8
19	A	1760	CLA	NC
19	A	1760	CLA	ND
19	A	1760	CLA	NA
19	A	1785	CLA	C8

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	1778	BCR	C21-C20-C19-C18
22	3	1220	BCR	C21-C20-C19-C18
22	I	1032	BCR	C20-C21-C22-C23
22	L	1169	BCR	C20-C21-C22-C37
22	A	1803	BCR	C21-C20-C19-C18

There are no ring outliers.

234 monomers are involved in 3581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1187	CLA	11	0
19	1	1188	CLA	7	0
19	1	1189	CLA	11	0
19	1	1190	CLA	5	0
19	1	1191	CLA	10	0
19	1	1192	CLA	9	0
19	1	1193	CLA	6	1
19	1	1194	CLA	5	0
19	1	1195	CLA	4	0
19	1	1196	CLA	6	0
19	1	1197	CLA	20	0
19	1	1198	CLA	20	0
19	1	1199	CLA	2	0
19	1	1200	CLA	11	0
20	1	1202	LMU	5	0
20	1	7004	LMU	10	0
19	2	1212	CLA	18	0
19	2	1213	CLA	13	0
19	2	1214	CLA	7	0
19	2	1215	CLA	24	0
19	2	1217	CLA	9	0
19	2	1218	CLA	7	0
19	2	1220	CLA	74	0
19	2	1222	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	1223	CLA	4	0
19	2	1224	CLA	7	0
20	2	1225	LMU	1	1
21	2	1226	SUC	10	0
20	2	7003	LMU	3	0
20	2	7006	LMU	11	0
19	3	1212	CLA	9	0
19	3	1213	CLA	1	0
19	3	1214	CLA	3	0
19	3	1215	CLA	17	0
19	3	1216	CLA	7	0
19	3	1217	CLA	8	0
19	3	1218	CLA	25	0
19	3	1219	CLA	18	0
22	3	1220	BCR	21	0
21	3	1221	SUC	14	0
19	3	3007	CLA	2	0
19	3	3008	CLA	17	0
19	3	3011	CLA	17	0
20	3	7005	LMU	3	0
19	4	1196	CLA	34	0
19	4	1197	CLA	2	0
19	4	1198	CLA	25	0
19	4	1199	CLA	22	0
19	4	1200	CLA	3	0
19	4	1201	CLA	25	0
19	4	1202	CLA	4	0
19	4	1204	CLA	8	0
19	4	1205	CLA	3	0
19	4	1206	CLA	2	0
19	4	1207	CLA	5	0
19	4	1208	CLA	8	0
19	4	1209	CLA	5	0
19	4	4014	CLA	11	0
19	A	1759	CLA	20	0
19	A	1760	CLA	29	0
19	A	1761	CLA	32	0
19	A	1762	CLA	18	0
19	A	1763	CLA	31	0
19	A	1764	CLA	26	0
19	A	1765	CLA	25	0
19	A	1766	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1767	CLA	23	0
19	A	1768	CLA	4	0
19	A	1769	CLA	22	0
19	A	1770	CLA	27	0
19	A	1771	CLA	13	0
19	A	1772	CLA	34	0
19	A	1773	CLA	11	0
19	A	1774	CLA	31	0
19	A	1776	CLA	47	0
19	A	1777	CLA	13	0
19	A	1778	CLA	11	0
19	A	1779	CLA	35	0
19	A	1780	CLA	17	0
19	A	1781	CLA	85	0
19	A	1782	CLA	81	0
19	A	1783	CLA	61	0
19	A	1784	CLA	18	0
19	A	1785	CLA	17	0
19	A	1786	CLA	9	0
19	A	1787	CLA	26	0
19	A	1788	CLA	40	0
19	A	1789	CLA	20	0
19	A	1790	CLA	16	0
19	A	1791	CLA	24	1
19	A	1792	CLA	22	0
19	A	1793	CLA	35	0
19	A	1794	CLA	21	0
19	A	1795	CLA	40	0
19	A	1796	CLA	63	0
19	A	1797	CLA	35	0
19	A	1798	CLA	29	0
19	A	1799	CLA	7	0
19	A	1800	CLA	31	0
19	A	1801	CLA	15	0
23	A	1802	PQN	12	0
