



wwPDB X-ray Structure Validation Summary Report

Sep 16, 2014 – 06:37 AM EDT

PDB ID : 4KT0
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.
Deposited on : 2013-05-19
Resolution : 2.80 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>

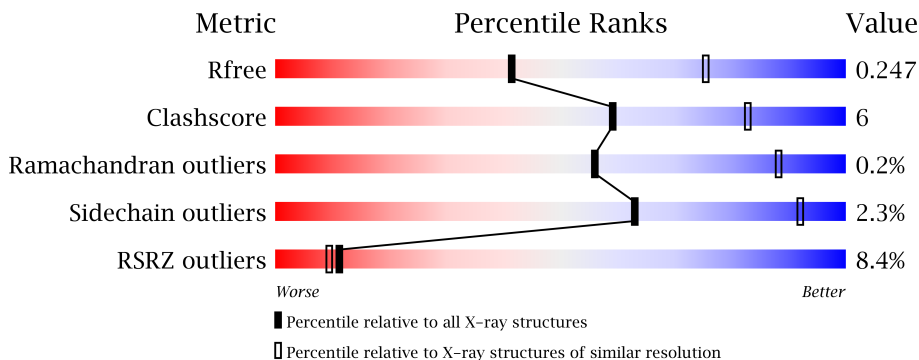
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	751	
2	B	731	
3	C	81	
4	D	141	
5	E	74	
6	F	165	
7	J	40	
8	K	128	
9	M	31	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	PQN	B	2002	-	X
11	SF4	A	3001	-	X
11	SF4	C	3003	-	X
12	LHG	A	5003	-	X
14	BCR	A	4002	-	X
14	BCR	A	4003	-	X
14	BCR	A	4007	-	X
14	BCR	A	4012	-	X
14	BCR	B	4006	-	X
14	BCR	B	4009	-	X
14	BCR	B	4017	-	X
14	BCR	J	4013	-	X
15	CLA	A	1106	-	X
15	CLA	A	1110	-	X
15	CLA	A	1121	-	X
15	CLA	A	1122	-	X
15	CLA	A	1801	-	X
15	CLA	F	1410	-	X
15	CLA	J	1302	-	X
15	CLA	J	1303	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 22051 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	739	Total	C	N	O	S	0	0	0
			5787	3791	984	985	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			

- 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
			600	369	103	117	11			

- Molecule 4 is a protein called Photosystem I subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	681	187	204	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	68	Total	C	N	O	0	0	0
			533	335	94	104			

- Molecule 6 is a protein called Photosystem I subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1099	711	183	200	5			

- Molecule 7 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			

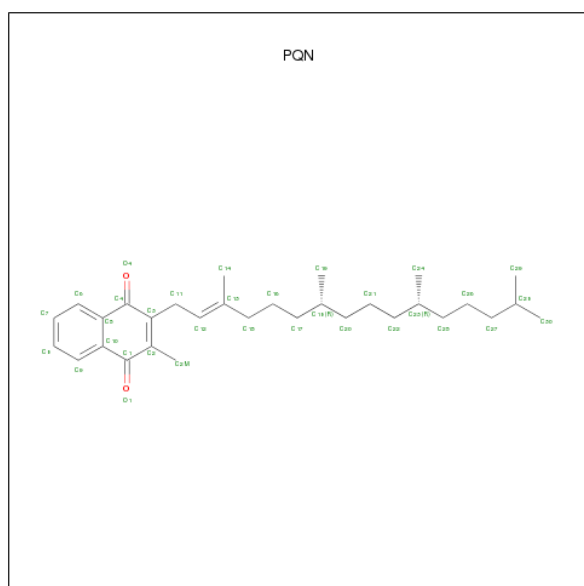
- Molecule 8 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	53	Total	C	N	O	S	0	0	0
			366	242	56	63	5			

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

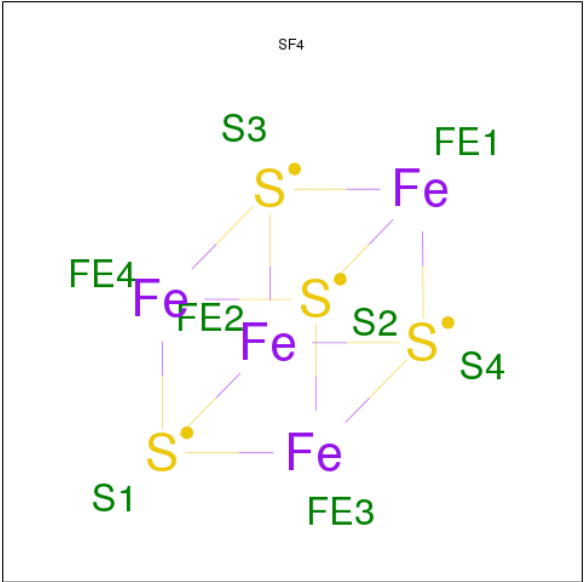
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	M	30	Total	C	N	O	0	0	0
			214	142	34	38			

- Molecule 10 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



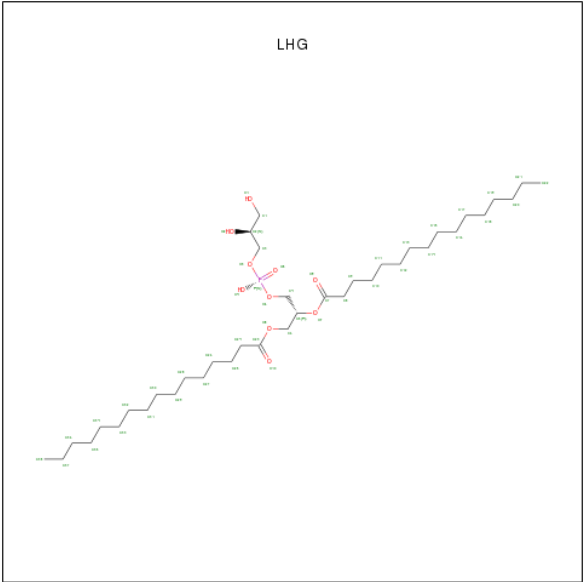
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			33	31	2		
10	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



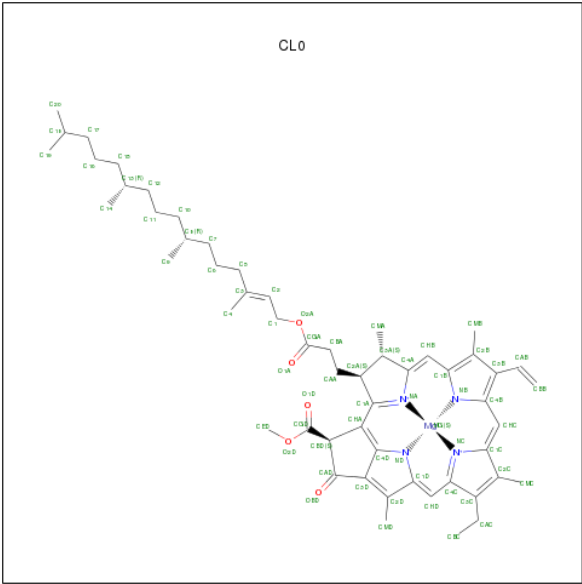
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



