



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:25 PM GMT

PDB ID : 4RKU
Title : Crystal structure of plant Photosystem I at 3 Angstrom resolution
Authors : Mazor, Y.; Borovikova, A.; Greenberg, I.; Nelson, N.
Deposited on : 2014-10-14
Resolution : 3.00 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

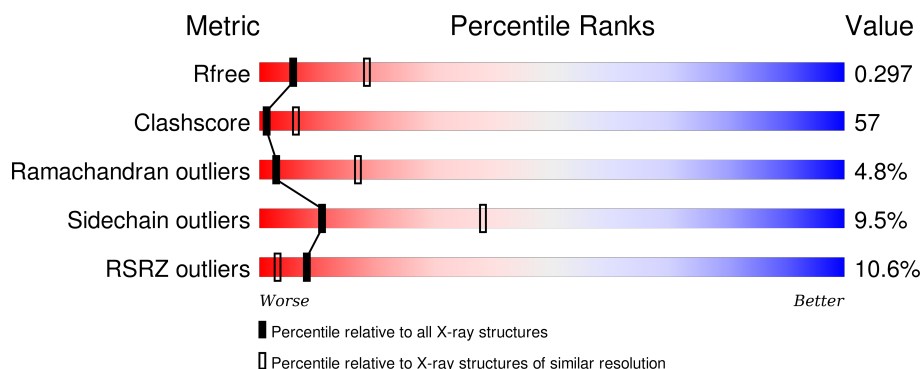
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	721	<div> <div>6%</div> <div>64%</div> <div>34%</div> <div>.</div> </div>
2	B	731	<div> <div>5%</div> <div>71%</div> <div>29%</div> <div>.</div> </div>
3	C	80	<div> <div>3%</div> <div>60%</div> <div>34%</div> <div>6%</div> </div>
4	D	137	<div> <div>14%</div> <div>43%</div> <div>44%</div> <div>11%</div> <div>.</div> </div>
5	E	63	<div> <div>19%</div> <div>44%</div> <div>41%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	152	
7	G	84	
8	H	82	
9	I	26	
10	J	40	
11	K	72	
12	L	163	
13	N	85	
14	1	182	
15	2	199	
16	3	275	
17	4	196	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	BCR	A	6002	-	-	-	X
19	BCR	A	6003	-	-	-	X
19	BCR	A	6007	-	-	-	X
19	BCR	B	6004	-	-	-	X
19	BCR	I	6020	-	-	-	X
19	BCR	J	6012	-	-	-	X
19	BCR	J	6013	-	-	-	X
20	LHG	1	1801	-	-	X	X
20	LHG	2	2801	-	-	X	-
20	LHG	B	7004	-	-	-	X
21	CLA	1	1001	X	-	X	-
21	CLA	1	1002	X	-	X	-
21	CLA	1	1003	X	-	X	-
21	CLA	1	1004	X	-	X	-
21	CLA	1	1005	X	-	-	-
21	CLA	1	1006	X	-	X	X
21	CLA	1	1007	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	1008	X	-	X	X
21	CLA	1	1009	X	-	X	X
21	CLA	1	1010	X	-	X	X
21	CLA	1	1011	X	-	-	-
21	CLA	1	1012	X	-	X	-
21	CLA	1	1013	X	-	X	X
21	CLA	1	1014	X	-	X	-
21	CLA	2	2001	X	-	-	-
21	CLA	2	2002	X	-	X	-
21	CLA	2	2003	X	-	X	-
21	CLA	2	2004	X	-	X	-
21	CLA	2	2005	X	-	X	X
21	CLA	2	2006	X	-	X	-
21	CLA	2	2007	X	-	-	-
21	CLA	2	2008	X	-	X	X
21	CLA	2	2009	X	-	X	-
21	CLA	2	2010	X	-	-	-
21	CLA	2	2011	X	-	X	-
21	CLA	2	2012	X	-	X	-
21	CLA	2	2013	X	-	X	-
21	CLA	2	2014	X	-	-	-
21	CLA	3	3001	X	-	X	-
21	CLA	3	3002	X	-	-	-
21	CLA	3	3003	X	-	-	X
21	CLA	3	3004	X	-	-	X
21	CLA	3	3005	X	-	-	-
21	CLA	3	3006	X	-	-	X
21	CLA	3	3008	X	-	-	-
21	CLA	3	3009	X	-	X	-
21	CLA	3	3010	X	-	-	-
21	CLA	3	3011	X	-	X	-
21	CLA	3	3012	X	-	X	-
21	CLA	3	3013	X	-	-	-
21	CLA	3	3014	X	-	-	X
21	CLA	3	3015	X	-	-	-
21	CLA	3	3016	X	-	-	-
21	CLA	3	3017	X	-	-	X
21	CLA	4	4001	X	-	X	X
21	CLA	4	4002	X	-	X	-
21	CLA	4	4003	X	-	X	-
21	CLA	4	4004	X	-	X	-
21	CLA	4	4005	X	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	4	4006	X	-	-	-
21	CLA	4	4007	X	-	-	X
21	CLA	4	4008	X	-	X	-
21	CLA	4	4009	X	-	-	-
21	CLA	4	4010	X	-	-	-
21	CLA	4	4011	X	-	X	-
21	CLA	4	4012	X	-	X	-
21	CLA	4	4013	X	-	-	-
21	CLA	4	4014	X	-	X	-
21	CLA	4	4015	X	-	-	-
21	CLA	A	1101	X	-	-	-
21	CLA	A	1102	X	-	-	-
21	CLA	A	1103	X	-	-	-
21	CLA	A	1104	X	-	-	-
21	CLA	A	1105	X	-	-	-
21	CLA	A	1106	X	-	-	-
21	CLA	A	1107	X	-	-	-
21	CLA	A	1108	X	-	-	-
21	CLA	A	1109	X	-	-	-
21	CLA	A	1110	X	-	-	X
21	CLA	A	1111	X	-	-	-
21	CLA	A	1112	X	-	-	-
21	CLA	A	1113	X	-	-	-
21	CLA	A	1114	X	-	-	-
21	CLA	A	1115	X	-	-	-
21	CLA	A	1116	X	-	-	-
21	CLA	A	1117	X	-	-	-
21	CLA	A	1118	X	-	-	-
21	CLA	A	1119	X	-	-	-
21	CLA	A	1120	X	-	-	-
21	CLA	A	1121	X	-	-	-
21	CLA	A	1122	X	-	-	-
21	CLA	A	1123	X	-	-	-
21	CLA	A	1124	X	-	-	-
21	CLA	A	1125	X	-	-	-
21	CLA	A	1126	X	-	-	X
21	CLA	A	1127	X	-	-	-
21	CLA	A	1128	X	-	-	-
21	CLA	A	1129	X	-	X	-
21	CLA	A	1130	X	-	-	-
21	CLA	A	1131	X	-	-	-
21	CLA	A	1132	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	1133	X	-	-	-
21	CLA	A	1134	X	-	-	-
21	CLA	A	1135	X	-	-	-
21	CLA	A	1136	X	-	-	-
21	CLA	A	1137	X	-	-	-
21	CLA	A	1138	X	-	-	-
21	CLA	A	1139	X	-	-	-
21	CLA	A	1140	X	-	-	-
21	CLA	A	1141	X	-	-	-
21	CLA	A	1142	X	-	-	-
21	CLA	A	1143	X	-	-	-
21	CLA	A	9012	X	-	-	-
21	CLA	A	9013	X	-	-	-
21	CLA	B	1201	X	-	-	-
21	CLA	B	1202	X	-	-	-
21	CLA	B	1203	X	-	-	-
21	CLA	B	1204	X	-	-	-
21	CLA	B	1205	X	-	-	-
21	CLA	B	1206	X	-	-	X
21	CLA	B	1207	X	-	-	-
21	CLA	B	1208	X	-	-	-
21	CLA	B	1209	X	-	-	-
21	CLA	B	1210	X	-	-	-
21	CLA	B	1211	X	-	-	-
21	CLA	B	1212	X	-	-	X
21	CLA	B	1213	X	-	X	-
21	CLA	B	1214	X	-	-	-
21	CLA	B	1215	X	-	-	-
21	CLA	B	1216	X	-	-	X
21	CLA	B	1217	X	-	-	-
21	CLA	B	1218	X	-	-	-
21	CLA	B	1219	X	-	-	-
21	CLA	B	1220	X	-	-	-
21	CLA	B	1221	X	-	-	-
21	CLA	B	1222	X	-	-	-
21	CLA	B	1223	X	-	-	-
21	CLA	B	1224	X	-	-	-
21	CLA	B	1225	X	-	-	-
21	CLA	B	1226	X	-	-	-
21	CLA	B	1227	X	-	X	-
21	CLA	B	1228	X	-	-	-
21	CLA	B	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	1230	X	-	-	-
21	CLA	B	1231	X	-	-	-
21	CLA	B	1234	X	-	-	-
21	CLA	B	1235	X	-	-	-
21	CLA	B	1236	X	-	-	-
21	CLA	B	1237	X	-	-	-
21	CLA	B	1238	X	-	-	-
21	CLA	B	1239	X	-	-	-
21	CLA	B	1240	X	-	X	X
21	CLA	B	9010	X	-	X	-
21	CLA	B	9022	X	-	-	-
21	CLA	B	9023	X	-	-	-
21	CLA	F	1301	X	-	-	-
21	CLA	F	1302	X	-	-	X
21	CLA	F	1303	X	-	X	-
21	CLA	G	1001	X	-	-	-
21	CLA	G	1002	X	-	X	-
21	CLA	H	1000	X	-	-	-
21	CLA	J	1302	X	-	-	X
21	CLA	J	6014	X	-	-	-
21	CLA	J	6015	X	-	-	-
21	CLA	L	1501	X	-	X	-
21	CLA	L	1502	X	-	-	-
21	CLA	L	1503	X	-	-	-
23	CL0	A	9011	X	-	-	-
26	LUT	1	1501	X	-	X	-
26	LUT	1	1502	X	-	X	X
26	LUT	2	2501	X	-	X	X
26	LUT	2	2502	X	-	X	-
26	LUT	4	4501	X	-	X	X
26	LUT	4	4502	X	-	X	-
27	NEX	4	4503	-	-	X	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 34540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5675	3717	968	972	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	GLY	CONFLICT	UNP P05310
A	627	SER	THR	CONFLICT	UNP P05310
A	639	GLY	ALA	CONFLICT	UNP P05310

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5834	3833	989	998	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	LEU	ILE	CONFLICT	UNP P05311
B	273	MET	VAL	CONFLICT	UNP P05311
B	471	SER	THR	CONFLICT	UNP P05311
B	476	VAL	ILE	CONFLICT	UNP P05311
B	477	LEU	PRO	CONFLICT	UNP P05311
B	483	SER	GLY	CONFLICT	UNP P05311
B	491	SER	ASN	CONFLICT	UNP P05311
B	603	GLN	ARG	CONFLICT	UNP P05311
B	635	TYR	ILE	CONFLICT	UNP P05311

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

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

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	137	Total	C	N	O	S	0	0	0
			1070	685	187	195	3			

- Molecule 5 is a protein called Photosystem I reaction center subunit IV B, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	63	Total	C	N	O	0	0	0
			507	321	89	97			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	152	Total	C	N	O	S	0	0	0
			1196	776	206	212	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	0	0	0
			639	414	107	118			

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	82	Total	C	N	O	0	0	0
			628	415	95	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	26	Total	C	N	O	S	0	0	0
			197	137	29	30	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	40	Total	C	N	O	0	0	0
			316	214	49	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	66	Total	C	N	O	S	0	0	0
			459	291	78	87	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	52	SER	PRO	CONFLICT	UNP E1C9L3
K	55	VAL	LEU	CONFLICT	UNP E1C9L3
K	59	ALA	THR	CONFLICT	UNP E1C9L3
K	62	THR	SER	CONFLICT	UNP E1C9L3
K	88	ALA	VAL	CONFLICT	UNP E1C9L3
K	111	THR	VAL	CONFLICT	UNP E1C9L3

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	163	Total	C	N	O	S	0	0	0
			1214	800	195	218	1			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			684	438	114	128	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	86	SER	GLY	CONFLICT	UNP E1C9K7
N	88	PHE	ILE	CONFLICT	UNP E1C9K7
N	89	ASP	GLU	CONFLICT	UNP E1C9K7
N	90	ALA	GLU	CONFLICT	UNP E1C9K7
N	97	ALA	THR	CONFLICT	UNP E1C9K7
N	110	SER	THR	CONFLICT	UNP E1C9K7
N	121	GLN	GLU	CONFLICT	UNP E1C9K7
N	124	THR	SER	CONFLICT	UNP E1C9K7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	146	ILE	LEU	CONFLICT	UNP E1C9K7
N	148	GLU	ASP	CONFLICT	UNP E1C9K7
N	151	GLU	ASP	CONFLICT	UNP E1C9K7
N	160	PHE	TYR	CONFLICT	UNP E1C9K7

- Molecule 14 is a protein called Chlorophyll a-b binding protein 6A, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	171	Total	C	N	O	S	0	0	0
			1271	823	218	226	4			

- Molecule 15 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	146	Total	C	N	O	S	0	0	0
			1116	726	189	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	151	Total	C	N	O	S	0	0	0
			1118	730	184	199	5			

