



wwPDB X-ray Structure Validation Summary Report ⓘ

May 2, 2016 – 11:39 PM EDT

PDB ID : 1JB0
Title : Crystal Structure of Photosystem I: a Photosynthetic Reaction Center and Core Antenna System from Cyanobacteria
Authors : Jordan, P.; Fromme, P.; Witt, H.T.; Klukas, O.; Saenger, W.; Krauss, N.
Deposited on : 2001-06-01
Resolution : 2.50 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

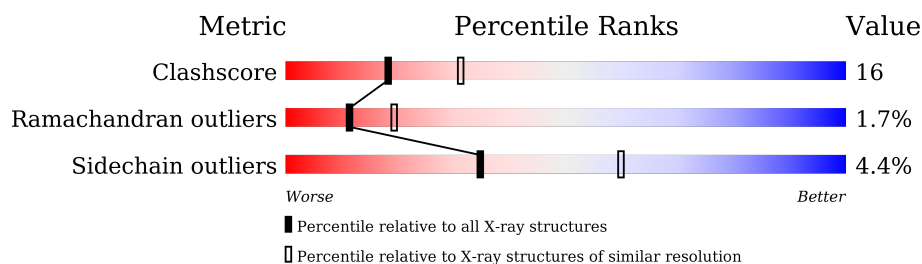
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)


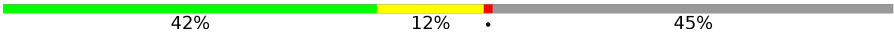



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	755	
2	B	740	
3	C	80	
4	D	138	
5	E	75	
6	F	164	
7	I	38	

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Mol	Chain	Length	Quality of chain
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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
14	CLA	A	1011	X	-	-	-
14	CLA	A	1013	X	-	-	-
14	CLA	A	1022	X	-	-	-
14	CLA	A	1101	X	-	-	-
14	CLA	A	1102	X	-	-	-
14	CLA	A	1103	X	-	-	-
14	CLA	A	1104	X	-	-	-
14	CLA	A	1105	X	-	-	-
14	CLA	A	1106	X	-	-	-
14	CLA	A	1107	X	-	-	-
14	CLA	A	1109	X	-	-	-
14	CLA	A	1110	X	-	-	-
14	CLA	A	1111	X	-	-	-
14	CLA	A	1112	X	-	-	-
14	CLA	A	1113	X	-	-	-
14	CLA	A	1114	X	-	-	-
14	CLA	A	1115	X	-	-	-
14	CLA	A	1116	X	-	-	-
14	CLA	A	1117	X	-	-	-
14	CLA	A	1118	X	-	-	-
14	CLA	A	1119	X	-	-	-
14	CLA	A	1120	X	-	-	-
14	CLA	A	1121	X	-	-	-
14	CLA	A	1122	X	-	-	-
14	CLA	A	1123	X	-	-	-
14	CLA	A	1124	X	-	-	-
14	CLA	A	1125	X	-	-	-
14	CLA	A	1126	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	1127	X	-	-	-
14	CLA	A	1128	X	-	-	-
14	CLA	A	1129	X	-	-	-
14	CLA	A	1130	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	X	-	-	-
14	CLA	A	1134	X	-	-	-
14	CLA	A	1135	X	-	-	-
14	CLA	A	1136	X	-	-	-
14	CLA	A	1137	X	-	-	-
14	CLA	A	1138	X	-	-	-
14	CLA	A	1139	X	-	-	-
14	CLA	A	1140	X	-	-	-
14	CLA	A	1237	X	-	-	-
14	CLA	A	1402	X	-	-	-
14	CLA	A	1801	X	-	-	-
14	CLA	B	1012	X	-	-	-
14	CLA	B	1021	X	-	-	-
14	CLA	B	1023	X	-	-	-
14	CLA	B	1201	X	-	-	-
14	CLA	B	1202	X	-	-	-
14	CLA	B	1203	X	-	-	-
14	CLA	B	1204	X	-	-	-
14	CLA	B	1205	X	-	-	-
14	CLA	B	1206	X	-	-	-
14	CLA	B	1207	X	-	-	-
14	CLA	B	1208	X	-	-	-
14	CLA	B	1209	X	-	-	-
14	CLA	B	1210	X	-	-	-
14	CLA	B	1211	X	-	-	-
14	CLA	B	1212	X	-	-	-
14	CLA	B	1213	X	-	-	-
14	CLA	B	1214	X	-	-	-
14	CLA	B	1215	X	-	-	-
14	CLA	B	1216	X	-	-	-
14	CLA	B	1217	X	-	-	-
14	CLA	B	1218	X	-	-	-
14	CLA	B	1219	X	-	-	-
14	CLA	B	1220	X	-	-	-
14	CLA	B	1221	X	-	-	-
14	CLA	B	1222	X	-	-	-
14	CLA	B	1223	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	1224	X	-	-	-
14	CLA	B	1225	X	-	-	-
14	CLA	B	1226	X	-	-	-
14	CLA	B	1227	X	-	-	-
14	CLA	B	1228	X	-	-	-
14	CLA	B	1229	X	-	-	-
14	CLA	B	1230	X	-	-	-
14	CLA	B	1231	X	-	-	-
14	CLA	B	1232	X	-	-	-
14	CLA	B	1233	X	-	-	-
14	CLA	B	1234	X	-	-	-
14	CLA	B	1235	X	-	-	-
14	CLA	B	1238	X	-	-	-
14	CLA	B	1239	X	-	-	-
14	CLA	F	1301	X	-	-	-
14	CLA	J	1302	X	-	-	-
14	CLA	J	1303	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	M	1601	X	-	-	-
14	CLA	X	1701	X	-	-	-
18	LHG	A	5003	X	-	-	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 24198 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	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

- Molecule 2 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

- 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
			598	367	103	117	11			

- Molecule 4 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

- Molecule 5 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			539	342	93	104			

- Molecule 6 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

- Molecule 8 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

- Molecule 9 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	S	0	0	0
			222	130	46	46				

- Molecule 10 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ARG	PRO	CONFLICT	UNP P25902
L	144	VAL	-	SEE REMARK 999	UNP P25902
L	145	VAL	-	SEE REMARK 999	UNP P25902
L	146	ASP	-	SEE REMARK 999	UNP P25902
L	147	GLY	-	SEE REMARK 999	UNP P25902
L	148	ILE	-	SEE REMARK 999	UNP P25902
L	149	MET	-	SEE REMARK 999	UNP P25902
L	150	THR	-	SEE REMARK 999	UNP P25902
L	151	GLY	-	SEE REMARK 999	UNP P25902
L	152	LEU	-	SEE REMARK 999	UNP P25902
L	153	PHE	-	SEE REMARK 999	UNP P25902
L	154	ASN	-	SEE REMARK 999	UNP P25902

