wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:36 AM GMT

PDB ID	:	3PCQ
Title	:	Femtosecond X-ray protein Nanocrystallography
Authors	:	Chapman, H.N.; Fromme, P.; Barty, A.; White, T.A.; Kirian, R.A.; Aquila, A.; Hunter, M.S.; Schulz, J.; Deponte, D.P.; Weierstall, U.; Doak, R.B.; Maia, F.R.N.C.; Martin, A.V.; Schlichting, I.; Lomb, L.; Coppola, N.; Shoeman, R.L.; Epp, S.W.; Hartmann, R.; Rolles, D.; Rudenko, A.; Foucar, L.; Kimmel, N.; Weidenspointner, G.; Holl, P.; Liang, M.; Barthelmess, M.; Caleman, C.; Boutet, S.; Bogan, M.J.; Krzywinski, J.; Bostedt, C.; Bajt, S.; Gumprecht, L.; Rudek, B.; Erk, B.; Schmidt, C.; Homke, A.; Reich, C.; Pietschner, D.; Struder, L.; Hauser, G.; Gorke, H.; Ullrich, J.; Herrmann, S.; Schaller, G.; Schopper, F.; Soltau, H.; Kuhnel, K.-U.; Messerschmidt, M.; Bozek, J.D.; Hau-Riege, S.P.; Frank, M.; Hampton, C.Y.; Sierra, R.; Starodub, D.; Williams, G.J.; Hajdu, J.; Timneanu, N.; Seibert, M.M.; Andreasson, J.; Rocker, A.; Jonsson, O.; Svenda, M.; Stern, S.; Nass, K.; Andritschke, R.; Schroter, C.-D.; Krasniqi, F.; Bott, M.; Schmidt, K.E.; Wang, X.; Grotjohann, I.; Holton, J.M.; Barends, T.R.M.; Neutze, R.; Marchesini, S.; Fromme, R.; Schorb, S.; Rupp, D.; Adolph, M.; Gorkhover, T.; Andersson, I.; Hirsemann, H.; Potdevin, G.; Graafsma, H.; Nilsson, B.; Spence, J.C.H.
Deposited on	:	2010-10-21
Resolution	:	8.98 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

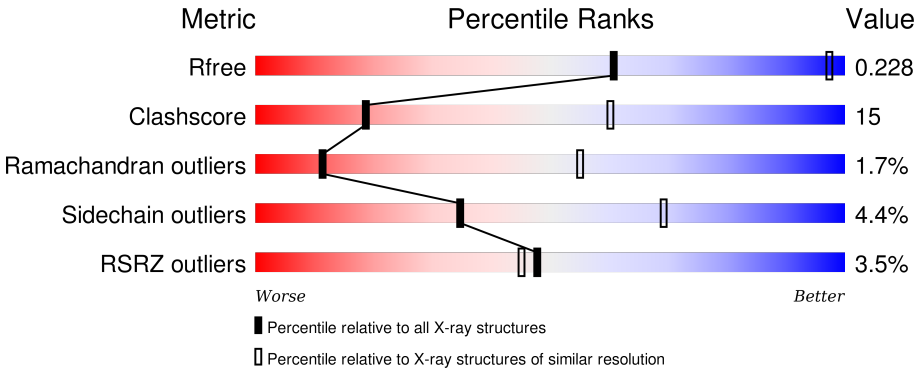
MolProbity : 4.02b-467

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 8.98 Å.

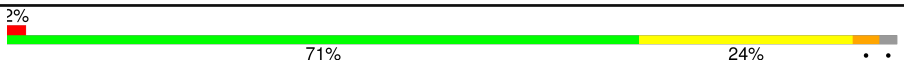
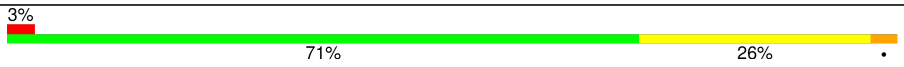
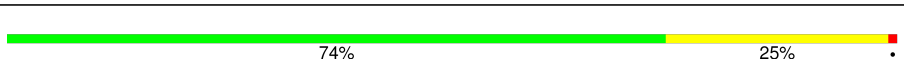
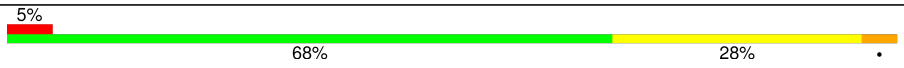
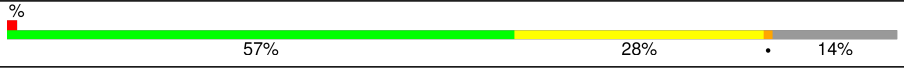
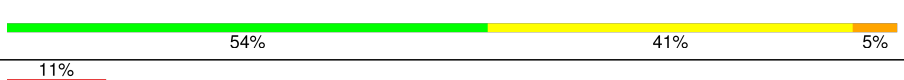
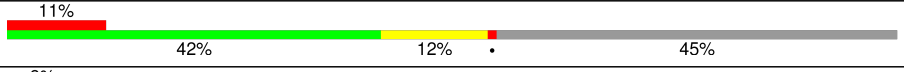
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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 <=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.

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

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	
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
13	CLA	A	801	X	-	-	-
13	CLA	A	802	X	-	-	X
13	CLA	A	803	X	-	-	X
13	CLA	A	804	X	-	-	X
13	CLA	A	805	X	-	-	X
13	CLA	A	806	X	-	-	X
13	CLA	A	807	X	-	-	X
13	CLA	A	808	X	-	-	X
13	CLA	A	809	X	-	-	X
13	CLA	A	810	X	-	-	X
13	CLA	A	812	X	-	-	X
13	CLA	A	813	X	-	-	X
13	CLA	A	814	X	-	-	X
13	CLA	A	815	X	-	-	-
13	CLA	A	816	X	-	-	X
13	CLA	A	817	X	-	-	X
13	CLA	A	818	X	-	-	X
13	CLA	A	819	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	820	X	-	-	X
13	CLA	A	821	X	-	-	X
13	CLA	A	822	X	-	-	X
13	CLA	A	823	X	-	-	X
13	CLA	A	824	X	-	-	X
13	CLA	A	825	X	-	-	X
13	CLA	A	826	X	-	-	X
13	CLA	A	827	X	-	-	X
13	CLA	A	828	X	-	-	X
13	CLA	A	829	X	-	-	X
13	CLA	A	830	X	-	-	X
13	CLA	A	831	X	-	-	X
13	CLA	A	832	X	-	-	X
13	CLA	A	833	X	-	-	X
13	CLA	A	834	-	-	-	X
13	CLA	A	835	X	-	-	X
13	CLA	A	836	X	-	-	X
13	CLA	A	837	X	-	-	X
13	CLA	A	838	X	-	-	X
13	CLA	A	839	X	-	-	X
13	CLA	A	840	X	-	-	X
13	CLA	A	841	X	-	-	X
13	CLA	A	842	X	-	-	X
13	CLA	A	843	X	-	-	X
13	CLA	A	844	X	-	-	X
13	CLA	A	845	X	-	-	X
13	CLA	A	846	X	-	-	X
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	X
13	CLA	B	803	X	-	-	X
13	CLA	B	804	X	-	-	X
13	CLA	B	805	X	-	-	X
13	CLA	B	806	X	-	-	X
13	CLA	B	807	X	-	-	X
13	CLA	B	808	X	-	-	X
13	CLA	B	809	X	-	-	X
13	CLA	B	810	X	-	-	X
13	CLA	B	811	X	-	-	X
13	CLA	B	812	X	-	-	X
13	CLA	B	813	X	-	-	X
13	CLA	B	814	X	-	-	X
13	CLA	B	815	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	816	X	-	-	X
13	CLA	B	817	X	-	-	X
13	CLA	B	818	X	-	-	X
13	CLA	B	819	X	-	-	X
13	CLA	B	820	X	-	-	X
13	CLA	B	821	X	-	-	X
13	CLA	B	822	X	-	-	-
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	X
13	CLA	B	825	X	-	-	X
13	CLA	B	826	X	-	-	X
13	CLA	B	827	X	-	-	X
13	CLA	B	828	X	-	-	X
13	CLA	B	829	X	-	-	X
13	CLA	B	830	X	-	-	X
13	CLA	B	831	X	-	-	X
13	CLA	B	832	X	-	-	X
13	CLA	B	833	X	-	-	X
13	CLA	B	834	X	-	-	X
13	CLA	B	835	X	-	-	X
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	X
13	CLA	B	839	-	-	-	X
13	CLA	B	840	X	-	-	X
13	CLA	B	841	X	-	-	X
13	CLA	F	1301	X	-	-	X
13	CLA	J	101	X	-	-	X
13	CLA	J	102	X	-	-	-
13	CLA	K	1401	X	-	-	X
13	CLA	L	1002	X	-	-	X
13	CLA	L	1003	X	-	-	X
13	CLA	L	1004	X	-	-	X
13	CLA	M	1601	X	-	-	X
13	CLA	X	1701	X	-	-	X
14	PQN	A	847	-	-	-	X
14	PQN	B	842	-	-	-	X
16	BCR	A	849	-	-	-	X
16	BCR	A	850	-	-	-	X
16	BCR	A	851	-	-	-	X
16	BCR	A	852	-	-	-	X
16	BCR	A	853	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	BCR	A	854	-	-	-	X
16	BCR	B	843	-	-	-	X
16	BCR	B	844	-	-	-	X
16	BCR	B	845	-	-	-	X
16	BCR	B	846	-	-	-	X
16	BCR	B	847	-	-	-	X
16	BCR	B	848	-	-	-	X
16	BCR	B	849	-	-	-	X
16	BCR	F	1302	-	-	-	X
16	BCR	I	101	-	-	-	X
16	BCR	I	102	-	-	-	X
16	BCR	J	103	-	-	-	X
16	BCR	J	104	-	-	-	X
16	BCR	J	105	-	-	-	X
16	BCR	L	1005	-	-	-	X
16	BCR	L	1006	-	-	-	X
16	BCR	M	1602	-	-	-	X
17	LHG	A	855	-	-	-	X
17	LHG	A	856	X	-	-	X
17	LHG	B	851	-	-	-	X
18	LMG	B	850	-	-	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 24196 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 I reaction center 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 I reaction center 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 I reaction center 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 I reaction center 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 I reaction center 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 I reaction center subunit PsaK.