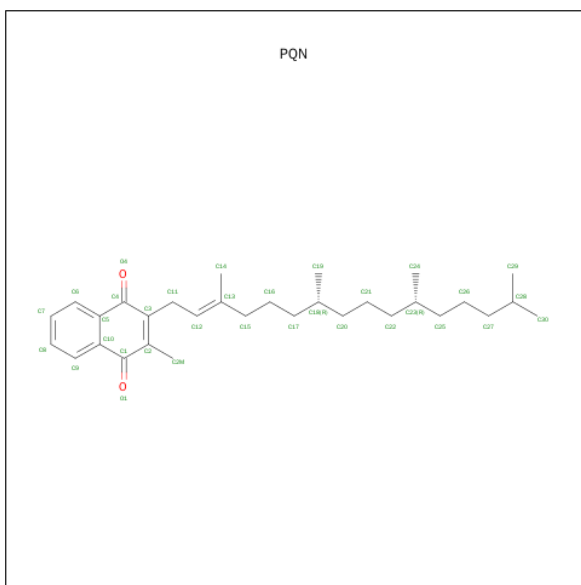
- Molecule 17 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	196	Total	C	N	O	S	0	0	0
			1439	934	242	260	3			

There are 2 discrepancies between the modelled and reference sequences:

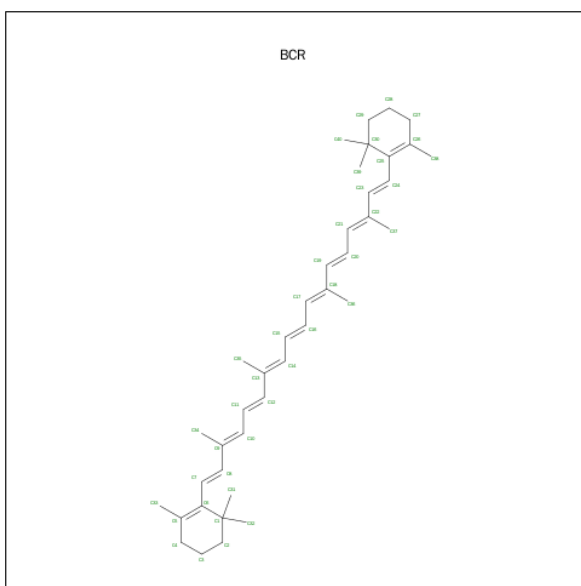
Chain	Residue	Modelled	Actual	Comment	Reference
4	129	ASP	ALA	CONFLICT	UNP Q9SQL2
4	151	PHE	SER	CONFLICT	UNP Q9SQL2

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



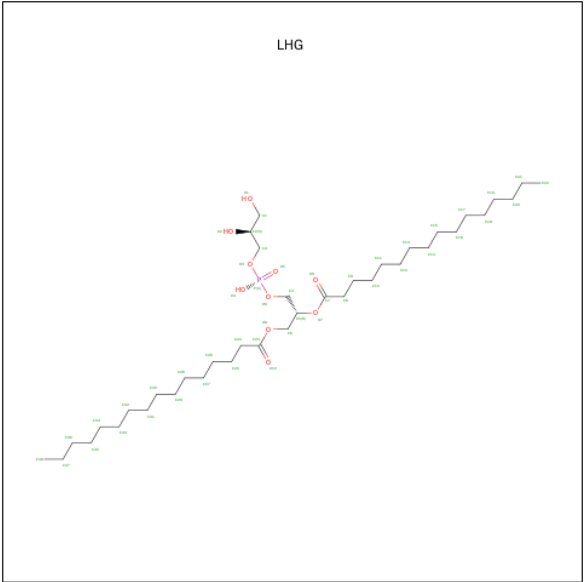
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0

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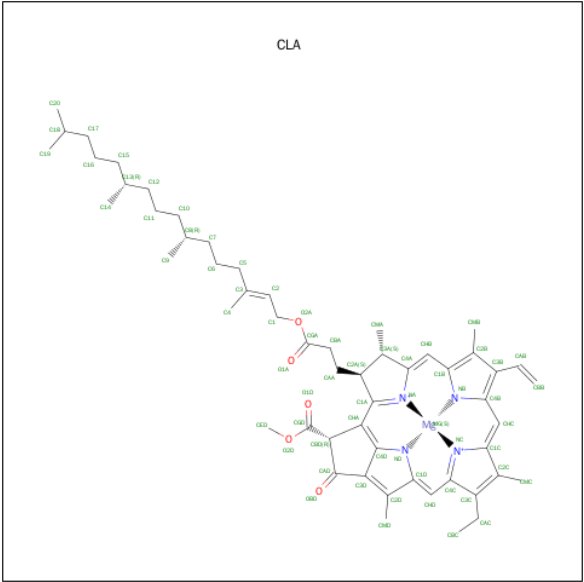
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 25 25	0	0
19	F	1	Total C 40 40	0	0
19	F	1	Total C 40 40	0	0
19	G	1	Total C 40 40	0	0
19	I	1	Total C 40 40	0	0
19	I	1	Total C 40 40	0	0
19	J	1	Total C 40 40	0	0
19	J	1	Total C 40 40	0	0
19	L	1	Total C 40 40	0	0
19	L	1	Total C 40 40	0	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			49	38	10	1		
20	A	1	Total	C	O	P	0	0
			49	38	10	1		
20	B	1	Total	C	O	P	0	0
			49	38	10	1		
20	1	1	Total	C	O	P	0	0
			49	38	10	1		
20	2	1	Total	C	O	P	0	0
			36	25	10	1		

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	F	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	F	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	F	1	Total 64	C 55	Mg 1	N 4	O 4	0	0
21	G	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	G	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	H	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	J	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
21	J	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
21	J	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	L	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	1	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
21	1	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N		0	0
			27	22	1	4			
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			59	50	1	4	4		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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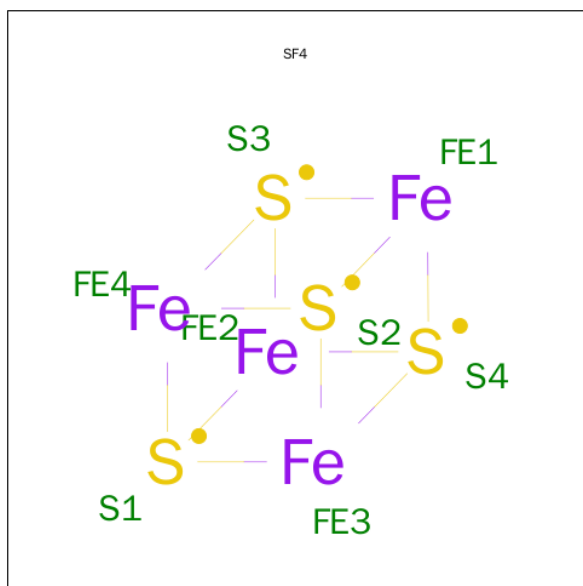
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	3	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	3	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	3	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
21	3	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	3	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	4	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



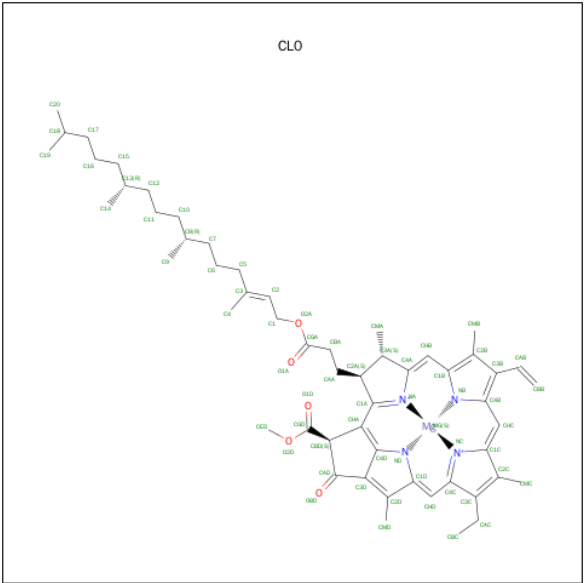
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	Fe	S	0	0
			8	4	4		
22	C	1	Total	Fe	S	0	0
			8	4	4		

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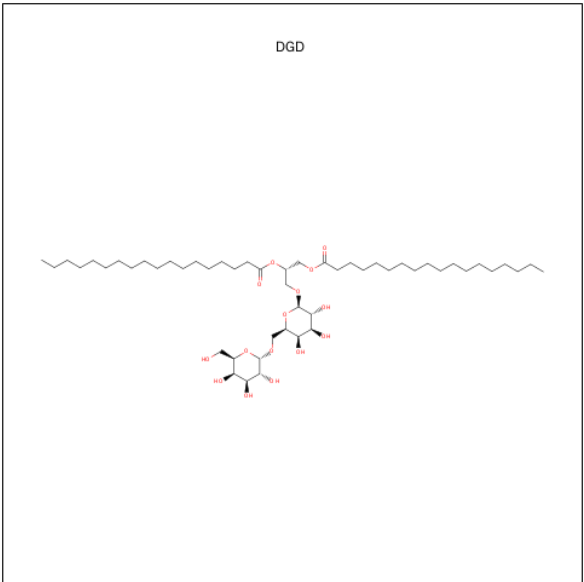
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
22	C	1	8	4	4	0	0

- Molecule 23 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



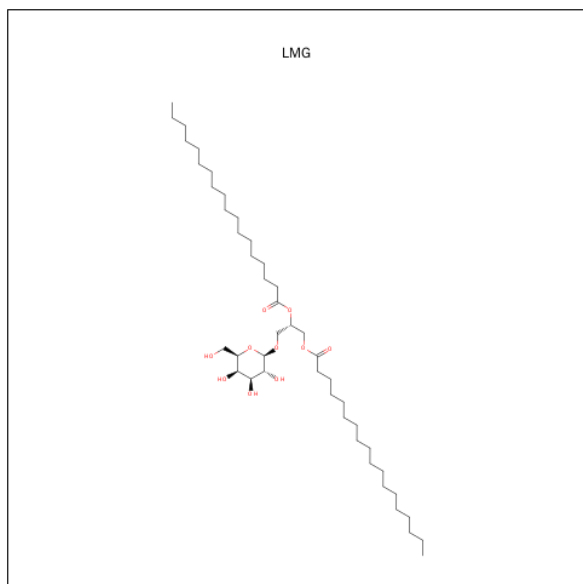
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	A	1	65	55	1	4	5	0	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



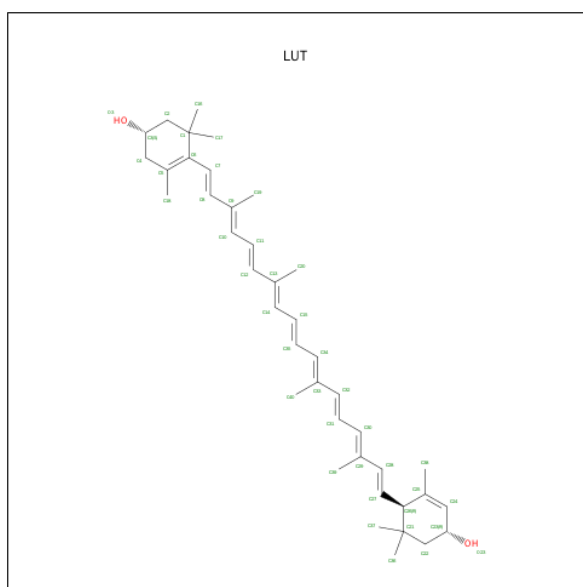
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			61	46	15		

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



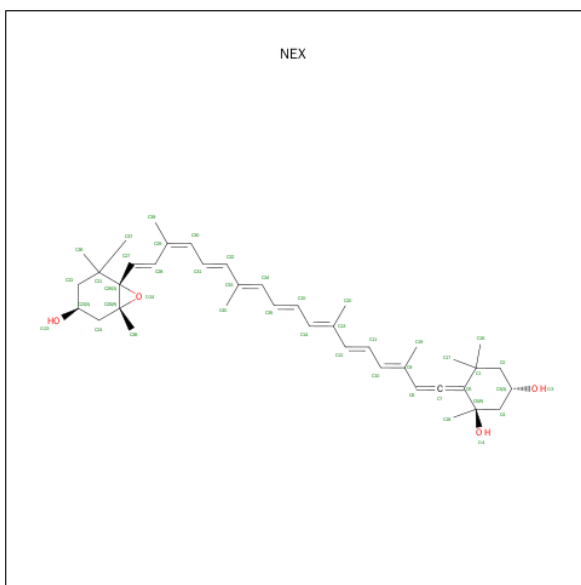
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	G	1	Total	C	O	0	0
			23	13	10		
25	J	1	Total	C	O	0	0
			35	25	10		

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



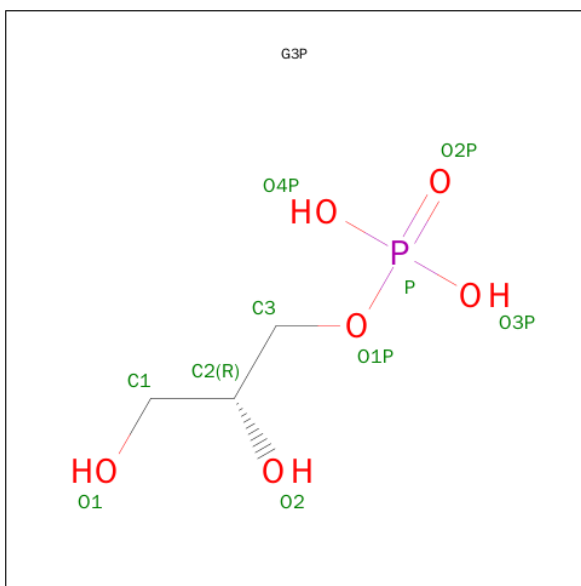
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	1	1	Total	C	O	0	0
			42	40	2		
26	1	1	Total	C	O	0	0
			42	40	2		
26	2	1	Total	C	O	0	0
			42	40	2		
26	2	1	Total	C	O	0	0
			42	40	2		
26	4	1	Total	C	O	0	0
			42	40	2		
26	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 27 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	4	1	Total	C	O	0	0
			44	40	4		

- Molecule 28 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $\text{C}_3\text{H}_9\text{O}_6\text{P}$).

