



wwPDB EM Validation Summary Report ⓘ

Jun 27, 2024 – 12:13 AM JST

PDB ID : 8H9T
EMDB ID : EMD-34581
Title : Human ATP synthase state 2 (combined)
Authors : Lai, Y.; Zhang, Y.; Liu, F.; Gao, Y.; Gong, H.; Rao, Z.
Deposited on : 2022-10-25
Resolution : 2.77 Å (reported)

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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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

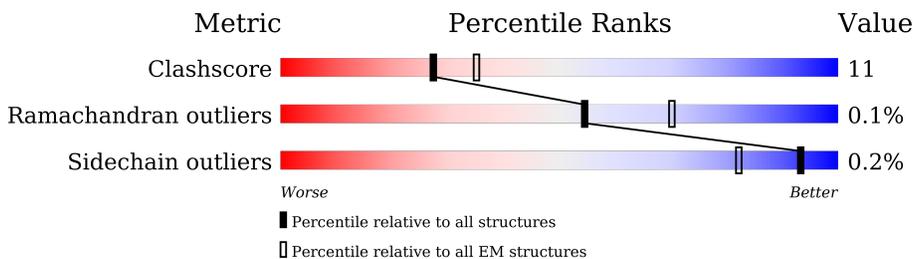
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	K	214	
2	L	108	
3	M	160	
4	1	75	
4	2	75	
4	3	75	
4	4	75	
4	5	75	

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Mol	Chain	Length	Quality of chain
4	6	75	81% 17%
4	7	75	84% 16%
4	8	75	79% 21%
5	H	146	59% 32% 10% 5%
6	I	51	65% 24% 12% 3%
7	N	226	69% 29%
8	P	58	53% 17% 29%
9	R	93	56% 24% 20%
10	S	102	35% 40% 25% 7%
11	T	69	30% 32% 36% 13%
12	Q	68	46% 29% 25%
13	A	510	75% 18% 6%
13	B	510	76% 19% 5%
13	C	510	77% 19%
14	D	482	67% 25% 8% 8%
14	E	482	78% 19%
14	F	482	79% 18%
15	G	273	73% 26% 9%
16	O	190	61% 37%

2 Entry composition i

There are 19 unique types of molecules in this entry. The entry contains 38255 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 F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	K	198	1573	1013	270	285	5	0	0

- Molecule 2 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	67	549	350	91	106	2	0	0

- Molecule 3 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	156	1259	813	199	243	4	0	0

- Molecule 4 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	75	534	353	83	94	4	0	0
4	7	75	534	353	83	94	4	0	0
4	8	75	534	353	83	94	4	0	0
4	1	75	534	353	83	94	4	0	0
4	2	75	534	353	83	94	4	0	0
4	3	75	534	353	83	94	4	0	0
4	4	75	534	353	83	94	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	75	Total	C	N	O	S	0	0
			534	353	83	94	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	132	Total	C	N	O	S	0	0
			975	614	164	195	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	45	Total	C	N	O	S	0	0
			354	225	64	64	1		

- Molecule 7 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	223	Total	C	N	O	S	0	0
			1718	1145	273	289	11		

- Molecule 8 is a protein called ATP synthase subunit ATP5MJ, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	41	Total	C	N	O	S	0	0
			344	234	53	54	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	74	Total	C	N	O	S	0	0
			621	411	104	103	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	77	Total	C	N	O	S	0	0
			604	401	96	106	1		

- Molecule 11 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	T	44	Total	C	N	O	0	0
			346	224	63	59		

- Molecule 12 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	51	Total	C	N	O	S	0	0
			422	281	67	68	6		

- Molecule 13 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	491	Total	C	N	O	S	0	0
			3745	2356	662	714	13		
13	A	477	Total	C	N	O	S	0	0
			3639	2290	645	692	12		
13	B	487	Total	C	N	O	S	0	0
			3714	2338	656	707	13		

- Molecule 14 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	466	Total	C	N	O	S	0	0
			3522	2234	597	678	13		
14	F	470	Total	C	N	O	S	0	0
			3562	2257	604	688	13		
14	D	442	Total	C	N	O	S	0	0
			3344	2118	571	643	12		

