



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 9, 2019 – 02:44 AM EST

PDB ID : 6RD8
EMDB ID: : EMD-4809
Title : CryoEM structure of Polytomella F-ATP synthase, c-ring position 2, focussed refinement of Fo and peripheral stalk
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on : 2019-04-12
Resolution : 3.08 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

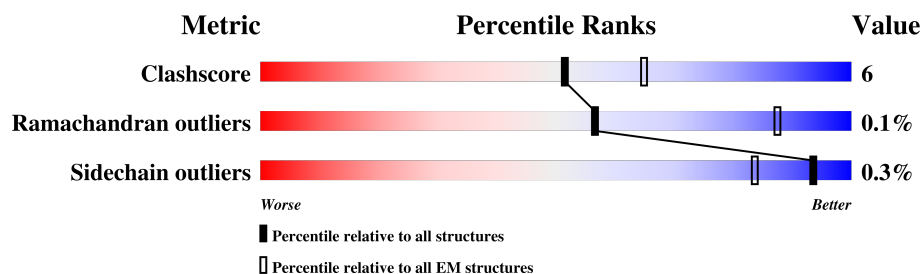
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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.



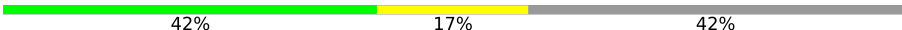
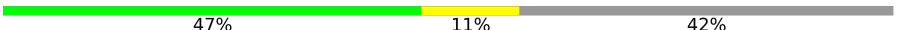
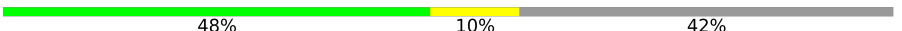
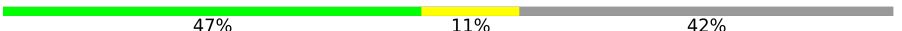



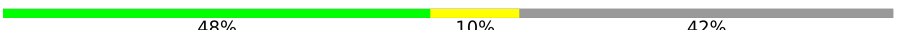

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	82	88% 11% .
2	1	618	86% 10% .
3	3	325	64% 11% 25%
4	5	123	90% 10%
5	6	151	74% 8% 18%
6	8	89	88% 10% ..
7	9	97	79% 16% ..
8	A	127	44% 14% 42%
8	B	127	45% 13% 42%

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Mol	Chain	Length	Quality of chain
8	C	127	 42%17%42%
8	D	127	 47%11%42%
8	E	127	 48%10%42%
8	F	127	 47%11%42%
8	G	127	 52%6%42%
8	H	127	 50%9%42%
8	I	127	 50%9%42%
8	J	127	 48%10%42%
9	M	327	 56%9%34%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17312 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	81	Total	C	N	O	S	0	0
			605	387	105	110	3		

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	595	Total	C	N	O	S	0	0
			4661	2958	798	900	5		

- Molecule 3 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	245	Total	C	N	O	S	0	0
			1874	1204	299	370	1		

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	123	Total	C	N	O	S	0	0
			986	640	172	170	4		

- Molecule 5 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 6 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	8	88	Total	C	N	O	0	0
			692	456	115	121		

- Molecule 7 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	96	Total	C	N	O	S	0	0
			768	510	122	130	6		

- Molecule 8 is a protein called Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	74	Total	C	N	O	S	0	0
			515	340	83	89	3		
8	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
8	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
8	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
8	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
8	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
8	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
8	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
8	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
8	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	M	1	Total	Zn	0
			1	1	

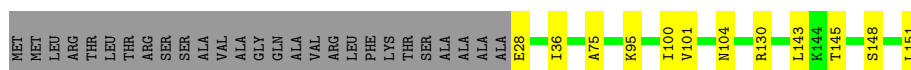
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	0	2	Total 2	O 2	0
11	1	1	Total 1	O 1	0
11	3	2	Total 2	O 2	0
11	5	2	Total 2	O 2	0
11	6	1	Total 1	O 1	0
11	A	1	Total 1	O 1	0
11	M	9	Total 9	O 9	0


- Molecule 1: ASA-10: Polytomella F-ATP synthase associated subunit 10



Chain 6:  74% 8% 18%




- Molecule 6: Mitochondrial ATP synthase subunit ASA8

Chain 8:  88% 10% ..