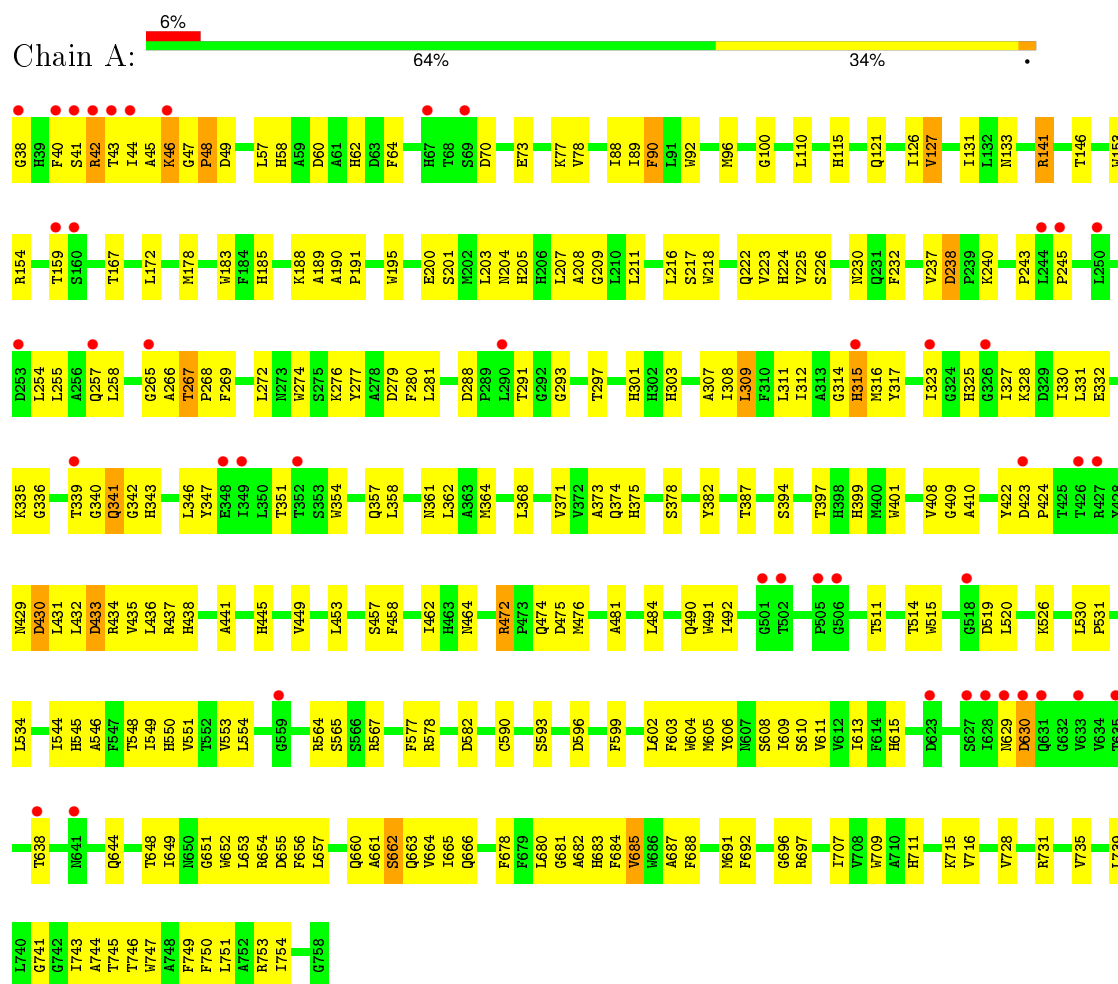


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	4	1	Total	C	O	P	0	0
			10	3	6	1		

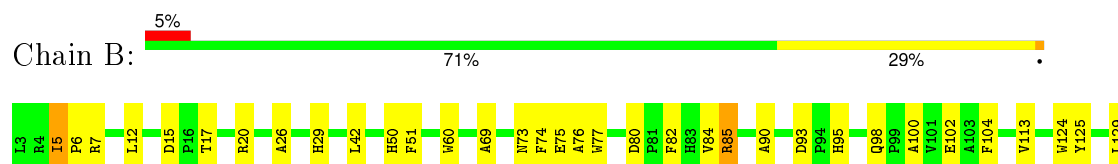
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

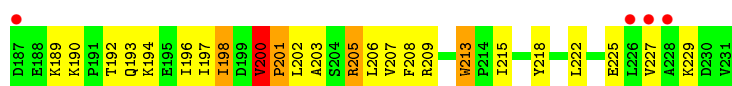
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



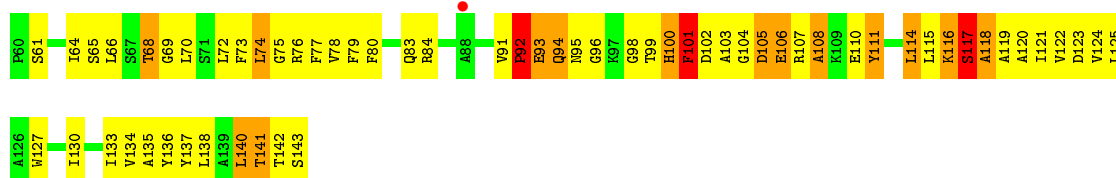
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



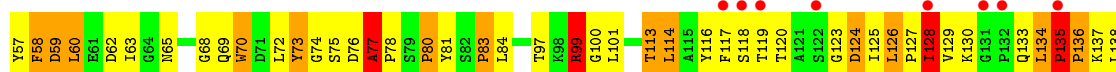




- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 8: Photosystem I reaction center subunit VI, chloroplastic



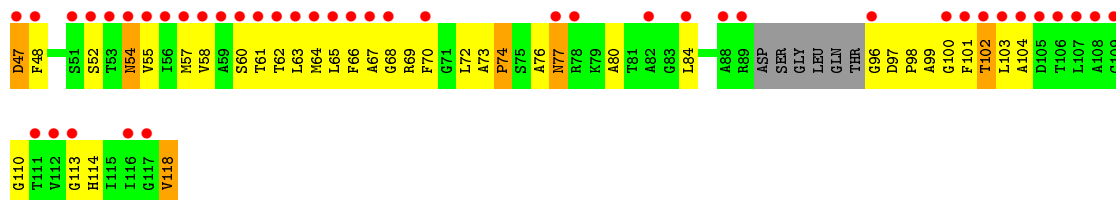
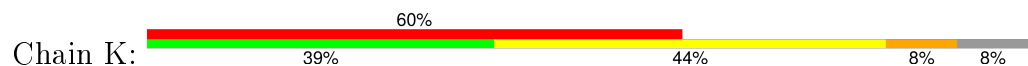
- Molecule 9: Photosystem I reaction center subunit VIII



- Molecule 10: Photosystem I reaction center subunit IX

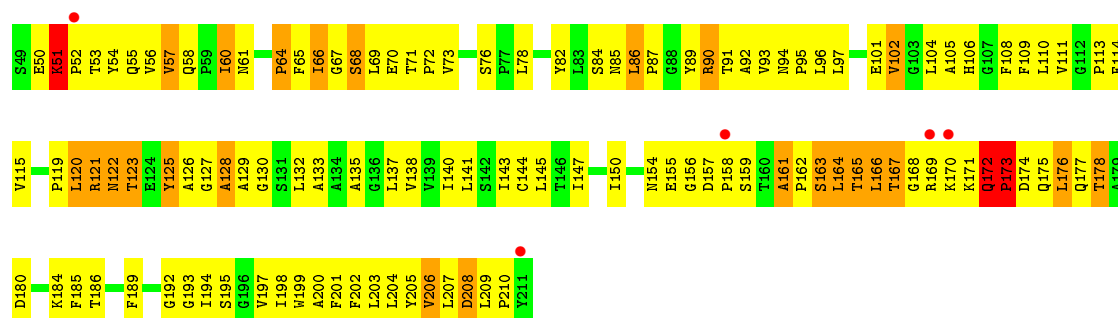


- Molecule 11: Photosystem I reaction center subunit X psaK

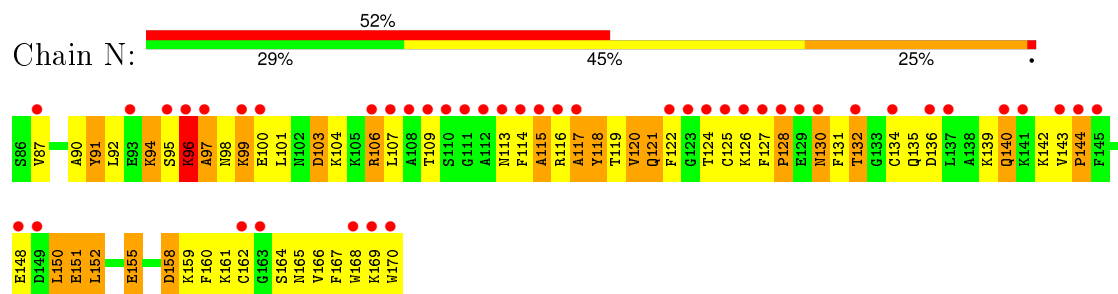


- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

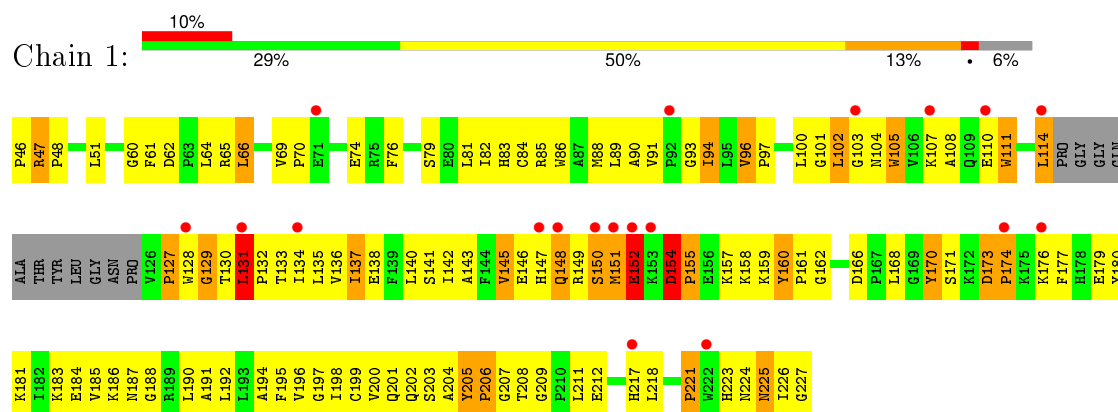




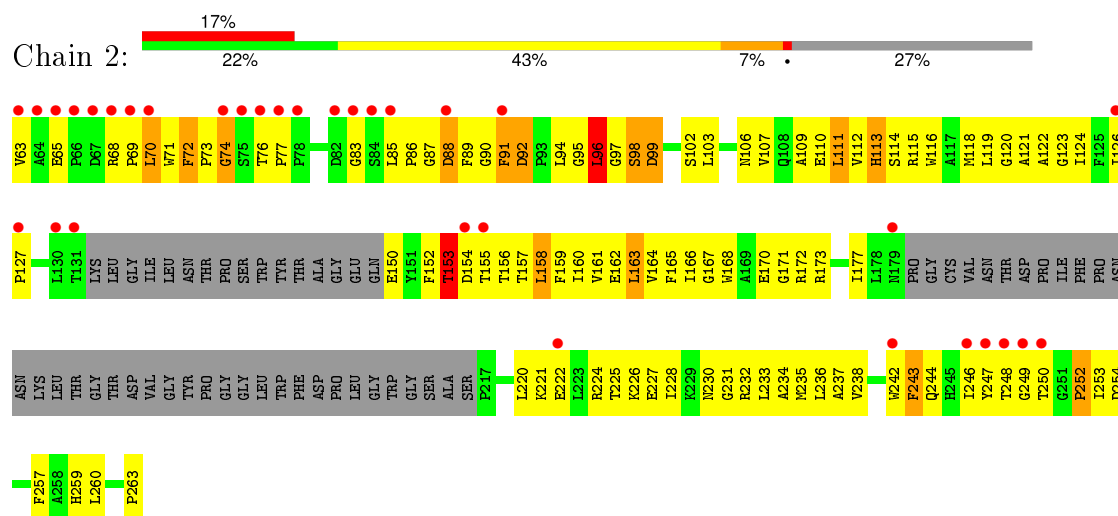
• Molecule 13: Photosystem I-N subunit



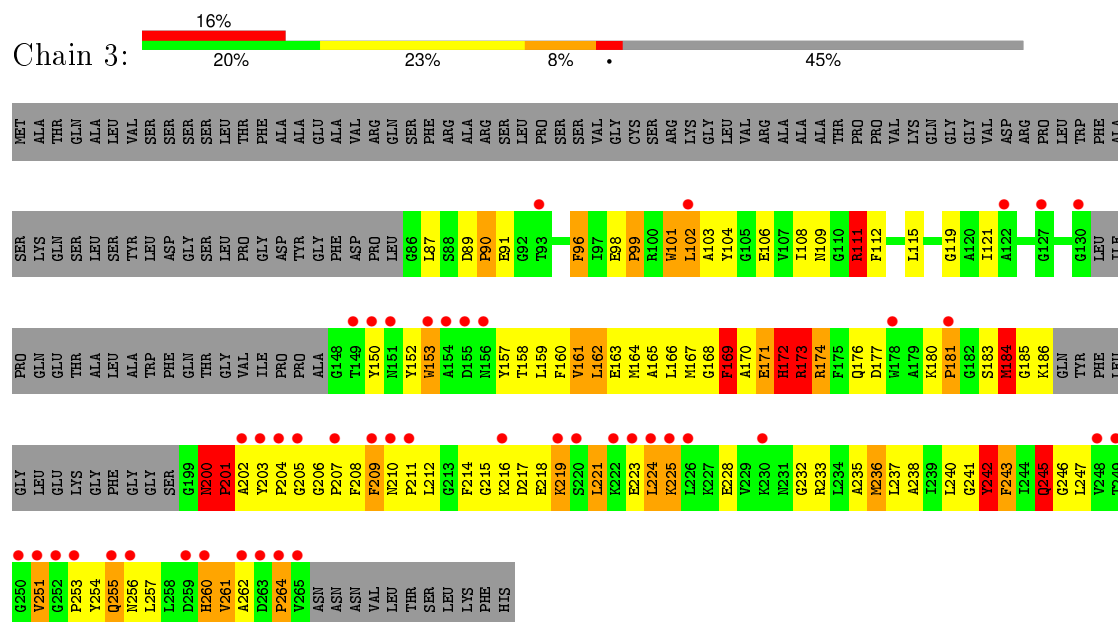
• Molecule 14: Chlorophyll a-b binding protein 6A, chloroplastic