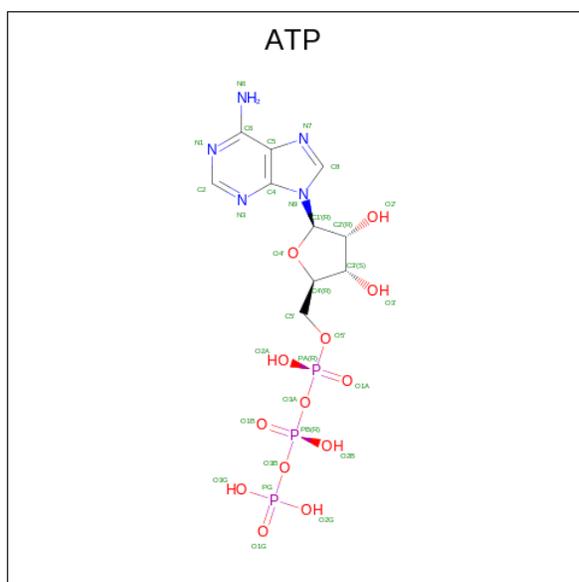
- Molecule 15 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	271	Total	C	N	O	S	0	0
			2103	1329	359	406	9		

- Molecule 16 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	187	Total	C	N	O	S	0	0
			1437	909	252	270	6		

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

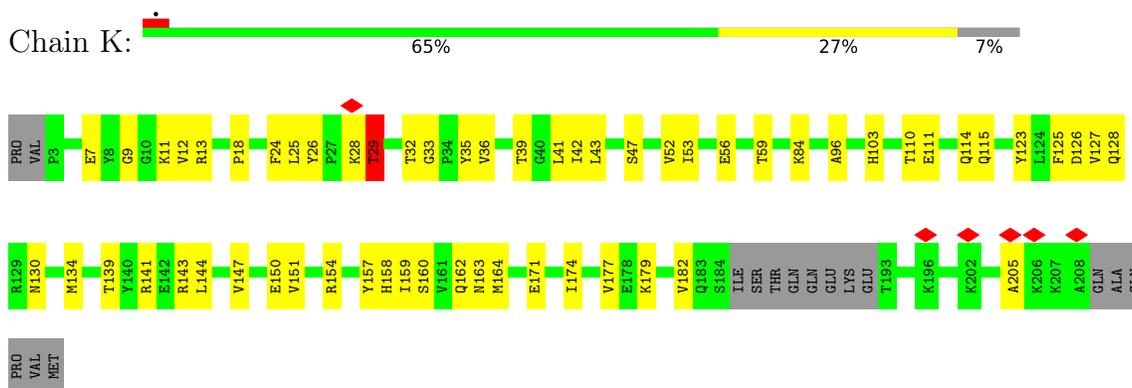
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
18	C	1	Total	Mg	0
			1	1	
18	A	1	Total	Mg	0
			1	1	
18	B	1	Total	Mg	0
			1	1	
18	F	1	Total	Mg	0
			1	1	
18	D	1	Total	Mg	0
			1	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

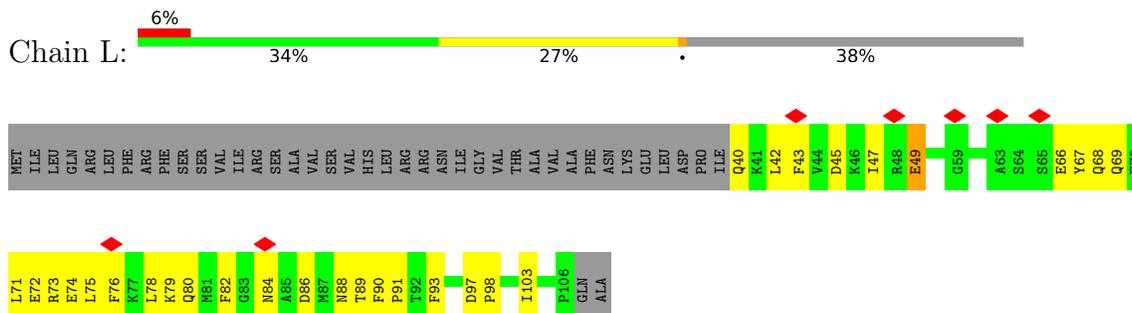
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