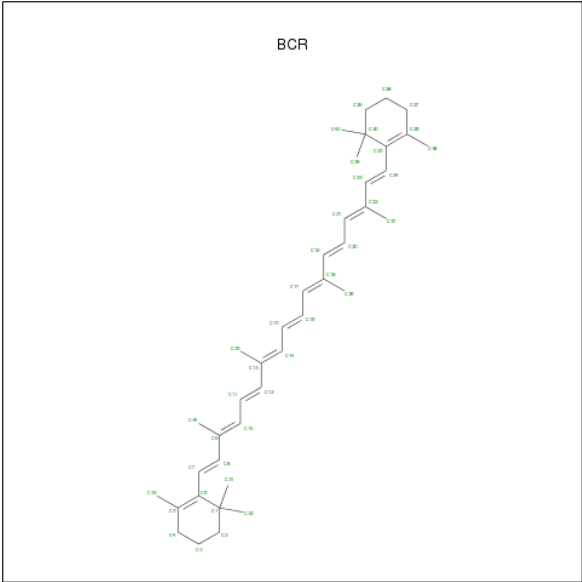
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			49	38	10	1		
12	A	1	Total	C	O	P	0	0
			49	38	10	1		
12	A	1	Total	C	O	P	0	0
			36	25	10	1		
12	B	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



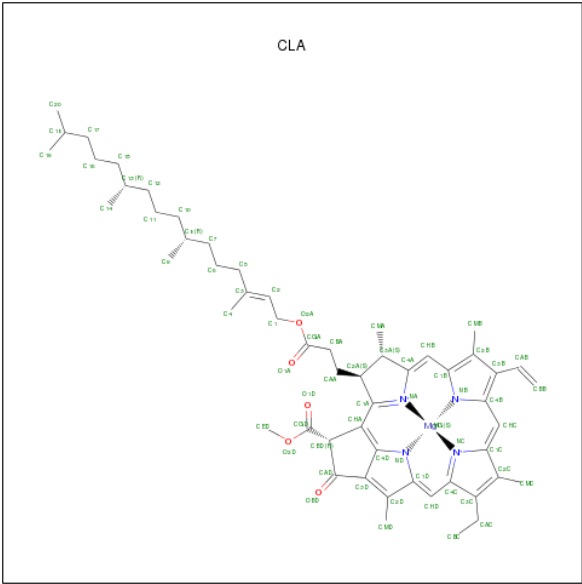
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	J	1	Total C 40 40	0	0

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C Mg N O 52 42 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0
15	A	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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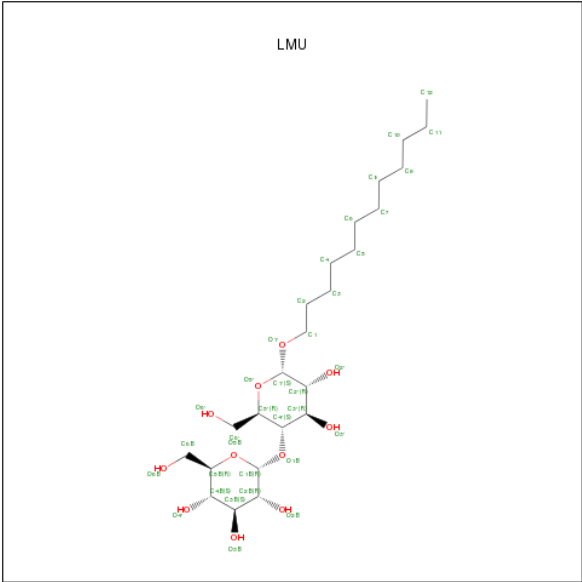
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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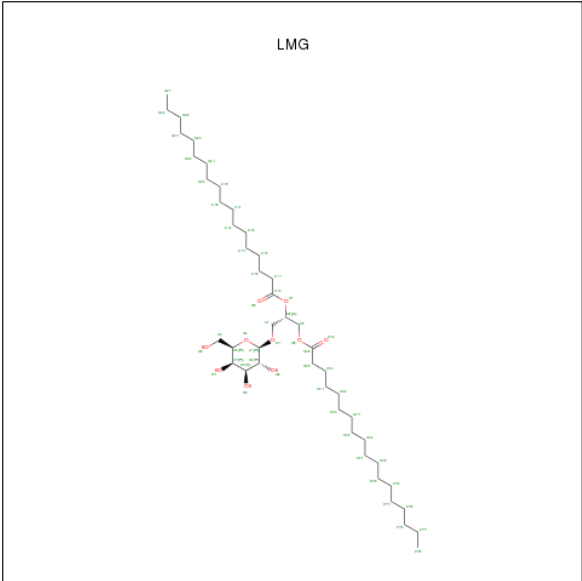
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	J	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			35	24	11		
16	J	1	Total	C	O	0	0
			35	24	11		

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	1	Total	Cl	0	0
			1	1		

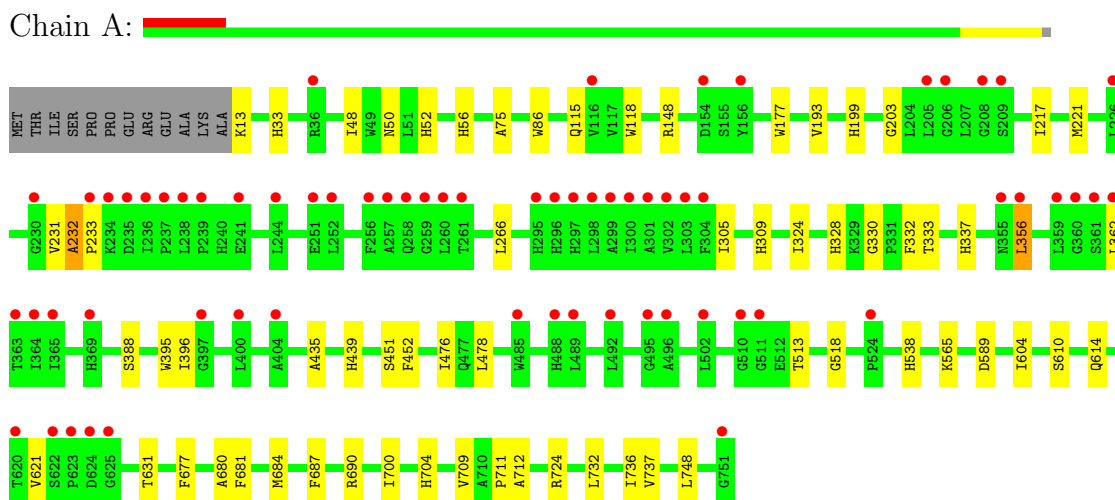
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	10	Total	O	0	0
			10	10		
19	B	15	Total	O	0	0
			15	15		
19	C	3	Total	O	0	0
			3	3		
19	F	1	Total	O	0	0
			1	1		