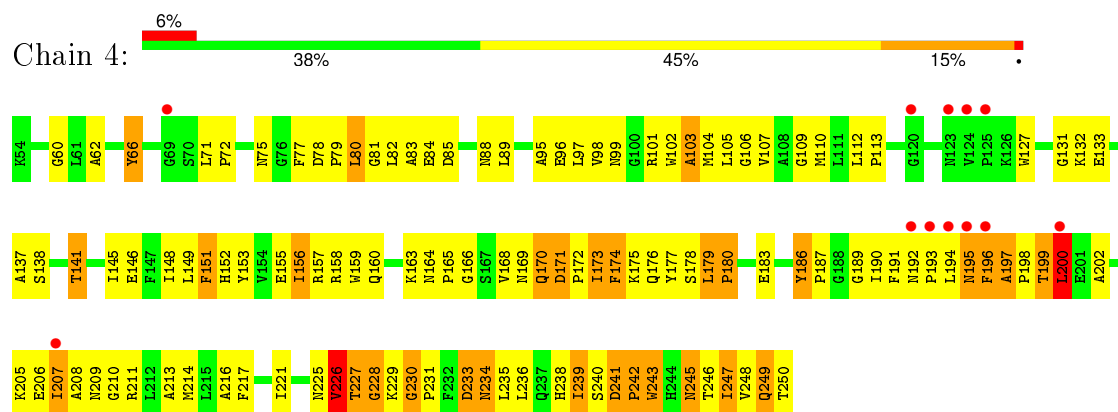
• Molecule 15: Type II chlorophyll a/b binding protein from photosystem I



● Molecule 16: Chlorophyll a-b binding protein 3, chloroplastic



● Molecule 17: Chlorophyll a-b binding protein P4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.63Å 189.17Å 129.67Å 90.00° 91.11° 90.00°	Depositor
Resolution (Å)	39.69 – 3.00 48.59 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.69-3.00) 91.2 (48.59-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.258 , 0.293 0.266 , 0.297	Depositor DCC
R_{free} test set	5774 reflections (5.74%)	DCC
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.5	EDS
Estimated twinning fraction	0.026 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 115991 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	34540	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: LHG, G3P, LUT, DGD, SF4, CLA, PQN, NEX, CL0, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/5867	0.48	2/8006 (0.0%)
2	B	0.39	0/6045	0.44	0/8259
3	C	0.32	0/625	0.49	1/846 (0.1%)
4	D	0.64	0/1097	0.84	3/1483 (0.2%)
5	E	0.62	0/518	0.75	2/704 (0.3%)
6	F	0.56	0/1223	0.61	2/1652 (0.1%)
7	G	0.77	0/653	0.93	2/885 (0.2%)
8	H	0.64	0/648	0.98	7/883 (0.8%)
9	I	0.26	0/203	0.62	0/276
10	J	0.60	0/325	0.66	1/445 (0.2%)
11	K	0.30	0/464	0.64	0/627
12	L	0.89	0/1250	0.97	6/1711 (0.4%)
13	N	0.37	0/699	0.77	1/935 (0.1%)
14	1	0.92	3/1308 (0.2%)	1.01	4/1783 (0.2%)
15	2	0.68	0/1153	0.77	1/1577 (0.1%)
16	3	0.54	0/1150	0.78	1/1562 (0.1%)
17	4	0.80	0/1483	0.82	2/2031 (0.1%)
All	All	0.58	3/24711 (0.0%)	0.67	35/33665 (0.1%)

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
2	B	0	1
5	E	0	1
8	H	0	1
11	K	0	1
13	N	0	2
16	3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	152	GLU	C-N	8.00	1.52	1.34
14	1	151	MET	C-N	-5.52	1.21	1.34
14	1	150	SER	C-N	5.16	1.46	1.34

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	67	GLY	N-CA-C	7.16	131.00	113.10
6	F	200	VAL	N-CA-C	-6.80	92.64	111.00
8	H	135	PRO	C-N-CD	6.56	142.17	128.40
8	H	134	LEU	CA-CB-CG	-6.49	100.37	115.30
8	H	136	PRO	CA-N-CD	-6.49	102.41	111.50

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	684	ARG	Sidechain
5	E	100	ARG	Sidechain
8	H	128	ILE	Peptide
11	K	97	ASP	Peptide
13	N	143	VAL	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	A	5675	0	5527	290	0
2	B	5834	0	5615	225	0
3	C	612	0	598	35	0
4	D	1070	0	1073	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	507	0	501	33	0
6	F	1196	0	1228	60	0
7	G	639	0	631	205	0
8	H	628	0	616	58	0
9	I	197	0	213	16	0
10	J	316	0	326	32	0
11	K	459	0	465	31	0
12	L	1214	0	1212	226	0
13	N	684	0	670	72	0
14	1	1271	0	1204	302	0
15	2	1116	0	1036	234	0
16	3	1118	0	1046	228	0
17	4	1439	0	1303	323	0
18	A	33	0	46	4	0
18	B	33	0	46	6	0
19	A	240	0	292	30	0
19	B	225	0	269	25	0
19	F	80	0	98	14	0
19	G	40	0	48	14	0
19	I	80	0	97	13	0
19	J	80	0	96	7	0
19	L	80	0	98	35	0
20	1	49	0	74	41	0
20	2	36	0	42	23	0
20	A	98	0	148	26	0
20	B	49	0	74	16	0
21	1	819	0	811	499	0
21	2	799	0	780	321	0
21	3	819	0	703	186	0
21	4	846	0	808	385	0
21	A	2538	0	2415	267	0
21	B	2467	0	2510	279	0
21	F	155	0	138	27	0
21	G	101	0	82	60	0
21	H	46	0	33	5	0
21	J	177	0	171	15	0
21	L	161	0	144	51	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	A	65	0	72	15	0
24	B	61	0	83	4	0
25	G	23	0	16	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	J	35	0	40	3	0
26	1	84	0	110	112	0
26	2	84	0	110	89	0
26	4	84	0	110	95	0
27	4	44	0	54	43	0
28	4	10	0	7	0	0
All	All	34540	0	33889	3868	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

The worst 5 of 3868 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)
1:A:43:THR:CB	1:A:46:LYS:HE3	1.47	1.45
1:A:43:THR:HB	1:A:46:LYS:CE	1.61	1.29
21:4:4011:CLA:HMB1	21:4:4011:CLA:HBB1	1.19	1.19
1:A:43:THR:CA	1:A:46:LYS:HE3	1.74	1.17
17:4:199:THR:HA	17:4:200:LEU:HD22	1.25	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	719/721 (100%)	666 (93%)	44 (6%)	9 (1%)	15 53
2	B	729/731 (100%)	702 (96%)	24 (3%)	3 (0%)	39 80
3	C	78/80 (98%)	69 (88%)	8 (10%)	1 (1%)	15 53
4	D	135/137 (98%)	104 (77%)	17 (13%)	14 (10%)	1 3
5	E	61/63 (97%)	51 (84%)	7 (12%)	3 (5%)	3 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	150/152 (99%)	128 (85%)	17 (11%)	5 (3%)	5	26
7	G	82/84 (98%)	65 (79%)	10 (12%)	7 (8%)	1	5
8	H	80/82 (98%)	67 (84%)	6 (8%)	7 (9%)	1	4
9	I	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
10	J	38/40 (95%)	36 (95%)	0	2 (5%)	2	14
11	K	62/72 (86%)	50 (81%)	10 (16%)	2 (3%)	5	27
12	L	161/163 (99%)	135 (84%)	14 (9%)	12 (8%)	1	6
13	N	83/85 (98%)	44 (53%)	20 (24%)	19 (23%)	0	0
14	1	167/182 (92%)	146 (87%)	10 (6%)	11 (7%)	1	8
15	2	140/199 (70%)	112 (80%)	18 (13%)	10 (7%)	1	7
16	3	145/275 (53%)	98 (68%)	26 (18%)	21 (14%)	0	1
17	4	193/196 (98%)	152 (79%)	22 (11%)	19 (10%)	1	3
All	All	3047/3288 (93%)	2648 (87%)	254 (8%)	145 (5%)	3	17

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
4	D	77	PRO
5	E	66	ILE
5	E	102	PRO
7	G	92	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	583/584 (100%)	553 (95%)	30 (5%)	29	69
2	B	596/600 (99%)	577 (97%)	19 (3%)	46	82
3	C	69/69 (100%)	65 (94%)	4 (6%)	25	63
4	D	114/117 (97%)	99 (87%)	15 (13%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	56/56 (100%)	47 (84%)	9 (16%)	3	14
6	F	124/125 (99%)	114 (92%)	10 (8%)	15	47
7	G	65/66 (98%)	52 (80%)	13 (20%)	1	8
8	H	67/68 (98%)	52 (78%)	15 (22%)	1	5
9	I	22/22 (100%)	19 (86%)	3 (14%)	5	20
10	J	33/33 (100%)	30 (91%)	3 (9%)	12	41
11	K	46/52 (88%)	41 (89%)	5 (11%)	8	30
12	L	126/129 (98%)	113 (90%)	13 (10%)	9	33
13	N	73/73 (100%)	62 (85%)	11 (15%)	3	17
14	1	123/148 (83%)	106 (86%)	17 (14%)	4	20
15	2	108/162 (67%)	92 (85%)	16 (15%)	4	17
16	3	103/213 (48%)	76 (74%)	27 (26%)	0	3
17	4	134/162 (83%)	113 (84%)	21 (16%)	3	15
All	All	2442/2679 (91%)	2211 (90%)	231 (10%)	11	38

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	70	TRP
12	L	102	VAL
17	4	151	PHE
8	H	99	ARG
9	I	14	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	172	GLN
14	1	202	GLN
17	4	244	HIS
14	1	201	GLN
14	1	217	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