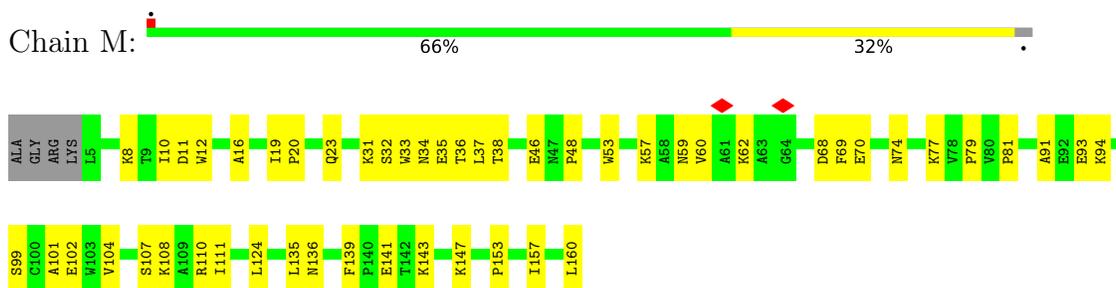
- Molecule 1: ATP synthase F(0) complex subunit B1, mitochondrial



- Molecule 2: ATP synthase-coupling factor 6, mitochondrial



- Molecule 3: ATP synthase subunit d, mitochondrial



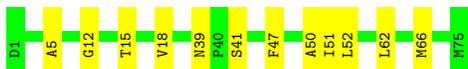
- Molecule 4: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 6:  81% 17%



• Molecule 4: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 7:  84% 16%



• Molecule 4: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 8:  79% 21%



• Molecule 4: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 1:  75% 25%



• Molecule 4: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 2:  77% 23%



• Molecule 4: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 3:  87% 12%



• Molecule 4: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 4:  88% 12%



- Molecule 4: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 5:  83% 17%



- Molecule 5: ATP synthase subunit delta, mitochondrial

Chain H:  5% 59% 32% 10%



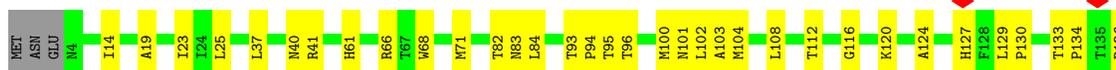
- Molecule 6: ATP synthase subunit epsilon, mitochondrial

Chain I:  65% 24% 12%



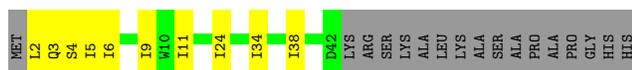
- Molecule 7: ATP synthase subunit a

Chain N:  69% 29%



- Molecule 8: ATP synthase subunit ATP5MJ, mitochondrial

Chain P:  53% 17% 29%

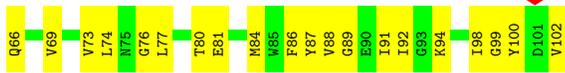
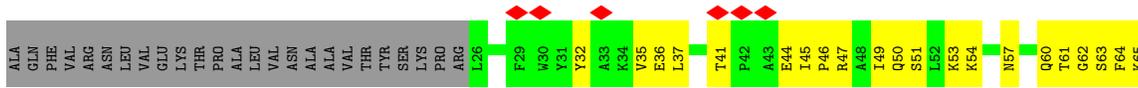


- Molecule 9: ATP synthase subunit f, mitochondrial

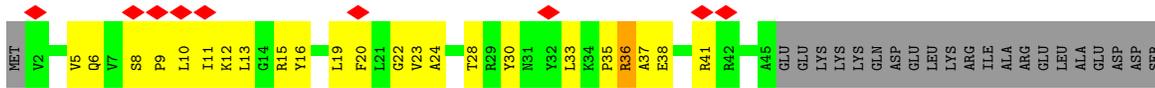
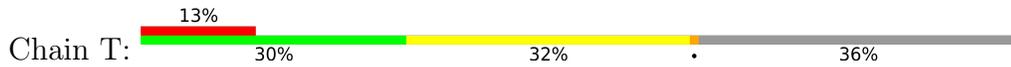
Chain R:  56% 24% 20%



