



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:22 PM GMT

PDB ID : 4FE1
Title : Improving the Accuracy of Macromolecular Structure Refinement at 7 Å Resolution
Authors : Fromme, R.; Adams, P.D.; Fromme, P.; Levitt, M.; Schroeder, G.F.; Brunger, A.T.
Deposited on : 2012-05-29
Resolution : 4.92 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

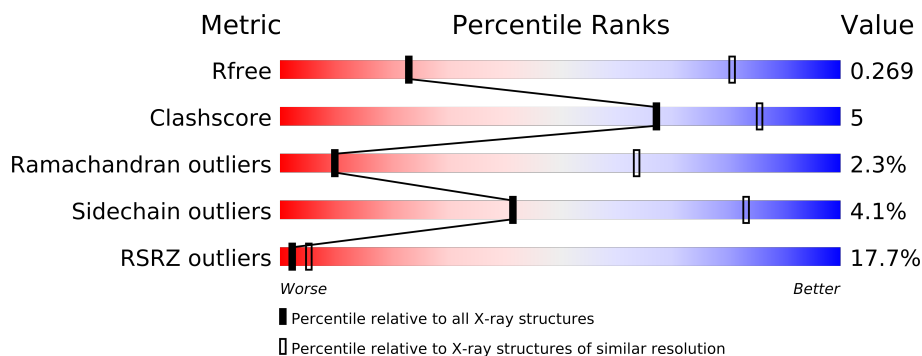
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.92 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}	66092	1047 (6.22-3.50)
Clashscore	79885	1321 (6.22-3.50)
Ramachandran outliers	78287	1237 (6.22-3.50)
Sidechain outliers	78261	1217 (6.22-3.50)
RSRZ outliers	66119	1046 (6.22-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
13	CLA	A	801	-	X
13	CLA	A	802	-	X
13	CLA	A	803	-	X
13	CLA	A	804	-	X
13	CLA	A	805	-	X
13	CLA	A	806	-	X
13	CLA	A	807	-	X
13	CLA	A	808	-	X
13	CLA	A	809	-	X
13	CLA	A	810	-	X
13	CLA	A	811	-	X
13	CLA	A	812	-	X
13	CLA	A	813	-	X
13	CLA	A	814	-	X
13	CLA	A	815	-	X
13	CLA	A	816	-	X
13	CLA	A	817	-	X
13	CLA	A	818	-	X
13	CLA	A	819	-	X
13	CLA	A	820	-	X
13	CLA	A	821	-	X
13	CLA	A	822	-	X
13	CLA	A	823	-	X
13	CLA	A	824	-	X
13	CLA	A	826	-	X
13	CLA	A	827	-	X
13	CLA	A	828	-	X
13	CLA	A	829	-	X
13	CLA	A	830	-	X
13	CLA	A	831	-	X
13	CLA	A	832	-	X
13	CLA	A	833	-	X
13	CLA	A	834	-	X
13	CLA	A	835	-	X
13	CLA	A	836	-	X
13	CLA	A	838	-	X
13	CLA	A	840	-	X
13	CLA	A	841	-	X
13	CLA	A	842	-	X
13	CLA	A	843	-	X
13	CLA	A	844	-	X
13	CLA	A	845	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
13	CLA	A	855	-	X
13	CLA	B	802	-	X
13	CLA	B	803	-	X
13	CLA	B	804	-	X
13	CLA	B	805	-	X
13	CLA	B	807	-	X
13	CLA	B	808	-	X
13	CLA	B	810	-	X
13	CLA	B	811	-	X
13	CLA	B	812	-	X
13	CLA	B	813	-	X
13	CLA	B	814	-	X
13	CLA	B	815	-	X
13	CLA	B	816	-	X
13	CLA	B	817	-	X
13	CLA	B	818	-	X
13	CLA	B	819	-	X
13	CLA	B	820	-	X
13	CLA	B	821	-	X
13	CLA	B	822	-	X
13	CLA	B	823	-	X
13	CLA	B	824	-	X
13	CLA	B	826	-	X
13	CLA	B	827	-	X
13	CLA	B	828	-	X
13	CLA	B	829	-	X
13	CLA	B	830	-	X
13	CLA	B	831	-	X
13	CLA	B	832	-	X
13	CLA	B	833	-	X
13	CLA	B	834	-	X
13	CLA	B	835	-	X
13	CLA	B	836	-	X
13	CLA	B	838	-	X
13	CLA	B	839	-	X
13	CLA	F	1301	-	X
13	CLA	J	1101	-	X
13	CLA	J	1102	-	X
13	CLA	J	1103	-	X
13	CLA	L	1003	-	X
13	CLA	L	1004	-	X
13	CLA	M	1201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
13	CLA	M	1202	-	X
13	CLA	X	102	-	X
14	PQN	A	846	-	X
14	PQN	B	840	-	X
15	BCR	A	847	-	X
15	BCR	A	848	-	X
15	BCR	A	849	-	X
15	BCR	A	850	-	X
15	BCR	A	851	-	X
15	BCR	A	852	-	X
15	BCR	B	841	-	X
15	BCR	B	842	-	X
15	BCR	B	843	-	X
15	BCR	B	844	-	X
15	BCR	B	845	-	X
15	BCR	B	846	-	X
15	BCR	B	847	-	X
15	BCR	B	849	-	X
15	BCR	B	850	-	X
15	BCR	F	1302	-	X
15	BCR	I	102	-	X
15	BCR	J	1104	-	X
15	BCR	J	1105	-	X
15	BCR	L	1005	-	X
15	BCR	M	1203	-	X
16	LHG	A	853	-	X
16	LHG	A	854	-	X
16	LHG	X	101	-	X
18	LMG	B	848	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 23997 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

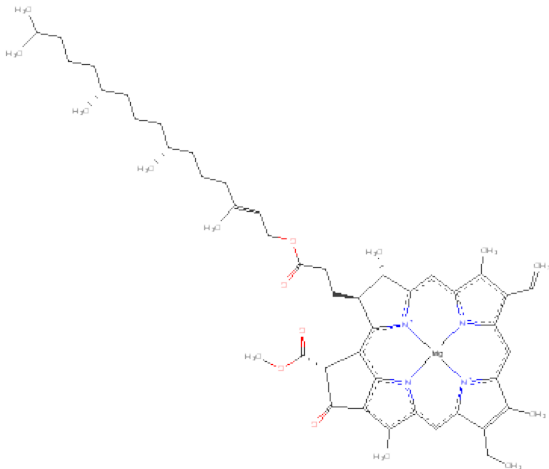
- Molecule 12 is a protein called Photosystem I 4.8K protein.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	32	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	33	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	34	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	35	ALA	-	EXPRESSION TAG	UNP Q8DKP6

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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
			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		

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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
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			60	50	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
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	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
			54	44	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
			61	51	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
			49	39	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
			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
			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
			50	40	1	4	5		

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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
			54	44	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
			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
			47	37	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
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	A	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
			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		