200 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
21	CLA	1	1001	14	45,63,73	1.91	12 (26%)	49,101,113	2.42	19 (38%)
21	CLA	1	1002	-	46,64,73	1.90	11 (23%)	50,102,113	2.44	17 (34%)
21	CLA	1	1003	14	55,73,73	1.68	12 (21%)	61,113,113	2.29	18 (29%)
21	CLA	1	1004	14	55,73,73	1.64	13 (23%)	61,113,113	2.28	14 (22%)
21	CLA	1	1005	-	46,64,73	1.82	12 (26%)	50,102,113	2.28	16 (32%)
21	CLA	1	1006	-	37,55,73	2.18	12 (32%)	42,91,113	2.74	16 (38%)
21	CLA	1	1007	20	45,63,73	1.89	12 (26%)	49,101,113	2.14	14 (28%)
21	CLA	1	1008	-	55,73,73	1.65	13 (23%)	61,113,113	2.18	13 (21%)
21	CLA	1	1009	-	55,73,73	1.65	11 (20%)	61,113,113	2.76	19 (31%)
21	CLA	1	1010	-	55,73,73	1.70	12 (21%)	61,113,113	2.01	13 (21%)
21	CLA	1	1011	-	55,73,73	1.68	13 (23%)	61,113,113	2.39	17 (27%)
21	CLA	1	1012	14	40,58,73	2.01	12 (30%)	44,95,113	2.36	17 (38%)
21	CLA	1	1013	-	55,73,73	1.73	12 (21%)	61,113,113	2.05	15 (24%)
21	CLA	1	1014	-	32,53,73	2.17	11 (34%)	37,89,113	2.68	11 (29%)
26	LUT	1	1501	-	41,43,43	2.39	2 (4%)	51,60,60	3.89	27 (52%)
26	LUT	1	1502	-	41,43,43	2.34	4 (9%)	51,60,60	4.41	28 (54%)
20	LHG	1	1801	21	48,48,48	0.87	2 (4%)	49,54,54	1.16	3 (6%)
21	CLA	2	2001	15	18,35,73	2.85	11 (61%)	22,60,113	3.54	14 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	2002	-	50,68,73	1.81	13 (26%)	55,107,113	2.34	16 (29%)
21	CLA	2	2003	-	55,73,73	1.78	12 (21%)	61,113,113	2.25	15 (24%)
21	CLA	2	2004	15	50,67,73	1.97	14 (28%)	56,105,113	2.31	14 (25%)
21	CLA	2	2005	-	55,73,73	1.65	10 (18%)	61,113,113	1.96	11 (18%)
21	CLA	2	2006	-	47,65,73	1.91	12 (25%)	50,103,113	2.38	13 (26%)
21	CLA	2	2007	20	45,63,73	1.85	12 (26%)	49,101,113	2.38	15 (30%)
21	CLA	2	2008	-	55,73,73	1.79	12 (21%)	61,113,113	2.28	16 (26%)
21	CLA	2	2009	15	36,54,73	2.21	12 (33%)	41,90,113	2.37	13 (31%)
21	CLA	2	2010	-	55,73,73	1.74	12 (21%)	61,113,113	2.15	14 (22%)
21	CLA	2	2011	-	50,68,73	1.81	13 (26%)	55,107,113	2.46	14 (25%)
21	CLA	2	2012	15	55,73,73	1.68	13 (23%)	61,113,113	2.04	15 (24%)
21	CLA	2	2013	-	55,73,73	1.63	12 (21%)	61,113,113	2.26	15 (24%)
21	CLA	2	2014	-	32,53,73	2.09	12 (37%)	37,89,113	2.73	14 (37%)
26	LUT	2	2501	-	41,43,43	2.39	3 (7%)	51,60,60	3.42	16 (31%)
26	LUT	2	2502	-	41,43,43	2.43	3 (7%)	51,60,60	2.43	14 (27%)
20	LHG	2	2801	21	35,35,48	1.10	3 (8%)	36,41,54	1.14	3 (8%)
21	CLA	3	3001	-	55,73,73	1.83	12 (21%)	61,113,113	2.05	11 (18%)
21	CLA	3	3002	-	45,63,73	2.04	11 (24%)	49,101,113	2.35	12 (24%)
21	CLA	3	3003	-	50,68,73	1.94	12 (24%)	55,107,113	2.05	13 (23%)
21	CLA	3	3004	-	32,53,73	2.25	11 (34%)	37,89,113	2.22	9 (24%)
21	CLA	3	3005	21	32,53,73	2.28	10 (31%)	37,89,113	2.41	9 (24%)
21	CLA	3	3006	-	55,73,73	1.85	12 (21%)	61,113,113	2.06	12 (19%)
21	CLA	3	3008	-	55,73,73	1.76	12 (21%)	61,113,113	2.15	17 (27%)
21	CLA	3	3009	-	36,54,73	2.31	12 (33%)	41,90,113	2.56	17 (41%)
21	CLA	3	3010	-	42,60,73	2.08	12 (28%)	45,97,113	2.45	14 (31%)
21	CLA	3	3011	-	36,54,73	2.31	12 (33%)	41,90,113	2.42	12 (29%)
21	CLA	3	3012	21,16	32,53,73	2.12	11 (34%)	37,89,113	3.06	17 (45%)
21	CLA	3	3013	-	40,58,73	2.13	13 (32%)	44,95,113	2.82	15 (34%)
21	CLA	3	3014	-	32,53,73	2.18	10 (31%)	37,89,113	2.49	14 (37%)
21	CLA	3	3015	-	32,53,73	2.28	11 (34%)	37,89,113	2.28	10 (27%)
21	CLA	3	3016	-	32,53,73	2.28	11 (34%)	37,89,113	2.29	9 (24%)
21	CLA	3	3017	-	32,53,73	2.25	11 (34%)	37,89,113	2.36	9 (24%)
21	CLA	4	4001	17	55,73,73	1.69	11 (20%)	61,113,113	2.26	14 (22%)
21	CLA	4	4002	-	46,64,73	1.91	13 (28%)	50,102,113	2.45	13 (26%)
21	CLA	4	4003	17	55,73,73	1.69	13 (23%)	61,113,113	1.87	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	4	4004	-	55,73,73	1.69	13 (23%)	61,113,113	2.27	13 (21%)
21	CLA	4	4005	17	32,53,73	2.08	12 (37%)	37,89,113	3.23	18 (48%)
21	CLA	4	4006	-	55,73,73	1.77	12 (21%)	61,113,113	2.29	21 (34%)
21	CLA	4	4007	-	55,73,73	1.69	12 (21%)	61,113,113	2.02	12 (19%)
21	CLA	4	4008	-	38,56,73	1.95	11 (28%)	42,92,113	3.17	19 (45%)
21	CLA	4	4009	17	40,58,73	1.93	11 (27%)	44,95,113	2.54	11 (25%)
21	CLA	4	4010	-	40,58,73	1.99	10 (25%)	44,95,113	2.65	15 (34%)
21	CLA	4	4011	-	55,73,73	1.59	13 (23%)	61,113,113	2.43	17 (27%)
21	CLA	4	4012	-	55,73,73	1.72	12 (21%)	61,113,113	2.16	13 (21%)
21	CLA	4	4013	-	41,59,73	1.83	12 (29%)	44,96,113	2.79	15 (34%)
21	CLA	4	4014	17	32,53,73	2.20	11 (34%)	37,89,113	2.56	14 (37%)
21	CLA	4	4015	-	36,54,73	2.11	10 (27%)	41,90,113	2.32	14 (34%)
26	LUT	4	4501	-	41,43,43	2.32	1 (2%)	51,60,60	3.75	24 (47%)
26	LUT	4	4502	-	41,43,43	2.37	5 (12%)	51,60,60	3.54	26 (50%)
27	NEX	4	4503	-	39,46,46	3.03	12 (30%)	48,70,70	2.27	17 (35%)
28	G3P	4	4505	-	9,9,9	0.60	0	10,12,12	0.66	0
21	CLA	A	1101	-	55,73,73	1.85	12 (21%)	61,113,113	2.08	12 (19%)
21	CLA	A	1102	-	40,58,73	2.16	12 (30%)	44,95,113	2.53	13 (29%)
21	CLA	A	1103	-	55,73,73	1.84	12 (21%)	61,113,113	2.03	14 (22%)
21	CLA	A	1104	1	55,73,73	1.83	11 (20%)	61,113,113	2.05	12 (19%)
21	CLA	A	1105	-	41,59,73	2.14	12 (29%)	44,96,113	2.34	13 (29%)
21	CLA	A	1106	1	55,73,73	1.86	12 (21%)	61,113,113	2.11	12 (19%)
21	CLA	A	1107	1	41,59,73	2.14	11 (26%)	44,96,113	2.45	13 (29%)
21	CLA	A	1108	-	36,54,73	2.38	12 (33%)	41,90,113	2.29	12 (29%)
21	CLA	A	1109	-	55,73,73	1.86	12 (21%)	61,113,113	2.02	14 (22%)
21	CLA	A	1110	-	45,63,73	2.00	12 (26%)	49,101,113	2.27	13 (26%)
21	CLA	A	1111	-	50,68,73	1.93	12 (24%)	55,107,113	2.15	13 (23%)
21	CLA	A	1112	-	36,54,73	2.37	13 (36%)	41,90,113	2.29	13 (31%)
21	CLA	A	1113	-	36,54,73	2.38	12 (33%)	41,90,113	2.31	12 (29%)
21	CLA	A	1114	-	36,54,73	2.41	12 (33%)	41,90,113	2.33	11 (26%)
21	CLA	A	1115	-	46,64,73	2.02	13 (28%)	50,102,113	2.12	10 (20%)
21	CLA	A	1116	-	44,62,73	2.05	13 (29%)	47,99,113	2.24	13 (27%)
21	CLA	A	1117	-	55,73,73	1.86	12 (21%)	61,113,113	2.07	12 (19%)
21	CLA	A	1118	-	36,54,73	2.31	12 (33%)	41,90,113	2.57	14 (34%)
21	CLA	A	1119	-	55,73,73	1.84	11 (20%)	61,113,113	2.02	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	1120	-	36,54,73	2.37	12 (33%)	41,90,113	2.29	12 (29%)
21	CLA	A	1121	-	36,54,73	2.38	11 (30%)	41,90,113	2.44	11 (26%)
21	CLA	A	1122	-	49,67,73	1.95	12 (24%)	53,105,113	2.22	11 (20%)
21	CLA	A	1123	-	55,73,73	1.86	13 (23%)	61,113,113	2.16	13 (21%)
21	CLA	A	1124	-	45,63,73	2.05	12 (26%)	49,101,113	2.24	12 (24%)
21	CLA	A	1125	-	45,63,73	1.78	11 (24%)	49,101,113	2.45	14 (28%)
21	CLA	A	1126	-	55,73,73	1.83	13 (23%)	61,113,113	2.06	15 (24%)
21	CLA	A	1127	-	55,73,73	1.84	12 (21%)	61,113,113	2.03	12 (19%)
21	CLA	A	1128	-	55,73,73	1.81	11 (20%)	61,113,113	2.06	14 (22%)
21	CLA	A	1129	-	40,58,73	2.13	11 (27%)	44,95,113	2.39	13 (29%)
21	CLA	A	1130	-	36,54,73	2.35	11 (30%)	41,90,113	2.25	12 (29%)
21	CLA	A	1131	-	55,73,73	1.69	12 (21%)	61,113,113	2.27	13 (21%)
21	CLA	A	1132	-	55,73,73	1.71	12 (21%)	61,113,113	2.02	14 (22%)
21	CLA	A	1133	-	36,54,73	2.25	12 (33%)	41,90,113	2.41	14 (34%)
21	CLA	A	1134	1	36,54,73	2.37	12 (33%)	41,90,113	2.35	11 (26%)
21	CLA	A	1135	-	41,59,73	2.12	12 (29%)	44,96,113	2.48	14 (31%)
21	CLA	A	1136	-	55,73,73	1.84	12 (21%)	61,113,113	2.10	14 (22%)
21	CLA	A	1137	-	45,63,73	2.02	12 (26%)	49,101,113	2.34	13 (26%)
21	CLA	A	1138	-	55,73,73	1.86	12 (21%)	61,113,113	2.02	13 (21%)
21	CLA	A	1139	-	55,73,73	1.85	12 (21%)	61,113,113	1.97	12 (19%)
21	CLA	A	1140	-	55,73,73	1.87	12 (21%)	61,113,113	2.03	12 (19%)
21	CLA	A	1141	20	41,59,73	2.16	13 (31%)	44,96,113	2.33	10 (22%)
21	CLA	A	1142	-	31,52,73	2.17	10 (32%)	37,88,113	2.29	9 (24%)
21	CLA	A	1143	-	32,53,73	2.28	11 (34%)	37,89,113	2.24	9 (24%)
18	PQN	A	5001	-	34,34,34	1.43	2 (5%)	44,45,45	1.08	2 (4%)
19	BCR	A	6002	-	41,41,41	2.80	6 (14%)	56,56,56	6.65	22 (39%)
19	BCR	A	6003	-	41,41,41	2.87	6 (14%)	56,56,56	6.34	25 (44%)
19	BCR	A	6007	-	41,41,41	2.74	6 (14%)	56,56,56	6.60	28 (50%)
19	BCR	A	6008	-	41,41,41	2.62	6 (14%)	56,56,56	7.61	38 (67%)
19	BCR	A	6011	-	41,41,41	2.77	6 (14%)	56,56,56	7.75	34 (60%)
19	BCR	A	6017	-	41,41,41	2.70	6 (14%)	56,56,56	6.40	25 (44%)
20	LHG	A	7001	-	48,48,48	0.92	2 (4%)	49,54,54	1.08	3 (6%)
20	LHG	A	7003	21	48,48,48	0.93	2 (4%)	49,54,54	1.01	3 (6%)
22	SF4	A	8001	-	0,12,12	0.00	-	0,24,24	0.00	-
23	CL0	A	9011	-	55,73,73	1.60	11 (20%)	61,113,113	2.26	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	9012	-	55,73,73	1.76	12 (21%)	61,113,113	2.16	15 (24%)
21	CLA	A	9013	-	55,73,73	1.67	11 (20%)	61,113,113	2.28	16 (26%)
21	CLA	B	1201	-	36,54,73	2.37	11 (30%)	41,90,113	2.39	12 (29%)
21	CLA	B	1202	-	55,73,73	1.85	12 (21%)	61,113,113	2.09	12 (19%)
21	CLA	B	1203	2	50,68,73	1.93	11 (22%)	55,107,113	2.09	11 (20%)
21	CLA	B	1204	-	45,63,73	2.04	12 (26%)	49,101,113	2.26	14 (28%)
21	CLA	B	1205	-	55,73,73	1.84	12 (21%)	61,113,113	2.19	12 (19%)
21	CLA	B	1206	2	55,73,73	1.82	12 (21%)	61,113,113	2.14	14 (22%)
21	CLA	B	1207	-	55,73,73	1.84	12 (21%)	61,113,113	2.15	13 (21%)
21	CLA	B	1208	-	45,63,73	2.05	13 (28%)	49,101,113	2.12	9 (18%)
21	CLA	B	1209	-	36,54,73	2.36	13 (36%)	41,90,113	2.28	11 (26%)
21	CLA	B	1210	-	55,73,73	1.90	12 (21%)	61,113,113	2.07	13 (21%)
21	CLA	B	1211	-	55,73,73	1.86	12 (21%)	61,113,113	2.08	13 (21%)
21	CLA	B	1212	-	36,54,73	2.38	12 (33%)	41,90,113	2.35	13 (31%)
21	CLA	B	1213	-	50,68,73	1.78	12 (24%)	55,107,113	2.27	14 (25%)
21	CLA	B	1214	-	49,67,73	1.95	11 (22%)	53,105,113	2.13	15 (28%)
21	CLA	B	1215	-	50,68,73	1.92	12 (24%)	55,107,113	2.17	12 (21%)
21	CLA	B	1216	-	55,73,73	1.83	12 (21%)	61,113,113	2.05	13 (21%)
21	CLA	B	1217	-	36,54,73	2.36	12 (33%)	41,90,113	2.36	13 (31%)
21	CLA	B	1218	-	50,68,73	1.93	11 (22%)	55,107,113	2.21	12 (21%)
21	CLA	B	1219	-	50,68,73	1.91	12 (24%)	55,107,113	2.11	15 (27%)
21	CLA	B	1220	-	55,73,73	1.85	11 (20%)	61,113,113	2.03	14 (22%)
21	CLA	B	1221	-	44,62,73	2.06	12 (27%)	47,99,113	2.44	13 (27%)
21	CLA	B	1222	-	55,73,73	1.86	12 (21%)	61,113,113	2.09	13 (21%)
21	CLA	B	1223	-	55,73,73	1.83	12 (21%)	61,113,113	2.15	12 (19%)
21	CLA	B	1224	-	55,73,73	1.85	12 (21%)	61,113,113	2.12	11 (18%)
21	CLA	B	1225	-	55,73,73	1.86	12 (21%)	61,113,113	2.05	12 (19%)
21	CLA	B	1226	-	55,73,73	1.67	11 (20%)	61,113,113	2.33	11 (18%)
21	CLA	B	1227	-	55,73,73	1.61	13 (23%)	61,113,113	2.31	16 (26%)
21	CLA	B	1228	-	41,59,73	1.98	12 (29%)	44,96,113	2.47	14 (31%)
21	CLA	B	1229	-	55,73,73	1.86	13 (23%)	61,113,113	2.05	11 (18%)
21	CLA	B	1230	-	48,66,73	1.96	12 (25%)	52,104,113	2.31	14 (26%)
21	CLA	B	1231	-	36,54,73	2.37	12 (33%)	41,90,113	2.37	11 (26%)
21	CLA	B	1234	-	50,68,73	1.94	12 (24%)	55,107,113	2.16	12 (21%)
21	CLA	B	1235	-	55,73,73	1.85	11 (20%)	61,113,113	2.07	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1236	-	45,63,73	2.03	11 (24%)	49,101,113	2.31	12 (24%)
21	CLA	B	1237	-	50,68,73	1.92	12 (24%)	55,107,113	2.11	13 (23%)
21	CLA	B	1238	-	55,73,73	1.86	12 (21%)	61,113,113	2.04	11 (18%)
21	CLA	B	1239	-	55,73,73	1.63	10 (18%)	61,113,113	2.31	17 (27%)
21	CLA	B	1240	20	55,73,73	1.70	13 (23%)	61,113,113	2.30	19 (31%)
18	PQN	B	5002	-	34,34,34	1.41	2 (5%)	44,45,45	1.01	4 (9%)
19	BCR	B	6004	-	41,41,41	2.88	7 (17%)	56,56,56	6.39	27 (48%)
19	BCR	B	6005	-	41,41,41	2.71	6 (14%)	56,56,56	7.00	28 (50%)
19	BCR	B	6006	-	41,41,41	2.76	6 (14%)	56,56,56	7.97	34 (60%)
19	BCR	B	6009	-	41,41,41	2.70	6 (14%)	56,56,56	6.27	22 (39%)
19	BCR	B	6010	-	41,41,41	2.70	6 (14%)	56,56,56	6.74	22 (39%)
19	BCR	B	6011	-	25,25,41	3.32	5 (20%)	33,33,56	8.25	16 (48%)
20	LHG	B	7004	21	48,48,48	0.94	3 (6%)	49,54,54	1.06	4 (8%)
24	DGD	B	7101	-	62,62,67	0.87	1 (1%)	76,76,81	1.39	11 (14%)
21	CLA	B	9010	-	55,73,73	1.70	12 (21%)	61,113,113	2.11	16 (26%)
21	CLA	B	9022	-	55,73,73	1.73	13 (23%)	61,113,113	2.48	19 (31%)
21	CLA	B	9023	-	55,73,73	1.67	12 (21%)	61,113,113	2.02	16 (26%)
22	SF4	C	8002	3	0,12,12	0.00	-	0,24,24	0.00	-
22	SF4	C	8003	-	0,12,12	0.00	-	0,24,24	0.00	-
21	CLA	F	1301	-	32,53,73	2.25	11 (34%)	37,89,113	2.23	8 (21%)
21	CLA	F	1302	-	36,54,73	2.38	12 (33%)	41,90,113	2.28	11 (26%)
21	CLA	F	1303	-	54,72,73	1.72	13 (24%)	61,111,113	1.97	16 (26%)
19	BCR	F	6014	-	41,41,41	2.68	6 (14%)	56,56,56	7.79	35 (62%)
19	BCR	F	6016	-	41,41,41	2.80	6 (14%)	56,56,56	7.75	36 (64%)
21	CLA	G	1001	-	45,63,73	1.88	13 (28%)	49,101,113	2.49	15 (30%)
21	CLA	G	1002	-	36,54,73	2.22	13 (36%)	41,90,113	2.54	15 (36%)
19	BCR	G	2011	-	41,41,41	2.93	6 (14%)	56,56,56	6.64	26 (46%)
25	LMG	G	2021	-	23,23,55	1.23	2 (8%)	31,31,63	1.83	6 (19%)
21	CLA	H	1000	8	36,54,73	2.30	12 (33%)	41,90,113	2.55	13 (31%)
19	BCR	I	6018	-	41,41,41	2.63	6 (14%)	56,56,56	7.65	33 (58%)
19	BCR	I	6020	-	41,41,41	2.81	6 (14%)	56,56,56	6.62	22 (39%)
21	CLA	J	1302	-	51,69,73	1.92	11 (21%)	56,108,113	2.19	13 (23%)
25	LMG	J	5001	-	35,35,55	1.07	2 (5%)	43,43,63	1.13	3 (6%)
19	BCR	J	6012	-	41,41,41	2.71	6 (14%)	56,56,56	7.48	30 (53%)
19	BCR	J	6013	-	41,41,41	2.78	6 (14%)	56,56,56	6.79	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	J	6014	-	51,69,73	1.93	12 (23%)	56,108,113	2.15	13 (23%)
21	CLA	J	6015	-	45,63,73	2.02	13 (28%)	49,101,113	2.37	15 (30%)
21	CLA	L	1501	12	36,54,73	2.34	11 (30%)	41,90,113	2.29	12 (29%)
21	CLA	L	1502	-	55,73,73	1.83	12 (21%)	61,113,113	2.04	13 (21%)
21	CLA	L	1503	-	40,58,73	2.13	12 (30%)	44,95,113	2.41	13 (29%)
19	BCR	L	6019	-	41,41,41	2.82	6 (14%)	56,56,56	6.34	26 (46%)
19	BCR	L	6020	-	41,41,41	2.80	6 (14%)	56,56,56	6.37	24 (42%)