• Molecule 10: ATP synthase subunit g, mitochondrial



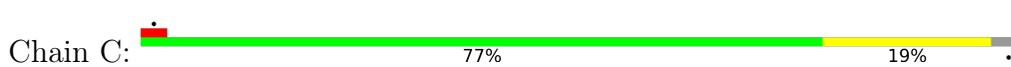
• Molecule 11: ATP synthase subunit e, mitochondrial



• Molecule 12: ATP synthase protein 8

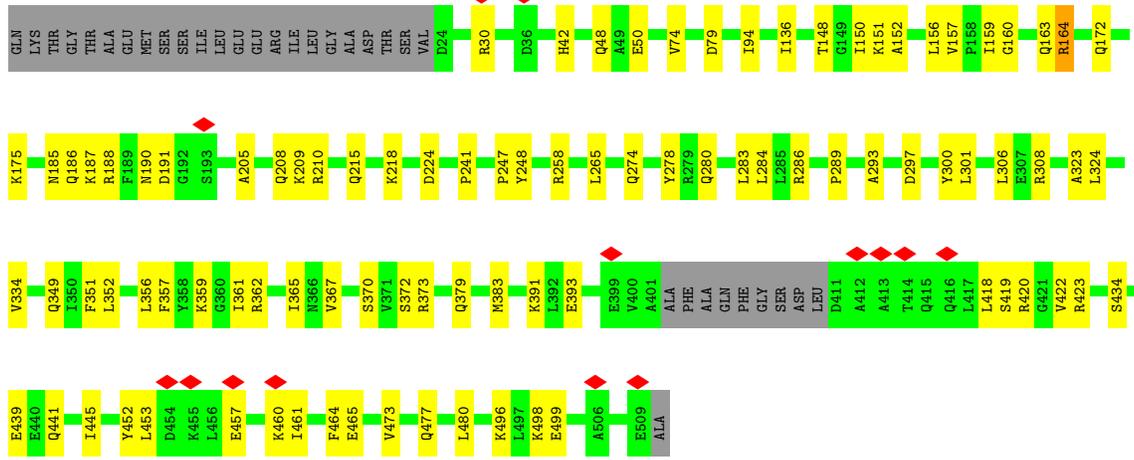


• Molecule 13: ATP synthase subunit alpha, mitochondrial



• Molecule 13: ATP synthase subunit alpha, mitochondrial

Chain A:  75% 18% 6%



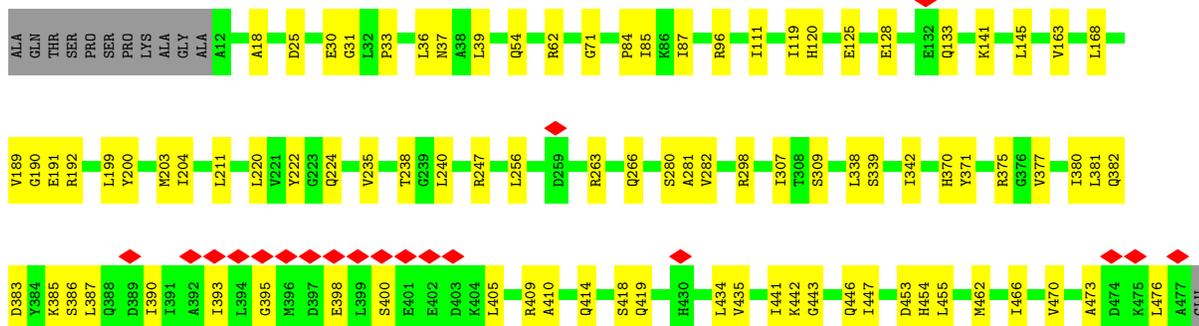
• Molecule 13: ATP synthase subunit alpha, mitochondrial