- Molecule 11 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			

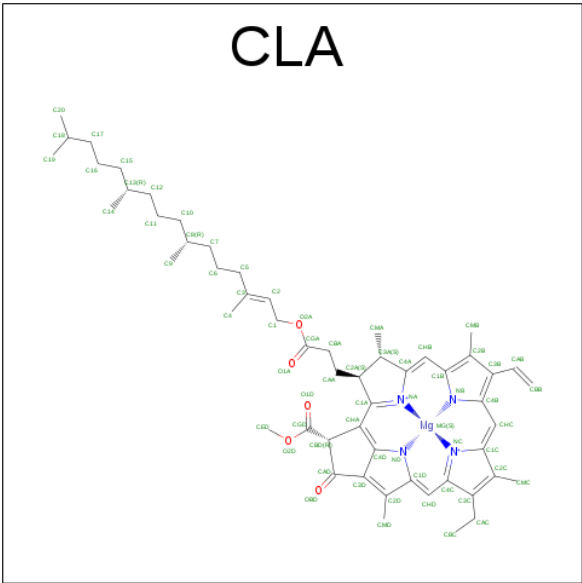
- Molecule 12 is a protein called PHOTOSYSTEM I SUBUNIT PSAX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O	0	0	0
			233	164	34	35			

- Molecule 13 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	1	Total	Ca	0	0
			1	1		

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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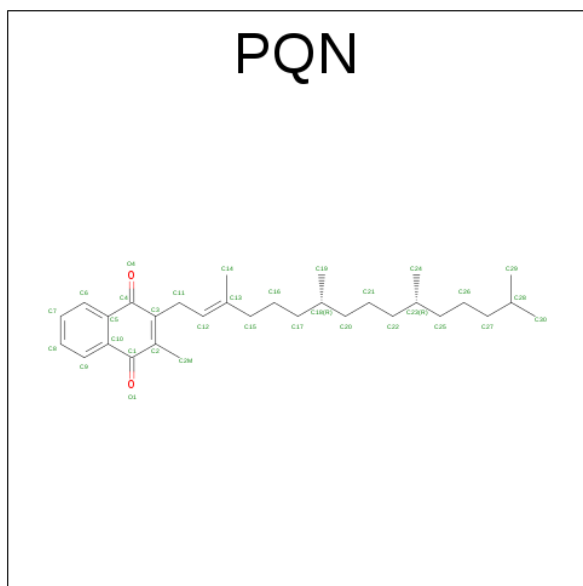
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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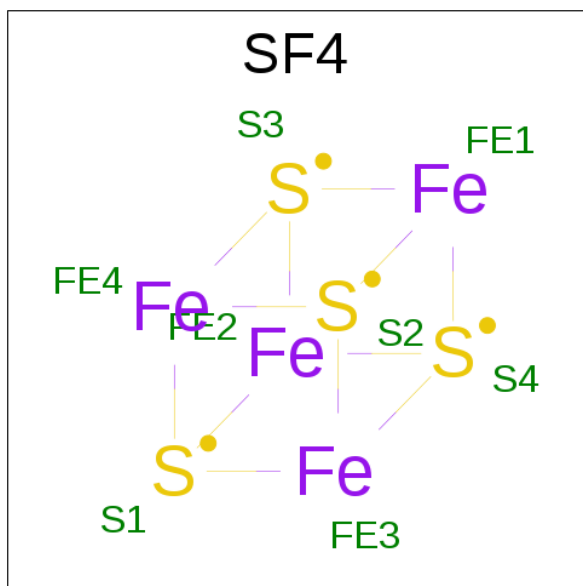
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
14	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



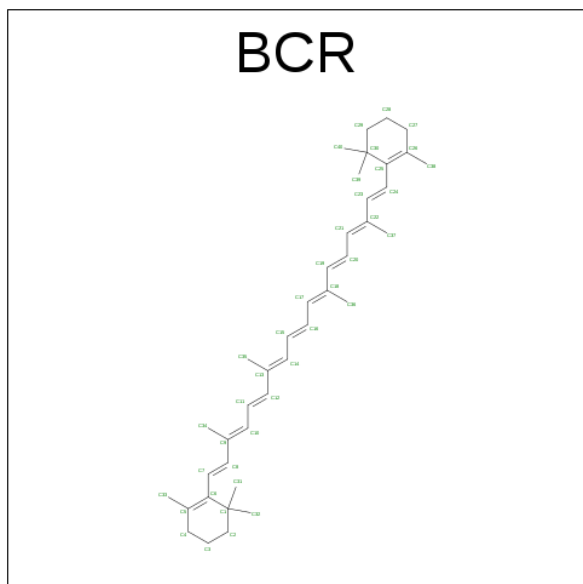
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			33	31	2		
15	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



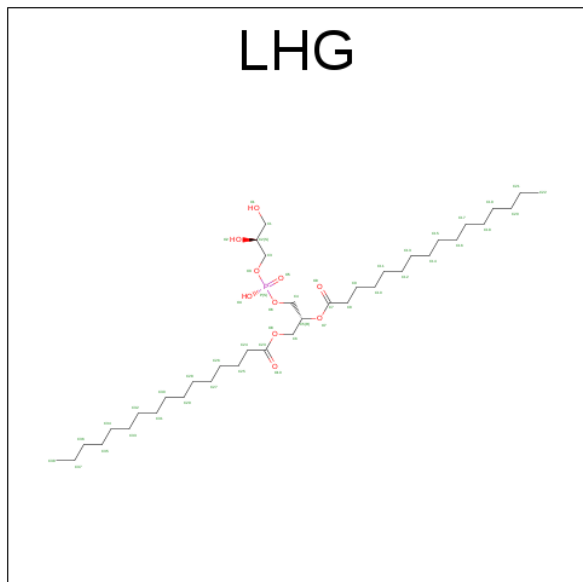
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	Fe	S	0	0
			8	4	4		
16	C	1	Total	Fe	S	0	0
			8	4	4		
16	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