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
21	CLA	1	1001	14	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	1	1002	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	1	1003	14	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1004	14	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1005	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	1	1006	-	3/3/16/25	0/16/114/135	0/0/9/9
21	CLA	1	1007	20	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	1	1008	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1009	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1010	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1011	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1012	14	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	1	1013	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1014	-	3/3/16/25	0/11/111/135	0/0/9/9
26	LUT	1	1501	-	1/1/12/27	0/29/67/67	0/2/2/2
26	LUT	1	1502	-	1/1/12/27	0/29/67/67	0/2/2/2
20	LHG	1	1801	21	-	0/53/53/53	0/0/0/0
21	CLA	2	2001	15	3/3/8/25	0/0/75/135	0/0/9/9
21	CLA	2	2002	-	3/3/19/25	1/31/129/135	0/0/9/9
21	CLA	2	2003	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	2004	15	3/3/18/25	0/31/125/135	0/0/9/9
21	CLA	2	2005	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	2006	-	3/3/18/25	1/28/126/135	0/0/9/9
21	CLA	2	2007	20	3/3/18/25	1/25/123/135	0/0/9/9
21	CLA	2	2008	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	2009	15	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	2	2010	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	2011	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	2	2012	15	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	2	2013	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	2014	-	3/3/16/25	0/11/111/135	0/0/9/9
26	LUT	2	2501	-	1/1/12/27	0/29/67/67	0/2/2/2
26	LUT	2	2502	-	1/1/12/27	1/29/67/67	0/2/2/2
20	LHG	2	2801	21	-	2/40/40/53	0/0/0/0
21	CLA	3	3001	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	3	3002	-	2/2/18/25	0/25/123/135	0/0/9/9
21	CLA	3	3003	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	3	3004	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3005	21	2/2/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3006	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	3	3008	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	3	3009	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	3	3010	-	3/3/17/25	0/22/120/135	0/0/9/9
21	CLA	3	3011	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	3	3012	21,16	3/3/16/25	1/11/111/135	0/0/9/9
21	CLA	3	3013	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	3	3014	-	2/2/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3015	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3016	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3017	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	4	4001	17	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4002	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	4	4003	17	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4004	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4005	17	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	4	4006	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	4007	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4008	-	3/3/16/25	0/17/115/135	0/0/9/9
21	CLA	4	4009	17	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	4	4010	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	4	4011	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4012	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4013	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	4	4014	17	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	4	4015	-	3/3/16/25	0/15/113/135	0/0/9/9
26	LUT	4	4501	-	1/1/12/27	0/29/67/67	0/2/2/2
26	LUT	4	4502	-	1/1/12/27	0/29/67/67	0/2/2/2
27	NEX	4	4503	-	-	1/27/83/83	0/2/3/3
28	G3P	4	4505	-	-	0/8/8/8	0/0/0/0
21	CLA	A	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1102	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	A	1103	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1104	1	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1105	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	A	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1107	1	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	A	1108	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1109	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1110	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	A	1111	-	2/2/19/25	0/31/129/135	0/0/9/9
21	CLA	A	1112	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1113	-	2/2/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1114	-	2/2/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1115	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	A	1116	-	2/2/17/25	0/24/122/135	0/0/9/9
21	CLA	A	1117	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1118	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1120	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1121	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1122	-	3/3/18/25	0/30/128/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	A	1125	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	A	1126	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1129	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	A	1130	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1131	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1133	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1134	1	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1135	-	1/1/17/25	0/21/119/135	0/0/9/9
21	CLA	A	1136	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1137	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	A	1138	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1139	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1141	20	3/3/17/25	1/21/119/135	0/0/9/9
21	CLA	A	1142	-	3/3/16/25	0/11/109/135	0/0/9/9
21	CLA	A	1143	-	3/3/16/25	0/11/111/135	0/0/9/9
18	PQN	A	5001	-	-	0/23/43/43	0/2/2/2
19	BCR	A	6002	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6003	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6007	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6008	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6011	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6017	-	-	0/29/63/63	0/2/2/2
20	LHG	A	7001	-	-	0/53/53/53	0/0/0/0
20	LHG	A	7003	21	-	0/53/53/53	0/0/0/0
22	SF4	A	8001	-	-	0/0/48/48	0/6/5/5
23	CL0	A	9011	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	9012	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	9013	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1201	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1202	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1203	2	2/2/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1204	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	B	1205	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1206	2	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1207	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1208	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	B	1209	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1211	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1212	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1213	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1214	-	2/2/18/25	0/30/128/135	0/0/9/9
21	CLA	B	1215	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1217	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1218	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1219	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1220	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
21	CLA	B	1222	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1223	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1224	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1227	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1228	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	B	1229	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1230	-	3/3/18/25	0/29/127/135	0/0/9/9
21	CLA	B	1231	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1234	-	2/2/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1235	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1236	-	2/2/18/25	0/25/123/135	0/0/9/9
21	CLA	B	1237	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1238	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1239	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1240	20	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	B	5002	-	-	0/23/43/43	0/2/2/2
19	BCR	B	6004	-	-	1/29/63/63	0/2/2/2
19	BCR	B	6005	-	-	2/29/63/63	0/2/2/2
19	BCR	B	6006	-	-	0/29/63/63	0/2/2/2
19	BCR	B	6009	-	-	0/29/63/63	0/2/2/2
19	BCR	B	6010	-	-	0/29/63/63	0/2/2/2
19	BCR	B	6011	-	-	0/18/35/63	0/1/1/2
20	LHG	B	7004	21	-	0/53/53/53	0/0/0/0
24	DGD	B	7101	-	-	0/50/90/95	0/2/2/2
21	CLA	B	9010	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	9022	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	9023	-	3/3/20/25	0/37/135/135	0/0/9/9
22	SF4	C	8002	3	-	0/0/48/48	0/6/5/5
22	SF4	C	8003	-	-	0/0/48/48	0/6/5/5
21	CLA	F	1301	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	F	1302	-	2/2/16/25	0/15/113/135	0/0/9/9
21	CLA	F	1303	-	3/3/19/25	0/35/133/135	0/0/9/9
19	BCR	F	6014	-	-	0/29/63/63	0/2/2/2
19	BCR	F	6016	-	-	0/29/63/63	0/2/2/2
21	CLA	G	1001	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	G	1002	-	3/3/16/25	0/15/113/135	0/0/9/9
19	BCR	G	2011	-	-	1/29/63/63	0/2/2/2
25	LMG	G	2021	-	-	1/16/36/70	0/1/1/1
21	CLA	H	1000	8	2/2/16/25	0/15/113/135	0/0/9/9
19	BCR	I	6018	-	-	0/29/63/63	0/2/2/2
19	BCR	I	6020	-	-	0/29/63/63	0/2/2/2
21	CLA	J	1302	-	2/2/19/25	0/33/131/135	0/0/9/9
25	LMG	J	5001	-	-	0/30/50/70	0/1/1/1
19	BCR	J	6012	-	-	0/29/63/63	0/2/2/2
19	BCR	J	6013	-	-	0/29/63/63	0/2/2/2
21	CLA	J	6014	-	3/3/19/25	0/33/131/135	0/0/9/9
21	CLA	J	6015	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	L	1501	12	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	L	1502	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	L	1503	-	3/3/17/25	0/19/117/135	0/0/9/9
19	BCR	L	6019	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	L	6020	-	-	0/29/63/63	0/2/2/2

The worst 5 of 2052 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	6003	BCR	C8-C9	-8.58	1.26	1.45
19	B	6011	BCR	C8-C9	-8.47	1.27	1.45
19	G	2011	BCR	C8-C9	-8.45	1.27	1.45
19	A	6002	BCR	C11-C10	-8.21	1.18	1.43
19	L	6019	BCR	C11-C10	-8.19	1.18	1.43

The worst 5 of 2891 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1502	LUT	C23-C24-C25	-21.29	105.32	125.22
26	2	2501	LUT	C23-C24-C25	-20.23	106.31	125.22
19	F	6016	BCR	C32-C1-C6	-18.88	80.71	110.30
19	B	6006	BCR	C32-C1-C6	-18.68	81.02	110.30
26	4	4501	LUT	C23-C24-C25	-18.63	107.81	125.22

5 of 457 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	4	4010	CLA	NC
21	4	4010	CLA	ND
21	4	4010	CLA	NA
21	B	1203	CLA	ND
21	B	1203	CLA	NA

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	6004	BCR	C10-C11-C12-C13
19	G	2011	BCR	C10-C11-C12-C13
27	4	4503	NEX	C34-C35-C15-C14
26	2	2502	LUT	C28-C27-C26-C21
19	B	6005	BCR	C11-C10-C9-C8

There are no ring outliers.