22	A	1803	BCR	41	0
22	A	1804	BCR	22	0
22	A	1805	BCR	48	0
22	A	1806	BCR	36	0
22	A	1807	BCR	62	0
22	A	1808	BCR	43	0
20	A	1809	LMU	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1810	LMU	4	0
19	A	1811	CLA	20	0
19	A	1812	CLA	35	0
19	A	1813	CLA	33	0
19	A	1815	CLA	19	0
19	A	1816	CLA	35	0
19	A	1817	CLA	9	0
20	A	7009	LMU	9	0
20	A	7010	LMU	8	0
20	A	7013	LMU	9	0
20	A	7016	LMU	42	0
20	A	7017	LMU	3	0
20	A	7019	LMU	2	0
20	A	7020	LMU	21	0
20	A	7021	LMU	24	0
20	A	7022	LMU	11	0
20	A	7023	LMU	26	0
20	A	7025	LMU	1	0
20	A	7026	LMU	20	0
20	A	7027	LMU	6	0
20	A	7028	LMU	4	0
20	A	7030	LMU	12	0
20	A	7031	LMU	4	0
20	A	7032	LMU	28	0
20	A	7033	LMU	19	0
20	A	7034	LMU	1	0
20	A	7036	LMU	19	0
20	A	7037	LMU	24	0
20	A	7038	LMU	13	0
20	A	7039	LMU	19	0
20	A	7040	LMU	4	0
20	A	7041	LMU	9	0
20	A	7042	LMU	35	0
20	A	7043	LMU	16	0
19	B	1735	CLA	33	0
19	B	1736	CLA	9	0
19	B	1737	CLA	24	0
19	B	1738	CLA	19	0
19	B	1739	CLA	22	0
19	B	1740	CLA	20	0
19	B	1741	CLA	6	0
19	B	1742	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1743	CLA	29	0
19	B	1744	CLA	20	0
19	B	1745	CLA	12	0
19	B	1746	CLA	23	0
19	B	1747	CLA	23	0
19	B	1748	CLA	14	0
19	B	1749	CLA	18	0
19	B	1750	CLA	9	0
19	B	1751	CLA	16	0
19	B	1752	CLA	14	0
19	B	1753	CLA	40	0
19	B	1754	CLA	23	0
19	B	1755	CLA	62	0
19	B	1756	CLA	46	0
19	B	1757	CLA	21	0
19	B	1758	CLA	34	0
19	B	1759	CLA	34	0
19	B	1760	CLA	10	0
19	B	1761	CLA	12	0
19	B	1762	CLA	28	0
19	B	1763	CLA	13	0
19	B	1764	CLA	21	0
19	B	1765	CLA	20	0
19	B	1766	CLA	3	0
19	B	1767	CLA	15	0
19	B	1768	CLA	48	0
19	B	1769	CLA	25	0
19	B	1770	CLA	24	0
19	B	1771	CLA	24	0
19	B	1772	CLA	2	0
23	B	1773	PQN	33	0
22	B	1774	BCR	8	0
22	B	1775	BCR	20	0
22	B	1776	BCR	20	0
22	B	1777	BCR	31	0
22	B	1778	BCR	30	0
22	B	1779	BCR	46	0
22	B	1780	BCR	53	0
22	B	1781	BCR	17	0
20	B	1782	LMU	1	0
24	B	1783	LMG	30	0
25	B	1784	SF4	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1785	CLA	22	0
19	B	1786	CLA	43	0
19	B	1787	CLA	50	0
21	B	8052	SUC	15	0
21	B	8053	SUC	1	0
21	B	8054	SUC	9	0
21	B	8055	SUC	9	0
21	B	8056	SUC	5	0
21	B	8059	SUC	18	0
21	B	8060	SUC	7	0
21	B	8061	SUC	1	0
21	B	8062	SUC	20	0
25	C	1082	SF4	5	0
25	C	1083	SF4	4	0
19	F	1155	CLA	1	0
19	F	1156	CLA	13	0
19	F	1157	CLA	13	0
19	G	1099	CLA	6	0
19	H	1079	CLA	19	0
21	H	1080	SUC	5	0
19	I	1031	CLA	11	0
22	I	1032	BCR	47	0
19	I	1033	CLA	15	0
19	J	1043	CLA	29	0
19	J	1044	CLA	40	0
19	J	1045	CLA	44	0
19	K	1085	CLA	26	0
