



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 21, 2017 – 01:54 PM EST

PDB ID : 6B2Z
EMDB ID: : EMD-7036
Title : Cryo-EM structure of the dimeric FO region of yeast mitochondrial ATP synthase
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : unknown
Resolution : 3.60 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

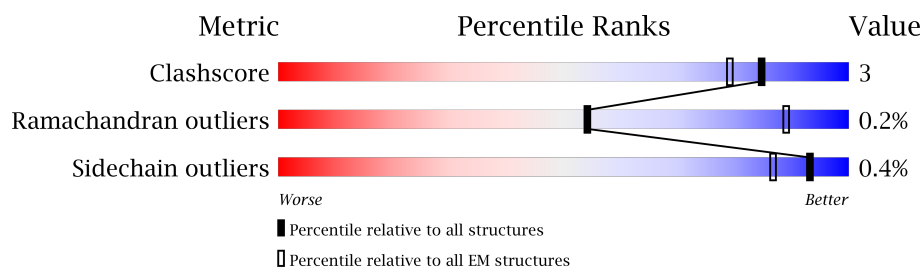
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



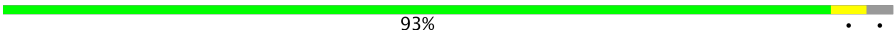
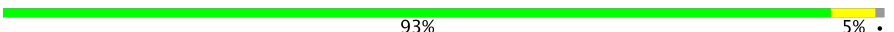
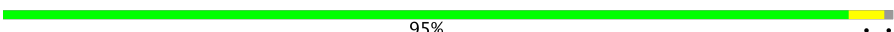









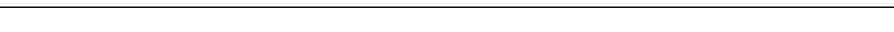

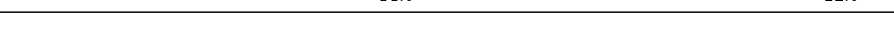
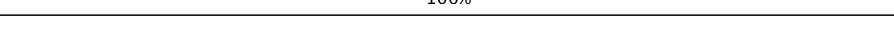
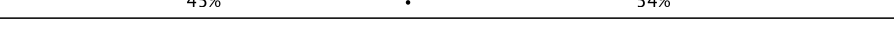



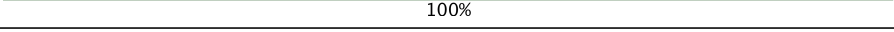
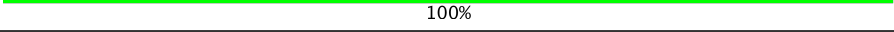


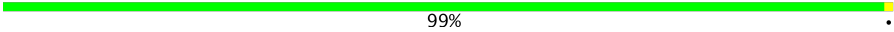
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	76	95% ..
1	1	76	96% ..
1	2	76	89% 8% ..
1	3	76	92% . . .
1	4	76	92% 7% .
1	5	76	91% 7% ..
1	6	76	89% 8% .
1	7	76	91% 5% .
1	8	76	95% ..

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Mol	Chain	Length	Quality of chain
1	9	76	 93% . .
1	B	76	 93% 5% .
1	C	76	 95% . .
1	D	76	 89% 8% ..
1	E	76	 91% 5% . .
1	F	76	 91% 8% .
1	G	76	 91% 7% ..
1	H	76	 89% 8% .
1	I	76	 91% 5% .
1	J	76	 95% . .
1	K	76	 92% 5% .
2	A	48	 88% 10% .
2	L	48	 83% 15% .
3	M	249	 88% 12%
3	a	249	 100%
4	N	209	 45% . 54%
4	b	209	 45% . 54%
5	O	173	 24% 6% . 69%
5	d	173	 29% . 69%
6	P	49	 100%
6	e	49	 100%
7	Q	95	 67% . 28%
7	f	95	 72% 28%
8	R	106	 99% .
8	g	106	 99% .