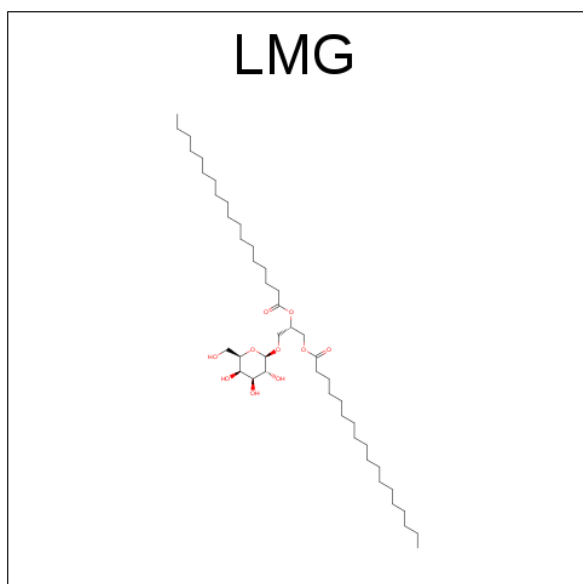
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	B	1	Total C 25 25	0	0
17	B	1	Total C 40 40	0	0
17	A	1	Total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

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			49	38	10	1		
18	A	1	Total	C	O	P	0	0
			27	16	10	1		
18	B	1	Total	C	O	P	0	0
			23	12	10	1		

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			55	45	10		

- Molecule 20 is water.

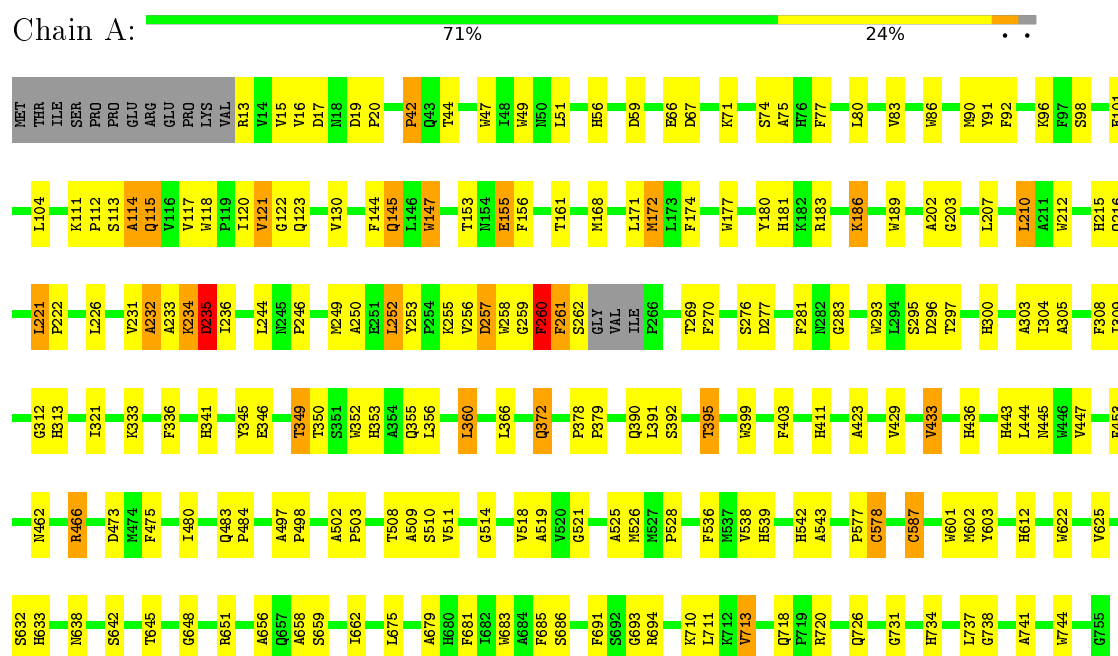
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	53	Total	O	0	0
			53	53		
20	B	65	Total	O	0	0
			65	65		
20	C	21	Total	O	0	0
			21	21		
20	D	17	Total	O	0	0
			17	17		
20	E	5	Total	O	0	0
			5	5		
20	F	6	Total	O	0	0
			6	6		
20	I	3	Total	O	0	0
			3	3		
20	J	1	Total	O	0	0
			1	1		
20	L	27	Total	O	0	0
			27	27		
20	M	3	Total	O	0	0
			3	3		

3 Residue-property plots

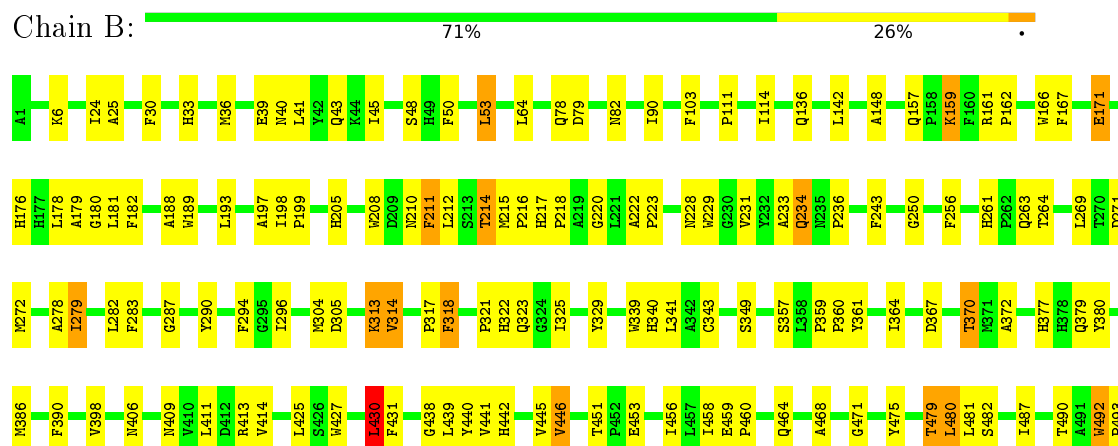
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

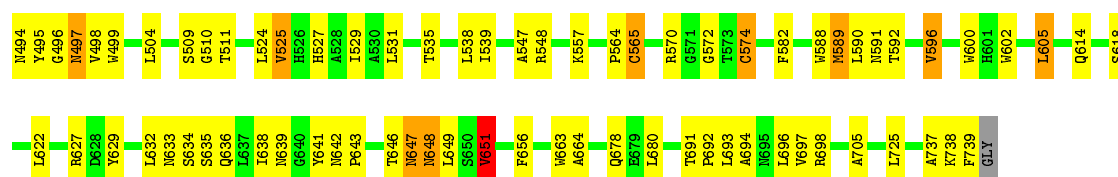
Note EDS was not executed.