20	K	1086	LMU	6	0
19	K	1142	CLA	20	1
19	K	1146	CLA	11	0
19	K	3009	CLA	3	0
19	L	1166	CLA	7	0
19	L	1167	CLA	18	0
19	L	1168	CLA	12	0
22	L	1169	BCR	48	0
22	L	1170	BCR	13	0
20	L	1171	LMU	3	0
19	L	1505	CLA	3	0
19	R	1054	CLA	11	0
19	R	1055	CLA	6	0
20	R	1056	LMU	19	0
20	R	1057	LMU	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	165/241 (68%)	0.85	25 (15%) 3 2	31, 61, 71, 72	0
2	2	176/269 (65%)	0.45	17 (9%) 10 9	33, 52, 64, 68	0
3	3	162/276 (58%)	0.76	22 (13%) 4 3	49, 79, 110, 112	0
4	4	166/251 (66%)	0.62	24 (14%) 3 3	21, 44, 57, 58	0
5	A	730/758 (96%)	0.22	28 (3%) 44 37	20, 20, 20, 20	0
6	B	733/734 (99%)	0.22	13 (1%) 71 65	20, 20, 20, 20	0
7	C	81/81 (100%)	0.75	12 (14%) 3 3	20, 20, 20, 20	0
8	D	138/212 (65%)	0.30	11 (7%) 15 12	20, 20, 20, 20	0
9	E	65/143 (45%)	0.47	7 (10%) 8 6	20, 20, 20, 20	0
10	F	154/231 (66%)	0.19	11 (7%) 19 15	20, 20, 20, 20	0
11	G	95/167 (56%)	0.45	8 (8%) 14 11	20, 20, 20, 20	0
12	H	69/144 (47%)	0.23	3 (4%) 39 32	20, 20, 20, 20	0
13	I	30/40 (75%)	-0.02	0 100 100	20, 20, 20, 20	0
14	J	42/44 (95%)	0.22	1 (2%) 62 55	20, 20, 20, 20	0
15	K	84/131 (64%)	1.41	23 (27%) 1 1	20, 20, 20, 20	0
16	L	161/216 (74%)	0.26	10 (6%) 24 19	20, 20, 20, 20	0
17	N	85/170 (50%)	0.20	3 (3%) 48 40	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3136/4161 (75%)	0.37	218 (6%) 19 16	20, 20, 65, 112	0

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	13.1
6	B	491	ASN	10.1
1	1	92	GLY	9.3

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Mol	Chain	Res	Type	RSRZ
3	3	42	PRO	8.7
2	2	123	PRO	8.1

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
22	BCR	A	1803	40/40	0.57	0.49	9.75	20,20,20,20	0
19	CLA	A	1801	55/65	0.61	0.40	5.26	20,20,20,20	0
19	CLA	2	1217	65/65	0.77	0.37	3.72	20,20,20,20	0
22	BCR	B	1775	40/40	0.80	0.35	3.49	20,20,20,20	0
22	BCR	I	1032	40/40	0.76	0.31	3.39	20,20,20,20	0
19	CLA	4	1202	25/65	0.69	0.34	2.91	20,20,20,20	0
19	CLA	B	1746	46/65	0.67	0.39	2.71	20,20,20,20	0
19	CLA	1	1197	51/65	0.71	0.52	2.69	20,20,20,20	0
19	CLA	A	1793	65/65	0.86	0.28	2.55	20,20,20,20	0
22	BCR	B	1781	40/40	0.87	0.27	2.39	20,20,20,20	0
19	CLA	1	1191	36/65	0.74	0.37	2.33	20,20,20,20	0
22	BCR	A	1806	40/40	0.79	0.35	2.19	20,20,20,20	0
22	BCR	A	1808	40/40	0.68	0.39	2.17	20,20,20,20	0
19	CLA	A	1777	51/65	0.82	0.40	2.06	20,20,20,20	0
19	CLA	4	1200	50/65	0.69	0.44	2.00	20,20,20,20	0
19	CLA	B	1755	58/65	0.68	0.41	1.89	20,20,20,20	0