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

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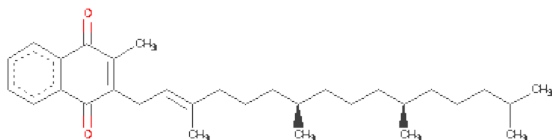
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 60	C 50	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 47	C 37	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	F	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	I	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	J	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	J	1	Total 37	C 31	Mg 1	N 4	O 1	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	M	1	Total 54	C 44	Mg 1	N 4	O 5	0	0

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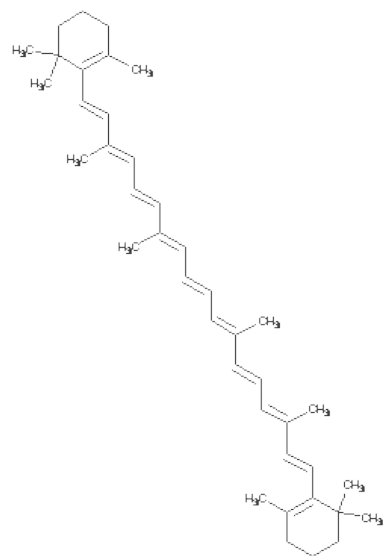
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



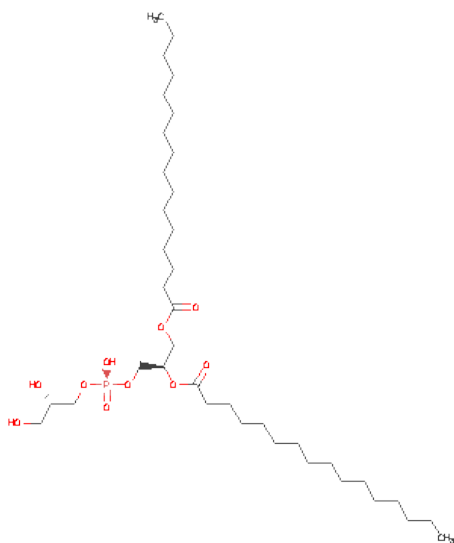
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 25 25	0	0
15	B	1	Total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

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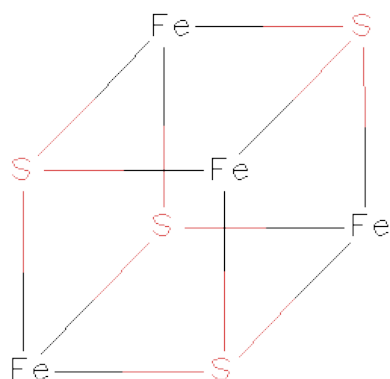
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 40 40	0	0
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	M	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



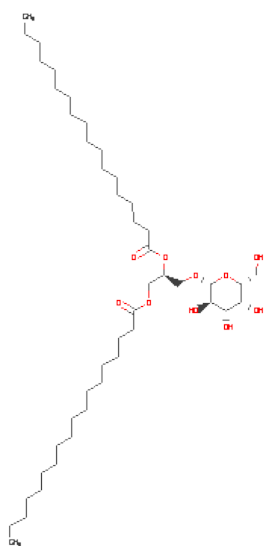
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 27 16 10 1	0	0
16	X	1	Total C O P 23 12 10 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



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		

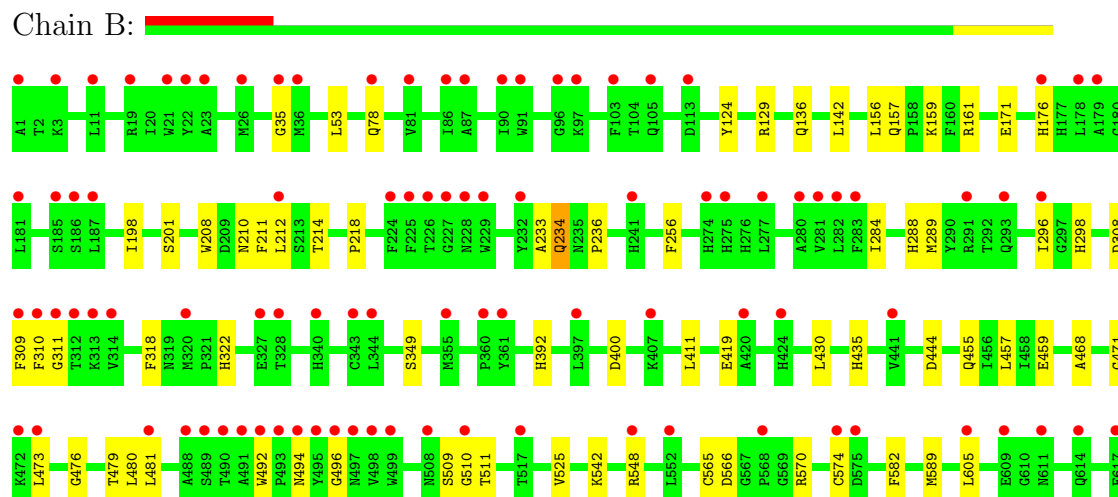
3 Residue-property plots

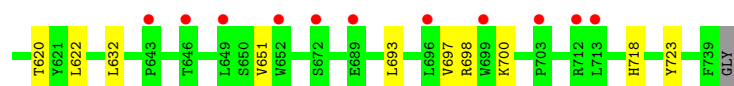
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





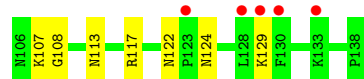
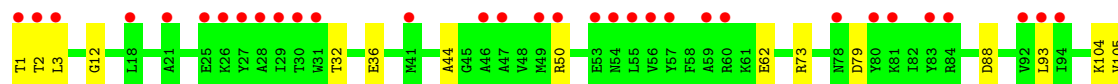
- Molecule 3: Photosystem I iron-sulfur center

Chain C:



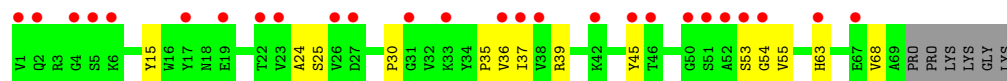
- Molecule 4: Photosystem I reaction center subunit II

Chain D:



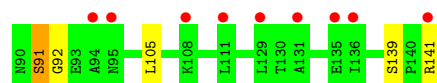
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:



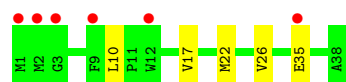
- Molecule 6: Photosystem I reaction center subunit III

Chain F:



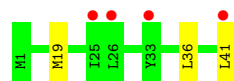
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



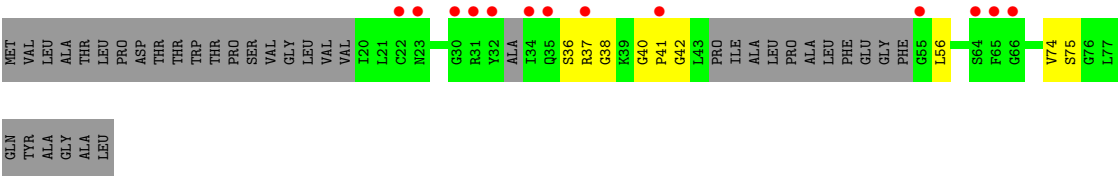
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:



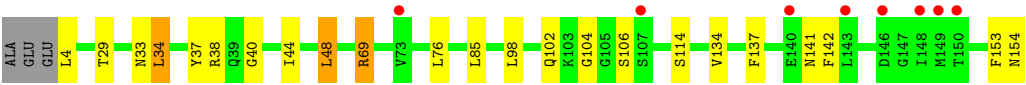
- Molecule 9: Photosystem I reaction center subunit Psak

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

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)	97.97 – 4.92 97.97 – 4.92	Depositor EDS
% Data completeness (in resolution range)	96.4 (97.97-4.92) 96.3 (97.97-4.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.35 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1058)	Depositor
R, R_{free}	0.274 , 0.315 0.240 , 0.269	Depositor DCC
R_{free} test set	1526 reflections (4.69%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 90.2	EDS
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	0 of 32897 reflections	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.38	0/5983	0.69	3/8158 (0.0%)
2	B	0.40	0/6096	0.68	2/8332 (0.0%)
3	C	0.39	0/608	0.76	0/824
4	D	0.35	0/1101	0.78	0/1492
5	E	0.42	0/551	0.85	1/750 (0.1%)
6	F	0.41	0/1087	0.76	0/1476
7	I	0.38	0/312	0.80	1/425 (0.2%)
8	J	0.40	0/350	0.80	1/477 (0.2%)
9	K	0.40	0/220	0.91	0/300
10	L	0.39	0/1148	0.79	2/1558 (0.1%)
11	M	0.47	0/244	0.91	1/332 (0.3%)
12	X	0.41	0/242	0.66	0/332
All	All	0.39	0/17942	0.72	11/24456 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD2	-8.44	110.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD1	8.11	125.60	118.30
10	L	76	LEU	CB-CG-CD2	7.19	123.22	111.00
7	I	26	VAL	CG1-CB-CG2	6.87	121.90	110.90
10	L	48	LEU	CB-CG-CD2	6.78	122.52	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	THR	Mainchain
2	B	35	GLY	Mainchain
4	D	88	ASP	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	0	46	0
2	B	5879	0	0	33	0
3	C	598	0	0	6	0
4	D	1075	0	0	8	0
5	E	539	0	0	3	0
6	F	1065	0	0	13	0
7	I	301	0	0	2	0
8	J	338	0	0	1	0
9	K	222	0	0	1	0
10	L	1119	0	0	7	1
11	M	241	0	0	2	0
12	X	233	0	0	1	0
13	A	2667	0	0	24	0
13	B	2230	0	0	14	0
13	F	45	0	0	1	0
13	I	65	0	0	1	0
13	J	147	0	0	0	0
13	L	195	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	99	0	0	1	0
13	X	45	0	0	0	0
14	A	33	0	0	0	0
14	B	33	0	0	0	0
15	A	240	0	0	0	0
15	B	345	0	0	0	0
15	F	40	0	0	0	0
15	I	40	0	0	0	0
15	J	80	0	0	0	0
15	L	80	0	0	1	0
15	M	40	0	0	0	0
16	A	76	0	0	0	0
16	X	23	0	0	0	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	55	0	0	0	0
19	L	1	0	0	0	0
All	All	23997	0	0	121	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 121 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:136:GLN:NE2	13:B:812:CLA:O1D	2.09	0.85
10:L:98:LEU:O	10:L:102:GLN:NE2	2.13	0.82
1:A:35:ASP:OD2	1:A:37:THR:OG1	2.02	0.78
1:A:501:THR:O	13:A:836:CLA:ND	2.20	0.74
6:F:91:SER:OG	6:F:92:GLY:N	2.24	0.70

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	Distance(Å)	Clash(Å)
10:L:40:GLY:O	10:L:114:SER:OG[3_665]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	685 (93%)	39 (5%)	12 (2%)	14	71
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	19	77
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	18	75
4	D	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	5	52
5	E	67/75 (89%)	53 (79%)	6 (9%)	8 (12%)	1	14
6	F	139/164 (85%)	127 (91%)	8 (6%)	4 (3%)	7	58
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	42/83 (51%)	30 (71%)	5 (12%)	7 (17%)	0	7
10	L	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	18	75
11	M	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	6	55
12	X	27/35 (77%)	21 (78%)	5 (18%)	1 (4%)	5	52
All	All	2215/2334 (95%)	2039 (92%)	126 (6%)	50 (2%)	10	63

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	235	ASP
2	B	211	PHE
2	B	234	GLN
2	B	480	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	567 (96%)	22 (4%)	45	85
2	B	595/597 (100%)	572 (96%)	23 (4%)	43	84
3	C	67/67 (100%)	65 (97%)	2 (3%)	53	88
4	D	115/115 (100%)	109 (95%)	6 (5%)	32	78
5	E	59/64 (92%)	58 (98%)	1 (2%)	73	94
6	F	109/128 (85%)	105 (96%)	4 (4%)	45	85
7	I	32/32 (100%)	31 (97%)	1 (3%)	52	88
8	J	36/36 (100%)	35 (97%)	1 (3%)	56	88
10	L	117/119 (98%)	109 (93%)	8 (7%)	22	69
11	M	26/26 (100%)	24 (92%)	2 (8%)	18	64
12	X	20/24 (83%)	18 (90%)	2 (10%)	11	51
All	All	1765/1811 (98%)	1693 (96%)	72 (4%)	41	83