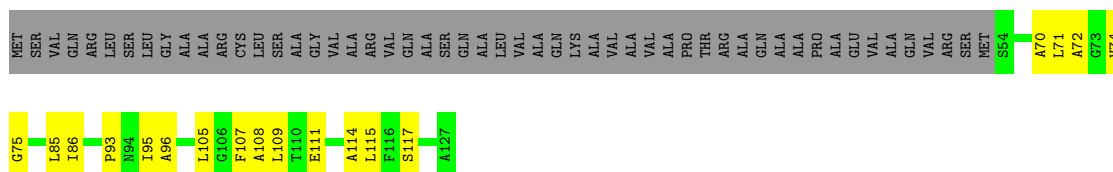
- Molecule 7: ASA-9: Polytomella F-ATP synthase associated subunit 9

Chain 9:  79% 16% ..



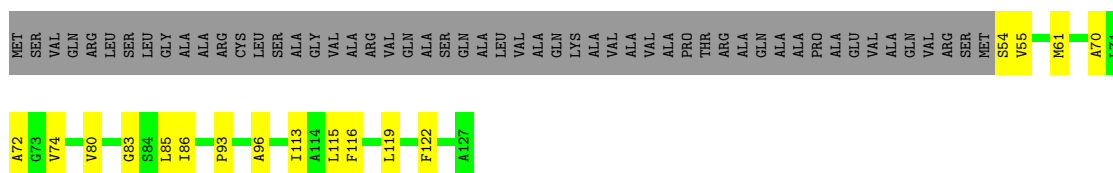
- Molecule 8: Mitochondrial ATP synthase subunit c

Chain A:  44% 14% 42%



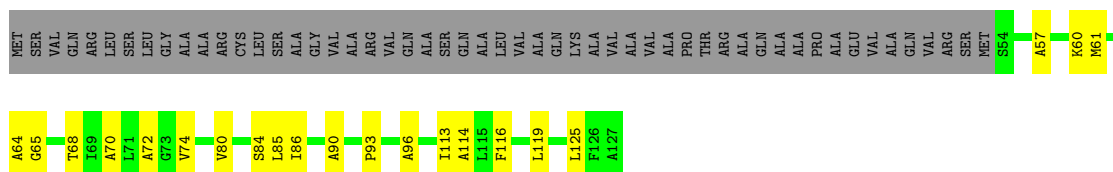
- Molecule 8: Mitochondrial ATP synthase subunit c

Chain B:  45% 13% 42%



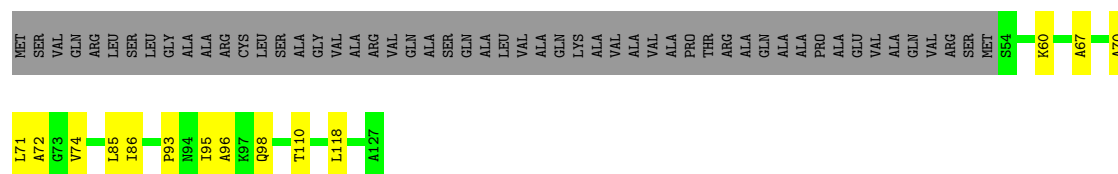
- Molecule 8: Mitochondrial ATP synthase subunit c

Chain C:  42% 17% 42%



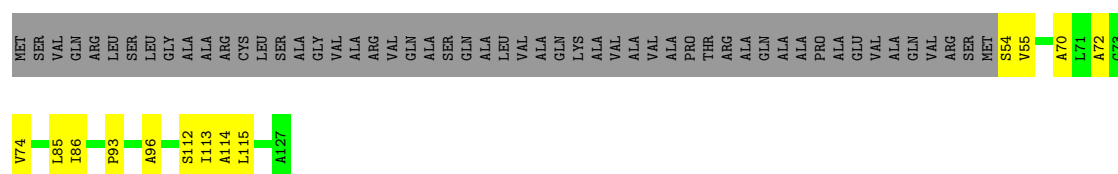
- Molecule 8: Mitochondrial ATP synthase subunit c

Chain D:  47% 11% 42%



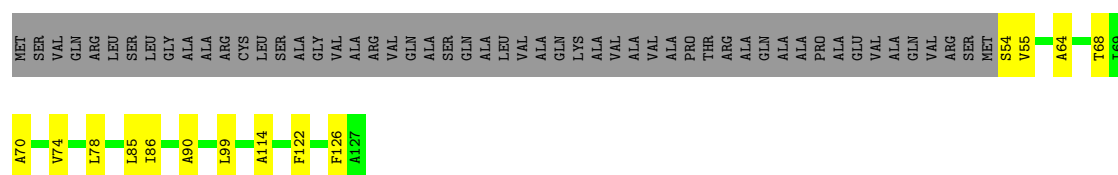
- Molecule 8: Mitochondrial ATP synthase subunit c