Chain B:  76% 19% 5%



• Molecule 14: ATP synthase subunit beta, mitochondrial

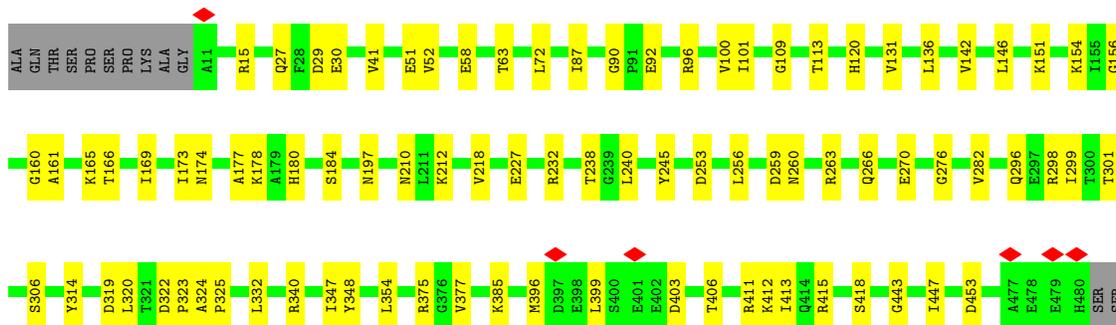
Chain E:  78% 19% 3%



GLU
HIS
SER
SER

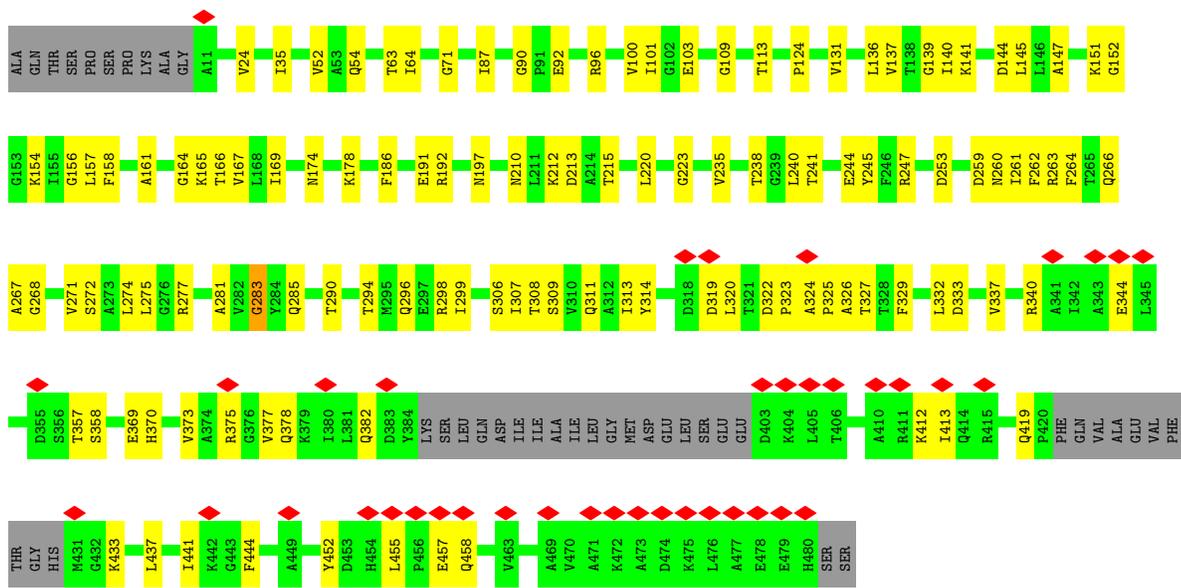
• Molecule 14: ATP synthase subunit beta, mitochondrial

Chain F:



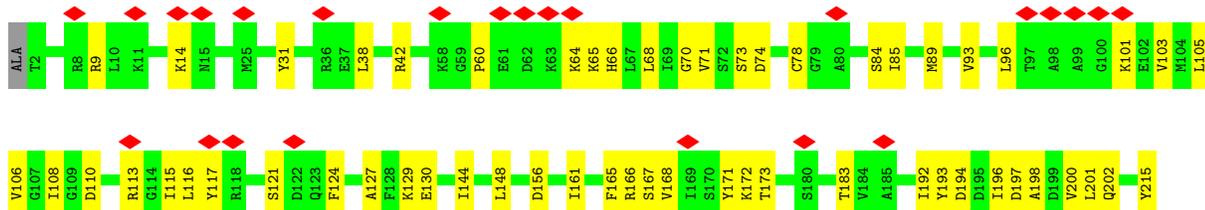
• Molecule 14: ATP synthase subunit beta, mitochondrial