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

- Molecule 10 is a protein called Photosystem I reaction center 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 is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	CONFLICT	UNP Q8DGB4

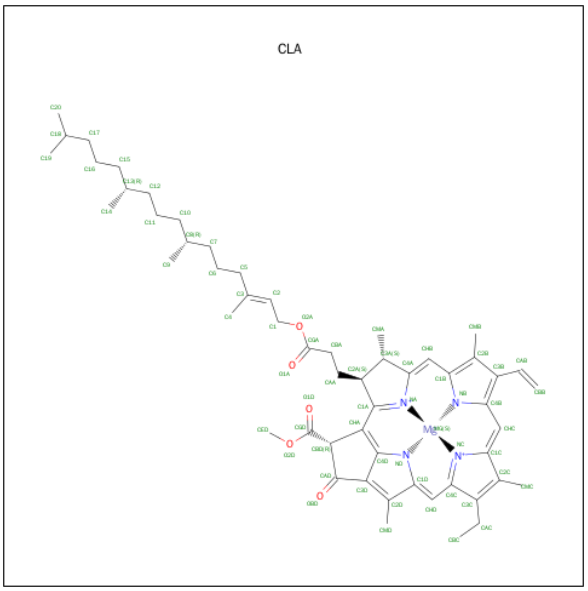
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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 4.8K protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O	0	0	0
			232	163	34	35			

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C Mg N O 45 35 1 4 5	0	0
13	A	1	Total C Mg N O 45 35 1 4 5	0	0
13	A	1	Total C Mg N O 49 39 1 4 5	0	0
13	A	1	Total C Mg N O 54 44 1 4 5	0	0
13	A	1	Total C Mg N O 54 44 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 61 51 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 49 39 1 4 5	0	0
13	A	1	Total C Mg N O 51 41 1 4 5	0	0
13	A	1	Total C Mg N O 59 49 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 50 40 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
13	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

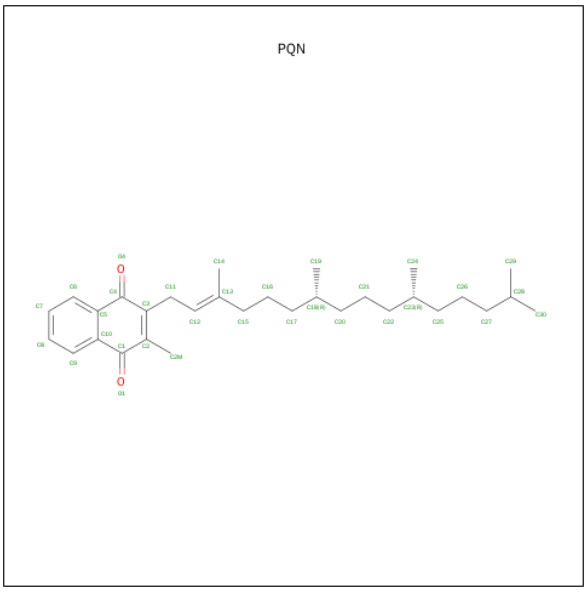
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

Continued on next page...

Continued from previous page...

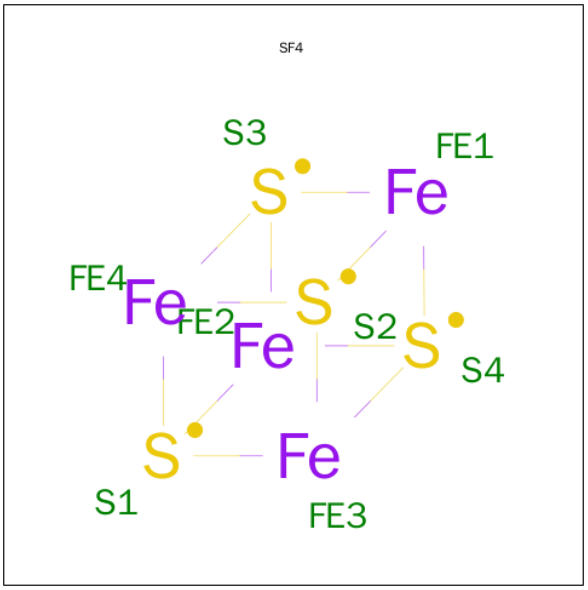
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
13	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



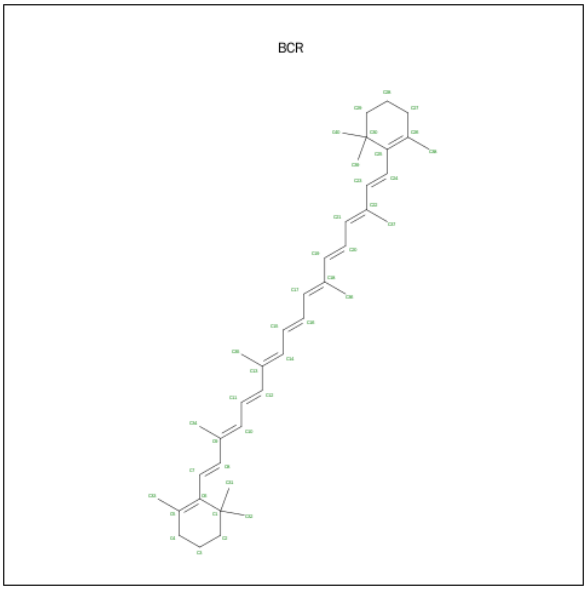
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Fe S 8 4 4	0	0
15	C	1	Total Fe S 8 4 4	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



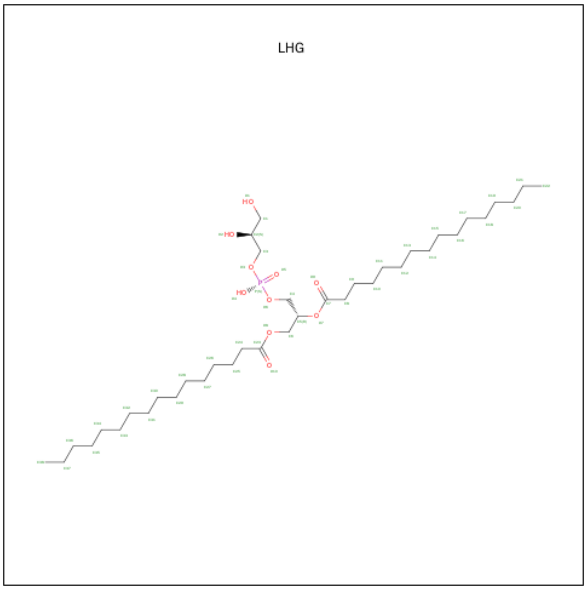
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 25 25	0	0

Continued on next page...

Continued from previous page...

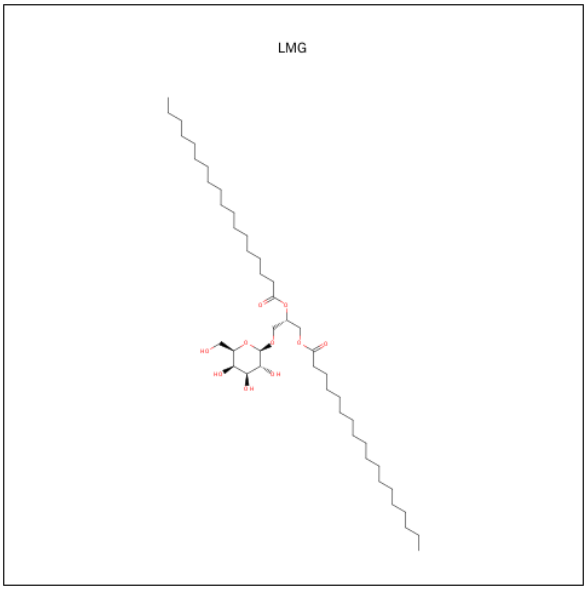
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	F	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	L	1	Total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

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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		

Continued on next page...