Chain E:  48% 10% 42%



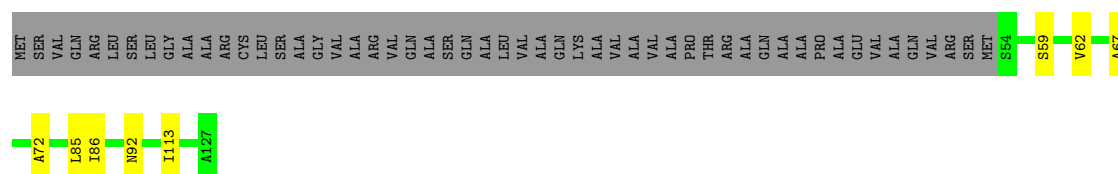
- Molecule 8: Mitochondrial ATP synthase subunit c

Chain F:  47% 11% 42%



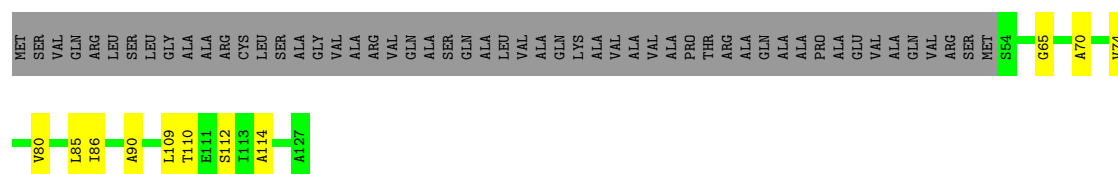
- Molecule 8: Mitochondrial ATP synthase subunit c

Chain G:  52% 6% 42%



- Molecule 8: Mitochondrial ATP synthase subunit c

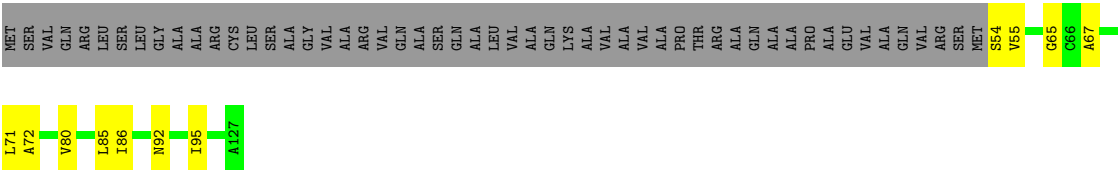
Chain H:  50% 9% 42%



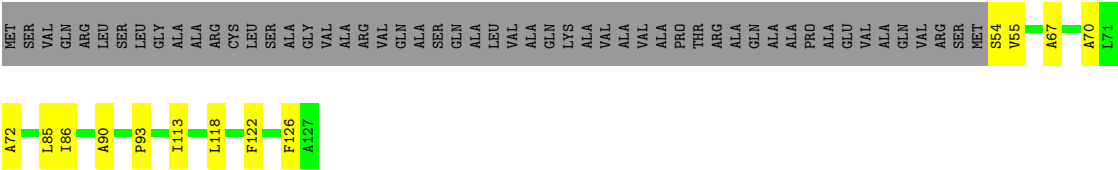
- Molecule 8: Mitochondrial ATP synthase subunit c