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Mol	Chain	Length	Quality of chain
9	S	59	<div><div></div><div>97%</div><div>.</div></div>
9	i	59	<div><div></div><div>100%</div><div></div></div>
10	T	68	<div><div></div><div>32%</div><div>.</div><div></div><div>65%</div></div>
10	k	68	<div><div></div><div>35%</div><div></div><div>65%</div></div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21436 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 ATP synthase subunit c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	2	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	3	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	4	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	5	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	6	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	7	73	Total	C	N	O	S	0	0
			522	348	81	89	4		
1	8	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	9	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	0	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	C	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	D	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	E	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	F	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	G	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	H	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	I	73	Total	C	N	O	S	0	0
			522	348	81	89	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
1	K	74	Total	C	N	O	S	0	0
			529	354	82	90	3		
1	B	75	Total	C	N	O	S	0	0
			537	359	83	91	4		

- Molecule 2 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	48	Total	C	N	O	S	0	0
			410	287	59	60	4		
2	L	48	Total	C	N	O	S	0	0
			410	287	59	60	4		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	249	Total	C	N	O	S	0	0
			1971	1338	296	326	11		
3	M	249	Total	C	N	O	S	0	0
			1971	1338	296	326	11		

- Molecule 4 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	97	Total	C	N	O	S	0	0
			639	407	107	124	1		
4	N	97	Total	C	N	O	S	0	0
			639	407	107	124	1		

- Molecule 5 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	53	Total	C	N	O	S	0	0
			411	262	69	78	2		
5	O	53	Total	C	N	O	S	0	0
			411	262	69	78	2		

- Molecule 6 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	49	Total	C	N	O	0	0
			245	147	49	49		
6	P	49	Total	C	N	O	0	0
			245	147	49	49		

- Molecule 7 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	68	Total	C	N	O	S	0	0
			528	349	92	86	1		
7	Q	68	Total	C	N	O	S	0	0
			528	349	92	86	1		

- Molecule 8 is a protein called ATP synthase subunit g.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	g	106	Total	C	N	O	0	0
			530	318	106	106		
8	R	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 9 is a protein called ATP synthase subunit j, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	59	Total	C	N	O	S	0	0
			473	313	78	80	2		
9	S	59	Total	C	N	O	S	0	0
			473	313	78	80	2		

- Molecule 10 is a protein called ATP synthase subunit k, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	24	Total	C	N	O	S	0	0
			180	122	30	27	1		
10	T	24	Total	C	N	O	S	0	0
			180	122	30	27	1		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

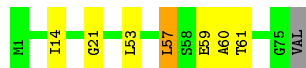
- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 1:  96% ..



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 2:  89% 8% ..



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 3:  92% ...



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 4:  92% 7% .




- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 5:  91% 7% ..



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 6:  89% 8% .



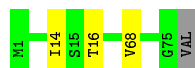
- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 7:  91% 5% .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 8:  95% . .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 9:  93% . .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain 0:  95% . .




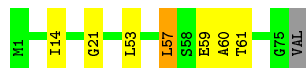
- Molecule 1: ATP synthase subunit c, mitochondrial

Chain C:  95% . .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain D:  89% 8% . .



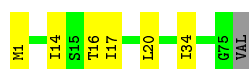
- Molecule 1: ATP synthase subunit c, mitochondrial

Chain E:  91% 5% . .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain F:  91% 8% .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain G: 91% 7% ..



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain H: 89% 8% .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain I: 91% 5% .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain J: 95% . .



- Molecule 1: ATP synthase subunit c, mitochondrial

Chain K: 92% 5% .



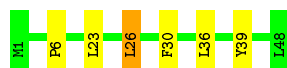
- Molecule 1: ATP synthase subunit c, mitochondrial

Chain B: 93% 5% .




- Molecule 2: ATP synthase protein 8

Chain A: 88% 10% .



- Molecule 2: ATP synthase protein 8

Chain L:  83% 15% .