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	349	SER
2	B	605	LEU
10	L	134	VAL
2	B	411	LEU
2	B	525	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	-	73,73,73	1.51	15 (20%)	95,113,113	1.95	20 (21%)
13	CLA	A	802	-	73,73,73	1.51	15 (20%)	95,113,113	1.46	13 (13%)
13	CLA	A	803	-	73,73,73	1.48	13 (17%)	95,113,113	1.64	16 (16%)
13	CLA	A	804	13	67,67,73	1.58	15 (22%)	86,105,113	1.69	16 (18%)
13	CLA	A	805	-	73,73,73	1.49	13 (17%)	95,113,113	1.58	14 (14%)
13	CLA	A	806	-	73,73,73	1.46	13 (17%)	95,113,113	1.54	16 (16%)
13	CLA	A	807	-	59,59,73	1.79	16 (27%)	77,96,113	1.84	15 (19%)
13	CLA	A	808	1	73,73,73	1.52	14 (19%)	95,113,113	1.93	20 (21%)
13	CLA	A	809	1	73,73,73	1.50	14 (19%)	95,113,113	1.87	22 (23%)
13	CLA	A	810	-	51,53,73	1.76	13 (25%)	68,89,113	2.01	14 (20%)
13	CLA	A	811	13	73,73,73	1.49	15 (20%)	95,113,113	1.74	16 (16%)
13	CLA	A	812	-	62,62,73	1.58	14 (22%)	80,99,113	1.85	16 (20%)
13	CLA	A	813	-	67,68,73	1.55	13 (19%)	87,107,113	1.82	22 (25%)
13	CLA	A	814	-	51,53,73	1.75	12 (23%)	68,89,113	1.89	12 (17%)
13	CLA	A	815	-	51,53,73	1.77	11 (21%)	68,89,113	1.86	12 (17%)
13	CLA	A	816	-	56,57,73	1.64	14 (25%)	73,93,113	1.75	14 (19%)
13	CLA	A	817	-	62,62,73	1.62	15 (24%)	80,99,113	1.70	15 (18%)
13	CLA	A	818	-	62,62,73	1.60	15 (24%)	80,99,113	1.88	18 (22%)
13	CLA	A	819	-	73,73,73	1.46	16 (21%)	95,113,113	1.78	20 (21%)
13	CLA	A	820	-	69,69,73	1.66	16 (23%)	89,108,113	1.62	17 (19%)
13	CLA	A	821	-	73,73,73	1.49	15 (20%)	95,113,113	1.65	18 (18%)
13	CLA	A	822	-	56,57,73	1.67	14 (25%)	73,93,113	2.08	15 (20%)
13	CLA	A	823	-	59,59,73	1.80	15 (25%)	77,96,113	1.51	14 (18%)
13	CLA	A	824	-	67,67,73	1.56	14 (20%)	86,105,113	2.13	20 (23%)
13	CLA	A	825	-	73,73,73	1.49	16 (21%)	95,113,113	1.61	18 (18%)
13	CLA	A	826	-	73,73,73	1.52	14 (19%)	95,113,113	1.69	19 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	827	-	73,73,73	1.47	14 (19%)	95,113,113	1.72	18 (18%)
13	CLA	A	828	-	73,73,73	1.49	15 (20%)	95,113,113	1.75	16 (16%)
13	CLA	A	829	-	73,73,73	1.47	14 (19%)	95,113,113	1.76	17 (17%)
13	CLA	A	830	-	73,73,73	1.46	15 (20%)	95,113,113	1.78	17 (17%)
13	CLA	A	831	-	58,58,73	1.66	14 (24%)	75,95,113	1.70	14 (18%)
13	CLA	A	832	-	73,73,73	1.48	14 (19%)	95,113,113	1.77	16 (16%)
13	CLA	A	833	-	73,73,73	1.49	15 (20%)	95,113,113	1.57	15 (15%)
13	CLA	A	834	-	73,73,73	1.49	14 (19%)	95,113,113	1.60	13 (13%)
13	CLA	A	835	-	62,62,73	1.62	14 (22%)	80,99,113	1.60	14 (17%)
13	CLA	A	836	1	51,53,73	1.76	11 (21%)	68,89,113	1.62	13 (19%)
13	CLA	A	837	-	59,59,73	1.85	15 (25%)	77,96,113	2.18	21 (27%)
13	CLA	A	838	-	73,73,73	1.50	14 (19%)	95,113,113	1.71	18 (18%)
13	CLA	A	839	-	54,55,73	1.61	12 (22%)	72,91,113	1.75	15 (20%)
13	CLA	A	840	-	73,73,73	1.48	16 (21%)	95,113,113	1.71	13 (13%)
13	CLA	A	841	-	59,59,73	1.80	15 (25%)	77,96,113	1.61	14 (18%)
13	CLA	A	842	-	73,73,73	1.52	16 (21%)	95,113,113	1.48	15 (15%)
13	CLA	A	843	-	73,73,73	1.45	14 (19%)	95,113,113	1.71	20 (21%)
13	CLA	A	844	-	47,49,73	3.17	12 (25%)	59,83,113	1.64	8 (13%)
13	CLA	A	845	16	60,60,73	1.64	14 (23%)	79,97,113	1.91	20 (25%)
14	PQN	A	846	-	34,34,34	1.01	1 (2%)	45,45,45	1.11	3 (6%)
15	BCR	A	847	-	41,41,41	2.20	22 (53%)	56,56,56	2.04	22 (39%)
15	BCR	A	848	-	41,41,41	2.20	20 (48%)	56,56,56	2.13	20 (35%)
15	BCR	A	849	-	41,41,41	2.06	17 (41%)	56,56,56	2.21	25 (44%)
15	BCR	A	850	-	41,41,41	2.25	21 (51%)	56,56,56	2.18	20 (35%)
15	BCR	A	851	-	41,41,41	2.17	21 (51%)	56,56,56	2.16	19 (33%)
15	BCR	A	852	-	41,41,41	2.22	20 (48%)	56,56,56	2.25	18 (32%)
16	LHG	A	853	-	48,48,48	0.87	2 (4%)	54,54,54	1.01	2 (3%)
16	LHG	A	854	13	26,26,48	4.10	4 (15%)	31,32,54	1.59	3 (9%)
13	CLA	A	855	-	51,53,73	1.77	12 (23%)	68,89,113	1.83	14 (20%)
17	SF4	A	856	1,2	12,12,12	21.02	12 (100%)	0,24,24	0.00	-
13	CLA	B	801	-	73,73,73	1.50	13 (17%)	95,113,113	1.79	20 (21%)
13	CLA	B	802	-	73,73,73	1.51	15 (20%)	95,113,113	2.04	19 (20%)
13	CLA	B	803	-	73,73,73	1.50	15 (20%)	95,113,113	1.78	19 (20%)
13	CLA	B	804	-	73,73,73	1.47	15 (20%)	95,113,113	1.61	16 (16%)
13	CLA	B	805	-	73,73,73	1.47	14 (19%)	95,113,113	1.51	17 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	806	-	73,73,73	1.48	15 (20%)	95,113,113	1.65	17 (17%)