Chain I:  50% 9% 42%

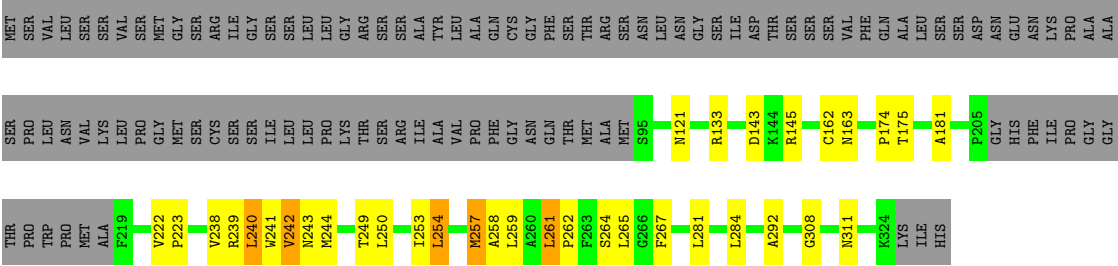




● Molecule 8: Mitochondrial ATP synthase subunit c



● Molecule 9: Mitochondrial ATP synthase subunit 6



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	136422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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 >2	RMSZ	# Z >2
1	0	0.37	0/625	0.48	0/851
2	1	0.41	0/4750	0.48	0/6434
3	3	0.42	0/1911	0.51	1/2601 (0.0%)
4	5	0.45	0/1011	0.49	0/1376
5	6	0.40	0/946	0.49	0/1287
6	8	0.47	0/715	0.56	1/974 (0.1%)
7	9	0.44	0/794	0.49	0/1073
8	A	0.43	0/521	0.53	0/704
8	B	0.37	0/520	0.44	0/704
8	C	0.36	0/520	0.44	0/704
8	D	0.36	0/520	0.43	0/704
8	E	0.35	0/520	0.49	0/704
8	F	0.34	0/520	0.44	0/704
8	G	0.33	0/520	0.51	0/704
8	H	0.33	0/520	0.52	0/704
8	I	0.32	0/520	0.45	0/704
8	J	0.35	0/520	0.52	0/704
9	M	0.46	0/1683	0.56	0/2295
All	All	0.41	0/17636	0.50	2/23931 (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
7	9	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	77	PRO	N-CA-CB	6.00	110.50	103.30
6	8	8	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	57	PHE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	605	0	589	7	0
2	1	4661	0	4695	44	0
3	3	1874	0	1826	26	0
4	5	986	0	1021	11	0
5	6	926	0	941	11	0
6	8	692	0	694	8	0
7	9	768	0	749	16	0
8	A	515	0	554	28	0
8	B	514	0	554	24	0
8	C	514	0	554	17	0
8	D	514	0	554	12	0
8	E	514	0	554	10	0
8	F	514	0	554	11	0
8	G	514	0	554	7	0
8	H	514	0	554	9	0
8	I	514	0	554	10	0
8	J	514	0	554	11	0
9	M	1640	0	1665	48	0
10	M	1	0	0	0	0
11	0	2	0	0	0	0
11	1	1	0	0	0	0
11	3	2	0	0	0	0
11	5	2	0	0	0	0
11	6	1	0	0	0	0
11	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	9	0	0	0	0
All	All	17312	0	17720	219	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 219 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:115:LEU:HB3	9:M:242:VAL:HG11	1.25	1.16
8:A:115:LEU:HD22	9:M:242:VAL:CG1	1.75	1.15
8:A:115:LEU:HD22	9:M:242:VAL:HG12	1.26	1.14
7:9:56:ASN:O	7:9:56:ASN:OD1	1.79	1.01
8:A:115:LEU:CB	9:M:242:VAL:HG11	2.00	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	0	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
2	1	593/618 (96%)	579 (98%)	14 (2%)	0	100	100
3	3	243/325 (75%)	234 (96%)	9 (4%)	0	100	100
4	5	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
5	6	122/151 (81%)	119 (98%)	3 (2%)	0	100	100
6	8	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
7	9	94/97 (97%)	84 (89%)	7 (7%)	3 (3%)	4	23
8	A	72/127 (57%)	71 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	B	72/127 (57%)	72 (100%)	0	0	100	100
8	C	72/127 (57%)	72 (100%)	0	0	100	100
8	D	72/127 (57%)	72 (100%)	0	0	100	100
8	E	72/127 (57%)	72 (100%)	0	0	100	100
8	F	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
8	G	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
8	H	72/127 (57%)	72 (100%)	0	0	100	100
8	I	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
8	J	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
9	M	213/327 (65%)	210 (99%)	3 (1%)	0	100	100
All	All	2271/3082 (74%)	2215 (98%)	53 (2%)	3 (0%)	56	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	9	76	THR
7	9	58	PRO
7	9	66	ILE

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 PDB entries followed by that with respect to all EM entries.

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	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	493 (100%)	0	100	100
3	3	195/258 (76%)	195 (100%)	0	100	100
4	5	107/107 (100%)	107 (100%)	0	100	100
5	6	96/115 (84%)	96 (100%)	0	100	100
6	8	71/72 (99%)	71 (100%)	0	100	100
7	9	78/79 (99%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A	50/86 (58%)	50 (100%)	0	100	100
8	B	50/86 (58%)	50 (100%)	0	100	100
8	C	50/86 (58%)	50 (100%)	0	100	100
8	D	50/86 (58%)	50 (100%)	0	100	100
8	E	50/86 (58%)	50 (100%)	0	100	100
8	F	50/86 (58%)	50 (100%)	0	100	100
8	G	50/86 (58%)	50 (100%)	0	100	100
8	H	50/86 (58%)	50 (100%)	0	100	100
8	I	50/86 (58%)	50 (100%)	0	100	100
8	J	50/86 (58%)	50 (100%)	0	100	100
9	M	178/272 (65%)	172 (97%)	6 (3%)	40	73
All	All	1781/2339 (76%)	1775 (100%)	6 (0%)	93	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	M	254	LEU
9	M	264	SER
9	M	257	MET
9	M	242	VAL
9	M	261	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
4	5	29	GLN
5	6	40	ASN
9	M	163	ASN
4	5	79	ASN
6	8	26	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.