- Molecule 3: ATP synthase subunit a

Chain a:  100%



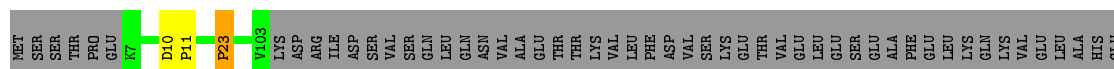
- Molecule 3: ATP synthase subunit a

Chain M:  88% 12%



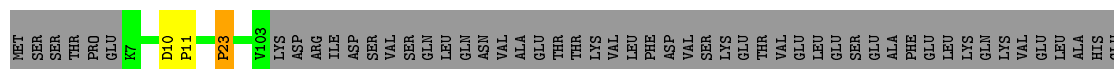
- Molecule 4: ATP synthase subunit b

Chain b:  45% 54%



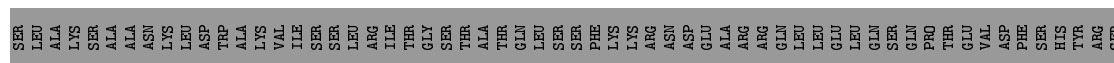
- Molecule 4: ATP synthase subunit b

Chain N:  45% 54%



- Molecule 5: ATP synthase subunit d, mitochondrial

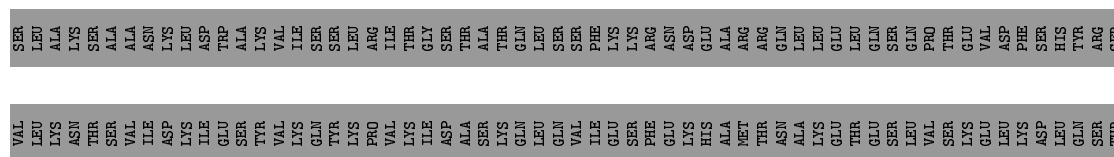
Chain d:  29% 69%





- Molecule 5: ATP synthase subunit d, mitochondrial

Chain O: 24% 6% 69%



- Molecule 6: ATP synthase subunit e, mitochondrial

Chain e: 100%

There are no outlier residues recorded for this chain.

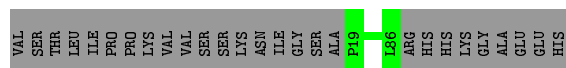
- Molecule 6: ATP synthase subunit e, mitochondrial

Chain P: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: ATP synthase subunit f, mitochondrial

Chain f: 72% 28%



- Molecule 7: ATP synthase subunit f, mitochondrial

Chain Q: 67% 28%



- Molecule 8: ATP synthase subunit g

Chain g: 99%



- Molecule 8: ATP synthase subunit g

Chain R: 99%



- Molecule 9: ATP synthase subunit j, mitochondrial

Chain i: 100%

There are no outlier residues recorded for this chain.

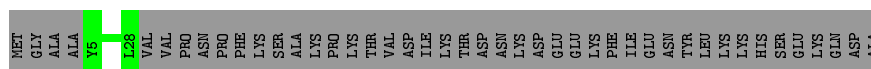
- Molecule 9: ATP synthase subunit j, mitochondrial

Chain S: 97%



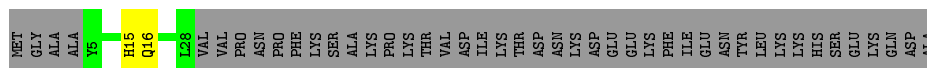
- Molecule 10: ATP synthase subunit k, mitochondrial