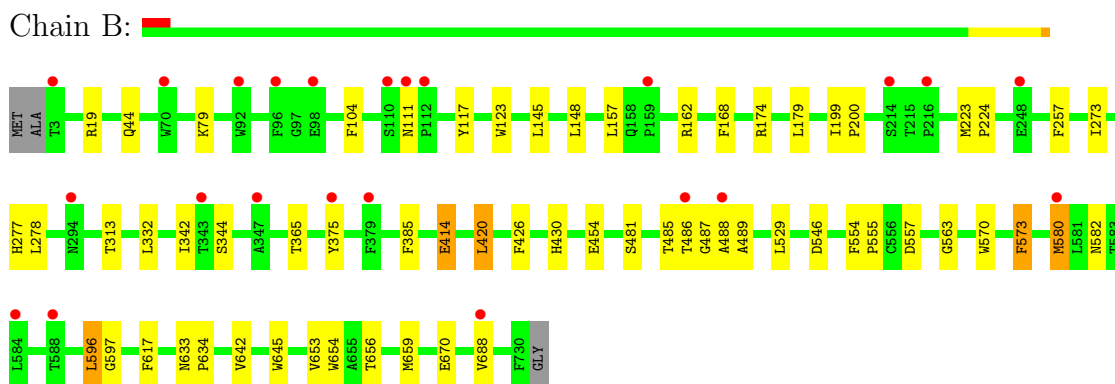
3 Residue-property plots

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

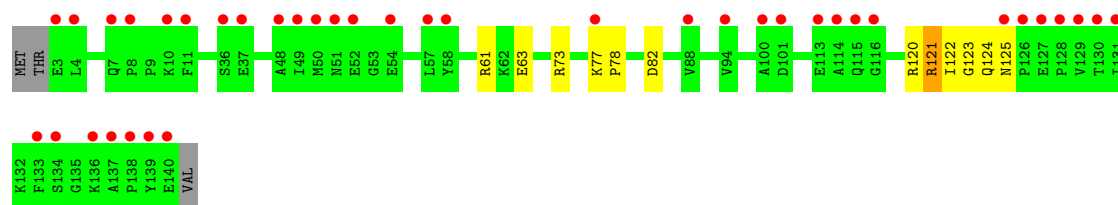


- Molecule 3: Photosystem I iron-sulfur center



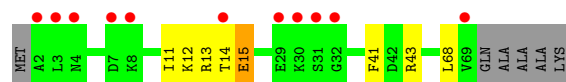
- Molecule 4: Photosystem I subunit II





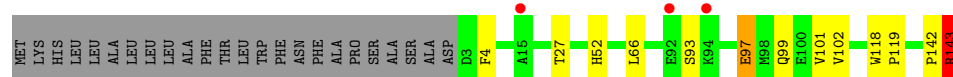
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



• Molecule 6: Photosystem I subunit III

Chain F:



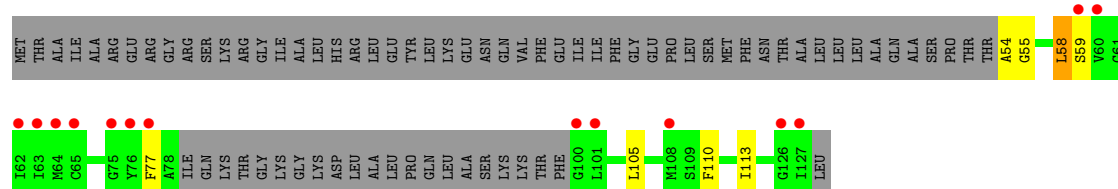
• Molecule 7: Photosystem I reaction center subunit IX

Chain J:



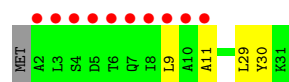
• Molecule 8: Photosystem I reaction center subunit PsaK

Chain K:



• Molecule 9: Photosystem I reaction center subunit XII

Chain M:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.18Å 173.31Å 179.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.80 48.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.98-2.80) 79.2 (48.55-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.198 , 0.245 0.201 , 0.247	Depositor DCC
R_{free} test set	3915 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.4	EDS
Estimated twinning fraction	0.001 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 114217 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22051	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, CL, SF4, LMU, PQN, CLA, CL0, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/5985	0.38	0/8158
2	B	0.23	0/5976	0.40	0/8173
3	C	0.24	0/610	0.45	0/826
4	D	0.23	0/1099	0.40	0/1482
5	E	0.24	0/542	0.45	0/733
6	F	0.23	0/1129	0.40	0/1535
7	J	0.26	0/328	0.38	0/443
8	K	0.25	0/371	0.39	0/499
9	M	0.22	0/217	0.35	0/295
All	All	0.23	0/16257	0.39	0/22144

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
4	D	0	1
6	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	121	ARG	Sidechain
6	F	143	ARG	Sidechain

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	5787	0	5646	60	0
2	B	5765	0	5544	56	0
3	C	600	0	581	4	0
4	D	1075	0	1069	7	0
5	E	533	0	517	8	0
6	F	1099	0	1096	7	0
7	J	319	0	328	4	0
8	K	366	0	376	7	0
9	M	214	0	213	2	0
10	A	33	0	46	1	0
10	B	33	0	46	3	0
11	A	8	0	0	0	0
11	C	16	0	0	0	0
12	A	134	0	190	18	0
12	B	49	0	74	2	0
13	A	110	0	105	12	0
14	A	240	0	294	17	0
14	B	320	0	390	26	0
14	F	80	0	97	8	0
14	J	40	0	49	3	0
15	A	2352	0	2285	69	0
15	B	2365	0	2272	58	0
15	F	175	0	177	3	0
15	J	91	0	66	2	0
15	K	92	0	66	2	0
16	B	35	0	46	0	0
16	J	35	0	46	2	0
17	B	55	0	86	2	0
18	B	1	0	0	0	0
19	A	10	0	0	5	0
19	B	15	0	0	6	0
19	C	3	0	0	0	0
19	F	1	0	0	1	0
All	All	22051	0	21705	267	0

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 6.

The worst 5 of 267 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:A:1011:CL0:CMA	19:A:9109:HOH:O	1.91	1.19
13:A:1011:CL0:H6	19:A:9109:HOH:O	1.48	1.11
14:B:4004:BCR:H403	14:B:4004:BCR:H23C	1.51	0.92
13:A:1011:CL0:H71	19:A:9109:HOH:O	1.71	0.88
15:A:1110:CLA:HBD	15:A:1110:CLA:HBA1	1.57	0.86

There are no symmetry-related clashes.