13	CLA	B	807	-	73,73,73	1.50	16 (21%)	95,113,113	1.70	15 (15%)
13	CLA	B	808	2	73,73,73	1.49	15 (20%)	95,113,113	1.79	19 (20%)
13	CLA	B	809	-	51,53,73	1.74	12 (23%)	68,89,113	1.99	13 (19%)
13	CLA	B	810	-	51,53,73	1.85	11 (21%)	68,89,113	1.61	12 (17%)
13	CLA	B	811	-	73,73,73	1.52	14 (19%)	95,113,113	1.79	20 (21%)
13	CLA	B	812	-	73,73,73	1.49	15 (20%)	95,113,113	1.80	17 (17%)
13	CLA	B	813	-	51,53,73	1.79	11 (21%)	68,89,113	2.00	14 (20%)
13	CLA	B	814	-	62,63,73	1.59	15 (24%)	81,101,113	1.88	18 (22%)
13	CLA	B	815	-	67,67,73	1.57	14 (20%)	86,105,113	1.60	17 (19%)
13	CLA	B	816	-	67,68,73	1.57	12 (17%)	87,107,113	1.73	16 (18%)
13	CLA	B	817	-	73,73,73	1.48	17 (23%)	95,113,113	1.55	13 (13%)
13	CLA	B	818	-	54,55,73	1.64	12 (22%)	72,91,113	1.79	15 (20%)
13	CLA	B	819	-	51,53,73	1.81	12 (23%)	68,89,113	2.00	15 (22%)
13	CLA	B	820	-	62,63,73	1.62	16 (25%)	81,101,113	1.63	17 (20%)
13	CLA	B	821	-	51,53,73	1.83	13 (25%)	68,89,113	1.78	14 (20%)
13	CLA	B	822	-	62,62,73	1.64	16 (25%)	80,99,113	1.84	19 (23%)
13	CLA	B	823	-	53,54,73	1.62	13 (24%)	71,90,113	1.84	18 (25%)
13	CLA	B	824	-	73,73,73	1.49	14 (19%)	95,113,113	1.81	19 (20%)
13	CLA	B	825	-	73,73,73	1.52	15 (20%)	95,113,113	1.57	15 (15%)
13	CLA	B	826	-	73,73,73	1.48	13 (17%)	95,113,113	1.42	11 (11%)
13	CLA	B	827	-	73,73,73	1.48	14 (19%)	95,113,113	1.90	19 (20%)
13	CLA	B	828	-	51,53,73	1.80	12 (23%)	68,89,113	1.91	14 (20%)
13	CLA	B	829	-	56,57,73	1.64	15 (26%)	73,93,113	1.67	12 (16%)
13	CLA	B	830	-	73,73,73	1.51	14 (19%)	95,113,113	1.59	13 (13%)
13	CLA	B	831	-	65,66,73	1.56	14 (21%)	85,104,113	2.14	19 (22%)
13	CLA	B	832	-	51,53,73	1.77	13 (25%)	68,89,113	1.88	13 (19%)
13	CLA	B	833	-	51,53,73	1.77	13 (25%)	68,89,113	1.81	14 (20%)
13	CLA	B	834	-	51,53,73	1.80	13 (25%)	68,89,113	1.88	14 (20%)
13	CLA	B	835	-	67,68,73	1.57	12 (17%)	87,107,113	1.93	20 (22%)
13	CLA	B	836	-	73,73,73	1.50	15 (20%)	95,113,113	1.60	16 (16%)
13	CLA	B	837	-	54,55,73	1.63	14 (25%)	72,91,113	1.82	15 (20%)
13	CLA	B	838	-	73,73,73	1.48	14 (19%)	95,113,113	1.74	20 (21%)
13	CLA	B	839	-	73,73,73	1.47	13 (17%)	95,113,113	1.58	16 (16%)
14	PQN	B	840	-	34,34,34	0.94	1 (2%)	45,45,45	1.28	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	B	841	-	41,41,41	2.17	22 (53%)	56,56,56	2.09	21 (37%)
15	BCR	B	842	-	41,41,41	2.22	21 (51%)	56,56,56	2.27	20 (35%)
15	BCR	B	843	-	41,41,41	2.14	20 (48%)	56,56,56	2.39	25 (44%)
15	BCR	B	844	-	24,25,41	2.48	13 (54%)	31,33,56	2.29	13 (41%)
15	BCR	B	845	-	41,41,41	2.14	20 (48%)	56,56,56	2.34	21 (37%)
15	BCR	B	846	-	41,41,41	2.18	21 (51%)	56,56,56	2.06	21 (37%)
15	BCR	B	847	-	41,41,41	2.17	21 (51%)	56,56,56	2.27	23 (41%)
18	LMG	B	848	-	55,55,55	1.02	6 (10%)	63,63,63	1.18	3 (4%)
15	BCR	B	849	-	41,41,41	2.09	18 (43%)	56,56,56	2.33	22 (39%)
15	BCR	B	850	-	41,41,41	2.18	20 (48%)	56,56,56	2.36	23 (41%)
17	SF4	C	101	3	12,12,12	20.95	12 (100%)	0,24,24	0.00	-
17	SF4	C	102	3	12,12,12	20.83	12 (100%)	0,24,24	0.00	-
13	CLA	F	1301	-	51,53,73	1.89	12 (23%)	68,89,113	1.92	17 (25%)
15	BCR	F	1302	-	41,41,41	2.15	20 (48%)	56,56,56	2.19	21 (37%)
13	CLA	I	101	-	73,73,73	1.49	15 (20%)	95,113,113	1.72	16 (16%)
15	BCR	I	102	-	41,41,41	2.06	17 (41%)	56,56,56	2.32	24 (42%)
13	CLA	J	1101	-	73,73,73	1.47	14 (19%)	95,113,113	1.70	22 (23%)
13	CLA	J	1102	8	51,53,73	1.79	12 (23%)	68,89,113	2.02	14 (20%)
13	CLA	J	1103	-	44,45,73	3.14	13 (29%)	55,78,113	1.61	7 (12%)
15	BCR	J	1104	-	41,41,41	2.20	21 (51%)	56,56,56	2.23	23 (41%)
15	BCR	J	1105	-	41,41,41	2.19	21 (51%)	56,56,56	2.13	22 (39%)
13	CLA	L	1002	10	73,73,73	1.49	14 (19%)	95,113,113	1.77	16 (16%)
13	CLA	L	1003	-	73,73,73	1.47	12 (16%)	95,113,113	1.85	17 (17%)
13	CLA	L	1004	-	73,73,73	1.47	13 (17%)	95,113,113	1.66	17 (17%)
15	BCR	L	1005	-	41,41,41	2.14	22 (53%)	56,56,56	2.24	22 (39%)
15	BCR	L	1006	-	41,41,41	2.19	20 (48%)	56,56,56	2.01	19 (33%)
13	CLA	M	1201	-	62,62,73	1.64	17 (27%)	80,99,113	1.88	19 (23%)
13	CLA	M	1202	-	51,53,73	1.84	13 (25%)	68,89,113	1.97	15 (22%)
15	BCR	M	1203	-	41,41,41	2.13	19 (46%)	56,56,56	2.27	19 (33%)
16	LHG	X	101	-	21,22,48	3.37	3 (14%)	26,28,54	1.04	2 (7%)
13	CLA	X	102	12	51,53,73	1.82	12 (23%)	68,89,113	2.20	14 (20%)