Continued from previous page...

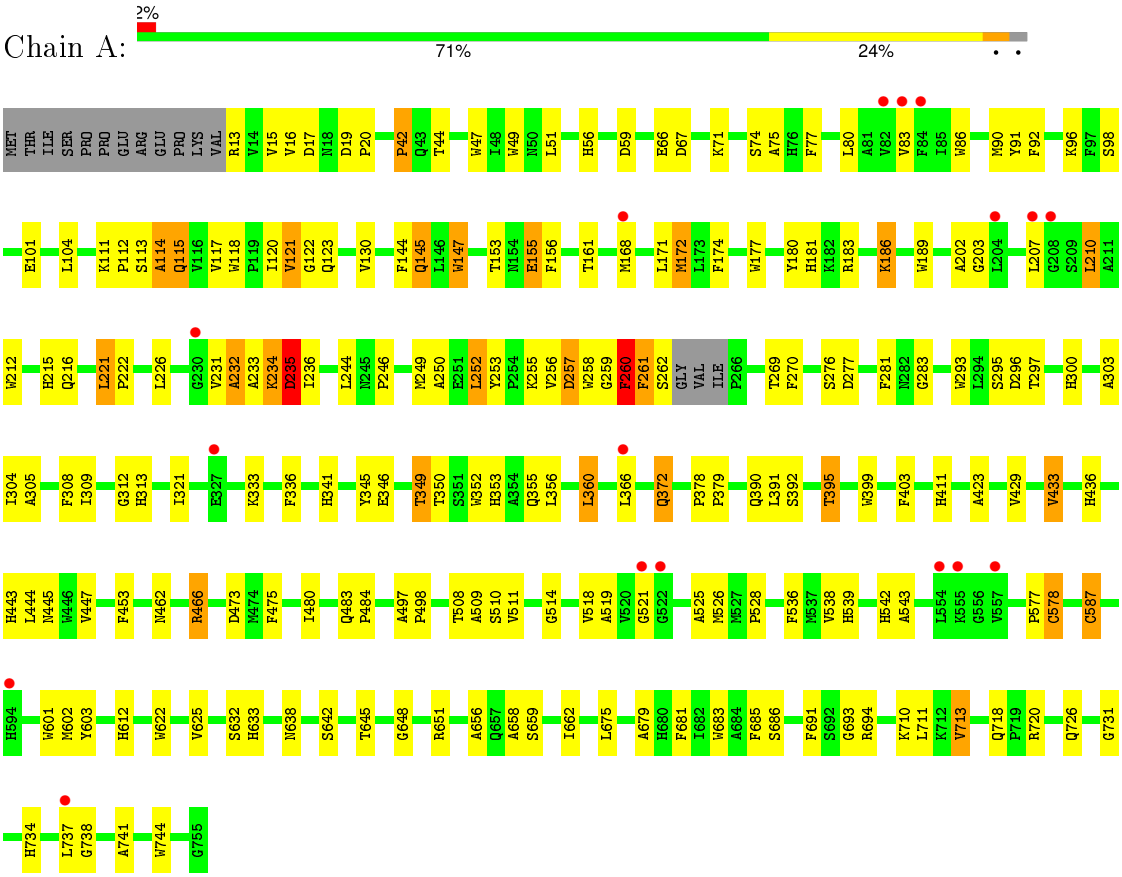
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	21	Total O 21 21	0	0
20	D	17	Total O 17 17	0	0
20	E	5	Total O 5 5	0	0
20	F	6	Total O 6 6	0	0
20	I	3	Total O 3 3	0	0
20	J	1	Total O 1 1	0	0
20	L	27	Total O 27 27	0	0
20	M	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

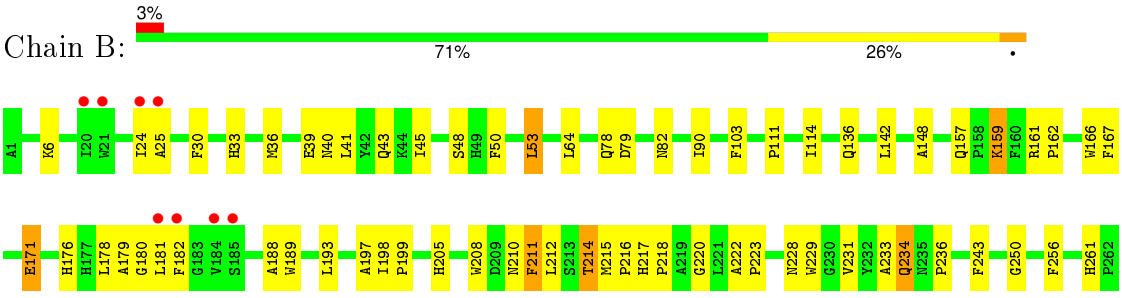
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

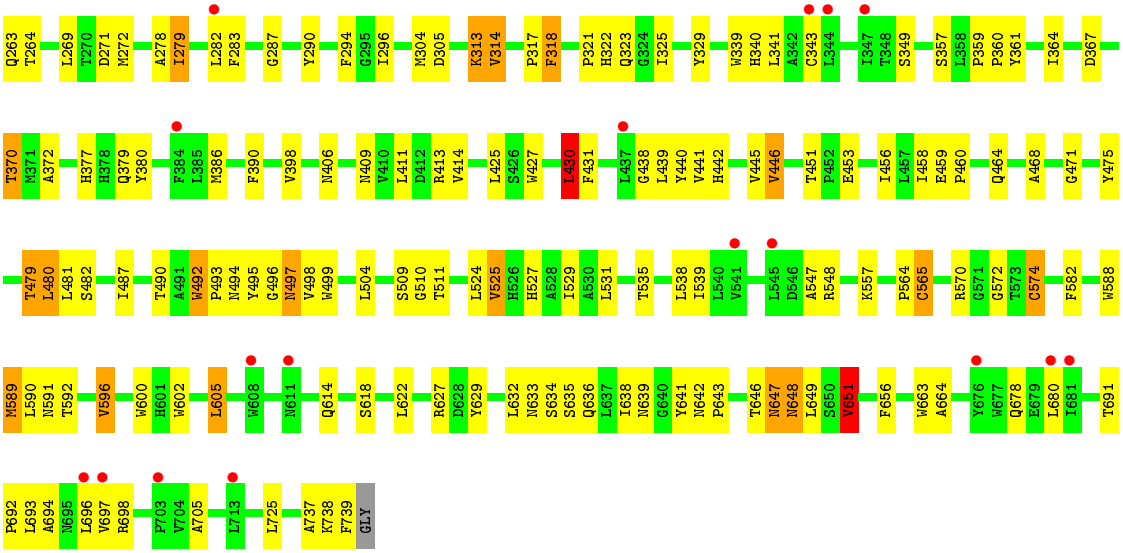
Chain A:



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

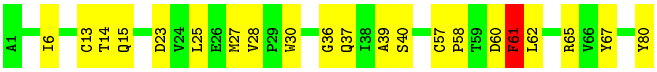
Chain B:





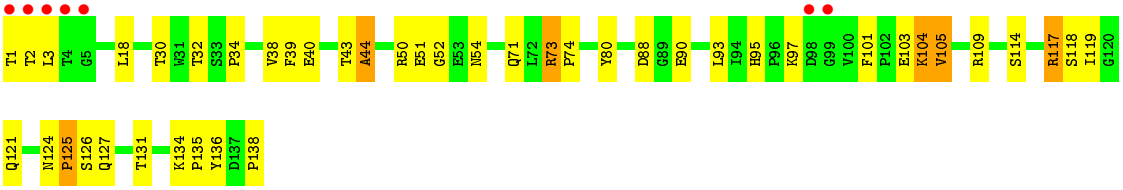
- Molecule 3: Photosystem I iron-sulfur center

Chain C:



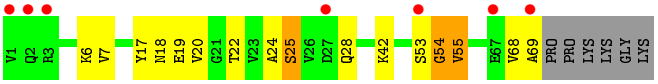
- Molecule 4: Photosystem I reaction center subunit II

Chain D:



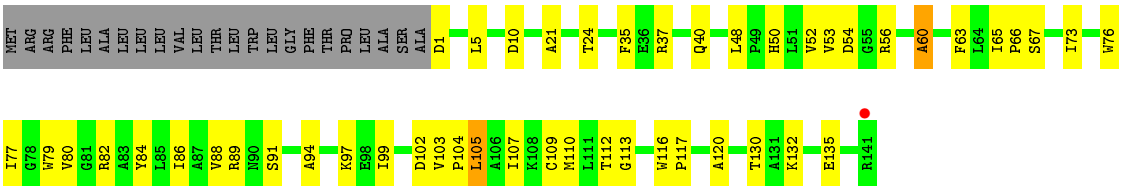
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:



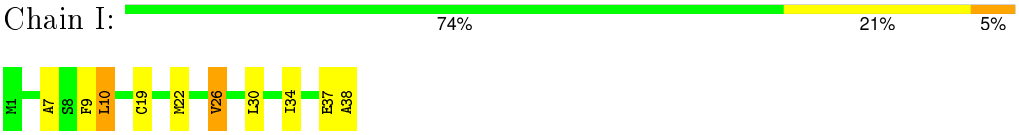
- Molecule 6: Photosystem I reaction center subunit III

Chain F:



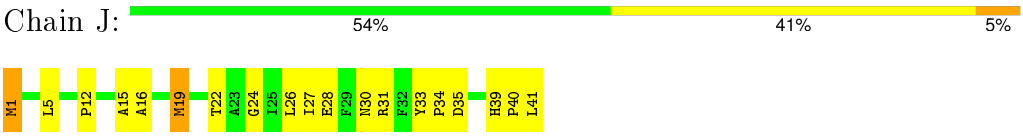
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



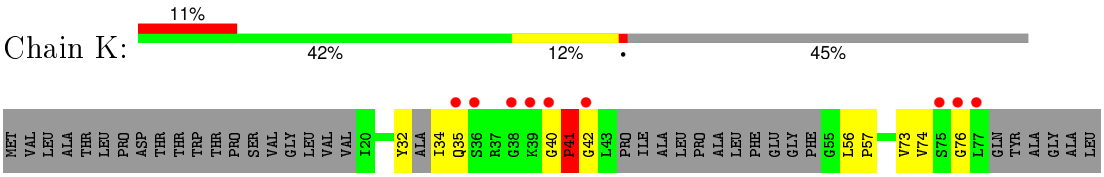
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:



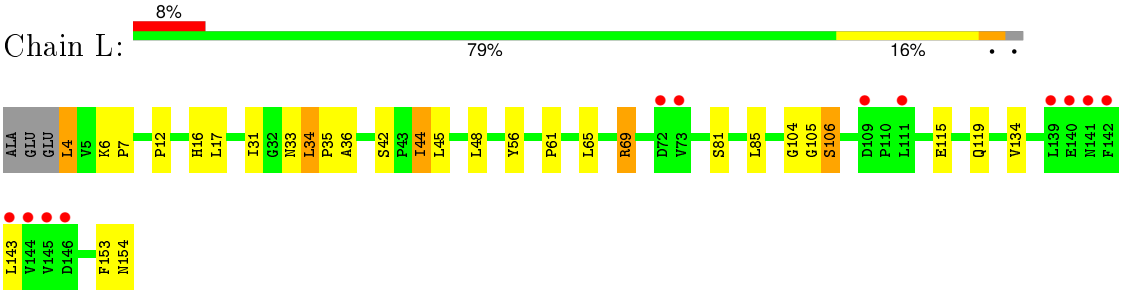
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



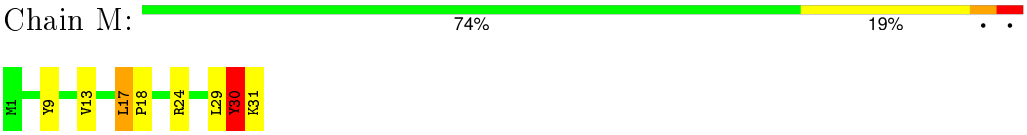
- Molecule 10: Photosystem I reaction center subunit XI

Chain L:



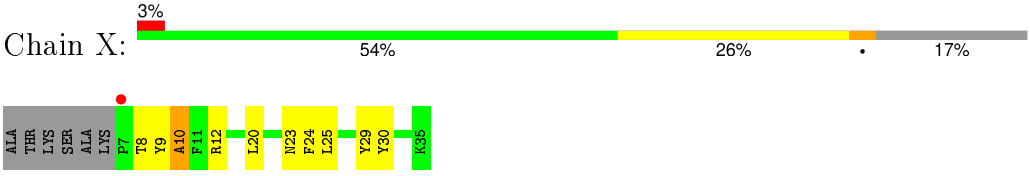
- Molecule 11: Photosystem I reaction center subunit XII

Chain M:



- Molecule 12: Photosystem I 4.8K protein

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.12 – 8.98 81.12 – 9.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (81.12-8.98) 99.1 (81.12-9.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.89 (at 8.41Å)	Xtriage
Refinement program	REFMAC 5.6.0076	Depositor
R, R_{free}	0.252 , 0.232 0.246 , 0.228	Depositor DCC
R_{free} test set	187 reflections (3.46%)	DCC
Wilson B-factor (Å^2)	203.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.500 for H, K, L 0.500 for K, H, -L 0.499 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.16$, $< L^2 > = 0.04$	Xtriage
Outliers	0 of 5591 reflections	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	24196	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 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	0.67	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	0.54	0/241	0.67	0/330
All	All	0.55	0/17940	0.70	15/24451 (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(^{o})	Ideal(^{o})
3	C	80	TYR	CA-C-O	9.93	140.96	120.10
11	M	30	TYR	N-CA-C	7.84	132.17	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.51	131.88	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	GLY	N-CA-C	-6.42	97.05	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

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	214	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	39	0
5	E	539	0	528	10	1
6	F	1065	0	1079	41	1
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	2
11	M	241	0	264	13	0
12	X	232	0	220	6	0
13	A	2687	0	2675	139	0
13	B	2349	0	2304	151	0
13	F	45	0	33	1	0
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	11	0
13	M	45	0	33	1	0
13	X	45	0	33	1	0
14	A	33	0	46	1	0
14	B	33	0	46	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
16	A	240	0	336	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	265	0	369	17	0
16	F	40	0	56	2	0
16	I	80	0	112	3	0
16	J	120	0	168	16	0
16	L	80	0	112	1	0
16	M	40	0	56	2	0
17	A	76	0	98	6	0
17	B	23	0	16	1	0
18	B	55	0	86	5	0
19	L	1	0	0	0	1
20	A	53	0	0	5	1
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	2
20	M	2	0	0	1	0
All	All	24196	0	23793	736	5

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 15.

The worst 5 of 736 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	16:J:104:BCR:H312	1.26	1.17
2:B:622:LEU:HD12	13:B:802:CLA:H11	1.28	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	1.04
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01

All (5) 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:1126:HOH:O	20:L:1126:HOH:O[2_655]	1.08	1.12
10:L:153:PHE:O	19:L:1001:CA:CA[3_665]	1.57	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:28:GLN:OE1	6:F:1:ASP:N[4_664]	2.00	0.20
10:L:154:ASN:OXT	20:A:950:HOH:O[3_665]	2.07	0.13
20:L:1108:HOH:O	20:L:1117:HOH:O[2_655]	2.07	0.13

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 58
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	16 61
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	15 60
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	8 49
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	2 26
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	8 49
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 21
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	15 60
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	5 40
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	4 38
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	11 55

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 71
2	B	595/597 (100%)	567 (95%)	28 (5%)	32 68
3	C	67/67 (100%)	66 (98%)	1 (2%)	72 88
4	D	115/115 (100%)	107 (93%)	8 (7%)	19 56
5	E	59/64 (92%)	59 (100%)	0	100 100
6	F	109/128 (85%)	107 (98%)	2 (2%)	66 87
7	I	32/32 (100%)	30 (94%)	2 (6%)	22 59
8	J	36/36 (100%)	34 (94%)	2 (6%)	26 62
10	L	117/119 (98%)	109 (93%)	8 (7%)	20 57
11	M	26/26 (100%)	25 (96%)	1 (4%)	40 73
12	X	20/27 (74%)	18 (90%)	2 (10%)	9 38
All	All	1765/1814 (97%)	1687 (96%)	78 (4%)	35 69

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 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	263	GLN
2	B	494	ASN
6	F	40	GLN
2	B	336	GLN
2	B	340	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