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	737/751 (98%)	694 (94%)	40 (5%)	3 (0%)	43	80
2	B	726/731 (99%)	695 (96%)	31 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	136/141 (96%)	123 (90%)	13 (10%)	0	100	100
5	E	66/74 (89%)	57 (86%)	9 (14%)	0	100	100
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100	100
7	J	38/40 (95%)	38 (100%)	0	0	100	100
8	K	49/128 (38%)	46 (94%)	3 (6%)	0	100	100
9	M	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
All	All	1997/2142 (93%)	1887 (94%)	107 (5%)	3 (0%)	56	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN

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Mol	Chain	Res	Type
1	A	232	ALA
1	A	233	PRO

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/603 (98%)	584 (98%)	9 (2%)	76	96
2	B	582/583 (100%)	571 (98%)	11 (2%)	69	94
3	C	68/69 (99%)	67 (98%)	1 (2%)	76	96
4	D	112/116 (97%)	110 (98%)	2 (2%)	71	94
5	E	57/60 (95%)	54 (95%)	3 (5%)	32	67
6	F	118/137 (86%)	112 (95%)	6 (5%)	33	69
7	J	35/35 (100%)	35 (100%)	0	100	100
8	K	37/100 (37%)	33 (89%)	4 (11%)	9	26
9	M	19/25 (76%)	18 (95%)	1 (5%)	32	67
All	All	1621/1728 (94%)	1584 (98%)	37 (2%)	63	92

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	573	PHE
3	C	66	ARG
8	K	105	LEU
2	B	580	MET
2	B	596	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	614	GLN
4	D	95	GLN
2	B	114	ASN

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Mol	Chain	Res	Type
1	A	538	HIS
2	B	34	HIS