190 monomers are involved in 2349 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	1001	CLA	72	0
21	1	1002	CLA	71	0
21	1	1003	CLA	52	0
21	1	1004	CLA	29	0
21	1	1005	CLA	20	0
21	1	1006	CLA	61	0
21	1	1007	CLA	22	0
21	1	1008	CLA	26	0
21	1	1009	CLA	72	0
21	1	1010	CLA	28	0
21	1	1011	CLA	19	0
21	1	1012	CLA	25	0
21	1	1013	CLA	69	0
21	1	1014	CLA	29	0
26	1	1501	LUT	51	0
26	1	1502	LUT	61	0
20	1	1801	LHG	41	0
21	2	2001	CLA	19	0
21	2	2002	CLA	49	0
21	2	2003	CLA	41	0
21	2	2004	CLA	36	0
21	2	2005	CLA	24	0
21	2	2006	CLA	23	0
21	2	2007	CLA	8	0
21	2	2008	CLA	21	0
21	2	2009	CLA	25	0
21	2	2010	CLA	20	0
21	2	2011	CLA	22	0
21	2	2012	CLA	26	0
21	2	2013	CLA	22	0
21	2	2014	CLA	15	0
26	2	2501	LUT	65	0
26	2	2502	LUT	24	0
20	2	2801	LHG	23	0
21	3	3001	CLA	25	0
21	3	3002	CLA	3	0
21	3	3003	CLA	12	0
21	3	3005	CLA	4	0
21	3	3006	CLA	3	0
21	3	3008	CLA	18	0
21	3	3009	CLA	22	0
21	3	3010	CLA	17	0
21	3	3011	CLA	35	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	3012	CLA	35	0
21	3	3013	CLA	15	0
21	3	3014	CLA	4	0
21	3	3017	CLA	5	0
21	4	4001	CLA	53	0
21	4	4002	CLA	46	0
21	4	4003	CLA	38	0
21	4	4004	CLA	46	0
21	4	4005	CLA	48	0
21	4	4006	CLA	20	0
21	4	4007	CLA	15	0
21	4	4008	CLA	29	0
21	4	4009	CLA	11	0
21	4	4010	CLA	10	0
21	4	4011	CLA	21	0
21	4	4012	CLA	32	0
21	4	4013	CLA	16	0
21	4	4014	CLA	32	0
21	4	4015	CLA	18	0
26	4	4501	LUT	41	0
26	4	4502	LUT	54	0
27	4	4503	NEX	43	0
21	A	1101	CLA	7	0
21	A	1102	CLA	7	0
21	A	1103	CLA	7	0
21	A	1104	CLA	6	0
21	A	1105	CLA	2	0
21	A	1106	CLA	11	0
21	A	1107	CLA	7	0
21	A	1108	CLA	4	0
21	A	1109	CLA	9	0
21	A	1110	CLA	3	0
21	A	1111	CLA	6	0
21	A	1112	CLA	3	0
21	A	1113	CLA	1	0
21	A	1114	CLA	3	0
21	A	1115	CLA	7	0
21	A	1116	CLA	3	0
21	A	1117	CLA	7	0
21	A	1118	CLA	4	0
21	A	1119	CLA	3	0
21	A	1120	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1121	CLA	1	0
21	A	1122	CLA	7	0
21	A	1123	CLA	8	0
21	A	1124	CLA	9	0
21	A	1125	CLA	18	0
21	A	1126	CLA	14	0
21	A	1127	CLA	4	0
21	A	1128	CLA	15	0
21	A	1129	CLA	23	0
21	A	1130	CLA	17	0
21	A	1131	CLA	8	0
21	A	1132	CLA	16	0
21	A	1133	CLA	4	0
21	A	1135	CLA	5	0
21	A	1136	CLA	10	0
21	A	1137	CLA	9	0
21	A	1138	CLA	9	0
21	A	1139	CLA	3	0
21	A	1140	CLA	5	0
21	A	1141	CLA	4	0
18	A	5001	PQN	4	0
19	A	6002	BCR	3	0
19	A	6003	BCR	2	0
19	A	6007	BCR	2	0
19	A	6008	BCR	7	0
19	A	6011	BCR	11	0
19	A	6017	BCR	6	0
20	A	7001	LHG	10	0
20	A	7003	LHG	16	0
23	A	9011	CL0	15	0
21	A	9012	CLA	19	0
21	A	9013	CLA	11	0
21	B	1201	CLA	2	0
21	B	1202	CLA	4	0
21	B	1203	CLA	3	0
21	B	1204	CLA	3	0
21	B	1205	CLA	7	0
21	B	1206	CLA	13	0
21	B	1207	CLA	15	0
21	B	1208	CLA	7	0
21	B	1209	CLA	7	0
21	B	1210	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	1211	CLA	3	0
21	B	1212	CLA	2	0
21	B	1213	CLA	26	0
21	B	1214	CLA	6	0
21	B	1215	CLA	4	0
21	B	1216	CLA	5	0
21	B	1217	CLA	5	0
21	B	1218	CLA	2	0
21	B	1219	CLA	7	0
21	B	1220	CLA	10	0
21	B	1221	CLA	7	0
21	B	1222	CLA	7	0
21	B	1223	CLA	5	0
21	B	1224	CLA	8	0
21	B	1225	CLA	8	0
21	B	1226	CLA	11	0
21	B	1227	CLA	26	0
21	B	1228	CLA	8	0
21	B	1229	CLA	10	0
21	B	1230	CLA	5	0
21	B	1231	CLA	3	0
21	B	1234	CLA	6	0
21	B	1235	CLA	8	0
21	B	1236	CLA	4	0
21	B	1237	CLA	1	0
21	B	1238	CLA	3	0
21	B	1239	CLA	13	0
21	B	1240	CLA	21	0
18	B	5002	PQN	6	0
19	B	6004	BCR	8	0
19	B	6005	BCR	4	0
19	B	6006	BCR	5	0
19	B	6009	BCR	5	0
19	B	6010	BCR	2	0
19	B	6011	BCR	1	0
20	B	7004	LHG	16	0
24	B	7101	DGD	4	0
21	B	9010	CLA	21	0
21	B	9022	CLA	9	0
21	B	9023	CLA	13	0
21	F	1301	CLA	3	0
21	F	1302	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	1303	CLA	21	0
19	F	6014	BCR	6	0
19	F	6016	BCR	8	0
21	G	1001	CLA	16	0
21	G	1002	CLA	44	0
19	G	2011	BCR	14	0
25	G	2021	LMG	12	0
21	H	1000	CLA	5	0
19	I	6018	BCR	10	0
19	I	6020	BCR	4	0
21	J	1302	CLA	1	0
25	J	5001	LMG	3	0
19	J	6012	BCR	5	0
19	J	6013	BCR	3	0
21	J	6014	CLA	4	0
21	J	6015	CLA	11	0
21	L	1501	CLA	25	0
21	L	1502	CLA	8	0
21	L	1503	CLA	18	0
19	L	6019	BCR	19	0
19	L	6020	BCR	16	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	721/721 (100%)	0.21	44 (6%) 25 9	34, 73, 146, 307	0
2	B	731/731 (100%)	0.01	37 (5%) 32 12	30, 58, 139, 288	0
3	C	80/80 (100%)	-0.04	2 (2%) 61 30	42, 62, 98, 112	0
4	D	137/137 (100%)	0.48	19 (13%) 4 1	52, 80, 137, 204	0
5	E	63/63 (100%)	0.99	12 (19%) 2 1	42, 86, 124, 170	0
6	F	152/152 (100%)	-0.22	4 (2%) 59 29	44, 73, 135, 225	0
7	G	84/84 (100%)	-0.22	1 (1%) 81 55	63, 98, 122, 147	0
8	H	82/82 (100%)	0.51	8 (9%) 10 4	57, 97, 150, 184	0
9	I	26/26 (100%)	0.32	0 100 100	47, 68, 91, 112	0
10	J	40/40 (100%)	-0.59	0 100 100	47, 69, 110, 138	0
11	K	66/72 (91%)	4.26	43 (65%) 0 0	171, 246, 287, 303	0
12	L	163/163 (100%)	-0.13	5 (3%) 52 24	51, 79, 157, 195	0
13	N	85/85 (100%)	2.62	44 (51%) 0 0	177, 229, 289, 321	0
14	1	171/182 (93%)	0.40	19 (11%) 7 3	63, 103, 176, 315	0
15	2	146/199 (73%)	0.91	33 (22%) 1 1	74, 125, 214, 316	0
16	3	151/275 (54%)	1.55	45 (29%) 1 0	109, 193, 274, 335	0
17	4	196/196 (100%)	0.21	12 (6%) 25 9	59, 93, 182, 301	0
All	All	3094/3288 (94%)	0.39	328 (10%) 8 3	30, 80, 228, 335	0

The worst 5 of 328 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	102	THR	20.2
14	1	152	GLU	16.4
16	3	265	VAL	15.3
1	A	43	THR	15.1

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Mol	Chain	Res	Type	RSRZ
15	2	76	THR	14.7