• Molecule 1: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



• Molecule 2: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2





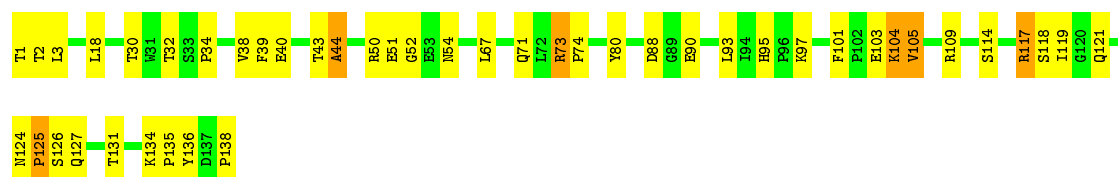
• Molecule 3: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C: 74% 25%



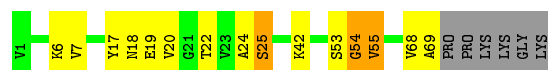
• Molecule 4: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II

Chain D: 67% 28%



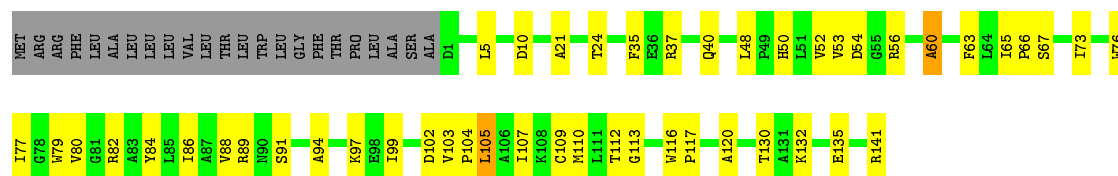
• Molecule 5: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV

Chain E: 72% 16% 8%



• Molecule 6: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III

Chain F: 57% 28% 14%



• Molecule 7: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII

Chain I: 74% 21% 5%

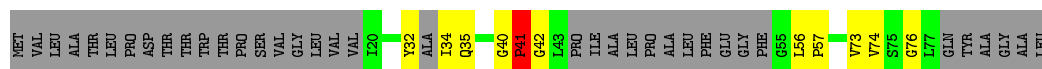


• Molecule 8: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX

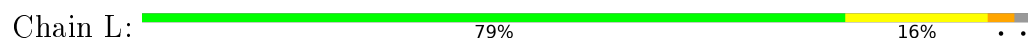
Chain J: 54% 41% 5%



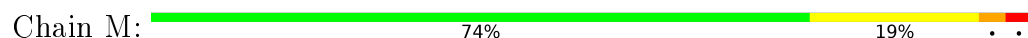
- Molecule 9: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X



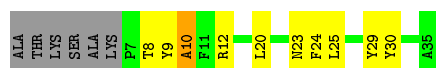
- Molecule 10: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI



- Molecule 11: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII



- Molecule 12: PHOTOSYSTEM I SUBUNIT PSAX



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00 Å 281.00 Å 165.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (30.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.199 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24198	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, SF4, CLA, PQN, CA, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/5983	0.66	2/8158 (0.0%)
2	B	0.56	0/6096	0.67	2/8332 (0.0%)
3	C	0.74	0/608	0.96	4/824 (0.5%)
4	D	0.57	0/1101	0.81	1/1492 (0.1%)
5	E	0.57	0/551	0.84	2/750 (0.3%)
6	F	0.47	0/1087	0.66	0/1476
7	I	0.66	0/312	0.75	0/425
8	J	0.45	0/350	0.65	0/477
9	K	0.52	0/219	0.86	3/297 (1.0%)
10	L	0.67	0/1148	0.75	0/1558
11	M	0.63	0/244	0.85	1/332 (0.3%)
12	X	0.55	0/242	0.67	0/332
All	All	0.55	0/17941	0.70	15/24453 (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
3	C	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	TYR	CA-C-O	9.95	140.99	120.10
11	M	30	TYR	N-CA-C	7.84	132.18	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.52	131.91	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	A	521	GLY	N-CA-C	-6.39	97.13	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

5.2 Too-close contacts [i](#)

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	5784	0	5639	215	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	40	0
5	E	539	0	528	10	0
6	F	1065	0	1079	42	0
7	I	301	0	306	7	0
8	J	338	0	347	23	0
9	K	222	0	110	4	0
10	L	1119	0	1125	22	0
11	M	241	0	264	13	0
12	X	233	0	231	6	0
13	L	1	0	0	0	0
14	A	2687	0	2675	143	0
14	B	2349	0	2304	152	0
14	F	45	0	33	1	0
14	J	82	0	58	1	0
14	K	45	0	33	1	0
14	L	195	0	216	11	0
14	M	45	0	33	1	0
14	X	45	0	33	1	0
15	A	33	0	46	1	0
15	B	33	0	46	1	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A	240	0	336	22	0
17	B	265	0	369	17	0
17	F	40	0	56	2	0
17	I	80	0	112	3	0
17	J	120	0	168	16	0
17	L	80	0	112	1	0
17	M	40	0	56	2	0
18	A	76	0	98	6	0
18	B	23	0	16	1	0
19	B	55	0	86	5	0
20	A	53	0	0	5	0
20	B	65	0	0	3	0
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	1
20	M	3	0	0	1	0
All	All	24198	0	23804	743	1

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 16.

The worst 5 of 743 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)
8:J:31:ARG:HD3	17:J:4013:BCR:H312	1.25	1.17
2:B:622:LEU:HD12	14:B:1012:CLA:H11	1.29	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.05
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:4048:HOH:O	20:L:4048:HOH:O[2_655]	1.94	0.26

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	736/755 (98%)	695 (94%)	31 (4%)	10 (1%)	14	24
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	16	29
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	15	26
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	8	13
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	2	2
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	8	13
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	1
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	15	26
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	5	6
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	4	5
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	11	19

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE
1	A	261	PHE
2	B	234	GLN

5.3.2 Protein sidechains [i](#)

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	589/603 (98%)	565 (96%)	24 (4%)	37	63
2	B	595/597 (100%)	567 (95%)	28 (5%)	32	56
3	C	67/67 (100%)	66 (98%)	1 (2%)	72	91
4	D	115/115 (100%)	107 (93%)	8 (7%)	19	34
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	107 (98%)	2 (2%)	66	88
7	I	32/32 (100%)	30 (94%)	2 (6%)	22	40
8	J	36/36 (100%)	34 (94%)	2 (6%)	26	47
10	L	117/119 (98%)	109 (93%)	8 (7%)	20	36
11	M	26/26 (100%)	25 (96%)	1 (4%)	40	67
12	X	20/24 (83%)	18 (90%)	2 (10%)	9	18
All	All	1765/1811 (98%)	1687 (96%)	78 (4%)	35	60