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 122 ligands modelled in this entry, 1 is monoatomic - leaving 121 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	CL0	A	1011	-	73,73,73	2.18	19 (26%)	96,113,113	2.32	24 (25%)
15	CLA	A	1012	19	73,73,73	2.21	21 (28%)	96,113,113	2.37	28 (29%)
15	CLA	A	1022	19	73,73,73	2.21	20 (27%)	96,113,113	2.33	23 (23%)
15	CLA	A	1101	-	73,73,73	2.22	20 (27%)	96,113,113	2.40	27 (28%)
15	CLA	A	1102	15	73,73,73	2.23	20 (27%)	96,113,113	2.32	25 (26%)
15	CLA	A	1103	-	73,73,73	2.21	19 (26%)	96,113,113	2.24	27 (28%)
15	CLA	A	1104	-	73,73,73	2.19	20 (27%)	96,113,113	2.33	26 (27%)
15	CLA	A	1105	-	73,73,73	2.18	20 (27%)	96,113,113	2.40	24 (25%)
15	CLA	A	1106	1	73,73,73	2.22	20 (27%)	96,113,113	2.37	29 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1107	1	58,58,73	2.50	23 (39%)	76,95,113	2.60	27 (35%)
13	CL0	A	1108	-	51,53,73	2.62	20 (39%)	69,89,113	2.44	22 (31%)
15	CLA	A	1109	15	73,73,73	2.23	20 (27%)	96,113,113	2.38	28 (29%)
15	CLA	A	1110	-	62,62,73	2.36	22 (35%)	81,99,113	2.53	24 (29%)
15	CLA	A	1111	-	67,68,73	2.29	20 (29%)	88,107,113	2.38	26 (29%)
15	CLA	A	1112	-	51,53,73	2.61	21 (41%)	69,89,113	2.45	23 (33%)
15	CLA	A	1113	-	51,53,73	2.61	20 (39%)	69,89,113	2.44	21 (30%)
15	CLA	A	1114	-	56,57,73	2.53	20 (35%)	74,93,113	2.53	23 (31%)
15	CLA	A	1115	-	53,54,73	2.52	19 (35%)	72,90,113	2.47	20 (27%)
15	CLA	A	1116	-	62,62,73	2.39	20 (32%)	81,99,113	2.51	26 (32%)
15	CLA	A	1117	-	73,73,73	2.21	20 (27%)	96,113,113	2.26	25 (26%)
15	CLA	A	1118	-	53,54,73	2.49	18 (33%)	72,90,113	2.51	20 (27%)
15	CLA	A	1119	-	71,72,73	2.29	22 (30%)	91,111,113	2.32	24 (26%)
15	CLA	A	1120	-	56,57,73	2.53	21 (37%)	74,93,113	2.55	25 (33%)
15	CLA	A	1121	-	53,54,73	2.52	19 (35%)	72,90,113	2.52	20 (27%)
15	CLA	A	1122	-	73,73,73	2.23	20 (27%)	96,113,113	2.31	25 (26%)
15	CLA	A	1123	-	73,73,73	2.19	20 (27%)	96,113,113	2.30	28 (29%)
15	CLA	A	1124	-	62,63,73	2.39	20 (32%)	82,101,113	2.50	24 (29%)
15	CLA	A	1125	-	60,60,73	2.52	20 (33%)	80,97,113	2.60	30 (37%)
15	CLA	A	1126	-	73,73,73	2.22	21 (28%)	96,113,113	2.36	29 (30%)
15	CLA	A	1127	-	73,73,73	2.20	19 (26%)	96,113,113	2.29	28 (29%)
15	CLA	A	1128	-	73,73,73	2.19	20 (27%)	96,113,113	2.27	26 (27%)
15	CLA	A	1129	-	53,54,73	2.50	19 (35%)	72,90,113	2.56	24 (33%)
15	CLA	A	1130	-	62,63,73	2.40	21 (33%)	82,101,113	2.48	25 (30%)
15	CLA	A	1131	-	62,63,73	2.43	21 (33%)	82,101,113	2.50	25 (30%)
15	CLA	A	1132	-	70,70,73	2.33	20 (28%)	92,109,113	2.37	25 (27%)
15	CLA	A	1133	-	53,54,73	2.50	19 (35%)	72,90,113	2.50	25 (34%)
15	CLA	A	1134	1	53,54,73	2.52	19 (35%)	72,90,113	2.51	22 (30%)
15	CLA	A	1135	-	62,63,73	2.38	20 (32%)	82,101,113	2.52	26 (31%)
15	CLA	A	1136	-	73,73,73	2.19	20 (27%)	96,113,113	2.29	23 (23%)
15	CLA	A	1137	-	58,58,73	2.48	21 (36%)	76,95,113	2.53	25 (32%)
15	CLA	A	1138	-	73,73,73	2.25	20 (27%)	96,113,113	2.29	27 (28%)
15	CLA	A	1140	-	73,73,73	2.21	20 (27%)	96,113,113	2.22	24 (25%)
15	CLA	A	1801	12	60,60,73	2.55	23 (38%)	80,97,113	2.53	28 (35%)
10	PQN	A	2001	-	34,34,34	1.38	2 (5%)	45,45,45	1.00	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SF4	A	3001	1,2	12,12,12	6.48	12 (100%)	0,24,24	0.00	-
14	BCR	A	4001	-	41,41,41	2.75	6 (14%)	56,56,56	6.05	25 (44%)
14	BCR	A	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.25	25 (44%)
14	BCR	A	4003	-	41,41,41	2.72	6 (14%)	56,56,56	6.28	25 (44%)
14	BCR	A	4007	-	41,41,41	2.71	6 (14%)	56,56,56	6.49	24 (42%)
14	BCR	A	4008	-	41,41,41	2.72	7 (17%)	56,56,56	6.56	24 (42%)
14	BCR	A	4012	-	41,41,41	2.79	6 (14%)	56,56,56	5.98	22 (39%)
12	LHG	A	5001	-	48,48,48	0.89	2 (4%)	54,54,54	1.05	3 (5%)
12	LHG	A	5003	15	48,48,48	0.90	2 (4%)	54,54,54	1.08	3 (5%)
12	LHG	A	5005	-	35,35,48	1.74	4 (11%)	41,41,54	1.11	3 (7%)
15	CLA	B	1013	-	73,73,73	2.20	20 (27%)	96,113,113	2.42	27 (28%)
15	CLA	B	1021	-	73,73,73	2.20	21 (28%)	96,113,113	2.28	27 (28%)
15	CLA	B	1023	-	73,73,73	2.17	22 (30%)	96,113,113	2.27	25 (26%)
15	CLA	B	1201	-	53,54,73	2.51	19 (35%)	72,90,113	2.54	23 (31%)
15	CLA	B	1202	-	73,73,73	2.21	20 (27%)	96,113,113	2.32	26 (27%)
15	CLA	B	1203	-	73,73,73	2.19	20 (27%)	96,113,113	2.29	25 (26%)
15	CLA	B	1204	-	53,54,73	2.50	19 (35%)	72,90,113	2.57	23 (31%)
15	CLA	B	1205	-	62,63,73	2.37	19 (30%)	82,101,113	2.45	23 (28%)
15	CLA	B	1206	2	53,54,73	2.52	19 (35%)	72,90,113	2.54	24 (33%)
15	CLA	B	1207	-	53,54,73	2.52	19 (35%)	72,90,113	2.54	21 (29%)
15	CLA	B	1208	-	51,53,73	2.61	20 (39%)	69,89,113	2.43	18 (26%)
15	CLA	B	1209	-	51,53,73	2.57	20 (39%)	69,89,113	2.48	25 (36%)
15	CLA	B	1210	-	73,73,73	2.20	20 (27%)	96,113,113	2.29	27 (28%)
15	CLA	B	1211	-	53,54,73	2.50	19 (35%)	72,90,113	2.48	22 (30%)
15	CLA	B	1212	-	51,53,73	2.60	20 (39%)	69,89,113	2.44	20 (28%)
15	CLA	B	1213	-	58,58,73	2.52	22 (37%)	76,95,113	2.51	24 (31%)
15	CLA	B	1214	-	73,73,73	2.21	20 (27%)	96,113,113	2.35	26 (27%)
15	CLA	B	1215	-	73,73,73	2.21	20 (27%)	96,113,113	2.43	27 (28%)
15	CLA	B	1216	-	73,73,73	2.20	20 (27%)	96,113,113	2.23	25 (26%)
15	CLA	B	1217	-	54,55,73	2.88	21 (38%)	73,91,113	2.58	25 (34%)
15	CLA	B	1218	-	59,59,73	2.55	21 (35%)	78,96,113	2.56	27 (34%)
15	CLA	B	1219	-	62,63,73	2.43	21 (33%)	82,101,113	2.56	27 (32%)
15	CLA	B	1220	-	64,64,73	2.50	22 (34%)	84,102,113	2.43	25 (29%)
15	CLA	B	1221	-	73,73,73	2.19	21 (28%)	96,113,113	2.31	24 (25%)
15	CLA	B	1222	-	64,64,73	2.45	20 (31%)	84,102,113	2.48	25 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1223	-	73,73,73	2.19	20 (27%)	96,113,113	2.33	27 (28%)
15	CLA	B	1224	-	73,73,73	2.19	19 (26%)	96,113,113	2.32	25 (26%)
15	CLA	B	1225	-	73,73,73	2.18	20 (27%)	96,113,113	2.33	25 (26%)
15	CLA	B	1226	-	73,73,73	2.18	19 (26%)	96,113,113	2.29	24 (25%)
15	CLA	B	1227	-	51,53,73	2.56	21 (41%)	69,89,113	2.49	19 (27%)
15	CLA	B	1228	-	73,73,73	2.23	22 (30%)	96,113,113	2.25	24 (25%)
15	CLA	B	1229	-	73,73,73	2.18	20 (27%)	96,113,113	2.29	24 (25%)
15	CLA	B	1230	-	73,73,73	2.20	21 (28%)	96,113,113	2.41	30 (31%)
15	CLA	B	1231	-	73,73,73	2.22	20 (27%)	96,113,113	2.33	27 (28%)
15	CLA	B	1232	-	51,53,73	2.55	20 (39%)	69,89,113	2.40	21 (30%)
15	CLA	B	1234	-	73,73,73	2.20	20 (27%)	96,113,113	2.32	27 (28%)
15	CLA	B	1235	-	73,73,73	2.20	20 (27%)	96,113,113	2.28	26 (27%)
15	CLA	B	1236	-	58,58,73	2.49	21 (36%)	76,95,113	2.59	26 (34%)
15	CLA	B	1237	19	62,63,73	2.39	20 (32%)	82,101,113	2.47	28 (34%)
15	CLA	B	1238	19	52,52,73	3.40	20 (38%)	68,87,113	2.41	20 (29%)
15	CLA	B	1239	-	53,54,73	2.52	20 (37%)	72,90,113	2.55	22 (30%)
15	CLA	B	1240	12	51,53,73	2.61	21 (41%)	69,89,113	2.43	21 (30%)
16	LMU	B	1301	-	36,36,36	0.44	0	47,47,47	0.92	4 (8%)
10	PQN	B	2002	-	34,34,34	1.38	2 (5%)	45,45,45	1.10	4 (8%)
14	BCR	B	4004	-	41,41,41	2.74	6 (14%)	56,56,56	6.13	28 (50%)
14	BCR	B	4005	-	41,41,41	2.73	6 (14%)	56,56,56	6.20	23 (41%)
14	BCR	B	4006	-	41,41,41	2.82	6 (14%)	56,56,56	6.46	24 (42%)
14	BCR	B	4009	-	41,41,41	2.73	7 (17%)	56,56,56	6.55	24 (42%)
14	BCR	B	4010	-	41,41,41	2.71	6 (14%)	56,56,56	6.42	23 (41%)
14	BCR	B	4011	-	41,41,41	2.75	6 (14%)	56,56,56	6.51	25 (44%)
14	BCR	B	4014	-	41,41,41	2.73	6 (14%)	56,56,56	6.44	21 (37%)
14	BCR	B	4017	-	41,41,41	2.71	6 (14%)	56,56,56	6.35	24 (42%)
17	LMG	B	5002	-	55,55,55	0.88	2 (3%)	63,63,63	0.98	2 (3%)
12	LHG	B	5004	15	48,48,48	0.90	2 (4%)	54,54,54	1.13	3 (5%)
11	SF4	C	3002	3	12,12,12	6.40	12 (100%)	0,24,24	0.00	-
11	SF4	C	3003	3	12,12,12	6.54	12 (100%)	0,24,24	0.00	-
15	CLA	F	1139	19	73,73,73	2.22	21 (28%)	96,113,113	2.23	22 (22%)
15	CLA	F	1301	-	51,53,73	2.59	20 (39%)	69,89,113	2.43	20 (28%)
15	CLA	F	1410	6	73,73,73	2.20	20 (27%)	96,113,113	2.38	28 (29%)
14	BCR	F	4015	-	41,41,41	2.73	7 (17%)	56,56,56	6.41	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	F	4016	-	41,41,41	2.72	6 (14%)	56,56,56	6.50	24 (42%)
15	CLA	J	1302	7	51,53,73	2.61	20 (39%)	69,89,113	2.42	18 (26%)
15	CLA	J	1303	-	53,54,73	2.53	20 (37%)	72,90,113	2.53	21 (29%)
16	LMU	J	1304	-	36,36,36	0.41	0	47,47,47	0.64	1 (2%)
14	BCR	J	4013	-	41,41,41	2.71	6 (14%)	56,56,56	6.40	28 (50%)
15	CLA	K	1401	-	53,54,73	2.51	19 (35%)	72,90,113	2.59	24 (33%)
15	CLA	K	1402	-	53,54,73	2.51	19 (35%)	72,90,113	2.51	21 (29%)