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	$\#\|Z\| > 2$
13	CLA	A	801	-	55,73,73	0.88	1 (1%)	61,113,113	2.24	10 (16%)
13	CLA	A	802	20	55,73,73	0.86	3 (5%)	61,113,113	1.41	10 (16%)
13	CLA	A	803	-	55,73,73	0.96	4 (7%)	61,113,113	1.46	11 (18%)
13	CLA	A	804	-	55,73,73	0.84	3 (5%)	61,113,113	1.49	8 (13%)
13	CLA	A	805	13	49,67,73	0.89	2 (4%)	53,105,113	1.69	12 (22%)
13	CLA	A	806	-	55,73,73	0.84	2 (3%)	61,113,113	1.60	11 (18%)
13	CLA	A	807	-	55,73,73	0.87	2 (3%)	61,113,113	1.66	14 (22%)
13	CLA	A	808	-	41,59,73	1.07	3 (7%)	44,96,113	1.63	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	A	809	1	55,73,73	1.06	4 (7%)	61,113,113	1.57	11 (18%)
13	CLA	A	810	1	55,73,73	0.79	1 (1%)	61,113,113	1.54	11 (18%)
13	CLA	A	811	-	32,53,73	0.99	3 (9%)	37,89,113	1.63	8 (21%)
13	CLA	A	812	13	55,73,73	0.88	3 (5%)	61,113,113	1.38	9 (14%)
13	CLA	A	813	-	44,62,73	1.02	4 (9%)	47,99,113	1.62	9 (19%)
13	CLA	A	814	-	50,68,73	0.86	2 (4%)	55,107,113	1.58	10 (18%)
13	CLA	A	815	-	32,53,73	1.07	3 (9%)	37,89,113	1.72	8 (21%)
13	CLA	A	816	-	32,53,73	0.86	1 (3%)	37,89,113	1.84	9 (24%)
13	CLA	A	817	20	39,57,73	0.94	2 (5%)	43,93,113	1.70	8 (18%)
13	CLA	A	818	-	44,62,73	0.99	3 (6%)	47,99,113	1.55	8 (17%)
13	CLA	A	819	-	44,62,73	1.08	4 (9%)	47,99,113	1.67	12 (25%)
13	CLA	A	820	-	55,73,73	0.99	4 (7%)	61,113,113	1.57	13 (21%)
13	CLA	A	821	-	51,69,73	0.99	4 (7%)	56,108,113	1.62	12 (21%)
13	CLA	A	822	20	55,73,73	0.89	4 (7%)	61,113,113	1.57	14 (22%)
13	CLA	A	823	-	39,57,73	0.98	2 (5%)	43,93,113	1.83	12 (27%)
13	CLA	A	824	-	41,59,73	1.03	3 (7%)	44,96,113	1.72	8 (18%)
13	CLA	A	825	-	49,67,73	0.90	2 (4%)	53,105,113	1.53	12 (22%)
13	CLA	A	826	20	55,73,73	0.90	2 (3%)	61,113,113	1.50	9 (14%)
13	CLA	A	827	20	55,73,73	0.86	2 (3%)	61,113,113	1.43	10 (16%)
13	CLA	A	828	-	55,73,73	0.94	2 (3%)	61,113,113	1.51	9 (14%)
13	CLA	A	829	-	55,73,73	0.83	2 (3%)	61,113,113	1.38	11 (18%)
13	CLA	A	830	-	55,73,73	0.78	1 (1%)	61,113,113	1.51	9 (14%)
13	CLA	A	831	-	55,73,73	0.97	4 (7%)	61,113,113	1.50	11 (18%)
13	CLA	A	832	-	40,58,73	1.08	3 (7%)	44,95,113	1.88	13 (29%)
13	CLA	A	833	-	55,73,73	0.78	0	61,113,113	1.50	11 (18%)
13	CLA	A	834	-	55,73,73	0.73	0	61,113,113	1.43	10 (16%)
13	CLA	A	835	-	55,73,73	0.98	3 (5%)	61,113,113	1.60	11 (18%)
13	CLA	A	836	-	44,62,73	1.00	4 (9%)	47,99,113	1.67	10 (21%)
13	CLA	A	837	1	32,53,73	0.95	2 (6%)	37,89,113	1.72	9 (24%)
13	CLA	A	838	-	41,59,73	0.84	0	44,96,113	1.69	11 (25%)
13	CLA	A	839	-	55,73,73	0.95	3 (5%)	61,113,113	1.32	7 (11%)
13	CLA	A	840	-	37,55,73	1.05	3 (8%)	42,91,113	1.74	10 (23%)
13	CLA	A	841	-	55,73,73	0.87	4 (7%)	61,113,113	1.43	12 (19%)
13	CLA	A	842	20	41,59,73	1.04	4 (9%)	44,96,113	1.63	10 (22%)
13	CLA	A	843	-	55,73,73	0.99	2 (3%)	61,113,113	1.51	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	A	844	20	55,73,73	1.02	5 (9%)	61,113,113	1.44	11 (18%)
13	CLA	A	845	-	29,49,73	1.08	3 (10%)	32,83,113	1.44	3 (9%)
13	CLA	A	846	17	42,60,73	1.15	5 (11%)	45,97,113	1.88	11 (24%)
14	PQN	A	847	-	34,34,34	3.59	17 (50%)	44,45,45	2.21	3 (6%)
15	SF4	A	848	1,2	0,12,12	0.00	-	0,24,24	0.00	-
16	BCR	A	849	-	41,41,41	1.33	5 (12%)	56,56,56	1.92	16 (28%)
16	BCR	A	850	-	41,41,41	1.24	4 (9%)	56,56,56	1.81	16 (28%)
16	BCR	A	851	-	41,41,41	1.38	6 (14%)	56,56,56	1.98	18 (32%)
16	BCR	A	852	-	41,41,41	1.34	6 (14%)	56,56,56	1.82	15 (26%)
16	BCR	A	853	-	41,41,41	1.25	7 (17%)	56,56,56	1.94	17 (30%)
16	BCR	A	854	-	41,41,41	1.34	6 (14%)	56,56,56	2.07	21 (37%)
17	LHG	A	855	-	48,48,48	1.67	6 (12%)	49,54,54	1.25	3 (6%)
17	LHG	A	856	13	26,26,48	2.19	5 (19%)	27,32,54	1.51	4 (14%)
13	CLA	B	801	-	55,73,73	0.91	3 (5%)	61,113,113	1.38	10 (16%)
13	CLA	B	802	20	55,73,73	0.85	1 (1%)	61,113,113	1.59	9 (14%)
13	CLA	B	803	-	55,73,73	1.09	4 (7%)	61,113,113	1.37	10 (16%)
13	CLA	B	804	-	44,62,73	1.04	2 (4%)	47,99,113	1.77	9 (19%)
13	CLA	B	805	-	55,73,73	0.87	3 (5%)	61,113,113	1.47	9 (14%)
13	CLA	B	806	-	55,73,73	0.80	1 (1%)	61,113,113	1.34	9 (14%)
13	CLA	B	807	-	55,73,73	0.95	3 (5%)	61,113,113	1.50	9 (14%)
13	CLA	B	808	-	55,73,73	0.91	3 (5%)	61,113,113	1.66	11 (18%)
13	CLA	B	809	2	55,73,73	0.70	0	61,113,113	1.42	10 (16%)
13	CLA	B	810	2	55,73,73	0.82	1 (1%)	61,113,113	1.39	10 (16%)
13	CLA	B	811	-	32,53,73	1.04	4 (12%)	37,89,113	1.64	8 (21%)
13	CLA	B	812	-	32,53,73	0.88	1 (3%)	37,89,113	1.71	9 (24%)
13	CLA	B	813	-	55,73,73	0.84	2 (3%)	61,113,113	1.49	9 (14%)
13	CLA	B	814	-	55,73,73	0.94	4 (7%)	61,113,113	1.53	9 (14%)
13	CLA	B	815	-	32,53,73	1.02	3 (9%)	37,89,113	1.76	7 (18%)
13	CLA	B	816	-	45,63,73	1.11	6 (13%)	49,101,113	1.61	11 (22%)
13	CLA	B	817	-	49,67,73	1.01	4 (8%)	53,105,113	1.58	11 (20%)
13	CLA	B	818	-	50,68,73	1.01	3 (6%)	55,107,113	1.67	12 (21%)
13	CLA	B	819	20	55,73,73	0.90	3 (5%)	61,113,113	1.43	10 (16%)
13	CLA	B	820	-	37,55,73	0.89	2 (5%)	42,91,113	1.88	12 (28%)
13	CLA	B	821	-	32,53,73	0.97	1 (3%)	37,89,113	1.85	10 (27%)
13	CLA	B	822	20	45,63,73	1.03	2 (4%)	49,101,113	1.55	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	B	823	-	32,53,73	0.97	2 (6%)	37,89,113	1.64	8 (21%)
13	CLA	B	824	2	44,62,73	1.15	5 (11%)	47,99,113	1.71	11 (23%)
13	CLA	B	825	20	36,54,73	0.85	2 (5%)	41,90,113	1.84	11 (26%)
13	CLA	B	826	-	55,73,73	0.82	2 (3%)	61,113,113	1.50	10 (16%)
13	CLA	B	827	-	55,73,73	1.03	3 (5%)	61,113,113	1.64	12 (19%)
13	CLA	B	828	-	55,73,73	1.11	6 (10%)	61,113,113	1.53	11 (18%)
13	CLA	B	829	-	55,73,73	0.86	3 (5%)	61,113,113	1.61	10 (16%)
13	CLA	B	830	-	32,53,73	1.08	4 (12%)	37,89,113	1.81	10 (27%)
13	CLA	B	831	-	39,57,73	1.06	3 (7%)	43,93,113	1.70	10 (23%)
13	CLA	B	832	-	55,73,73	0.94	2 (3%)	61,113,113	1.53	9 (14%)
13	CLA	B	833	-	48,66,73	1.02	4 (8%)	52,104,113	1.67	11 (21%)
13	CLA	B	834	-	32,53,73	1.10	3 (9%)	37,89,113	1.70	10 (27%)
13	CLA	B	835	20	32,53,73	1.14	4 (12%)	37,89,113	1.63	8 (21%)
13	CLA	B	836	20	32,53,73	0.88	2 (6%)	37,89,113	1.60	8 (21%)
13	CLA	B	837	-	50,68,73	1.03	3 (6%)	55,107,113	1.53	9 (16%)
13	CLA	B	838	-	55,73,73	0.93	3 (5%)	61,113,113	1.55	14 (22%)
13	CLA	B	839	-	37,55,73	1.00	3 (8%)	42,91,113	1.60	10 (23%)
13	CLA	B	840	20	55,73,73	0.93	2 (3%)	61,113,113	1.33	8 (13%)
13	CLA	B	841	-	55,73,73	0.83	4 (7%)	61,113,113	1.48	11 (18%)
14	PQN	B	842	-	34,34,34	3.52	15 (44%)	44,45,45	2.07	3 (6%)
16	BCR	B	843	-	41,41,41	1.49	5 (12%)	56,56,56	2.08	16 (28%)
16	BCR	B	844	-	41,41,41	1.54	8 (19%)	56,56,56	2.14	18 (32%)
16	BCR	B	845	-	41,41,41	1.24	5 (12%)	56,56,56	2.05	20 (35%)
16	BCR	B	846	-	25,25,41	1.35	4 (16%)	33,33,56	1.89	11 (33%)
16	BCR	B	847	-	41,41,41	1.22	5 (12%)	56,56,56	1.92	19 (33%)
16	BCR	B	848	-	41,41,41	1.22	4 (9%)	56,56,56	2.03	20 (35%)
16	BCR	B	849	-	41,41,41	1.26	6 (14%)	56,56,56	1.77	17 (30%)
18	LMG	B	850	-	55,55,55	0.86	2 (3%)	63,63,63	1.26	3 (4%)
17	LHG	B	851	-	22,22,48	2.63	4 (18%)	23,28,54	1.05	1 (4%)
15	SF4	C	101	3	0,12,12	0.00	-	0,24,24	0.00	-
15	SF4	C	102	3	0,12,12	0.00	-	0,24,24	0.00	-
13	CLA	F	1301	20	32,53,73	0.92	1 (3%)	37,89,113	1.64	9 (24%)
16	BCR	F	1302	-	41,41,41	1.25	3 (7%)	56,56,56	1.85	14 (25%)
16	BCR	I	101	-	41,41,41	1.29	7 (17%)	56,56,56	1.83	15 (26%)
16	BCR	I	102	-	41,41,41	1.26	6 (14%)	56,56,56	1.85	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	J	101	8	32,53,73	1.01	3 (9%)	37,89,113	1.81	9 (24%)
13	CLA	J	102	-	27,45,73	1.11	2 (7%)	29,78,113	1.67	9 (31%)
16	BCR	J	103	-	41,41,41	1.26	5 (12%)	56,56,56	1.93	16 (28%)
16	BCR	J	104	-	41,41,41	1.23	3 (7%)	56,56,56	1.85	21 (37%)