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	411	LEU
2	B	596	VAL
10	L	69	ARG
2	B	430	LEU
2	B	525	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	263	GLN
2	B	494	ASN
6	F	40	GLN
2	B	340	HIS
2	B	611	ASN

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 ⓘ

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 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	$\# Z > 2$
14	CLA	A	1011	1	57,73,73	1.20	2 (3%)	61,113,113	2.30	10 (16%)
14	CLA	A	1013	1	57,73,73	1.21	4 (7%)	61,113,113	1.48	10 (16%)
14	CLA	A	1022	20	57,73,73	1.09	4 (7%)	61,113,113	1.45	10 (16%)
14	CLA	A	1101	1	57,73,73	1.11	4 (7%)	61,113,113	1.49	9 (14%)
14	CLA	A	1102	1,14	51,67,73	1.19	3 (5%)	53,105,113	1.69	13 (24%)
14	CLA	A	1103	1	57,73,73	1.15	3 (5%)	61,113,113	1.61	12 (19%)
14	CLA	A	1104	1	57,73,73	1.16	3 (5%)	61,113,113	1.76	15 (24%)
14	CLA	A	1105	1	43,59,73	1.44	4 (9%)	43,96,113	1.63	9 (20%)
14	CLA	A	1106	1	57,73,73	1.30	5 (8%)	61,113,113	1.56	11 (18%)
14	CLA	A	1107	1	57,73,73	1.11	3 (5%)	61,113,113	1.52	12 (19%)
14	CLA	A	1108	1	34,53,73	1.38	5 (14%)	37,89,113	1.63	9 (24%)
14	CLA	A	1109	1,14	57,73,73	1.15	5 (8%)	61,113,113	1.39	9 (14%)
14	CLA	A	1110	1	46,62,73	1.36	5 (10%)	47,99,113	1.62	11 (23%)
14	CLA	A	1111	1	52,68,73	1.17	3 (5%)	55,107,113	1.58	10 (18%)
14	CLA	A	1112	1	34,53,73	1.39	4 (11%)	37,89,113	1.72	9 (24%)
14	CLA	A	1113	1	34,53,73	1.46	2 (5%)	37,89,113	1.84	11 (29%)
14	CLA	A	1114	20	41,57,73	1.29	4 (9%)	43,93,113	1.70	9 (20%)
14	CLA	A	1115	1	46,62,73	1.25	4 (8%)	47,99,113	1.55	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	1116	1	46,62,73	1.39	5 (10%)	47,99,113	1.69	13 (27%)
14	CLA	A	1117	1	57,73,73	1.16	7 (12%)	61,113,113	1.56	15 (24%)
14	CLA	A	1118	1	53,69,73	1.33	5 (9%)	55,108,113	1.62	11 (20%)
14	CLA	A	1119	20	57,73,73	1.14	5 (8%)	61,113,113	1.58	13 (21%)
14	CLA	A	1120	1	41,57,73	1.35	4 (9%)	43,93,113	1.84	12 (27%)
14	CLA	A	1121	1	43,59,73	1.35	6 (13%)	43,96,113	1.71	9 (20%)
14	CLA	A	1122	1	51,67,73	1.21	3 (5%)	53,105,113	1.54	11 (20%)
14	CLA	A	1123	20	57,73,73	1.19	3 (5%)	61,113,113	1.49	10 (16%)
14	CLA	A	1124	20	57,73,73	1.14	4 (7%)	61,113,113	1.39	8 (13%)
14	CLA	A	1125	1	57,73,73	1.25	4 (7%)	61,113,113	1.52	10 (16%)
14	CLA	A	1126	1	57,73,73	1.02	3 (5%)	61,113,113	1.37	12 (19%)
14	CLA	A	1127	1	57,73,73	1.20	2 (3%)	61,113,113	1.51	9 (14%)
14	CLA	A	1128	1	57,73,73	1.20	5 (8%)	61,113,113	1.51	11 (18%)
14	CLA	A	1129	1	42,58,73	1.37	4 (9%)	44,95,113	1.85	13 (29%)
14	CLA	A	1130	1	57,73,73	1.18	1 (1%)	61,113,113	1.50	12 (19%)
14	CLA	A	1131	1	57,73,73	1.05	1 (1%)	61,113,113	1.47	11 (18%)
14	CLA	A	1132	1	57,73,73	1.17	5 (8%)	61,113,113	1.58	10 (16%)
14	CLA	A	1133	1	46,62,73	1.35	5 (10%)	47,99,113	1.68	13 (27%)
14	CLA	A	1134	1	34,53,73	1.48	4 (11%)	37,89,113	1.69	9 (24%)
14	CLA	A	1135	1	43,59,73	1.40	1 (2%)	43,96,113	1.68	10 (23%)
14	CLA	A	1136	1	57,73,73	1.15	5 (8%)	61,113,113	1.32	7 (11%)
14	CLA	A	1137	1	39,55,73	1.45	4 (10%)	42,91,113	1.75	10 (23%)
14	CLA	A	1138	1	57,73,73	1.12	4 (7%)	61,113,113	1.43	12 (19%)
14	CLA	A	1139	20	43,59,73	1.48	4 (9%)	43,96,113	1.67	11 (25%)
14	CLA	A	1140	1	57,73,73	1.26	3 (5%)	61,113,113	1.50	11 (18%)
14	CLA	A	1237	20	57,73,73	1.25	6 (10%)	61,113,113	1.43	11 (18%)
14	CLA	A	1402	-	31,49,73	1.59	5 (16%)	30,83,113	1.60	7 (23%)
14	CLA	A	1801	18	44,60,73	1.38	6 (13%)	45,97,113	1.87	11 (24%)
15	PQN	A	2001	-	34,34,34	3.38	17 (50%)	45,45,45	2.21	3 (6%)
16	SF4	A	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
17	BCR	A	4001	-	41,41,41	1.33	5 (12%)	56,56,56	1.89	15 (26%)
17	BCR	A	4002	-	41,41,41	1.23	4 (9%)	56,56,56	1.79	16 (28%)
17	BCR	A	4003	-	41,41,41	1.37	6 (14%)	56,56,56	1.96	18 (32%)
17	BCR	A	4007	-	41,41,41	1.33	4 (9%)	56,56,56	1.81	15 (26%)
17	BCR	A	4008	-	41,41,41	1.24	6 (14%)	56,56,56	1.91	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	A	4011	-	41,41,41	1.35	6 (14%)	56,56,56	2.06	20 (35%)
18	LHG	A	5001	-	48,48,48	1.70	6 (12%)	49,54,54	1.26	3 (6%)
18	LHG	A	5003	14	26,26,48	2.24	5 (19%)	27,32,54	1.49	4 (14%)
14	CLA	B	1012	20	57,73,73	1.16	2 (3%)	61,113,113	1.60	10 (16%)
14	CLA	B	1021	2	57,73,73	1.22	3 (5%)	61,113,113	1.42	9 (14%)
14	CLA	B	1023	2	57,73,73	1.24	4 (7%)	61,113,113	1.39	10 (16%)
14	CLA	B	1201	2	46,62,73	1.31	5 (10%)	47,99,113	1.75	9 (19%)