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	-	-	0/37/135/135	0/0/9/9
13	CLA	A	802	-	-	0/37/135/135	0/0/9/9
13	CLA	A	803	-	-	0/37/135/135	0/0/9/9
13	CLA	A	804	13	-	0/29/128/135	0/0/9/9
13	CLA	A	805	-	-	0/37/135/135	0/0/9/9
13	CLA	A	806	-	-	0/37/135/135	0/0/9/9
13	CLA	A	807	-	-	0/21/119/135	0/0/9/9
13	CLA	A	808	1	-	0/37/135/135	0/0/9/9
13	CLA	A	809	1	-	0/37/135/135	0/0/9/9
13	CLA	A	810	-	-	0/11/111/135	0/0/9/9
13	CLA	A	811	13	-	0/37/135/135	0/0/9/9
13	CLA	A	812	-	-	0/23/122/135	0/0/9/9
13	CLA	A	813	-	-	0/31/129/135	0/0/9/9
13	CLA	A	814	-	-	0/11/111/135	0/0/9/9
13	CLA	A	815	-	-	0/11/111/135	0/0/9/9
13	CLA	A	816	-	-	0/17/116/135	0/0/9/9
13	CLA	A	817	-	-	0/23/122/135	0/0/9/9
13	CLA	A	818	-	-	0/23/122/135	0/0/9/9
13	CLA	A	819	-	-	0/37/135/135	0/0/9/9
13	CLA	A	820	-	-	0/33/131/135	0/0/9/9
13	CLA	A	821	-	-	0/37/135/135	0/0/9/9
13	CLA	A	822	-	-	0/17/116/135	0/0/9/9
13	CLA	A	823	-	-	0/21/119/135	0/0/9/9
13	CLA	A	824	-	-	0/29/128/135	0/0/9/9
13	CLA	A	825	-	-	0/37/135/135	0/0/9/9
13	CLA	A	826	-	-	0/37/135/135	0/0/9/9
13	CLA	A	827	-	-	0/37/135/135	0/0/9/9
13	CLA	A	828	-	-	0/37/135/135	0/0/9/9
13	CLA	A	829	-	-	0/37/135/135	0/0/9/9
13	CLA	A	830	-	-	0/37/135/135	0/0/9/9
13	CLA	A	831	-	-	0/19/117/135	0/0/9/9
13	CLA	A	832	-	-	0/37/135/135	0/0/9/9
13	CLA	A	833	-	-	0/37/135/135	0/0/9/9
13	CLA	A	834	-	-	0/37/135/135	0/0/9/9
13	CLA	A	835	-	-	0/23/122/135	0/0/9/9
13	CLA	A	836	1	-	0/11/111/135	0/0/9/9
13	CLA	A	837	-	-	0/21/119/135	0/0/9/9
13	CLA	A	838	-	-	0/37/135/135	0/0/9/9
13	CLA	A	839	-	-	0/16/114/135	0/0/9/9
13	CLA	A	840	-	-	0/37/135/135	0/0/9/9
13	CLA	A	841	-	-	0/21/119/135	0/0/9/9
13	CLA	A	842	-	-	0/37/135/135	0/0/9/9
13	CLA	A	843	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	844	-	-	0/5/101/135	0/0/9/9
13	CLA	A	845	16	-	0/22/120/135	0/0/9/9
14	PQN	A	846	-	-	0/23/43/43	0/0/2/2
15	BCR	A	847	-	-	0/29/63/63	0/2/2/2
15	BCR	A	848	-	-	0/29/63/63	0/2/2/2
15	BCR	A	849	-	-	0/29/63/63	0/2/2/2
15	BCR	A	850	-	-	0/29/63/63	0/2/2/2
15	BCR	A	851	-	-	0/29/63/63	0/2/2/2
15	BCR	A	852	-	-	0/29/63/63	0/2/2/2
16	LHG	A	853	-	-	0/53/53/53	0/0/0/0
16	LHG	A	854	13	-	0/31/31/53	0/0/0/0
13	CLA	A	855	-	-	0/11/111/135	0/0/9/9
17	SF4	A	856	1,2	-	0/0/48/48	0/0/5/5
13	CLA	B	801	-	-	0/37/135/135	0/0/9/9
13	CLA	B	802	-	-	0/37/135/135	0/0/9/9
13	CLA	B	803	-	-	0/37/135/135	0/0/9/9
13	CLA	B	804	-	-	0/37/135/135	0/0/9/9
13	CLA	B	805	-	-	0/37/135/135	0/0/9/9
13	CLA	B	806	-	-	0/37/135/135	0/0/9/9
13	CLA	B	807	-	-	0/37/135/135	0/0/9/9
13	CLA	B	808	2	-	0/37/135/135	0/0/9/9
13	CLA	B	809	-	-	0/11/111/135	0/0/9/9
13	CLA	B	810	-	-	0/11/111/135	0/0/9/9
13	CLA	B	811	-	-	0/37/135/135	0/0/9/9
13	CLA	B	812	-	-	0/37/135/135	0/0/9/9
13	CLA	B	813	-	-	0/11/111/135	0/0/9/9
13	CLA	B	814	-	-	0/25/123/135	0/0/9/9
13	CLA	B	815	-	-	0/29/128/135	0/0/9/9
13	CLA	B	816	-	-	0/31/129/135	0/0/9/9
13	CLA	B	817	-	-	0/37/135/135	0/0/9/9
13	CLA	B	818	-	-	0/16/114/135	0/0/9/9
13	CLA	B	819	-	-	0/11/111/135	0/0/9/9
13	CLA	B	820	-	-	0/25/123/135	0/0/9/9
13	CLA	B	821	-	-	0/11/111/135	0/0/9/9
13	CLA	B	822	-	-	0/23/122/135	0/0/9/9
13	CLA	B	823	-	-	0/15/113/135	0/0/9/9
13	CLA	B	824	-	-	0/37/135/135	0/0/9/9
13	CLA	B	825	-	-	0/37/135/135	0/0/9/9
13	CLA	B	826	-	-	0/37/135/135	0/0/9/9
13	CLA	B	827	-	-	0/37/135/135	0/0/9/9
13	CLA	B	828	-	-	0/11/111/135	0/0/9/9
13	CLA	B	829	-	-	0/17/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	830	-	-	0/37/135/135	0/0/9/9
13	CLA	B	831	-	-	0/29/127/135	0/0/9/9
13	CLA	B	832	-	-	0/11/111/135	0/0/9/9
13	CLA	B	833	-	-	0/11/111/135	0/0/9/9
13	CLA	B	834	-	-	0/11/111/135	0/0/9/9
13	CLA	B	835	-	-	0/31/129/135	0/0/9/9
13	CLA	B	836	-	-	0/37/135/135	0/0/9/9
13	CLA	B	837	-	-	0/16/114/135	0/0/9/9
13	CLA	B	838	-	-	0/37/135/135	0/0/9/9
13	CLA	B	839	-	-	0/37/135/135	0/0/9/9
14	PQN	B	840	-	-	0/23/43/43	0/0/2/2
15	BCR	B	841	-	-	0/29/63/63	0/2/2/2
15	BCR	B	842	-	-	0/29/63/63	0/2/2/2
15	BCR	B	843	-	-	0/29/63/63	0/2/2/2
15	BCR	B	844	-	-	0/18/35/63	0/1/1/2
15	BCR	B	845	-	-	0/29/63/63	0/2/2/2
15	BCR	B	846	-	-	0/29/63/63	0/2/2/2
15	BCR	B	847	-	-	0/29/63/63	0/2/2/2
18	LMG	B	848	-	-	0/50/70/70	0/1/1/1
15	BCR	B	849	-	-	0/29/63/63	0/2/2/2
15	BCR	B	850	-	-	0/29/63/63	0/2/2/2
17	SF4	C	101	3	-	0/0/48/48	0/0/5/5
17	SF4	C	102	3	-	0/0/48/48	0/0/5/5
13	CLA	F	1301	-	-	0/11/111/135	0/0/9/9
15	BCR	F	1302	-	-	0/29/63/63	0/2/2/2
13	CLA	I	101	-	-	0/37/135/135	0/0/9/9
15	BCR	I	102	-	-	0/29/63/63	0/2/2/2
13	CLA	J	1101	-	-	0/37/135/135	0/0/9/9
13	CLA	J	1102	8	-	0/11/111/135	0/0/9/9
13	CLA	J	1103	-	-	0/2/96/135	0/0/9/9
15	BCR	J	1104	-	-	0/29/63/63	0/2/2/2
15	BCR	J	1105	-	-	0/29/63/63	0/2/2/2
13	CLA	L	1002	10	-	0/37/135/135	0/0/9/9
13	CLA	L	1003	-	-	0/37/135/135	0/0/9/9
13	CLA	L	1004	-	-	0/37/135/135	0/0/9/9
15	BCR	L	1005	-	-	0/29/63/63	0/2/2/2
15	BCR	L	1006	-	-	0/29/63/63	0/2/2/2
13	CLA	M	1201	-	-	0/23/122/135	0/0/9/9
13	CLA	M	1202	-	-	0/11/111/135	0/0/9/9
15	BCR	M	1203	-	-	0/29/63/63	0/2/2/2
16	LHG	X	101	-	-	0/26/26/53	0/0/0/0
13	CLA	X	102	12	-	0/11/111/135	0/0/9/9