19	CLA	B	1772	36/65	0.77	0.30	1.86	20,20,20,20	0
22	BCR	B	1779	40/40	0.83	0.31	1.75	20,20,20,20	0
19	CLA	H	1079	65/65	0.79	0.29	1.68	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	BCR	L	1170	40/40	0.88	0.26	1.62	20,20,20,20	0
19	CLA	A	1781	65/65	0.80	0.30	1.56	20,20,20,20	0
19	CLA	A	1776	65/65	0.82	0.32	1.52	20,20,20,20	0
24	LMG	B	1783	49/55	0.77	0.34	1.51	20,20,20,20	0
22	BCR	L	1169	40/40	0.72	0.42	1.48	20,20,20,20	0
22	BCR	B	1777	40/40	0.85	0.33	1.47	20,20,20,20	0
19	CLA	A	1787	65/65	0.81	0.28	1.46	20,20,20,20	0
22	BCR	B	1778	40/40	0.85	0.32	1.46	20,20,20,20	0
22	BCR	A	1804	40/40	0.76	0.33	1.35	20,20,20,20	0
19	CLA	A	1785	65/65	0.83	0.31	1.33	20,20,20,20	0
19	CLA	A	1764	65/65	0.90	0.33	1.30	20,20,20,20	0
22	BCR	A	1805	40/40	0.74	0.34	1.25	20,20,20,20	0
19	CLA	B	1759	65/65	0.87	0.32	1.23	20,20,20,20	0
19	CLA	B	1749	61/65	0.86	0.28	1.18	20,20,20,20	0
19	CLA	A	1774	65/65	0.82	0.32	1.17	20,20,20,20	0
22	BCR	B	1780	40/40	0.80	0.36	1.17	20,20,20,20	0
19	CLA	B	1764	45/65	0.79	0.29	1.16	20,20,20,20	0
19	CLA	B	1771	65/65	0.86	0.33	1.16	20,20,20,20	0
19	CLA	B	1735	65/65	0.83	0.30	1.14	20,20,20,20	0
19	CLA	A	1762	57/65	0.85	0.30	1.13	20,20,20,20	0
19	CLA	A	1795	51/65	0.85	0.26	1.06	20,20,20,20	0
19	CLA	A	1760	55/65	0.84	0.29	1.01	20,20,20,20	0
19	CLA	B	1762	65/65	0.80	0.32	0.99	20,20,20,20	0
19	CLA	A	1780	65/65	0.78	0.34	0.95	20,20,20,20	0
19	CLA	B	1787	65/65	0.86	0.31	0.94	20,20,20,20	0
19	CLA	3	1212	36/65	0.73	0.36	0.93	20,20,20,20	0
22	BCR	A	1807	40/40	0.80	0.37	0.93	20,20,20,20	0
19	CLA	I	1031	60/65	0.85	0.23	0.83	20,20,20,20	0
19	CLA	B	1748	60/65	0.88	0.30	0.83	20,20,20,20	0
19	CLA	B	1751	46/65	0.75	0.34	0.81	20,20,20,20	0
19	CLA	A	1775	36/65	0.70	0.29	0.79	20,20,20,20	0
19	CLA	L	1167	47/65	0.86	0.23	0.77	20,20,20,20	0
19	CLA	B	1757	65/65	0.90	0.28	0.75	20,20,20,20	0
19	CLA	B	1741	54/65	0.82	0.30	0.73	20,20,20,20	0
19	CLA	A	1770	45/65	0.70	0.39	0.72	20,20,20,20	0
19	CLA	B	1740	65/65	0.85	0.30	0.72	20,20,20,20	0
19	CLA	B	1758	65/65	0.89	0.30	0.72	20,20,20,20	0
19	CLA	L	1166	50/65	0.81	0.27	0.70	20,20,20,20	0
19	CLA	B	1739	65/65	0.90	0.28	0.68	20,20,20,20	0
22	BCR	B	1774	40/40	0.79	0.34	0.68	20,20,20,20	0
19	CLA	G	1099	51/65	0.70	0.35	0.67	20,20,20,20	0
19	CLA	A	1792	51/65	0.83	0.28	0.66	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	SUC	2	1226	22/23	0.77	0.27	0.66	20,20,20,20	0