Chain D:



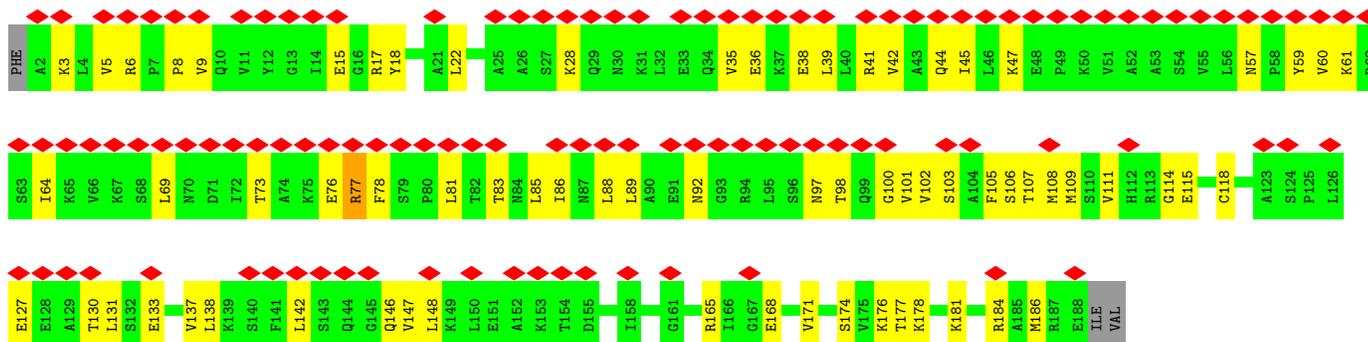
• Molecule 15: ATP synthase subunit gamma, mitochondrial

Chain G:





● Molecule 16: ATP synthase subunit O, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37480	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	38.103	Depositor
Minimum map value	-23.201	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.075	Depositor
Recommended contour level	4.5	Depositor
Map size (\AA)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG

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	K	0.39	0/1605	0.48	0/2169
2	L	0.34	0/560	0.59	0/748
3	M	0.36	0/1291	0.46	0/1755
4	1	0.41	0/543	0.50	0/732
4	2	0.41	0/543	0.50	0/732
4	3	0.41	0/543	0.50	0/732
4	4	0.41	0/543	0.49	0/732
4	5	0.41	0/543	0.50	0/732
4	6	0.41	0/543	0.49	0/732
4	7	0.41	0/543	0.50	0/732
4	8	0.41	0/543	0.50	0/732
5	H	0.35	0/987	0.51	0/1344
6	I	0.38	0/359	0.45	0/482
7	N	0.43	0/1755	0.54	0/2403
8	P	0.46	0/354	0.50	0/478
9	R	0.45	0/640	0.48	0/858
10	S	0.36	0/618	0.50	0/841
11	T	0.31	0/354	0.58	0/480
12	Q	0.42	0/437	0.56	0/598
13	A	0.38	0/3687	0.47	0/4973
13	B	0.40	0/3762	0.47	0/5073
13	C	0.39	0/3792	0.48	0/5112
14	D	0.35	0/3398	0.47	0/4607
14	E	0.39	0/3580	0.48	0/4857
14	F	0.40	0/3621	0.47	0/4911
15	G	0.36	0/2129	0.47	0/2860
16	O	0.32	0/1453	0.52	0/1958
All	All	0.39	0/38726	0.49	0/52363

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	3	0	1
4	6	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	3	38	ARG	Sidechain
4	6	38	ARG	Sidechain