Chain k: 35% 65%



- Molecule 10: ATP synthase subunit k, mitochondrial

Chain T: 32% 65%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	238848	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 ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	47170	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.34	0/545	0.61	0/737
1	1	0.35	0/545	0.55	0/737
1	2	0.38	0/545	0.67	1/737 (0.1%)
1	3	0.37	0/537	0.61	1/727 (0.1%)
1	4	0.34	0/545	0.60	0/737
1	5	0.32	0/545	0.58	0/737
1	6	0.33	0/537	0.60	0/727
1	7	0.31	0/529	0.56	0/716
1	8	0.31	0/545	0.56	0/737
1	9	0.32	0/537	0.57	0/727
1	B	0.34	0/545	0.60	0/737
1	C	0.34	0/545	0.55	0/737
1	D	0.38	0/545	0.67	1/737 (0.1%)
1	E	0.37	0/537	0.61	1/727 (0.1%)
1	F	0.34	0/545	0.60	0/737
1	G	0.32	0/545	0.58	0/737
1	H	0.33	0/537	0.60	0/727
1	I	0.31	0/529	0.56	0/716
1	J	0.31	0/545	0.56	0/737
1	K	0.32	0/537	0.57	0/727
10	T	0.28	0/185	0.68	0/250
10	k	0.28	0/185	0.68	0/250
2	A	0.50	0/422	0.77	1/570 (0.2%)
2	L	0.50	0/422	0.77	1/570 (0.2%)
3	M	0.45	0/2023	0.70	0/2758
3	a	0.45	0/2023	0.70	0/2758
4	N	0.34	0/646	0.58	2/883 (0.2%)
4	b	0.34	0/646	0.58	2/883 (0.2%)
5	O	0.37	0/418	0.60	1/563 (0.2%)
5	d	0.37	0/418	0.60	1/563 (0.2%)
7	Q	0.38	0/546	0.59	0/738
7	f	0.38	0/546	0.59	0/738
9	S	0.42	0/488	0.60	0/659
9	i	0.42	0/488	0.60	0/659

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
All	All	0.38	0/20276	0.62	12/27480 (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
8	R	0	2
8	g	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	281	LEU	CA-CB-CG	7.81	133.26	115.30
5	O	281	LEU	CA-CB-CG	7.81	133.26	115.30
2	A	26	LEU	CA-CB-CG	7.72	133.06	115.30
2	L	26	LEU	CA-CB-CG	7.71	133.03	115.30
1	2	57	LEU	CA-CB-CG	5.79	128.62	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	R	80	UNK	Mainchain,Peptide
8	g	80	UNK	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	537	0	582	4	0
1	1	537	0	582	3	0
1	2	537	0	582	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	529	0	570	4	0
1	4	537	0	582	5	0
1	5	537	0	582	5	0
1	6	529	0	570	5	0
1	7	522	0	570	4	0
1	8	537	0	582	4	0
1	9	529	0	570	4	0
1	B	537	0	582	5	0
1	C	537	0	582	4	0
1	D	537	0	582	6	0
1	E	529	0	570	5	0
1	F	537	0	582	6	0
1	G	537	0	582	5	0
1	H	529	0	570	5	0
1	I	522	0	570	4	0
1	J	537	0	582	4	0
1	K	529	0	570	5	0
2	A	410	0	444	3	0
2	L	410	0	444	5	0
3	M	1971	0	2071	17	0
3	a	1971	0	2071	0	0
4	N	639	0	555	0	0
4	b	639	0	555	0	0
5	O	411	0	397	7	0
5	d	411	0	397	0	0
6	P	245	0	51	0	0
6	e	245	0	51	0	0
7	Q	528	0	494	2	0
7	f	528	0	494	0	0
8	R	530	0	108	0	0
8	g	530	0	108	0	0
9	S	473	0	476	1	0
9	i	473	0	476	0	0
10	T	180	0	192	1	0
10	k	180	0	192	0	0
All	All	21436	0	21120	85	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 3.

The worst 5 of 85 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)
3:M:27:THR:H	3:M:30:SER:HB3	1.61	0.66
1:8:14:ILE:HG21	1:9:14:ILE:HD13	1.83	0.61
1:J:14:ILE:HG21	1:K:14:ILE:HD13	1.83	0.60
1:F:17:ILE:HB	1:G:17:ILE:HG12	1.87	0.57
3:M:211:VAL:HG23	3:M:212:PRO:HD3	1.87	0.56