19	CLA	3	3002	25/65	0.75	0.31	0.64	20,20,20,20	0
19	CLA	A	1779	55/65	0.88	0.23	0.63	20,20,20,20	0
19	CLA	A	1789	65/65	0.85	0.27	0.59	20,20,20,20	0
19	CLA	A	1761	65/65	0.83	0.29	0.57	20,20,20,20	0
19	CLA	B	1770	65/65	0.85	0.30	0.56	20,20,20,20	0
19	CLA	B	1736	45/65	0.81	0.27	0.56	20,20,20,20	0
19	CLA	A	1759	50/65	0.88	0.25	0.56	20,20,20,20	0
19	CLA	A	1783	65/65	0.91	0.30	0.56	20,20,20,20	0
19	CLA	A	1769	54/65	0.83	0.27	0.56	20,20,20,20	0
23	PQN	A	1802	33/33	0.87	0.31	0.56	20,20,20,20	0
19	CLA	B	1744	65/65	0.83	0.30	0.55	20,20,20,20	0
19	CLA	A	1811	65/65	0.89	0.31	0.53	20,20,20,20	0
19	CLA	B	1769	47/65	0.87	0.29	0.51	20,20,20,20	0
19	CLA	B	1786	65/65	0.90	0.27	0.49	20,20,20,20	0
19	CLA	B	1767	60/65	0.84	0.28	0.47	20,20,20,20	0
19	CLA	B	1785	65/65	0.86	0.30	0.45	20,20,20,20	0
19	CLA	A	1763	46/65	0.74	0.36	0.40	20,20,20,20	0
19	CLA	A	1800	65/65	0.86	0.27	0.38	20,20,20,20	0
19	CLA	A	1794	47/65	0.87	0.27	0.38	20,20,20,20	0
19	CLA	B	1737	65/65	0.89	0.25	0.37	20,20,20,20	0
19	CLA	A	1812	65/65	0.85	0.31	0.35	20,20,20,20	0
19	CLA	K	3009	65/65	0.72	0.34	0.33	20,20,20,20	0
19	CLA	4	1204	55/65	0.79	0.24	0.32	20,20,20,20	0
19	CLA	B	1753	65/65	0.85	0.25	0.32	20,20,20,20	0
19	CLA	A	1773	52/65	0.83	0.24	0.29	20,20,20,20	0
19	CLA	B	1756	65/65	0.82	0.32	0.27	20,20,20,20	0
19	CLA	B	1750	50/65	0.83	0.26	0.27	20,20,20,20	0
19	CLA	4	1199	55/65	0.74	0.31	0.27	20,20,20,20	0
20	LMU	L	1171	35/35	0.77	0.24	0.26	20,20,20,20	0
19	CLA	B	1761	50/65	0.85	0.25	0.26	20,20,20,20	0
19	CLA	A	1784	55/65	0.85	0.28	0.26	20,20,20,20	0
19	CLA	B	1760	50/65	0.89	0.24	0.26	20,20,20,20	0
19	CLA	B	1738	65/65	0.90	0.27	0.22	20,20,20,20	0
19	CLA	2	1222	50/65	0.84	0.28	0.20	20,20,20,20	0
19	CLA	A	1813	65/65	0.85	0.29	0.20	20,20,20,20	0
19	CLA	B	1765	45/65	0.67	0.39	0.19	20,20,20,20	0
22	BCR	B	1776	40/40	0.77	0.33	0.18	20,20,20,20	0
20	LMU	A	7047	35/35	0.72	0.25	0.18	20,20,20,20	0
23	PQN	B	1773	33/33	0.91	0.29	0.16	20,20,20,20	0
19	CLA	B	1763	50/65	0.84	0.27	0.15	20,20,20,20	0
19	CLA	A	1788	65/65	0.88	0.27	0.15	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	B	1745	60/65	0.76	0.31	0.13	20,20,20,20	0
19	CLA	B	1768	65/65	0.89	0.26	0.04	20,20,20,20	0
19	CLA	1	1192	61/65	0.80	0.26	0.04	20,20,20,20	0
19	CLA	B	1742	55/65	0.82	0.26	-0.09	20,20,20,20	0
19	CLA	A	1798	55/65	0.72	0.29	-0.12	20,20,20,20	0
19	CLA	A	1786	50/65	0.88	0.21	-0.12	20,20,20,20	0