16	BCR	J	105	-	41,41,41	1.39	6 (14%)	56,56,56	1.92	13 (23%)
13	CLA	K	1401	-	32,53,73	1.03	3 (9%)	37,89,113	1.68	8 (21%)
13	CLA	L	1002	10	55,73,73	0.88	2 (3%)	61,113,113	1.57	10 (16%)
13	CLA	L	1003	-	55,73,73	1.02	5 (9%)	61,113,113	1.45	11 (18%)
13	CLA	L	1004	20	55,73,73	0.90	1 (1%)	61,113,113	1.47	9 (14%)
16	BCR	L	1005	-	41,41,41	1.39	6 (14%)	56,56,56	1.85	15 (26%)
16	BCR	L	1006	-	41,41,41	1.56	8 (19%)	56,56,56	1.77	11 (19%)
13	CLA	M	1601	20	32,53,73	0.99	2 (6%)	37,89,113	1.81	10 (27%)
16	BCR	M	1602	-	41,41,41	1.30	6 (14%)	56,56,56	1.82	13 (23%)
13	CLA	X	1701	12	32,53,73	0.88	1 (3%)	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
13	CLA	A	801	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	802	20	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	803	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	804	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	805	13	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	A	806	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	807	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	808	-	2/2/17/25	0/21/119/135	0/0/9/9
13	CLA	A	809	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	810	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	811	-	-	0/11/111/135	0/0/9/9
13	CLA	A	812	13	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	813	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	814	-	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	A	815	-	3/3/16/25	0/11/111/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	816	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	817	20	3/3/16/25	1/18/116/135	0/0/9/9
13	CLA	A	818	-	1/1/17/25	0/24/122/135	0/0/9/9
13	CLA	A	819	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	820	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	821	-	3/3/19/25	0/33/131/135	0/0/9/9
13	CLA	A	822	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	823	-	3/3/16/25	0/18/116/135	0/0/9/9
13	CLA	A	824	-	2/2/17/25	0/21/119/135	0/0/9/9
13	CLA	A	825	-	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	A	826	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	827	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	828	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	829	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	A	830	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	831	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	832	-	3/3/17/25	0/19/117/135	0/0/9/9
13	CLA	A	833	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	834	-	-	0/37/135/135	0/0/9/9
13	CLA	A	835	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	836	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	837	1	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	838	-	3/3/17/25	0/21/119/135	0/0/9/9
13	CLA	A	839	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	840	-	1/1/16/25	0/16/114/135	0/0/9/9
13	CLA	A	841	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	842	20	3/3/17/25	0/21/119/135	0/0/9/9
13	CLA	A	843	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	844	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	845	-	3/3/14/25	0/5/101/135	0/0/9/9
13	CLA	A	846	17	3/3/17/25	0/22/120/135	0/0/9/9
14	PQN	A	847	-	-	0/23/43/43	0/2/2/2
15	SF4	A	848	1,2	-	0/0/48/48	0/6/5/5
16	BCR	A	849	-	-	0/29/63/63	0/2/2/2
16	BCR	A	850	-	-	0/29/63/63	0/2/2/2
16	BCR	A	851	-	-	0/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	A	852	-	-	0/29/63/63	0/2/2/2
16	BCR	A	853	-	-	0/29/63/63	0/2/2/2
16	BCR	A	854	-	-	0/29/63/63	0/2/2/2
17	LHG	A	855	-	-	0/53/53/53	0/0/0/0
17	LHG	A	856	13	1/1/5/5	0/31/31/53	0/0/0/0
13	CLA	B	801	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	802	20	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	803	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	804	-	2/2/17/25	0/24/122/135	0/0/9/9
13	CLA	B	805	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	806	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	807	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	808	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	809	2	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	810	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	811	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	812	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	813	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	814	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	815	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	816	-	3/3/18/25	0/25/123/135	0/0/9/9
13	CLA	B	817	-	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	B	818	-	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	B	819	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	820	-	3/3/16/25	0/16/114/135	0/0/9/9
13	CLA	B	821	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	822	20	3/3/18/25	0/25/123/135	0/0/9/9
13	CLA	B	823	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	824	2	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	B	825	20	3/3/16/25	0/15/113/135	0/0/9/9
13	CLA	B	826	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	827	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	828	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	829	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	830	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	831	-	3/3/16/25	0/18/116/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	832	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	833	-	3/3/18/25	0/29/127/135	0/0/9/9
13	CLA	B	834	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	835	20	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	836	20	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	837	-	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	B	838	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	839	-	-	0/16/114/135	0/0/9/9
13	CLA	B	840	20	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	841	-	2/2/20/25	0/37/135/135	0/0/9/9
14	PQN	B	842	-	-	0/23/43/43	0/2/2/2
16	BCR	B	843	-	-	0/29/63/63	0/2/2/2
16	BCR	B	844	-	-	0/29/63/63	0/2/2/2
16	BCR	B	845	-	-	0/29/63/63	0/2/2/2
16	BCR	B	846	-	-	0/18/35/63	0/1/1/2
16	BCR	B	847	-	-	0/29/63/63	0/2/2/2
16	BCR	B	848	-	-	0/29/63/63	0/2/2/2
16	BCR	B	849	-	-	0/29/63/63	0/2/2/2
18	LMG	B	850	-	-	0/50/70/70	0/1/1/1
17	LHG	B	851	-	-	0/26/26/53	0/0/0/0
15	SF4	C	101	3	-	0/0/48/48	0/6/5/5
15	SF4	C	102	3	-	0/0/48/48	0/6/5/5
13	CLA	F	1301	20	3/3/16/25	0/11/111/135	0/0/9/9
16	BCR	F	1302	-	-	0/29/63/63	0/2/2/2
16	BCR	I	101	-	-	0/29/63/63	0/2/2/2
16	BCR	I	102	-	-	0/29/63/63	0/2/2/2
13	CLA	J	101	8	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	J	102	-	3/3/13/25	0/2/96/135	0/0/9/9
16	BCR	J	103	-	-	0/29/63/63	0/2/2/2
16	BCR	J	104	-	-	0/29/63/63	0/2/2/2
16	BCR	J	105	-	-	0/29/63/63	0/2/2/2
13	CLA	K	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	L	1002	10	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	L	1003	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	L	1004	20	3/3/20/25	0/37/135/135	0/0/9/9
16	BCR	L	1005	-	-	0/29/63/63	0/2/2/2
16	BCR	L	1006	-	-	0/29/63/63	0/2/2/2
13	CLA	M	1601	20	3/3/16/25	0/11/111/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	M	1602	-	-	0/29/63/63	0/2/2/2
13	CLA	X	1701	12	3/3/16/25	0/11/111/135	0/0/9/9