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	CL0	A	1011	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1012	19	-	0/37/135/135	0/0/9/9
15	CLA	A	1022	19	-	0/37/135/135	0/0/9/9
15	CLA	A	1101	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1102	15	-	0/37/135/135	0/0/9/9
15	CLA	A	1103	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1104	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1105	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1106	1	-	0/37/135/135	0/0/9/9
15	CLA	A	1107	1	-	0/19/117/135	0/0/9/9
13	CL0	A	1108	-	-	0/11/111/135	0/0/9/9
15	CLA	A	1109	15	-	0/37/135/135	0/0/9/9
15	CLA	A	1110	-	-	0/23/122/135	0/0/9/9
15	CLA	A	1111	-	-	0/31/129/135	0/0/9/9
15	CLA	A	1112	-	-	0/11/111/135	0/0/9/9
15	CLA	A	1113	-	-	0/11/111/135	0/0/9/9
15	CLA	A	1114	-	-	0/17/116/135	0/0/9/9
15	CLA	A	1115	-	-	0/15/113/135	0/0/9/9
15	CLA	A	1116	-	-	0/23/122/135	0/0/9/9
15	CLA	A	1117	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1118	-	-	0/15/113/135	0/0/9/9
15	CLA	A	1119	-	-	0/33/133/135	0/0/9/9
15	CLA	A	1120	-	-	0/17/116/135	0/0/9/9
15	CLA	A	1121	-	-	0/15/113/135	0/0/9/9
15	CLA	A	1122	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1123	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1124	-	-	0/25/123/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1125	-	-	0/22/120/135	0/0/9/9
15	CLA	A	1126	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1127	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1128	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1129	-	-	0/15/113/135	0/0/9/9
15	CLA	A	1130	-	-	0/25/123/135	0/0/9/9
15	CLA	A	1131	-	-	0/25/123/135	0/0/9/9
15	CLA	A	1132	-	-	0/34/132/135	0/0/9/9
15	CLA	A	1133	-	-	0/15/113/135	0/0/9/9
15	CLA	A	1134	1	-	0/15/113/135	0/0/9/9
15	CLA	A	1135	-	-	0/25/123/135	0/0/9/9
15	CLA	A	1136	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1137	-	-	0/19/117/135	0/0/9/9
15	CLA	A	1138	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1140	-	-	0/37/135/135	0/0/9/9
15	CLA	A	1801	12	-	0/22/120/135	0/0/9/9
10	PQN	A	2001	-	-	0/23/43/43	0/2/2/2
11	SF4	A	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4008	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4012	-	-	0/29/63/63	0/2/2/2
12	LHG	A	5001	-	-	0/53/53/53	0/0/0/0
12	LHG	A	5003	15	-	0/53/53/53	0/0/0/0
12	LHG	A	5005	-	-	0/40/40/53	0/0/0/0
15	CLA	B	1013	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1021	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1023	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1201	-	-	0/15/113/135	0/0/9/9
15	CLA	B	1202	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1203	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1204	-	-	0/15/113/135	0/0/9/9
15	CLA	B	1205	-	-	0/25/123/135	0/0/9/9
15	CLA	B	1206	2	-	0/15/113/135	0/0/9/9
15	CLA	B	1207	-	-	0/15/113/135	0/0/9/9
15	CLA	B	1208	-	-	0/11/111/135	0/0/9/9
15	CLA	B	1209	-	-	0/11/111/135	0/0/9/9
15	CLA	B	1210	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1211	-	-	0/15/113/135	0/0/9/9
15	CLA	B	1212	-	-	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1213	-	-	0/19/117/135	0/0/9/9
15	CLA	B	1214	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1215	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1216	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1217	-	-	0/16/114/135	0/0/9/9
15	CLA	B	1218	-	-	0/21/119/135	0/0/9/9
15	CLA	B	1219	-	-	0/25/123/135	0/0/9/9
15	CLA	B	1220	-	-	0/27/125/135	0/0/9/9
15	CLA	B	1221	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1222	-	-	0/27/125/135	0/0/9/9
15	CLA	B	1223	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1224	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1225	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1226	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1227	-	-	0/11/111/135	0/0/9/9
15	CLA	B	1228	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1229	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1230	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1231	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1232	-	-	0/11/111/135	0/0/9/9
15	CLA	B	1234	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1235	-	-	0/37/135/135	0/0/9/9
15	CLA	B	1236	-	-	0/19/117/135	0/0/9/9
15	CLA	B	1237	19	-	0/25/123/135	0/0/9/9
15	CLA	B	1238	19	-	0/11/110/135	0/0/9/9
15	CLA	B	1239	-	-	0/15/113/135	0/0/9/9
15	CLA	B	1240	12	-	0/11/111/135	0/0/9/9
16	LMU	B	1301	-	-	0/21/61/61	0/2/2/2
10	PQN	B	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4006	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4009	-	-	2/29/63/63	0/2/2/2
14	BCR	B	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4014	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4017	-	-	0/29/63/63	0/2/2/2
17	LMG	B	5002	-	-	0/50/70/70	0/1/1/1
12	LHG	B	5004	15	-	0/53/53/53	0/0/0/0
11	SF4	C	3002	3	-	0/0/48/48	0/6/5/5
11	SF4	C	3003	3	-	0/0/48/48	0/6/5/5
15	CLA	F	1139	19	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	F	1301	-	-	0/11/111/135	0/0/9/9
15	CLA	F	1410	6	-	0/37/135/135	0/0/9/9
14	BCR	F	4015	-	-	0/29/63/63	0/2/2/2
14	BCR	F	4016	-	-	0/29/63/63	0/2/2/2
15	CLA	J	1302	7	-	0/11/111/135	0/0/9/9
15	CLA	J	1303	-	-	0/15/113/135	0/0/9/9
16	LMU	J	1304	-	-	0/21/61/61	0/2/2/2
14	BCR	J	4013	-	-	0/29/63/63	0/2/2/2
15	CLA	K	1401	-	-	0/15/113/135	0/0/9/9
15	CLA	K	1402	-	-	0/15/113/135	0/0/9/9