14	CLA	B	1202	2	57,73,73	1.17	4 (7%)	61,113,113	1.48	10 (16%)
14	CLA	B	1203	2	57,73,73	1.09	2 (3%)	61,113,113	1.37	8 (13%)
14	CLA	B	1204	2	57,73,73	1.26	4 (7%)	61,113,113	1.49	10 (16%)
14	CLA	B	1205	2	57,73,73	1.05	4 (7%)	61,113,113	1.64	12 (19%)
14	CLA	B	1206	2	57,73,73	1.03	1 (1%)	61,113,113	1.44	10 (16%)
14	CLA	B	1207	2	57,73,73	1.18	3 (5%)	61,113,113	1.38	8 (13%)
14	CLA	B	1208	2	34,53,73	1.37	5 (14%)	37,89,113	1.66	9 (24%)
14	CLA	B	1209	2	34,53,73	1.51	2 (5%)	37,89,113	1.67	8 (21%)
14	CLA	B	1210	2	57,73,73	1.06	3 (5%)	61,113,113	1.48	10 (16%)
14	CLA	B	1211	2	57,73,73	1.20	5 (8%)	61,113,113	1.54	9 (14%)
14	CLA	B	1212	2	34,53,73	1.37	4 (11%)	37,89,113	1.74	8 (21%)
14	CLA	B	1213	2	47,63,73	1.36	8 (17%)	49,101,113	1.61	11 (22%)
14	CLA	B	1214	2	51,67,73	1.25	5 (9%)	53,105,113	1.60	12 (22%)
14	CLA	B	1215	2	52,68,73	1.27	4 (7%)	55,107,113	1.67	12 (21%)
14	CLA	B	1216	20	57,73,73	1.16	4 (7%)	61,113,113	1.43	11 (18%)
14	CLA	B	1217	2	39,55,73	1.41	3 (7%)	42,91,113	1.85	13 (30%)
14	CLA	B	1218	2	34,53,73	1.42	2 (5%)	37,89,113	1.83	9 (24%)
14	CLA	B	1219	20	47,63,73	1.36	3 (6%)	49,101,113	1.54	12 (24%)
14	CLA	B	1220	2	34,53,73	1.37	3 (8%)	37,89,113	1.64	8 (21%)
14	CLA	B	1221	2	46,62,73	1.33	6 (13%)	47,99,113	1.71	11 (23%)
14	CLA	B	1222	20	38,54,73	1.27	3 (7%)	41,90,113	1.87	11 (26%)
14	CLA	B	1223	2	57,73,73	1.25	3 (5%)	61,113,113	1.50	11 (18%)
14	CLA	B	1224	2	57,73,73	1.26	4 (7%)	61,113,113	1.62	12 (19%)
14	CLA	B	1225	2	57,73,73	1.31	8 (14%)	61,113,113	1.52	12 (19%)
14	CLA	B	1226	2	57,73,73	1.22	5 (8%)	61,113,113	1.62	10 (16%)
14	CLA	B	1227	2	34,53,73	1.47	5 (14%)	37,89,113	1.79	10 (27%)
14	CLA	B	1228	2	41,57,73	1.31	4 (9%)	43,93,113	1.66	9 (20%)
14	CLA	B	1229	2	57,73,73	1.16	4 (7%)	61,113,113	1.51	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	1230	2	50,66,73	1.42	4 (8%)	52,104,113	1.65	10 (19%)
14	CLA	B	1231	2	34,53,73	1.55	5 (14%)	37,89,113	1.75	9 (24%)
14	CLA	B	1232	20	34,53,73	1.43	5 (14%)	37,89,113	1.65	9 (24%)
14	CLA	B	1233	20	34,53,73	1.47	3 (8%)	37,89,113	1.61	8 (21%)
14	CLA	B	1234	2	52,68,73	1.37	3 (5%)	55,107,113	1.51	11 (20%)
14	CLA	B	1235	2	57,73,73	1.22	4 (7%)	61,113,113	1.53	14 (22%)
14	CLA	B	1236	2	39,55,73	1.30	4 (10%)	42,91,113	1.61	9 (21%)
14	CLA	B	1238	20	57,73,73	1.17	5 (8%)	61,113,113	1.36	9 (14%)
14	CLA	B	1239	2	57,73,73	1.20	5 (8%)	61,113,113	1.46	12 (19%)
15	PQN	B	2002	-	34,34,34	3.30	15 (44%)	45,45,45	2.06	3 (6%)
17	BCR	B	4004	-	41,41,41	1.48	5 (12%)	56,56,56	2.04	17 (30%)
17	BCR	B	4005	-	41,41,41	1.53	7 (17%)	56,56,56	2.11	18 (32%)
17	BCR	B	4006	-	41,41,41	1.22	5 (12%)	56,56,56	2.04	20 (35%)
17	BCR	B	4009	-	25,25,41	1.33	4 (16%)	32,33,56	1.87	10 (31%)
17	BCR	B	4010	-	41,41,41	1.21	4 (9%)	56,56,56	1.90	19 (33%)
17	BCR	B	4014	-	41,41,41	1.20	4 (9%)	56,56,56	2.01	20 (35%)
17	BCR	B	4017	-	41,41,41	1.24	4 (9%)	56,56,56	1.75	16 (28%)
19	LMG	B	5002	-	55,55,55	0.86	2 (3%)	63,63,63	1.27	3 (4%)
18	LHG	B	5004	-	22,22,48	2.70	4 (18%)	23,28,54	1.08	1 (4%)
16	SF4	C	3002	3	0,12,12	0.00	-	0,24,24	0.00	-
16	SF4	C	3003	3	0,12,12	0.00	-	0,24,24	0.00	-
14	CLA	F	1301	20	34,53,73	1.42	3 (8%)	37,89,113	1.64	10 (27%)
17	BCR	F	4016	-	41,41,41	1.23	3 (7%)	56,56,56	1.83	15 (26%)
17	BCR	I	4018	-	41,41,41	1.28	6 (14%)	56,56,56	1.81	15 (26%)
17	BCR	I	4020	-	41,41,41	1.24	6 (14%)	56,56,56	1.84	16 (28%)
14	CLA	J	1302	8	34,53,73	1.54	4 (11%)	37,89,113	1.80	9 (24%)
14	CLA	J	1303	8	29,45,73	1.72	3 (10%)	28,78,113	1.75	9 (32%)
17	BCR	J	4012	-	41,41,41	1.25	5 (12%)	56,56,56	1.92	16 (28%)
17	BCR	J	4013	-	41,41,41	1.24	3 (7%)	56,56,56	1.85	21 (37%)
17	BCR	J	4015	-	41,41,41	1.36	5 (12%)	56,56,56	1.90	13 (23%)
14	CLA	K	1401	-	34,53,73	1.43	4 (11%)	37,89,113	1.65	9 (24%)
14	CLA	L	1501	10	57,73,73	1.18	4 (7%)	61,113,113	1.54	11 (18%)
14	CLA	L	1502	10	57,73,73	1.17	6 (10%)	61,113,113	1.48	12 (19%)
14	CLA	L	1503	20	57,73,73	1.15	3 (5%)	61,113,113	1.44	9 (14%)
17	BCR	L	4019	-	41,41,41	1.39	7 (17%)	56,56,56	1.83	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	L	4022	-	41,41,41	1.57	7 (17%)	56,56,56	1.75	11 (19%)
14	CLA	M	1601	20	34,53,73	1.53	3 (8%)	37,89,113	1.78	9 (24%)
17	BCR	M	4021	-	41,41,41	1.30	6 (14%)	56,56,56	1.80	14 (25%)
14	CLA	X	1701	12	34,53,73	1.48	2 (5%)	37,89,113	1.72	10 (27%)