19	CLA	A	1772	65/65	0.83	0.23	-0.16	2,35,60,60	0
19	CLA	2	1215	50/65	0.73	0.27	-0.19	20,20,20,20	0
19	CLA	A	1767	65/65	0.85	0.28	-0.19	20,20,20,20	0
19	CLA	1	1189	47/65	0.75	0.27	-0.20	20,20,20,20	0
19	CLA	3	1218	65/65	0.72	0.28	-0.22	20,20,20,20	0
19	CLA	B	1754	54/65	0.90	0.23	-0.24	20,20,20,20	0
19	CLA	A	1790	50/65	0.86	0.23	-0.25	20,20,20,20	0
20	LMU	A	1809	35/35	0.75	0.20	-0.26	20,20,20,20	0
19	CLA	A	1782	65/65	0.86	0.23	-0.28	20,20,20,20	0
19	CLA	A	1771	50/65	0.79	0.29	-0.29	20,20,20,20	0
19	CLA	F	1155	36/65	0.88	0.20	-0.29	20,20,20,20	0
19	CLA	A	1778	42/65	0.72	0.30	-0.29	20,20,20,20	0
19	CLA	B	1747	59/65	0.86	0.24	-0.29	20,20,20,20	0
19	CLA	A	1796	65/65	0.84	0.29	-0.29	20,20,20,20	0
19	CLA	B	1752	55/65	0.86	0.22	-0.31	20,20,20,20	0
19	CLA	2	1221	25/65	0.78	0.31	-0.32	20,20,20,20	0
19	CLA	A	1766	45/65	0.81	0.26	-0.37	20,20,20,20	0
19	CLA	F	1156	41/65	0.74	0.28	-0.38	20,20,20,20	0
19	CLA	A	1765	55/65	0.86	0.26	-0.39	20,20,20,20	0
19	CLA	L	1168	50/65	0.81	0.23	-0.47	20,20,20,20	0
19	CLA	4	1197	36/65	0.81	0.24	-0.51	20,20,20,20	0
19	CLA	3	1214	25/65	0.58	0.27	-0.58	20,20,20,20	0
19	CLA	1	1199	25/65	0.73	0.25	-0.60	20,20,20,20	0
19	CLA	B	1743	65/65	0.89	0.22	-0.62	20,20,20,20	0
20	LMU	A	1810	35/35	0.77	0.17	-0.65	20,20,20,20	0
19	CLA	1	1195	36/65	0.83	0.27	-0.68	20,20,20,20	0
19	CLA	4	1207	36/65	0.85	0.21	-0.70	20,20,20,20	0
19	CLA	3	1215	25/65	0.76	0.26	-0.85	20,20,20,20	0
19	CLA	1	1196	36/65	0.81	0.25	-0.88	20,20,20,20	0
19	CLA	4	1206	25/65	0.88	0.17	-1.04	20,20,20,20	0
19	CLA	4	1201	52/65	0.83	0.20	-1.12	20,20,20,20	0
19	CLA	4	1196	55/65	0.75	0.25	-1.28	20,20,20,20	0
19	CLA	1	1190	46/65	0.82	0.22	-1.33	20,20,20,20	0
19	CLA	3	1213	25/65	0.78	0.19	-1.70	20,20,20,20	0
25	SF4	B	1784	8/8	0.98	0.06	-1.75	20,20,20,20	0
25	SF4	C	1082	8/8	0.97	0.09	-2.05	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	SF4	C	1083	8/8	0.98	0.06	-3.35	20,20,20,20	0
19	CLA	2	1223	50/65	0.77	0.26	-	20,20,20,20	0
19	CLA	4	1208	25/65	0.81	0.18	-	20,20,20,20	0
19	CLA	4	1203	25/65	0.75	0.24	-	20,20,20,20	0
20	LMU	R	1057	35/35	0.69	0.38	-	20,20,20,20	0
21	SUC	B	8060	23/23	0.87	0.28	-	20,20,20,20	0
21	SUC	B	8054	23/23	0.72	0.25	-	20,20,20,20	0
20	LMU	A	7033	35/35	0.77	0.21	-	20,20,20,20	0
19	CLA	1	1194	25/65	0.72	0.25	-	20,20,20,20	0
21	SUC	B	8052	23/23	0.72	0.45	-	20,20,20,20	0
20	LMU	A	7039	35/35	0.81	0.19	-	20,20,20,20	0