The worst 5 of 2012 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1238	CLA	O1A-CGA	16.37	1.22	1.11
15	B	1217	CLA	O2A-C1	10.62	1.60	1.45
14	A	4012	BCR	C11-C10	-8.24	1.18	1.43
14	B	4006	BCR	C11-C10	-8.22	1.18	1.43
14	F	4016	BCR	C11-C10	-8.12	1.18	1.43

The worst 5 of 2699 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4009	BCR	C16-C17-C18	26.43	165.49	127.29
14	F	4016	BCR	C20-C21-C22	25.03	163.47	127.29
14	B	4006	BCR	C20-C21-C22	23.66	161.49	127.29
14	A	4008	BCR	C20-C21-C22	22.96	160.48	127.29
14	A	4007	BCR	C20-C21-C22	22.96	160.48	127.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	4009	BCR	C11-C10-C9-C34
14	B	4009	BCR	C11-C10-C9-C8

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	739/751 (98%)	0.08	66 (8%) 10 8	43, 90, 141, 226	0
2	B	728/731 (99%)	-0.24	23 (3%) 45 46	53, 83, 126, 179	0
3	C	80/81 (98%)	-0.34	1 (1%) 74 75	60, 72, 95, 105	0
4	D	138/141 (97%)	1.10	39 (28%) 1 1	72, 90, 125, 161	0
5	E	68/74 (91%)	0.31	11 (16%) 2 2	59, 75, 109, 138	0
6	F	141/165 (85%)	-0.52	3 (2%) 60 61	64, 82, 111, 169	0
7	J	40/40 (100%)	-0.46	2 (5%) 28 28	66, 76, 124, 149	0
8	K	53/128 (41%)	0.99	14 (26%) 1 1	134, 160, 207, 253	0
9	M	30/31 (96%)	2.29	10 (33%) 1 1	109, 132, 158, 172	0
All	All	2017/2142 (94%)	0.03	169 (8%) 11 9	43, 86, 145, 253	0

The worst 5 of 169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	M	2	ALA	26.8
9	M	3	LEU	15.6
4	D	113	GLU	10.8
1	A	260	LEU	8.7
1	A	751	GLY	7.8