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
14	CLA	A	1011	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1013	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1022	20	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1101	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1102	1,14	3/3/18/25	0/30/128/135	0/0/9/9
14	CLA	A	1103	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1104	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1105	1	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1107	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1108	1	-	0/11/111/135	0/0/9/9
14	CLA	A	1109	1,14	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1110	1	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	A	1111	1	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	A	1112	1	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	A	1113	1	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	A	1114	20	3/3/16/25	1/18/116/135	0/0/9/9
14	CLA	A	1115	1	1/1/17/25	0/24/122/135	0/0/9/9
14	CLA	A	1116	1	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	A	1117	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1118	1	3/3/19/25	0/33/131/135	0/0/9/9
14	CLA	A	1119	20	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1120	1	3/3/16/25	0/18/116/135	0/0/9/9
14	CLA	A	1121	1	2/2/17/25	0/21/119/135	0/0/9/9
14	CLA	A	1122	1	3/3/18/25	0/30/128/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1123	20	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1124	20	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1125	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1126	1	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1127	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1128	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1129	1	3/3/17/25	0/19/117/135	0/0/9/9
14	CLA	A	1130	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1131	1	-	0/37/135/135	0/0/9/9
14	CLA	A	1132	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1133	1	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	A	1134	1	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	A	1135	1	3/3/17/25	0/21/119/135	0/0/9/9
14	CLA	A	1136	1	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1137	1	1/1/16/25	0/16/114/135	0/0/9/9
14	CLA	A	1138	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1139	20	3/3/17/25	0/21/119/135	0/0/9/9
14	CLA	A	1140	1	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1237	20	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	A	1402	-	3/3/14/25	0/5/101/135	0/0/9/9
14	CLA	A	1801	18	3/3/17/25	0/22/120/135	0/0/9/9
15	PQN	A	2001	-	-	0/23/43/43	0/2/2/2
16	SF4	A	3001	1,2	-	0/0/48/48	0/6/5/5
17	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4008	-	-	0/29/63/63	0/2/2/2
17	BCR	A	4011	-	-	0/29/63/63	0/2/2/2
18	LHG	A	5001	-	-	0/53/53/53	0/0/0/0
18	LHG	A	5003	14	1/1/5/5	0/31/31/53	0/0/0/0
14	CLA	B	1012	20	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1021	2	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1023	2	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1201	2	2/2/17/25	0/24/122/135	0/0/9/9
14	CLA	B	1202	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1203	2	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1204	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1205	2	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1206	2	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1207	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1208	2	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1209	2	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1210	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1211	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1212	2	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1213	2	3/3/18/25	0/25/123/135	0/0/9/9
14	CLA	B	1214	2	3/3/18/25	0/30/128/135	0/0/9/9
14	CLA	B	1215	2	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	B	1216	20	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1217	2	3/3/16/25	0/16/114/135	0/0/9/9
14	CLA	B	1218	2	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1219	20	3/3/18/25	0/25/123/135	0/0/9/9
14	CLA	B	1220	2	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1221	2	3/3/17/25	0/24/122/135	0/0/9/9
14	CLA	B	1222	20	3/3/16/25	0/15/113/135	0/0/9/9
14	CLA	B	1223	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1224	2	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1225	2	1/1/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1226	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1227	2	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1228	2	3/3/16/25	0/18/116/135	0/0/9/9
14	CLA	B	1229	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1230	2	3/3/18/25	0/29/127/135	0/0/9/9
14	CLA	B	1231	2	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1232	20	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1233	20	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	B	1234	2	3/3/19/25	0/31/129/135	0/0/9/9
14	CLA	B	1235	2	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1236	2	-	0/16/114/135	0/0/9/9
14	CLA	B	1238	20	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	B	1239	2	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PQN	B	2002	-	-	0/23/43/43	0/2/2/2
17	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4005	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4006	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4009	-	-	0/18/35/63	0/1/1/2
17	BCR	B	4010	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4014	-	-	0/29/63/63	0/2/2/2
17	BCR	B	4017	-	-	0/29/63/63	0/2/2/2
19	LMG	B	5002	-	-	0/50/70/70	0/1/1/1
18	LHG	B	5004	-	-	0/26/26/53	0/0/0/0
16	SF4	C	3002	3	-	0/0/48/48	0/6/5/5
16	SF4	C	3003	3	-	0/0/48/48	0/6/5/5
14	CLA	F	1301	20	3/3/16/25	0/11/111/135	0/0/9/9
17	BCR	F	4016	-	-	0/29/63/63	0/2/2/2
17	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
17	BCR	I	4020	-	-	0/29/63/63	0/2/2/2
14	CLA	J	1302	8	3/3/16/25	0/11/111/135	0/0/9/9
14	CLA	J	1303	8	3/3/13/25	0/2/96/135	0/0/9/9
17	BCR	J	4012	-	-	0/29/63/63	0/2/2/2
17	BCR	J	4013	-	-	0/29/63/63	0/2/2/2
17	BCR	J	4015	-	-	0/29/63/63	0/2/2/2
14	CLA	K	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
14	CLA	L	1501	10	3/3/20/25	0/37/135/135	0/0/9/9
14	CLA	L	1502	10	2/2/20/25	0/37/135/135	0/0/9/9
14	CLA	L	1503	20	3/3/20/25	0/37/135/135	0/0/9/9
17	BCR	L	4019	-	-	0/29/63/63	0/2/2/2
17	BCR	L	4022	-	-	0/29/63/63	0/2/2/2
14	CLA	M	1601	20	3/3/16/25	0/11/111/135	0/0/9/9
17	BCR	M	4021	-	-	0/29/63/63	0/2/2/2
14	CLA	X	1701	12	3/3/16/25	0/11/111/135	0/0/9/9