19	CLA	2	1219	25/65	0.75	0.23	-	20,20,20,20	0
21	SUC	B	8059	23/23	0.86	0.23	-	20,20,20,20	0
19	CLA	A	1768	54/65	0.83	0.23	-	20,20,20,20	0
20	LMU	A	7017	35/35	0.71	0.21	-	20,20,20,20	0
20	LMU	3	7005	35/35	0.71	0.31	-	20,20,20,20	0
19	CLA	4	1198	65/65	0.72	0.26	-	20,20,20,20	0
19	CLA	I	1033	55/65	0.68	0.28	-	20,20,20,20	0
20	LMU	A	7042	35/35	0.73	0.23	-	20,20,20,20	0
19	CLA	2	1227	25/65	0.69	0.56	-	20,20,20,20	0
19	CLA	1	1187	46/65	0.71	0.27	-	20,20,20,20	0
20	LMU	A	7010	35/35	0.73	0.32	-	20,20,20,20	0
21	SUC	B	8061	23/23	0.74	0.32	-	20,20,20,20	0
19	CLA	2	1213	56/65	0.79	0.22	-	20,20,20,20	0
19	CLA	K	1085	50/65	0.78	0.28	-	20,20,20,20	0
19	CLA	J	1043	61/65	0.73	0.30	-	20,20,20,20	0
19	CLA	4	1209	46/65	0.78	0.33	-	20,20,20,20	0
19	CLA	A	1817	46/65	0.72	0.33	-	20,20,20,20	0
19	CLA	2	1216	25/65	0.62	0.30	-	20,20,20,20	0
21	SUC	H	1080	23/23	0.71	0.30	-	20,20,20,20	0
19	CLA	3	3011	65/65	0.81	0.26	-	20,20,20,20	0
20	LMU	A	7032	35/35	0.82	0.33	-	20,20,20,20	0
19	CLA	A	1815	55/65	0.71	0.27	-	20,20,20,20	0
20	LMU	4	1210	35/35	0.77	0.29	-	20,20,20,20	0
19	CLA	2	1214	25/65	0.76	0.41	-	20,20,20,20	0
19	CLA	B	1766	51/65	0.62	0.39	-	20,20,20,20	0
19	CLA	R	1055	65/65	0.72	0.33	-	20,20,20,20	0
20	LMU	A	7038	35/35	0.66	0.37	-	20,20,20,20	0
20	LMU	B	1782	25/35	0.78	0.20	-	20,20,20,20	0
19	CLA	J	1046	25/65	0.50	0.56	-	5,42,60,60	0
21	SUC	B	8056	23/23	0.81	0.16	-	20,20,20,20	0
20	LMU	A	7024	35/35	0.80	0.18	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	1	1200	51/65	0.71	0.37	-	20,20,20,20	0
19	CLA	R	1054	57/65	0.72	0.28	-	20,20,20,20	0
19	CLA	1	1198	61/65	0.70	0.27	-	2,35,60,60	0
19	CLA	A	1816	55/65	0.74	0.32	-	20,20,20,20	0
21	SUC	B	8053	23/23	0.54	0.38	-	3,33,60,60	0
20	LMU	A	7035	35/35	0.81	0.26	-	20,20,20,20	0
20	LMU	A	7030	35/35	0.70	0.35	-	20,20,20,20	0
20	LMU	A	7022	35/35	0.77	0.20	-	20,20,20,20	0
20	LMU	2	1225	35/35	0.59	0.30	-	20,20,20,20	0
20	LMU	A	7020	35/35	0.81	0.23	-	20,20,20,20	0
19	CLA	A	1799	50/65	0.69	0.40	-	20,20,20,20	0
19	CLA	L	1505	55/65	0.62	0.36	-	20,20,20,20	0
20	LMU	A	7043	35/35	0.71	0.19	-	20,20,20,20	0
19	CLA	1	1188	47/65	0.80	0.26	-	20,20,20,20	0
20	LMU	A	7040	35/35	0.75	0.20	-	20,20,20,20	0
20	LMU	R	1056	35/35	0.80	0.22	-	20,20,20,20	0
19	CLA	2	1224	65/65	0.81	0.23	-	20,20,20,20	0
20	LMU	A	7009	34/35	0.69	0.33	-	20,20,20,20	0
19	CLA	2	1218	65/65	0.70	0.28	-	20,20,20,20	0
20	LMU	A	7025	35/35	0.69	0.24	-	20,20,20,20	0