The worst 5 of 429 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	847	PQN	C2M-C2	-6.92	1.36	1.50
14	B	842	PQN	C2M-C2	-6.60	1.37	1.50
14	B	842	PQN	C16-C15	-4.52	1.35	1.52
14	A	847	PQN	C16-C15	-4.38	1.35	1.52
13	B	807	CLA	C3B-C2B	-3.76	1.35	1.40

The worst 5 of 1335 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	842	PQN	C11-C12-C13	-7.97	113.20	126.70
14	A	847	PQN	C11-C12-C13	-7.86	113.38	126.70
14	A	847	PQN	C15-C13-C12	-7.70	106.45	121.05
13	A	801	CLA	O1D-CGD-CBD	-7.61	113.72	124.62
14	B	842	PQN	C15-C13-C12	-6.52	108.68	121.05

5 of 249 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	L	1004	CLA	NC
13	L	1004	CLA	ND
13	L	1004	CLA	NA
13	A	829	CLA	ND
13	A	820	CLA	NC

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	817	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

114 monomers are involved in 334 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	801	CLA	9	0
13	A	802	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	803	CLA	10	0
13	A	804	CLA	2	0
13	A	805	CLA	1	0
13	A	806	CLA	6	0
13	A	807	CLA	4	0
13	A	808	CLA	2	0
13	A	809	CLA	6	0
13	A	810	CLA	4	0
13	A	811	CLA	4	0
13	A	812	CLA	1	0
13	A	814	CLA	1	0
13	A	815	CLA	5	0
13	A	817	CLA	2	0
13	A	819	CLA	4	0
13	A	820	CLA	6	0
13	A	821	CLA	5	0
13	A	822	CLA	4	0
13	A	823	CLA	2	0
13	A	824	CLA	1	0
13	A	825	CLA	2	0
13	A	826	CLA	4	0
13	A	827	CLA	5	0
13	A	828	CLA	3	0
13	A	829	CLA	13	0
13	A	830	CLA	1	0
13	A	831	CLA	6	0
13	A	832	CLA	1	0
13	A	833	CLA	1	0
13	A	835	CLA	4	0
13	A	836	CLA	4	0
13	A	837	CLA	2	0
13	A	838	CLA	2	0
13	A	839	CLA	6	0
13	A	840	CLA	3	0
13	A	841	CLA	2	0
13	A	843	CLA	8	0
13	A	844	CLA	5	0
13	A	845	CLA	1	0
13	A	846	CLA	5	0
14	A	847	PQN	1	0
16	A	849	BCR	2	0
16	A	850	BCR	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	851	BCR	1	0
16	A	852	BCR	4	0
16	A	853	BCR	1	0
16	A	854	BCR	13	0
17	A	855	LHG	4	0
17	A	856	LHG	2	0
13	B	801	CLA	8	0
13	B	802	CLA	17	0
13	B	803	CLA	4	0
13	B	804	CLA	2	0
13	B	805	CLA	3	0
13	B	806	CLA	6	0
13	B	807	CLA	1	0
13	B	808	CLA	3	0
13	B	809	CLA	2	0
13	B	810	CLA	5	0
13	B	811	CLA	1	0
13	B	812	CLA	1	0
13	B	813	CLA	6	0
13	B	814	CLA	6	0
13	B	815	CLA	2	0
13	B	816	CLA	3	0
13	B	817	CLA	8	0
13	B	818	CLA	5	0
13	B	819	CLA	5	0
13	B	820	CLA	2	0
13	B	821	CLA	1	0
13	B	822	CLA	4	0
13	B	823	CLA	3	0
13	B	824	CLA	10	0
13	B	825	CLA	2	0
13	B	826	CLA	3	0
13	B	827	CLA	5	0
13	B	828	CLA	8	0
13	B	829	CLA	7	0
13	B	830	CLA	5	0
13	B	831	CLA	2	0
13	B	832	CLA	6	0
13	B	833	CLA	7	0
13	B	835	CLA	3	0
13	B	836	CLA	2	0
13	B	837	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	838	CLA	2	0
13	B	839	CLA	4	0
13	B	840	CLA	3	0
14	B	842	PQN	1	0
16	B	843	BCR	1	0
16	B	844	BCR	1	0
16	B	845	BCR	5	0
16	B	846	BCR	5	0
16	B	847	BCR	3	0
16	B	848	BCR	1	0
16	B	849	BCR	1	0
18	B	850	LMG	5	0
17	B	851	LHG	1	0
13	F	1301	CLA	1	0
16	F	1302	BCR	2	0
16	I	101	BCR	3	0
13	J	101	CLA	1	0
16	J	103	BCR	4	0
16	J	104	BCR	7	0
16	J	105	BCR	5	0
13	K	1401	CLA	1	0
13	L	1002	CLA	2	0
13	L	1003	CLA	8	0
13	L	1004	CLA	2	0
16	L	1006	BCR	1	0
13	M	1601	CLA	1	0
16	M	1602	BCR	2	0
13	X	1701	CLA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	740/755 (98%)	-0.20	17 (2%) 64 59	22, 45, 71, 93	0
2	B	739/740 (99%)	-0.09	25 (3%) 49 46	20, 38, 71, 89	0
3	C	80/80 (100%)	-0.59	0 100 100	22, 33, 45, 54	0
4	D	138/138 (100%)	-0.03	7 (5%) 32 32	27, 41, 56, 84	0
5	E	69/75 (92%)	0.48	7 (10%) 9 14	29, 46, 62, 76	0
6	F	141/164 (85%)	-0.20	1 (0%) 89 85	37, 57, 68, 72	0
7	I	38/38 (100%)	0.41	0 100 100	20, 33, 47, 53	0
8	J	41/41 (100%)	0.07	0 100 100	53, 60, 77, 86	0
9	K	46/83 (55%)	1.08	9 (19%) 1 7	72, 81, 96, 99	0
10	L	151/154 (98%)	0.31	12 (7%) 15 19	19, 26, 47, 67	0
11	M	31/31 (100%)	0.32	0 100 100	30, 38, 52, 62	0
12	X	29/35 (82%)	-0.00	1 (3%) 49 46	58, 63, 81, 88	0
All	All	2243/2334 (96%)	-0.06	79 (3%) 48 45	19, 42, 74, 99	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2	THR	7.8
4	D	3	LEU	6.3
4	D	4	THR	5.9
1	A	207	LEU	5.8
10	L	144	VAL	4.8