The worst 5 of 537 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	2001	PQN	C2M-C2	-6.78	1.36	1.50
15	B	2002	PQN	C2M-C2	-6.43	1.37	1.50
15	B	2002	PQN	C16-C15	-4.56	1.34	1.52
15	A	2001	PQN	C16-C15	-4.44	1.35	1.52
14	B	1204	CLA	C3B-C2B	-3.89	1.35	1.40

The worst 5 of 1366 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	2002	PQN	C11-C12-C13	-7.97	113.14	126.70
15	A	2001	PQN	C11-C12-C13	-7.85	113.34	126.70
15	A	2001	PQN	C15-C13-C12	-7.82	106.41	120.98
14	A	1011	CLA	O1D-CGD-CBD	-7.07	113.64	124.64
15	B	2002	PQN	C15-C13-C12	-6.64	108.62	120.98

5 of 249 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	F	1301	CLA	NC
14	F	1301	CLA	ND
14	F	1301	CLA	NA
14	A	1115	CLA	NA
14	B	1206	CLA	ND

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	1114	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

114 monomers are involved in 339 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1011	CLA	9	0
14	A	1013	CLA	10	0
14	A	1022	CLA	3	0
14	A	1101	CLA	2	0
14	A	1102	CLA	1	0
14	A	1103	CLA	6	0
14	A	1104	CLA	4	0
14	A	1105	CLA	2	0
14	A	1106	CLA	6	0
14	A	1107	CLA	4	0
14	A	1108	CLA	4	0
14	A	1109	CLA	1	0
14	A	1111	CLA	1	0
14	A	1112	CLA	5	0
14	A	1114	CLA	2	0
14	A	1116	CLA	5	0
14	A	1117	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1118	CLA	5	0
14	A	1119	CLA	4	0
14	A	1120	CLA	2	0
14	A	1121	CLA	1	0
14	A	1122	CLA	2	0
14	A	1123	CLA	4	0
14	A	1124	CLA	5	0
14	A	1125	CLA	3	0
14	A	1126	CLA	14	0
14	A	1127	CLA	1	0
14	A	1128	CLA	7	0
14	A	1129	CLA	1	0
14	A	1130	CLA	2	0
14	A	1132	CLA	4	0
14	A	1133	CLA	4	0
14	A	1134	CLA	2	0
14	A	1135	CLA	2	0
14	A	1136	CLA	7	0
14	A	1137	CLA	3	0
14	A	1138	CLA	2	0
14	A	1140	CLA	8	0
14	A	1237	CLA	5	0
14	A	1402	CLA	1	0
14	A	1801	CLA	5	0
15	A	2001	PQN	1	0
17	A	4001	BCR	2	0
17	A	4002	BCR	2	0
17	A	4003	BCR	1	0
17	A	4007	BCR	4	0
17	A	4008	BCR	1	0
17	A	4011	BCR	13	0
18	A	5001	LHG	4	0
18	A	5003	LHG	2	0
14	B	1012	CLA	17	0
14	B	1021	CLA	8	0
14	B	1023	CLA	4	0
14	B	1201	CLA	2	0
14	B	1202	CLA	3	0
14	B	1203	CLA	6	0
14	B	1204	CLA	1	0
14	B	1205	CLA	3	0
14	B	1206	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1207	CLA	5	0
14	B	1208	CLA	1	0
14	B	1209	CLA	1	0
14	B	1210	CLA	6	0
14	B	1211	CLA	6	0
14	B	1212	CLA	2	0
14	B	1213	CLA	3	0
14	B	1214	CLA	8	0
14	B	1215	CLA	6	0
14	B	1216	CLA	5	0
14	B	1217	CLA	2	0
14	B	1218	CLA	1	0
14	B	1219	CLA	4	0
14	B	1220	CLA	3	0
14	B	1221	CLA	10	0
14	B	1222	CLA	2	0
14	B	1223	CLA	3	0
14	B	1224	CLA	5	0
14	B	1225	CLA	8	0
14	B	1226	CLA	7	0
14	B	1227	CLA	5	0
14	B	1228	CLA	2	0
14	B	1229	CLA	6	0
14	B	1230	CLA	7	0
14	B	1232	CLA	3	0
14	B	1233	CLA	2	0
14	B	1234	CLA	3	0
14	B	1235	CLA	2	0
14	B	1236	CLA	4	0
14	B	1238	CLA	3	0
15	B	2002	PQN	1	0
17	B	4004	BCR	1	0
17	B	4005	BCR	1	0
17	B	4006	BCR	5	0
17	B	4009	BCR	5	0
17	B	4010	BCR	3	0
17	B	4014	BCR	1	0
17	B	4017	BCR	1	0
19	B	5002	LMG	5	0
18	B	5004	LHG	1	0
14	F	1301	CLA	1	0
17	F	4016	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	I	4018	BCR	3	0
14	J	1302	CLA	1	0
17	J	4012	BCR	4	0
17	J	4013	BCR	7	0
17	J	4015	BCR	5	0
14	K	1401	CLA	1	0
14	L	1501	CLA	2	0
14	L	1502	CLA	8	0
14	L	1503	CLA	2	0
17	L	4022	BCR	1	0
14	M	1601	CLA	1	0
17	M	4021	BCR	2	0
14	X	1701	CLA	1	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.