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
14	BCR	B	4009	40/40	0.39	9.83	72,103,147,151	0
15	CLA	A	1121	46/65	0.22	5.35	91,114,141,163	0
15	CLA	J	1303	46/65	0.33	5.28	94,114,141,159	0
11	SF4	C	3003	8/8	0.22	4.80	60,67,100,115	0
15	CLA	F	1410	65/65	0.23	3.70	69,96,135,147	0
11	SF4	A	3001	8/8	0.24	3.57	50,62,210,290	0
14	BCR	A	4007	40/40	0.36	3.48	69,86,137,139	0
15	CLA	J	1302	45/65	0.25	3.45	82,93,138,150	0
10	PQN	B	2002	33/33	0.28	3.40	59,79,99,105	0
15	CLA	A	1122	65/65	0.22	3.33	74,91,119,129	0
14	BCR	A	4003	40/40	0.40	3.11	69,111,146,146	0
15	CLA	A	1110	54/65	0.22	2.91	96,121,150,154	0
14	BCR	B	4017	40/40	0.20	2.71	70,87,101,104	0
14	BCR	J	4013	40/40	0.27	2.61	78,97,112,121	0
12	LHG	A	5003	49/49	0.33	2.40	91,121,142,143	0
15	CLA	A	1106	65/65	0.20	2.37	59,79,98,109	0
15	CLA	A	1801	52/65	0.35	2.30	100,122,154,158	0
14	BCR	A	4012	40/40	0.17	2.28	55,77,87,91	0
14	BCR	B	4006	40/40	0.24	2.10	86,109,141,142	0
14	BCR	A	4002	40/40	0.31	2.02	88,109,128,130	0
14	BCR	B	4005	40/40	0.29	1.98	73,93,125,128	0
15	CLA	A	1111	60/65	0.26	1.94	78,96,107,112	0
13	CL0	A	1108	45/65	0.27	1.86	86,113,154,170	0
14	BCR	F	4015	40/40	0.21	1.79	52,73,107,111	0
14	BCR	B	4004	40/40	0.30	1.73	101,115,147,151	0
15	CLA	B	1240	45/65	0.28	1.69	71,83,124,151	0
15	CLA	A	1136	65/65	0.31	1.67	78,105,139,142	0
17	LMG	B	5002	55/55	0.27	1.38	71,101,130,137	0
15	CLA	A	1138	65/65	0.20	1.33	47,55,69,77	0
15	CLA	B	1229	65/65	0.18	1.32	50,62,86,107	0
15	CLA	B	1228	65/65	0.19	1.32	54,74,105,114	0
15	CLA	A	1101	65/65	0.18	1.32	55,73,89,96	0
15	CLA	B	1231	65/65	0.22	1.23	66,89,115,138	0
15	CLA	B	1214	65/65	0.23	1.21	72,89,119,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	CLA	F	1139	65/65	0.20	1.13	47,58,90,98	0
16	LMU	J	1304	35/35	0.32	1.13	91,159,172,173	0
15	CLA	B	1023	65/65	0.23	1.09	55,79,111,119	0
12	LHG	B	5004	49/49	0.21	1.08	59,88,99,106	0
15	CLA	B	1230	65/65	0.15	1.05	53,68,118,125	0
15	CLA	A	1022	65/65	0.23	1.04	53,78,96,103	0
15	CLA	A	1127	65/65	0.36	1.04	67,79,100,106	0
15	CLA	A	1126	65/65	0.23	1.02	63,80,101,116	0
14	BCR	F	4016	40/40	0.15	1.01	59,72,89,94	0
11	SF4	C	3002	8/8	0.21	1.01	60,88,151,152	0
15	CLA	K	1401	46/65	0.30	1.00	120,155,169,173	0
15	CLA	B	1234	65/65	0.25	0.98	56,73,108,120	0
15	CLA	A	1135	55/65	0.25	0.95	70,98,132,135	0
15	CLA	A	1012	65/65	0.23	0.94	47,60,86,93	0
10	PQN	A	2001	33/33	0.19	0.89	45,57,68,74	0
15	CLA	A	1132	62/65	0.15	0.85	74,105,153,156	0
14	BCR	B	4011	40/40	0.19	0.84	49,67,84,91	0
15	CLA	K	1402	46/65	0.32	0.77	163,187,214,221	0
15	CLA	A	1102	65/65	0.17	0.77	55,81,107,112	0
15	CLA	B	1219	55/65	0.17	0.75	74,86,119,142	0
15	CLA	B	1216	65/65	0.17	0.72	67,91,106,118	0
15	CLA	A	1116	54/65	0.37	0.69	84,113,130,141	0
15	CLA	F	1301	45/65	0.17	0.65	54,75,97,131	0
15	CLA	B	1224	65/65	0.27	0.63	60,78,98,108	0
15	CLA	B	1215	65/65	0.24	0.62	72,85,104,106	0
15	CLA	A	1105	65/65	0.19	0.50	70,96,111,120	0
15	CLA	B	1021	65/65	0.22	0.50	49,69,80,84	0
15	CLA	B	1218	51/65	0.19	0.50	86,98,125,159	0
15	CLA	A	1117	65/65	0.37	0.48	80,100,111,113	0
15	CLA	B	1210	65/65	0.20	0.47	75,95,108,120	0
15	CLA	A	1103	65/65	0.24	0.45	61,80,108,118	0
15	CLA	A	1140	65/65	0.18	0.44	52,73,103,116	0
15	CLA	A	1123	65/65	0.25	0.43	75,88,98,104	0
15	CLA	A	1130	55/65	0.15	0.39	82,106,133,139	0
12	LHG	A	5001	49/49	0.19	0.37	49,70,91,100	0
15	CLA	B	1217	47/65	0.19	0.30	96,114,132,157	0
13	CL0	A	1011	65/65	0.18	0.27	51,69,81,99	0
15	CLA	B	1227	45/65	0.15	0.27	54,72,94,98	0
15	CLA	B	1013	65/65	0.20	0.27	46,53,77,89	0
14	BCR	A	4008	40/40	0.29	0.24	67,93,105,115	0
14	BCR	B	4014	40/40	0.17	0.24	46,62,88,89	0
15	CLA	A	1109	65/65	0.17	0.20	66,81,105,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	CLA	B	1220	56/65	0.14	0.18	61,77,111,119	0
15	CLA	B	1201	46/65	0.17	0.15	72,83,107,123	0
15	CLA	A	1133	46/65	0.25	0.13	86,103,118,128	0
15	CLA	A	1125	52/65	0.26	0.13	76,98,124,133	0
14	BCR	B	4010	40/40	0.17	0.12	55,74,102,113	0
15	CLA	A	1119	64/65	0.24	0.12	78,97,115,137	0
15	CLA	A	1118	46/65	0.17	0.11	99,113,135,154	0
15	CLA	A	1124	55/65	0.29	0.10	61,92,120,129	0
14	BCR	A	4001	40/40	0.25	0.09	111,127,138,140	0
15	CLA	B	1212	45/65	0.20	0.09	101,117,128,143	0
15	CLA	B	1208	45/65	0.17	0.09	88,114,130,140	0
15	CLA	B	1205	55/65	0.16	0.06	68,87,100,112	0
15	CLA	A	1128	65/65	0.20	0.06	54,74,90,101	0
15	CLA	B	1235	65/65	0.17	0.05	55,66,85,92	0
12	LHG	A	5005	36/49	0.21	0.03	103,143,182,188	0
15	CLA	B	1237	55/65	0.16	-0.01	71,82,117,132	0
15	CLA	A	1131	55/65	0.16	-0.01	78,107,126,140	0
15	CLA	B	1226	65/65	0.18	-0.02	54,79,133,144	0
15	CLA	B	1223	65/65	0.22	-0.02	59,77,94,98	0
15	CLA	B	1202	65/65	0.18	-0.03	67,82,99,106	0
15	CLA	B	1213	50/65	0.16	-0.06	89,104,128,136	0
15	CLA	A	1104	65/65	0.23	-0.10	58,72,83,96	0
15	CLA	B	1203	65/65	0.21	-0.16	62,83,99,104	0
15	CLA	B	1238	44/65	0.15	-0.16	68,80,92,111	0
15	CLA	B	1211	46/65	0.15	-0.16	90,106,116,133	0
15	CLA	A	1120	49/65	0.19	-0.16	101,116,140,156	0
15	CLA	B	1225	65/65	0.21	-0.19	66,80,100,104	0
15	CLA	B	1239	46/65	0.19	-0.20	62,78,107,141	0
15	CLA	B	1236	50/65	0.18	-0.21	52,72,106,114	0
15	CLA	A	1137	50/65	0.18	-0.24	72,94,128,134	0
16	LMU	B	1301	35/35	0.20	-0.28	120,136,148,154	0
15	CLA	B	1232	45/65	0.16	-0.32	72,89,109,115	0
15	CLA	B	1221	65/65	0.17	-0.36	68,79,105,125	0
15	CLA	B	1207	46/65	0.31	-0.36	118,164,185,189	0
15	CLA	A	1113	45/65	0.24	-0.38	112,129,158,162	0
15	CLA	B	1206	46/65	0.17	-0.38	78,100,119,149	0
15	CLA	A	1134	46/65	0.22	-0.42	109,127,151,186	0
15	CLA	A	1115	46/65	0.22	-0.48	109,129,140,151	0
15	CLA	A	1129	46/65	0.16	-0.51	76,92,115,151	0
15	CLA	A	1107	50/65	0.14	-0.51	56,64,98,112	0
15	CLA	A	1112	45/65	0.16	-0.62	89,115,127,130	0
15	CLA	B	1209	45/65	0.15	-0.66	102,113,134,148	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	CLA	B	1204	46/65	0.16	-0.69	79,96,115,137	0
15	CLA	B	1222	56/65	0.22	-0.73	52,66,101,108	0
15	CLA	A	1114	49/65	0.20	-0.85	98,124,137,150	0
18	CL	B	6000	1/1	0.09	-1.70	82,82,82,82	0

6.5 Other polymers ⓘ

There are no such residues in this entry.