20	LMU	A	7026	35/35	0.75	0.29	-	20,20,20,20	0
20	LMU	A	7023	35/35	0.82	0.24	-	20,20,20,20	0
19	CLA	4	4007	52/65	0.69	0.36	-	20,20,20,20	0
19	CLA	3	3014	25/65	0.66	0.50	-	20,20,20,20	0
19	CLA	F	1157	53/65	0.73	0.37	-	20,20,20,20	0
21	SUC	B	8062	23/23	0.82	0.29	-	20,20,20,20	0
20	LMU	K	1086	35/35	0.77	0.21	-	20,20,20,20	0
26	UNL	B	8057	23/-	0.80	0.17	-	20,20,20,20	0
22	BCR	3	1220	40/40	0.71	0.25	-	20,20,20,20	0
19	CLA	2	2010	25/65	0.76	0.29	-	20,20,20,20	0
19	CLA	1	1201	25/65	0.77	0.27	-	20,20,20,20	0
19	CLA	3	1219	65/65	0.66	0.46	-	20,20,20,20	0
19	CLA	J	1044	61/65	0.66	0.32	-	20,20,20,20	0
20	LMU	A	7036	34/35	0.80	0.28	-	20,20,20,20	0
19	CLA	4	1205	25/65	0.79	0.23	-	20,20,20,20	0
20	LMU	A	7021	35/35	0.72	0.26	-	20,20,20,20	0
19	CLA	2	1220	56/65	0.69	0.27	-	2,36,60,60	0
20	LMU	A	7037	35/35	0.66	0.24	-	20,20,20,20	0
19	CLA	K	1142	45/65	0.69	0.26	-	20,20,20,20	0
20	LMU	1	7004	35/35	0.62	0.43	-	20,20,20,20	0
20	LMU	A	7015	35/35	0.66	0.40	-	20,20,20,20	0
20	LMU	A	7019	35/35	0.78	0.20	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	4	4003	25/65	0.58	0.31	-	20,20,20,20	0
19	CLA	3	3008	50/65	0.78	0.31	-	20,20,20,20	0
20	LMU	A	7028	35/35	0.81	0.18	-	20,20,20,20	0
19	CLA	3	3015	25/65	0.75	0.33	-	20,20,20,20	0
20	LMU	A	7034	35/35	0.74	0.25	-	20,20,20,20	0
20	LMU	A	7013	35/35	0.57	0.31	-	20,20,20,20	0
19	CLA	3	3007	42/65	0.75	0.30	-	20,20,20,20	0
20	LMU	A	7027	35/35	0.76	0.22	-	20,20,20,20	0
19	CLA	4	4014	47/65	0.68	0.32	-	20,20,20,20	0
21	SUC	B	8051	23/23	0.77	0.33	-	20,20,20,20	0
19	CLA	3	1217	25/65	0.62	0.25	-	20,20,20,20	0
20	LMU	A	7031	35/35	0.70	0.28	-	20,20,20,20	0
19	CLA	A	1797	65/65	0.65	0.27	-	20,20,20,20	0
19	CLA	J	1045	55/65	0.79	0.22	-	2,33,60,60	0
20	LMU	2	7006	35/35	0.78	0.21	-	20,20,20,20	0
21	SUC	3	1221	23/23	0.83	0.30	-	20,20,20,20	0
20	LMU	2	7003	35/35	0.74	0.24	-	20,20,20,20	0
20	LMU	A	7041	35/35	0.66	0.23	-	20,20,20,20	0
19	CLA	K	1146	50/65	0.72	0.30	-	20,20,20,20	0
19	CLA	3	1216	25/65	0.74	0.20	-	20,20,20,20	0
21	SUC	B	8055	23/23	0.86	0.26	-	20,20,20,20	0
20	LMU	A	7016	35/35	0.81	0.24	-	20,20,20,20	0
20	LMU	1	1202	35/35	0.72	0.34	-	20,20,20,20	0
19	CLA	1	1193	51/65	0.74	0.37	-	20,20,20,20	0
19	CLA	A	1791	45/65	0.74	0.27	-	20,20,20,20	0
19	CLA	2	1212	51/65	0.64	0.27	-	20,20,20,20	0
19	CLA	3	3001	25/65	0.78	0.31	-	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.