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
27	NEX	4	4503	44/44	0.58	0.66	9.28	72,110,128,133	0
19	BCR	J	6013	40/40	0.57	0.60	7.89	119,143,153,153	0
20	LHG	B	7004	49/49	0.88	0.41	7.15	68,98,111,124	0
21	CLA	J	1302	61/65	0.71	0.33	6.49	59,117,149,153	0
21	CLA	1	1013	65/65	0.66	0.70	3.86	94,119,138,148	0
19	BCR	A	6002	40/40	0.73	0.46	3.66	72,103,133,133	0
21	CLA	2	2008	65/65	0.61	0.45	3.62	103,135,158,161	0
19	BCR	A	6007	40/40	0.80	0.33	3.35	69,91,97,98	0
21	CLA	3	3004	45/65	0.55	0.65	3.14	260,267,271,309	0
19	BCR	A	6003	40/40	0.74	0.43	3.14	80,97,123,124	0
21	CLA	4	4007	65/65	0.56	0.39	3.10	103,123,140,244	0
21	CLA	3	3014	45/65	0.53	0.66	2.96	242,261,265,271	0
21	CLA	2	2005	65/65	0.90	0.32	2.92	89,112,126,128	0
21	CLA	4	4005	45/65	0.56	0.32	2.84	107,130,142,144	0
21	CLA	1	1008	65/65	0.89	0.27	2.80	64,84,124,129	0
20	LHG	1	1801	49/49	0.87	0.23	2.67	68,88,119,122	0
26	LUT	1	1502	42/42	0.87	0.34	2.55	65,87,109,118	0
21	CLA	1	1009	65/65	0.79	0.28	2.53	58,78,104,108	0
21	CLA	B	1216	65/65	0.90	0.23	2.47	43,56,94,97	0
21	CLA	A	1110	55/65	0.73	0.37	2.36	129,148,161,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	F	1302	46/65	0.90	0.30	2.34	52,85,98,151	0
26	LUT	2	2501	42/42	0.74	0.40	2.32	106,121,131,138	0
19	BCR	I	6020	40/40	0.92	0.26	2.30	44,51,65,75	0
21	CLA	A	1126	65/65	0.88	0.35	2.29	59,79,95,106	0
19	BCR	B	6004	40/40	0.86	0.43	2.23	54,75,81,82	0
21	CLA	B	1240	65/65	0.91	0.28	2.21	42,72,83,97	0
21	CLA	1	1006	47/65	0.56	0.49	2.11	116,133,148,152	0
19	BCR	J	6012	40/40	0.92	0.26	2.10	45,67,98,109	0
21	CLA	B	1206	65/65	0.93	0.27	2.08	38,50,78,84	0
21	CLA	4	4001	65/65	0.80	0.60	1.96	73,91,124,131	0
19	BCR	G	2011	40/40	0.88	0.31	1.91	55,78,120,121	0
20	LHG	A	7001	49/49	0.91	0.31	1.90	47,72,94,97	0
21	CLA	F	1301	45/65	0.91	0.20	1.86	48,63,77,148	0
21	CLA	B	1215	60/65	0.88	0.36	1.85	51,69,81,84	0
19	BCR	A	6008	40/40	0.76	0.39	1.84	57,87,105,112	0
19	BCR	B	6009	40/40	0.86	0.31	1.83	30,52,68,73	0
21	CLA	A	1107	51/65	0.85	0.28	1.80	52,74,99,104	0
26	LUT	4	4502	42/42	0.90	0.27	1.75	56,76,84,88	0
21	CLA	4	4012	65/65	0.93	0.22	1.62	54,62,89,107	0
21	CLA	1	1007	55/65	0.91	0.36	1.45	76,100,121,139	0
21	CLA	A	1106	65/65	0.93	0.25	1.40	39,55,76,81	0
18	PQN	B	5002	33/33	0.90	0.31	1.40	41,50,76,79	0
21	CLA	G	1001	55/65	0.89	0.31	1.35	74,93,113,123	0
21	CLA	A	1138	65/65	0.93	0.23	1.33	32,49,60,65	0
19	BCR	L	6019	40/40	0.86	0.35	1.33	40,59,79,87	0
21	CLA	B	1224	65/65	0.90	0.29	1.31	32,54,93,95	0
21	CLA	L	1501	46/65	0.93	0.34	1.30	66,80,103,115	0
21	CLA	A	1117	65/65	0.93	0.38	1.30	59,78,92,123	0
26	LUT	1	1501	42/42	0.86	0.29	1.28	83,94,104,107	0
25	LMG	J	5001	35/55	0.86	0.31	1.27	62,91,103,104	0
21	CLA	B	1212	46/65	0.87	0.49	1.25	64,85,98,109	0
21	CLA	G	1002	46/65	0.84	0.25	1.25	112,128,140,145	0
21	CLA	B	9022	65/65	0.93	0.24	1.17	32,47,62,86	0
21	CLA	F	1303	64/65	0.91	0.29	1.16	52,65,104,149	0
19	BCR	B	6006	40/40	0.78	0.40	1.11	45,63,110,110	0
21	CLA	B	1214	59/65	0.90	0.34	1.09	44,61,102,119	0
23	CL0	A	9011	65/65	0.95	0.24	1.07	30,39,53,73	0
21	CLA	3	3006	65/65	0.51	0.48	1.07	144,177,194,197	0
21	CLA	A	1132	65/65	0.94	0.21	1.04	39,50,80,85	0
21	CLA	B	1236	55/65	0.93	0.25	1.01	51,61,122,125	0
19	BCR	B	6005	40/40	0.79	0.36	1.00	51,69,122,123	0
21	CLA	B	1209	46/65	0.93	0.18	0.98	52,63,84,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	PQN	A	5001	33/33	0.93	0.28	0.97	38,57,67,71	0
21	CLA	4	4014	45/65	0.83	0.35	0.97	71,105,128,134	0
21	CLA	A	1122	59/65	0.89	0.23	0.97	57,78,98,103	0
21	CLA	A	9012	65/65	0.91	0.26	0.96	36,63,75,78	0
24	DGD	B	7101	61/66	0.87	0.26	0.95	40,70,96,104	0
21	CLA	A	1112	46/65	0.84	0.36	0.93	68,88,99,101	0
21	CLA	A	1137	55/65	0.91	0.33	0.93	63,81,99,106	0
21	CLA	4	4004	65/65	0.88	0.31	0.91	56,81,91,96	0
21	CLA	A	1131	65/65	0.94	0.28	0.89	39,55,72,90	0
21	CLA	A	1111	60/65	0.88	0.26	0.88	60,86,114,117	0
21	CLA	3	3005	45/65	0.65	0.39	0.88	197,209,213,274	0
21	CLA	B	9023	65/65	0.93	0.28	0.87	36,54,62,89	0
21	CLA	3	3003	60/65	0.63	0.55	0.85	190,224,234,252	0
21	CLA	4	4010	50/65	0.87	0.24	0.85	57,93,132,147	0
21	CLA	L	1502	65/65	0.90	0.23	0.84	54,66,88,91	0
21	CLA	2	2007	55/65	0.82	0.36	0.83	113,130,142,149	0
19	BCR	B	6010	40/40	0.80	0.33	0.82	47,67,81,88	0
21	CLA	B	1210	65/65	0.90	0.24	0.81	46,56,73,101	0
21	CLA	B	1220	65/65	0.94	0.23	0.80	32,48,101,106	0
21	CLA	1	1010	65/65	0.74	0.42	0.78	108,123,152,154	0
21	CLA	4	4011	65/65	0.91	0.26	0.78	66,74,104,108	0
21	CLA	2	2013	65/65	0.86	0.27	0.77	91,119,135,146	0
19	BCR	A	6011	40/40	0.89	0.27	0.74	32,48,74,81	0
21	CLA	A	1141	51/65	0.88	0.28	0.73	91,124,133,137	0
21	CLA	A	1109	65/65	0.88	0.30	0.70	81,105,133,147	0
21	CLA	2	2012	65/65	0.91	0.23	0.69	72,88,117,121	0
19	BCR	F	6016	40/40	0.94	0.23	0.69	35,51,76,82	0
21	CLA	A	1139	65/65	0.92	0.20	0.68	33,51,81,88	0
21	CLA	A	1124	55/65	0.87	0.31	0.65	48,60,83,91	0
21	CLA	A	1136	65/65	0.86	0.26	0.63	59,82,108,155	0
21	CLA	B	1229	65/65	0.94	0.22	0.63	36,50,73,85	0
26	LUT	4	4501	42/42	0.76	0.42	0.62	77,95,99,107	0
21	CLA	B	1202	65/65	0.94	0.22	0.62	33,53,71,92	0
19	BCR	A	6017	40/40	0.90	0.29	0.61	34,52,79,93	0
26	LUT	2	2502	42/42	0.83	0.31	0.58	83,99,106,109	0
21	CLA	A	1103	65/65	0.91	0.25	0.58	63,80,90,111	0
21	CLA	A	1127	65/65	0.92	0.32	0.58	52,63,79,85	0
21	CLA	A	1104	65/65	0.92	0.28	0.57	47,69,81,87	0
21	CLA	A	1116	54/65	0.88	0.27	0.54	73,89,105,111	0
21	CLA	B	1234	60/65	0.88	0.29	0.54	39,56,98,104	0
21	CLA	B	1217	46/65	0.93	0.19	0.54	52,70,92,109	0
20	LHG	A	7003	49/49	0.87	0.27	0.52	81,113,121,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	A	1135	51/65	0.88	0.29	0.49	47,62,87,88	0
21	CLA	A	1105	51/65	0.92	0.22	0.49	67,81,98,103	0
21	CLA	J	6015	55/65	0.48	0.31	0.49	122,143,159,160	0
21	CLA	B	1230	58/65	0.90	0.23	0.46	38,59,73,77	0
21	CLA	B	1237	60/65	0.90	0.27	0.44	41,60,87,101	0
21	CLA	A	1133	46/65	0.84	0.25	0.42	77,90,112,119	0
21	CLA	1	1004	65/65	0.92	0.19	0.41	57,77,83,113	0
20	LHG	2	2801	36/49	0.79	0.39	0.39	112,132,147,150	0
21	CLA	B	1204	55/65	0.94	0.18	0.35	38,61,77,78	0
21	CLA	1	1003	65/65	0.87	0.19	0.32	53,72,97,108	0
21	CLA	A	1119	65/65	0.87	0.28	0.32	78,91,99,105	0
19	BCR	L	6020	40/40	0.92	0.19	0.32	60,75,82,83	0
21	CLA	B	1201	46/65	0.95	0.21	0.31	34,46,78,91	0
21	CLA	A	1129	50/65	0.86	0.25	0.28	51,83,90,93	0
19	BCR	F	6014	40/40	0.93	0.22	0.27	38,56,64,66	0
21	CLA	A	9013	65/65	0.91	0.25	0.26	35,61,71,110	0
21	CLA	2	2011	60/65	0.87	0.17	0.26	80,97,144,158	0
21	CLA	B	1239	65/65	0.93	0.23	0.25	32,47,65,73	0
21	CLA	B	1235	65/65	0.95	0.20	0.23	36,53,68,73	0
21	CLA	A	1128	65/65	0.93	0.24	0.23	44,66,81,96	0
21	CLA	4	4006	65/65	0.53	0.34	0.23	116,133,155,160	0
21	CLA	2	2006	57/65	0.54	0.32	0.22	140,162,183,256	0
21	CLA	B	1227	65/65	0.93	0.20	0.19	39,63,89,92	0
21	CLA	A	1140	65/65	0.93	0.22	0.18	35,50,73,99	0
21	CLA	B	1221	54/65	0.93	0.22	0.16	33,57,71,86	0
21	CLA	A	1130	46/65	0.93	0.21	0.16	48,60,88,109	0
21	CLA	B	1238	65/65	0.92	0.24	0.15	35,51,74,86	0
21	CLA	2	2010	65/65	0.80	0.29	0.15	103,118,134,151	0
21	CLA	1	1001	55/65	0.91	0.23	0.13	81,103,129,170	0
21	CLA	B	1205	65/65	0.95	0.20	0.10	33,46,70,83	0
21	CLA	4	4009	50/65	0.91	0.20	0.09	64,83,103,105	0
21	CLA	B	1208	55/65	0.91	0.22	0.09	49,68,96,99	0
21	CLA	L	1503	50/65	0.87	0.22	0.04	58,77,98,105	0
21	CLA	B	1213	60/65	0.89	0.22	0.00	67,81,103,106	0
21	CLA	A	1123	65/65	0.86	0.29	-0.05	58,84,97,103	0
21	CLA	B	1207	65/65	0.93	0.19	-0.06	40,62,83,98	0
21	CLA	B	1211	65/65	0.91	0.22	-0.09	56,68,81,90	0
21	CLA	B	1225	65/65	0.93	0.23	-0.10	31,46,60,71	0
21	CLA	B	1218	60/65	0.91	0.20	-0.11	54,78,101,102	0
21	CLA	1	1011	65/65	0.87	0.27	-0.12	89,109,115,118	0
21	CLA	2	2003	65/65	0.61	0.31	-0.15	136,144,159,185	0
21	CLA	A	1101	65/65	0.93	0.20	-0.16	43,63,91,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	SF4	A	8001	8/8	0.96	0.21	-0.17	50,64,71,75	0
21	CLA	B	1226	65/65	0.95	0.23	-0.17	28,43,71,73	0
21	CLA	3	3011	46/65	0.76	0.31	-0.18	131,154,160,195	0
21	CLA	2	2004	59/65	0.87	0.23	-0.18	84,101,110,116	0
21	CLA	1	1012	50/65	0.91	0.22	-0.21	78,95,113,175	0
21	CLA	B	1219	60/65	0.88	0.23	-0.22	50,81,101,103	0
21	CLA	3	3013	50/65	0.73	0.26	-0.25	107,132,148,153	0
21	CLA	A	1134	46/65	0.85	0.28	-0.26	93,103,131,137	0
21	CLA	A	1108	46/65	0.84	0.23	-0.26	103,120,136,146	0
25	LMG	G	2021	23/55	0.62	0.31	-0.30	160,168,177,180	0
21	CLA	B	9010	65/65	0.96	0.19	-0.31	29,39,57,72	0
21	CLA	A	1113	46/65	0.85	0.29	-0.35	95,112,136,139	0
21	CLA	3	3001	65/65	0.67	0.38	-0.40	187,204,220,223	0
21	CLA	4	4008	48/65	0.85	0.16	-0.45	66,92,107,138	0
21	CLA	4	4013	51/65	0.92	0.17	-0.45	63,77,101,104	0
21	CLA	A	1118	46/65	0.88	0.26	-0.47	109,118,126,135	0
21	CLA	A	1102	50/65	0.94	0.18	-0.48	43,63,91,95	0
21	CLA	4	4003	65/65	0.89	0.16	-0.53	61,86,100,116	0
21	CLA	B	1222	65/65	0.89	0.30	-0.55	28,47,85,87	0
21	CLA	2	2009	46/65	0.81	0.30	-0.56	82,101,128,141	0
21	CLA	A	1115	56/65	0.86	0.24	-0.59	85,107,132,161	0
21	CLA	B	1203	60/65	0.95	0.20	-0.59	30,43,69,74	0
21	CLA	3	3017	45/65	0.58	0.50	-0.61	224,249,260,262	0
21	CLA	B	1223	65/65	0.92	0.28	-0.61	31,50,60,63	0
21	CLA	3	3012	45/65	0.77	0.18	-0.63	163,196,205,208	0
21	CLA	A	1125	55/65	0.89	0.24	-0.65	54,73,89,99	0
21	CLA	A	1114	46/65	0.88	0.30	-0.73	93,114,120,124	0
21	CLA	B	1231	46/65	0.88	0.24	-0.79	49,76,87,92	0
21	CLA	A	1121	46/65	0.85	0.24	-0.80	103,130,154,160	0
21	CLA	B	1228	51/65	0.95	0.16	-0.83	33,45,66,92	0
21	CLA	2	2001	27/65	0.90	0.15	-0.96	105,120,130,131	0
22	SF4	C	8002	8/8	0.98	0.13	-1.12	53,65,79,92	0
22	SF4	C	8003	8/8	0.98	0.10	-1.25	53,63,89,92	0
21	CLA	1	1014	45/65	0.53	0.69	-	115,160,167,171	0
21	CLA	4	4015	46/65	0.92	0.17	-	51,65,83,108	0
21	CLA	3	3015	45/65	0.32	1.17	-	250,262,271,285	0
21	CLA	A	1143	46/65	0.52	0.92	-	198,214,217,262	0
21	CLA	4	4002	56/65	0.84	0.32	-	76,94,112,128	0
19	BCR	B	6011	25/40	0.71	0.32	-	77,111,118,120	0
21	CLA	J	6014	61/65	0.61	0.25	-	191,215,220,289	0
21	CLA	3	3016	45/65	0.42	0.78	-	172,203,215,248	0
21	CLA	A	1142	44/65	0.57	0.28	-	186,199,202,274	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	G3P	4	4505	10/10	0.89	0.24	-	94,125,132,135	0
21	CLA	A	1120	46/65	0.77	0.49	-	97,128,144,149	0
21	CLA	3	3009	46/65	0.81	0.24	-	138,174,190,191	0
21	CLA	2	2014	45/65	0.70	0.24	-	104,135,145,168	0
21	CLA	2	2002	60/65	0.81	0.33	-	112,142,151,201	0
21	CLA	1	1005	56/65	0.92	0.21	-	54,69,80,85	0
19	BCR	I	6018	40/40	0.83	0.30	-	37,61,79,86	0
21	CLA	1	1002	56/65	0.88	0.32	-	101,113,133,140	0
21	CLA	3	3008	65/65	0.72	0.25	-	149,167,183,187	0
21	CLA	H	1000	46/65	0.89	0.39	-	69,106,123,134	0
21	CLA	3	3010	52/65	0.67	0.32	-	115,168,179,182	0
21	CLA	3	3002	55/65	0.75	0.47	-	181,189,204,206	0

6.5 Other polymers [i](#)

There are no such residues in this entry.