The worst 5 of 1826 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	856	SF4	S3-FE4	-21.72	2.18	2.33
17	C	101	SF4	S2-FE1	-21.57	2.18	2.33
17	A	856	SF4	S1-FE4	-21.53	2.18	2.33
17	C	102	SF4	S3-FE2	-21.39	2.18	2.33
17	C	102	SF4	S4-FE3	-21.37	2.18	2.33

The worst 5 of 2027 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	824	CLA	C3D-CAD-CBD	-8.86	95.07	107.60
13	B	831	CLA	C3D-CAD-CBD	-8.27	95.90	107.60
13	A	844	CLA	CHA-CBD-CAD	-8.23	102.11	109.72
13	B	835	CLA	C3D-CAD-CBD	-7.74	96.65	107.60
13	J	1103	CLA	CHA-CBD-CAD	-7.62	102.67	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	1.27	140 (18%) 2 4	42, 99, 157, 202	0
2	B	739/740 (99%)	1.09	106 (14%) 3 7	34, 76, 126, 215	0
3	C	80/80 (100%)	0.92	4 (5%) 28 27	46, 72, 126, 138	0
4	D	138/138 (100%)	1.51	37 (26%) 1 4	45, 72, 117, 137	0
5	E	69/75 (92%)	1.83	26 (37%) 1 2	77, 100, 148, 194	0
6	F	141/164 (85%)	1.04	16 (11%) 6 11	54, 83, 136, 158	0
7	I	38/38 (100%)	1.11	6 (15%) 3 6	10, 36, 74, 78	0
8	J	41/41 (100%)	1.15	4 (9%) 8 13	65, 89, 136, 165	0
9	K	46/83 (55%)	1.73	13 (28%) 1 3	55, 87, 141, 169	0
10	L	151/154 (98%)	0.79	8 (5%) 25 26	14, 49, 104, 140	0
11	M	31/31 (100%)	0.95	2 (6%) 18 22	31, 51, 80, 92	0
12	X	29/35 (82%)	1.04	5 (17%) 2 5	59, 80, 120, 155	0
All	All	2243/2334 (96%)	1.18	367 (16%) 2 6	10, 81, 141, 215	0