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
16	BCR	B	845	40/40	0.74	1.29	9.49	33,51,87,88	0
13	CLA	A	843	65/65	0.90	1.48	6.80	29,35,60,60	0
13	CLA	B	831	49/65	0.83	0.82	6.19	36,40,63,65	0
16	BCR	J	104	40/40	0.86	0.87	5.98	61,69,75,76	0
13	CLA	M	1601	45/65	0.78	0.87	5.20	96,97,99,100	0
13	CLA	A	836	54/65	0.92	0.59	4.88	46,50,64,64	0
16	BCR	B	844	40/40	0.69	1.82	4.71	56,68,93,93	0
16	BCR	A	852	40/40	0.57	1.14	4.68	47,60,96,96	0
16	BCR	A	854	40/40	0.93	1.45	4.64	29,39,50,53	0
16	BCR	M	1602	40/40	0.83	0.88	4.54	28,37,59,62	0
13	CLA	A	837	45/65	0.87	0.56	4.43	60,68,76,80	0
16	BCR	I	101	40/40	0.86	0.78	4.29	19,27,40,40	0
13	CLA	B	809	65/65	0.94	0.72	4.13	20,26,61,62	0
13	CLA	A	804	65/65	0.92	0.83	4.12	45,50,80,83	0
13	CLA	A	825	59/65	0.85	0.74	3.98	34,43,76,76	0
13	CLA	J	101	45/65	0.72	0.70	3.89	98,99,100,100	0
13	CLA	B	841	65/65	0.85	1.15	3.79	22,29,44,50	0
16	BCR	B	847	40/40	0.88	0.97	3.73	46,53,61,61	0
16	BCR	B	843	40/40	0.77	0.86	3.64	88,90,97,98	0
16	BCR	F	1302	40/40	0.88	0.77	3.57	43,49,60,60	0
16	BCR	J	103	40/40	0.89	1.37	3.53	55,58,60,60	0
16	BCR	L	1006	40/40	0.89	0.45	3.48	26,35,66,67	0
16	BCR	J	105	40/40	0.73	0.78	3.46	53,67,93,94	0
14	PQN	A	847	33/33	0.92	0.77	3.39	41,43,67,68	0
13	CLA	A	809	65/65	0.94	0.75	3.39	33,40,66,67	0
13	CLA	B	830	45/65	0.83	0.69	3.31	51,54,67,72	0
16	BCR	B	848	40/40	0.92	0.96	3.27	40,52,58,58	0
13	CLA	A	839	65/65	0.87	0.70	3.09	32,38,58,59	0
16	BCR	L	1005	40/40	0.84	1.37	2.97	20,24,29,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	CLA	A	845	41/65	0.73	0.82	2.61	87,90,92,93	0
13	CLA	B	828	65/65	0.90	1.11	2.57	31,35,48,52	0
13	CLA	B	840	65/65	0.74	1.10	2.56	13,18,41,42	0
13	CLA	B	834	45/65	0.96	0.47	2.56	40,47,53,56	0
13	CLA	B	839	47/65	0.84	0.55	2.56	41,47,55,60	0
13	CLA	B	832	65/65	0.88	0.63	2.53	37,43,65,66	0
16	BCR	A	853	40/40	0.76	1.16	2.53	30,37,59,60	0
13	CLA	A	844	65/65	0.78	0.93	2.48	17,22,43,47	0
13	CLA	B	833	58/65	0.77	0.70	2.45	36,47,77,78	0
16	BCR	B	849	40/40	0.84	1.07	2.42	23,27,30,31	0
13	CLA	B	815	45/65	0.76	0.55	2.40	57,62,73,77	0
13	CLA	A	834	65/65	0.84	1.04	2.40	24,28,43,44	0
13	CLA	X	1701	45/65	0.89	0.46	2.39	77,83,86,88	0
13	CLA	A	819	54/65	0.93	0.39	2.36	44,50,54,56	0
13	CLA	A	829	65/65	0.98	0.61	2.36	38,46,74,75	0
13	CLA	B	811	45/65	0.80	0.39	2.34	42,49,62,66	0
13	CLA	A	810	65/65	0.85	0.90	2.31	39,43,77,78	0
18	LMG	B	850	55/55	0.69	1.11	2.30	34,40,57,60	0
17	LHG	A	856	27/49	0.92	0.40	2.29	51,56,60,61	0
13	CLA	A	846	52/65	0.82	0.54	2.24	69,75,97,99	0
17	LHG	A	855	49/49	0.79	0.76	2.21	39,50,60,63	0
13	CLA	B	814	65/65	0.82	0.65	2.21	34,43,68,69	0
13	CLA	A	827	65/65	0.79	0.64	2.16	24,31,83,85	0
13	CLA	B	806	65/65	0.94	0.98	2.15	30,34,53,54	0
13	CLA	A	833	65/65	0.87	0.80	2.15	20,31,85,88	0
13	CLA	B	807	65/65	0.92	0.52	2.06	21,24,50,53	0
13	CLA	A	838	51/65	0.86	0.34	2.05	30,35,45,46	0
13	CLA	B	804	54/65	0.92	0.84	1.92	20,29,48,52	0
13	CLA	B	829	65/65	0.94	0.89	1.91	18,29,63,65	0
13	CLA	B	821	45/65	0.80	0.49	1.84	80,81,90,93	0
13	CLA	A	803	65/65	0.94	0.71	1.83	33,41,51,54	0
13	CLA	A	841	65/65	0.97	0.42	1.80	33,38,55,55	0
13	CLA	B	808	65/65	0.96	0.56	1.79	21,28,49,50	0
13	CLA	A	802	65/65	0.92	0.53	1.78	23,26,35,39	0
13	CLA	B	827	65/65	0.96	0.64	1.74	24,31,77,80	0
16	BCR	A	851	40/40	0.73	1.46	1.74	47,61,89,89	0
16	BCR	A	850	40/40	0.76	1.29	1.73	57,61,79,79	0
13	CLA	A	816	45/65	0.79	0.63	1.70	78,82,83,83	0
13	CLA	B	816	55/65	0.74	0.63	1.61	54,60,85,87	0
13	CLA	B	835	45/65	0.93	0.46	1.59	58,61,70,75	0
14	PQN	B	842	33/33	0.94	0.96	1.58	24,29,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	CLA	A	835	65/65	0.95	0.49	1.56	14,19,36,40	0
13	CLA	B	825	46/65	0.89	0.49	1.54	29,36,46,48	0
13	CLA	A	817	49/65	0.85	0.47	1.52	87,90,92,94	0
13	CLA	A	822	65/65	0.76	0.83	1.52	41,45,55,57	0
13	CLA	B	813	65/65	0.92	0.90	1.49	49,59,68,70	0
13	CLA	B	818	60/65	0.94	0.86	1.48	33,39,64,66	0
13	CLA	F	1301	45/65	0.82	0.53	1.48	75,77,82,83	0
13	CLA	A	830	65/65	0.93	0.72	1.47	33,40,52,55	0
16	BCR	B	846	25/40	0.82	0.98	1.46	64,66,69,70	0
16	BCR	A	849	40/40	0.83	0.80	1.46	62,69,79,79	0
13	CLA	B	802	65/65	0.96	0.53	1.41	28,39,55,59	0
13	CLA	B	819	65/65	0.84	0.74	1.40	78,82,99,100	0
13	CLA	A	842	51/65	0.94	0.45	1.34	38,43,70,71	0
13	CLA	L	1004	65/65	0.84	0.82	1.32	22,31,61,62	0
13	CLA	B	838	65/65	0.92	0.46	1.30	38,44,74,78	0
13	CLA	B	820	47/65	0.74	0.67	1.20	88,92,97,97	0
13	CLA	B	822	55/65	0.93	0.35	1.20	69,70,88,89	0
13	CLA	B	826	65/65	0.85	0.65	1.19	31,39,63,65	0
13	CLA	A	828	65/65	0.84	0.56	1.19	32,42,66,68	0
13	CLA	B	817	59/65	0.92	0.54	1.15	39,47,66,70	0
13	CLA	B	812	45/65	0.62	0.57	1.12	66,69,80,85	0
13	CLA	A	840	47/65	0.85	0.70	1.07	30,35,52,57	0
13	CLA	A	818	54/65	0.84	0.51	1.06	63,66,68,69	0
13	CLA	L	1003	65/65	0.89	0.79	1.05	17,23,66,67	0
13	CLA	A	820	65/65	0.93	0.59	1.04	43,48,56,58	0
13	CLA	A	824	51/65	0.78	0.66	1.03	53,59,77,77	0
13	CLA	A	812	65/65	0.81	0.45	1.00	63,65,72,74	0
16	BCR	I	102	40/40	0.92	0.59	0.96	19,26,31,32	0
13	CLA	A	807	65/65	0.91	0.77	0.96	38,43,51,52	0
13	CLA	A	821	61/65	0.82	0.74	0.95	56,62,85,85	0
13	CLA	A	831	65/65	0.94	0.53	0.93	35,43,52,53	0
13	CLA	B	837	60/65	0.95	0.33	0.91	42,48,70,71	0
13	CLA	B	803	65/65	0.86	0.62	0.87	24,29,35,36	0
13	CLA	L	1002	65/65	0.92	0.57	0.85	21,27,58,61	0
13	CLA	A	814	60/65	0.88	0.69	0.85	49,53,80,81	0
13	CLA	A	801	65/65	0.93	0.39	0.83	22,27,36,38	0
13	CLA	B	805	65/65	0.92	0.65	0.82	28,37,66,69	0
13	CLA	A	806	65/65	0.90	0.61	0.80	33,39,68,70	0
13	CLA	B	823	45/65	0.93	0.36	0.79	58,62,70,73	0
13	CLA	K	1401	45/65	0.80	0.66	0.78	70,74,81,84	0
13	CLA	A	808	51/65	0.81	0.46	0.75	55,58,79,79	0
15	SF4	C	101	8/8	0.97	0.24	0.74	24,25,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	CLA	A	805	59/65	0.89	0.46	0.71	40,46,85,86	0
17	LHG	B	851	23/49	0.83	0.47	0.66	79,89,92,93	0
13	CLA	A	832	50/65	0.94	0.43	0.64	32,37,58,59	0
13	CLA	A	826	65/65	0.90	0.45	0.60	45,49,62,63	0
13	CLA	B	810	65/65	0.90	0.53	0.59	15,23,43,44	0
13	CLA	A	811	45/65	0.77	0.39	0.56	68,71,75,76	0
13	CLA	A	815	45/65	0.89	0.36	0.53	64,66,67,68	0
13	CLA	A	813	54/65	0.84	0.56	0.39	44,47,76,77	0
13	CLA	B	801	65/65	0.92	0.31	0.35	22,30,38,46	0
13	CLA	B	824	54/65	0.91	0.51	0.18	54,59,69,71	0
13	CLA	A	823	49/65	0.71	0.50	0.08	64,68,82,83	0
15	SF4	C	102	8/8	0.93	0.21	-0.06	33,34,35,35	0
19	CA	L	1001	1/1	0.79	0.17	-0.88	27,27,27,27	0
15	SF4	A	848	8/8	0.99	0.18	-1.54	25,26,27,27	0
13	CLA	J	102	37/65	0.61	0.94	-	95,96,97,97	0
13	CLA	B	836	45/65	0.81	0.41	-	78,82,85,87	0

6.5 Other polymers (i)

There are no such residues in this entry.