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	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	3	72/76 (95%)	72 (100%)	0	0	100	100
1	4	73/76 (96%)	73 (100%)	0	0	100	100
1	5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	6	72/76 (95%)	72 (100%)	0	0	100	100
1	7	71/76 (93%)	71 (100%)	0	0	100	100
1	8	73/76 (96%)	73 (100%)	0	0	100	100
1	9	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
1	B	73/76 (96%)	73 (100%)	0	0	100	100
1	C	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	D	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	E	72/76 (95%)	72 (100%)	0	0	100	100
1	F	73/76 (96%)	73 (100%)	0	0	100	100
1	G	73/76 (96%)	72 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	72/76 (95%)	72 (100%)	0	0	100	100
1	I	71/76 (93%)	71 (100%)	0	0	100	100
1	J	73/76 (96%)	73 (100%)	0	0	100	100
1	K	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
2	A	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	8	47
2	L	46/48 (96%)	43 (94%)	2 (4%)	1 (2%)	8	47
3	M	247/249 (99%)	228 (92%)	19 (8%)	0	100	100
3	a	247/249 (99%)	228 (92%)	19 (8%)	0	100	100
4	N	95/209 (46%)	87 (92%)	6 (6%)	2 (2%)	8	48
4	b	95/209 (46%)	87 (92%)	6 (6%)	2 (2%)	8	48
5	O	51/173 (30%)	50 (98%)	1 (2%)	0	100	100
5	d	51/173 (30%)	50 (98%)	1 (2%)	0	100	100
7	Q	66/95 (70%)	58 (88%)	8 (12%)	0	100	100
7	f	66/95 (70%)	58 (88%)	8 (12%)	0	100	100
9	S	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
9	i	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
10	T	22/68 (32%)	19 (86%)	3 (14%)	0	100	100
10	k	22/68 (32%)	19 (86%)	3 (14%)	0	100	100
All	All	2618/3322 (79%)	2506 (96%)	106 (4%)	6 (0%)	54	85

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	b	10	ASP
4	N	10	ASP
2	A	6	PRO
4	b	23	PRO
2	L	6	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 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	55/56 (98%)	55 (100%)	0	100	100
1	1	55/56 (98%)	55 (100%)	0	100	100
1	2	55/56 (98%)	55 (100%)	0	100	100
1	3	54/56 (96%)	54 (100%)	0	100	100
1	4	55/56 (98%)	55 (100%)	0	100	100
1	5	55/56 (98%)	54 (98%)	1 (2%)	64	87
1	6	54/56 (96%)	54 (100%)	0	100	100
1	7	54/56 (96%)	54 (100%)	0	100	100
1	8	55/56 (98%)	55 (100%)	0	100	100
1	9	54/56 (96%)	54 (100%)	0	100	100
1	B	55/56 (98%)	55 (100%)	0	100	100
1	C	55/56 (98%)	55 (100%)	0	100	100
1	D	55/56 (98%)	55 (100%)	0	100	100
1	E	54/56 (96%)	54 (100%)	0	100	100
1	F	55/56 (98%)	55 (100%)	0	100	100
1	G	55/56 (98%)	54 (98%)	1 (2%)	64	87
1	H	54/56 (96%)	54 (100%)	0	100	100
1	I	54/56 (96%)	54 (100%)	0	100	100
1	J	55/56 (98%)	55 (100%)	0	100	100
1	K	54/56 (96%)	54 (100%)	0	100	100
2	A	47/47 (100%)	47 (100%)	0	100	100
2	L	47/47 (100%)	47 (100%)	0	100	100
3	M	217/217 (100%)	216 (100%)	1 (0%)	91	97
3	a	217/217 (100%)	216 (100%)	1 (0%)	91	97
4	N	48/182 (26%)	48 (100%)	0	100	100
4	b	48/182 (26%)	48 (100%)	0	100	100
5	O	42/158 (27%)	40 (95%)	2 (5%)	30	68
5	d	42/158 (27%)	40 (95%)	2 (5%)	30	68
7	Q	46/76 (60%)	46 (100%)	0	100	100
7	f	46/76 (60%)	46 (100%)	0	100	100
9	S	49/49 (100%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i	49/49 (100%)	49 (100%)	0	100	100
10	T	18/57 (32%)	18 (100%)	0	100	100
10	k	18/57 (32%)	18 (100%)	0	100	100
All	All	2026/2692 (75%)	2018 (100%)	8 (0%)	93	98

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	d	284	MET
5	O	284	MET
3	M	34	ILE
5	d	277	ARG
1	G	57	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	2	GLN
1	C	2	GLN

5.3.3 RNA [i](#)

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](#)

There are no ligands in this entry.

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.