The worst 5 of 367 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	52	ALA	5.8
9	K	31	ARG	5.5
1	A	244	LEU	5.3
1	A	207	LEU	5.0
1	A	210	LEU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	CLA	A	824	59/65	0.72	8.01	59,101,164,321	0
15	BCR	B	844	25/40	0.79	7.34	65,68,113,118	0
15	BCR	A	850	40/40	1.12	6.23	56,96,126,139	0
15	BCR	B	849	40/40	0.68	5.30	12,43,147,152	0
15	BCR	J	1104	40/40	1.38	5.27	64,78,113,120	0
15	BCR	B	846	40/40	1.10	4.61	75,91,131,137	0
15	BCR	A	852	40/40	1.11	4.45	78,107,149,162	0
15	BCR	J	1105	40/40	0.97	4.44	63,67,71,71	0
13	CLA	M	1202	45/65	0.94	4.44	51,149,183,198	0
15	BCR	B	847	40/40	0.72	4.16	40,51,116,126	0
15	BCR	B	843	40/40	0.90	4.09	45,59,82,86	0
15	BCR	A	849	40/40	1.65	4.05	95,136,179,183	0
15	BCR	F	1302	40/40	1.09	3.81	70,94,125,128	0
13	CLA	B	830	65/65	0.99	3.81	82,91,129,139	0
15	BCR	B	841	40/40	1.20	3.55	65,105,151,155	0
13	CLA	A	809	65/65	0.92	3.51	78,117,148,152	0
15	BCR	A	851	40/40	0.91	3.41	50,58,118,132	0
15	BCR	A	847	40/40	1.64	3.36	98,140,151,162	0
13	CLA	A	843	65/65	0.68	3.33	56,83,169,197	0
16	LHG	A	853	49/49	0.97	3.14	57,74,107,127	0
13	CLA	B	824	65/65	0.74	3.13	58,65,88,96	0
13	CLA	A	820	61/65	1.38	3.08	119,135,166,198	0
15	BCR	A	848	40/40	1.63	3.08	112,132,147,157	0
13	CLA	A	855	45/65	0.76	2.95	95,118,140,153	0
13	CLA	J	1101	65/65	0.87	2.93	77,129,178,357	0
13	CLA	B	818	47/65	0.84	2.91	56,99,146,292	0
15	BCR	B	850	40/40	0.88	2.90	83,107,144,146	0
13	CLA	A	826	65/65	0.69	2.85	53,80,112,127	0
15	BCR	M	1203	40/40	0.69	2.78	43,48,87,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	PQN	A	846	33/33	0.83	2.70	55,64,82,82	0
13	CLA	A	842	65/65	0.92	2.70	62,82,149,162	0
13	CLA	B	814	55/65	1.13	2.52	77,122,182,325	0
14	PQN	B	840	33/33	0.81	2.42	56,84,105,121	0
13	CLA	A	815	45/65	1.32	2.41	111,150,177,185	0
13	CLA	A	806	65/65	0.85	2.39	63,80,155,164	0
13	CLA	A	833	65/65	0.76	2.38	39,45,110,121	0
13	CLA	A	816	49/65	1.32	2.34	119,163,187,193	0
13	CLA	A	803	65/65	0.74	2.33	76,100,142,222	0
13	CLA	A	807	51/65	0.98	2.29	87,100,151,177	0
13	CLA	A	808	65/65	0.63	2.22	72,89,172,177	0
15	BCR	I	102	40/40	0.50	2.18	19,20,48,52	0
13	CLA	A	827	65/65	0.90	2.18	68,103,137,248	0
13	CLA	A	829	65/65	0.88	2.18	83,108,179,197	0
13	CLA	A	834	65/65	0.63	2.15	39,40,92,96	0
15	BCR	B	842	40/40	0.93	2.13	48,76,129,134	0
18	LMG	B	848	55/55	0.72	2.13	42,51,67,114	0
13	CLA	B	804	65/65	0.74	2.05	45,51,117,199	0
13	CLA	B	839	65/65	0.57	2.00	35,49,151,215	0
15	BCR	B	845	40/40	0.77	2.00	60,66,78,82	0
13	CLA	B	811	65/65	0.79	1.97	48,71,108,145	0
15	BCR	L	1006	40/40	0.39	1.96	16,24,64,78	0
13	CLA	B	822	54/65	0.78	1.93	61,86,118,158	0
13	CLA	A	823	51/65	0.65	1.92	74,129,153,156	0
13	CLA	A	828	65/65	0.68	1.92	59,74,127,289	0
13	CLA	F	1301	45/65	0.88	1.89	94,137,167,175	0
13	CLA	B	815	59/65	0.76	1.89	55,58,76,293	0
13	CLA	B	835	60/65	0.51	1.84	65,106,240,292	0
13	CLA	B	838	65/65	0.75	1.84	35,45,102,125	0
13	CLA	B	816	60/65	0.86	1.83	46,53,111,221	0
13	CLA	B	813	45/65	0.84	1.82	51,86,132,141	0
13	CLA	L	1002	65/65	0.49	1.82	29,65,103,148	0
13	CLA	B	817	65/65	0.81	1.80	57,65,113,125	0
13	CLA	A	821	65/65	0.82	1.77	72,100,164,266	0
13	CLA	A	832	65/65	0.56	1.74	42,45,81,134	0
13	CLA	A	838	65/65	0.52	1.74	45,81,109,114	0
13	CLA	B	812	65/65	0.62	1.73	37,42,111,117	0
13	CLA	A	805	65/65	0.83	1.70	85,98,117,126	0
13	CLA	B	823	46/65	0.52	1.69	59,68,120,137	0
13	CLA	B	802	65/65	0.57	1.64	61,82,112,165	0
13	CLA	B	831	58/65	0.77	1.64	80,101,148,333	0
13	CLA	A	812	54/65	1.05	1.62	136,181,240,396	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	CLA	A	819	65/65	0.88	1.60	97,140,181,328	0
13	CLA	A	845	52/65	0.55	1.55	56,78,188,214	0
13	CLA	B	803	65/65	0.61	1.54	40,68,95,180	0
13	CLA	A	844	41/65	1.11	1.53	116,136,148,281	0
13	CLA	A	840	65/65	0.68	1.51	77,87,117,198	0
13	CLA	B	836	65/65	0.66	1.49	69,98,146,234	0
13	CLA	B	826	65/65	0.68	1.49	42,47,127,149	0
13	CLA	B	819	45/65	0.69	1.48	98,131,171,173	0
13	CLA	B	809	45/65	0.50	1.47	39,95,125,308	0
13	CLA	A	813	60/65	0.89	1.46	115,146,178,366	0
15	BCR	L	1005	40/40	0.59	1.44	11,16,81,93	0
13	CLA	L	1003	65/65	0.55	1.42	16,52,179,216	0
13	CLA	A	830	65/65	0.74	1.38	59,71,105,119	0
13	CLA	A	802	65/65	0.54	1.38	40,77,110,230	0
13	CLA	A	801	65/65	0.50	1.32	44,53,82,89	0
13	CLA	B	821	45/65	0.60	1.30	63,69,105,191	0
13	CLA	B	827	65/65	0.54	1.27	44,66,95,108	0
13	CLA	X	102	45/65	0.53	1.24	67,104,127,283	0
13	CLA	A	817	54/65	0.82	1.24	83,104,164,172	0
13	CLA	M	1201	54/65	0.59	1.22	34,42,121,127	0
13	CLA	A	837	51/65	0.49	1.14	52,56,96,147	0
13	CLA	L	1004	65/65	0.59	1.12	21,31,64,72	0
13	CLA	A	831	50/65	0.52	1.11	45,76,105,144	0
13	CLA	B	810	45/65	0.62	1.11	47,84,145,182	0
16	LHG	A	854	27/49	0.51	1.10	49,58,88,122	0
13	CLA	B	829	49/65	0.69	1.04	80,85,125,141	0
13	CLA	B	805	65/65	0.51	1.03	41,48,97,150	0
13	CLA	A	804	59/65	0.88	1.01	83,99,117,144	0
13	CLA	B	807	65/65	0.61	0.97	38,65,106,122	0
13	CLA	A	811	65/65	0.84	0.95	95,134,173,321	0
13	CLA	B	808	65/65	0.62	0.94	36,41,97,103	0
13	CLA	J	1103	37/65	0.66	0.94	85,117,155,158	0
13	CLA	B	825	65/65	0.44	0.93	40,60,136,157	0
13	CLA	J	1102	45/65	0.69	0.93	75,111,128,280	0
13	CLA	B	801	65/65	0.41	0.87	57,68,123,322	0
13	CLA	A	841	51/65	0.55	0.84	80,105,182,204	0
13	CLA	B	806	65/65	0.49	0.79	33,63,107,170	0
13	CLA	A	818	54/65	0.67	0.78	92,136,168,207	0
13	CLA	I	101	65/65	0.48	0.75	33,57,85,338	0
13	CLA	B	832	45/65	0.62	0.68	71,121,142,247	0
13	CLA	B	820	55/65	0.68	0.61	77,105,141,146	0
13	CLA	A	835	54/65	0.72	0.51	54,79,117,204	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	CLA	A	822	49/65	0.75	0.40	102,126,157,235	0
13	CLA	B	834	45/65	0.74	0.39	91,118,151,158	0
13	CLA	A	825	65/65	0.47	0.38	74,102,152,193	0
13	CLA	A	814	45/65	0.71	0.32	108,150,172,174	0
13	CLA	B	828	45/65	0.63	0.28	70,80,132,193	0
16	LHG	X	101	23/49	0.61	0.16	78,81,207,208	0
13	CLA	A	836	45/65	0.70	0.10	63,96,163,234	0
13	CLA	A	810	45/65	0.61	0.03	109,136,151,223	0
13	CLA	A	839	47/65	0.41	0.03	48,51,119,202	0
13	CLA	B	833	45/65	0.71	-0.00	77,104,141,148	0
13	CLA	B	837	47/65	0.46	-0.11	65,71,119,193	0
17	SF4	A	856	8/8	0.27	-1.28	49,50,150,174	0
17	SF4	C	101	8/8	0.23	-1.97	48,48,49,62	0
17	SF4	C	102	8/8	0.18	-2.11	47,48,122,359	0
19	CA	L	1001	1/1	0.18	-2.53	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.