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	K	1573	0	1552	63	0
2	L	549	0	533	33	0
3	M	1259	0	1238	47	0
4	1	534	0	553	24	0
4	2	534	0	553	17	0
4	3	534	0	553	9	0
4	4	534	0	553	7	0
4	5	534	0	553	15	0
4	6	534	0	553	17	0
4	7	534	0	553	10	0
4	8	534	0	553	22	0
5	H	975	0	979	35	0
6	I	354	0	364	8	0
7	N	1718	0	1879	62	0
8	P	344	0	361	7	0
9	R	621	0	618	17	0
10	S	604	0	631	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	T	346	0	355	23	0
12	Q	422	0	450	21	0
13	A	3639	0	3741	66	0
13	B	3714	0	3825	68	0
13	C	3745	0	3854	66	0
14	D	3344	0	3395	92	0
14	E	3522	0	3572	56	0
14	F	3562	0	3609	54	0
15	G	2103	0	2174	52	0
16	O	1437	0	1536	61	0
17	A	31	0	12	1	0
17	B	31	0	12	1	0
17	C	31	0	12	0	0
18	A	1	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	D	1	0	0	0	0
18	F	1	0	0	0	0
19	D	27	0	12	5	0
19	F	27	0	12	1	0
All	All	38255	0	39150	837	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 11.

The worst 5 of 837 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:53:TRP:HE1	3:M:70:GLU:HG2	1.20	1.00
14:E:393:ILE:HG23	14:E:395:GLY:H	1.34	0.92
1:K:103:HIS:HB2	12:Q:41:PRO:HA	1.51	0.89
10:S:102:VAL:HG21	11:T:37:ALA:HB1	1.57	0.87
3:M:53:TRP:NE1	3:M:70:GLU:HG2	1.92	0.85

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 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	K	194/214 (91%)	188 (97%)	5 (3%)	1 (0%)	29	58
2	L	65/108 (60%)	56 (86%)	9 (14%)	0	100	100
3	M	154/160 (96%)	145 (94%)	9 (6%)	0	100	100
4	1	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
4	2	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
4	3	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
4	4	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
4	5	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
4	6	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
4	7	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
4	8	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
5	H	130/146 (89%)	124 (95%)	6 (5%)	0	100	100
6	I	43/51 (84%)	42 (98%)	1 (2%)	0	100	100
7	N	221/226 (98%)	205 (93%)	15 (7%)	1 (0%)	29	58
8	P	39/58 (67%)	37 (95%)	2 (5%)	0	100	100
9	R	72/93 (77%)	68 (94%)	4 (6%)	0	100	100
10	S	75/102 (74%)	72 (96%)	3 (4%)	0	100	100
11	T	42/69 (61%)	34 (81%)	8 (19%)	0	100	100
12	Q	49/68 (72%)	38 (78%)	11 (22%)	0	100	100
13	A	473/510 (93%)	456 (96%)	17 (4%)	0	100	100
13	B	483/510 (95%)	464 (96%)	18 (4%)	1 (0%)	47	76
13	C	485/510 (95%)	472 (97%)	13 (3%)	0	100	100
14	D	436/482 (90%)	406 (93%)	29 (7%)	1 (0%)	47	76
14	E	464/482 (96%)	434 (94%)	29 (6%)	1 (0%)	47	76
14	F	468/482 (97%)	445 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	G	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
16	O	185/190 (97%)	178 (96%)	7 (4%)	0	100	100
All	All	4931/5334 (92%)	4689 (95%)	237 (5%)	5 (0%)	54	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	E	282	VAL
1	K	29	THR
13	B	13	GLU
7	N	139	PRO
14	D	283	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	K	160/187 (86%)	159 (99%)	1 (1%)	86	95
2	L	60/98 (61%)	59 (98%)	1 (2%)	60	85
3	M	135/139 (97%)	135 (100%)	0	100	100
4	1	51/51 (100%)	51 (100%)	0	100	100
4	2	51/51 (100%)	51 (100%)	0	100	100
4	3	51/51 (100%)	51 (100%)	0	100	100
4	4	51/51 (100%)	51 (100%)	0	100	100
4	5	51/51 (100%)	51 (100%)	0	100	100
4	6	51/51 (100%)	51 (100%)	0	100	100
4	7	51/51 (100%)	51 (100%)	0	100	100
4	8	51/51 (100%)	51 (100%)	0	100	100
5	H	103/108 (95%)	103 (100%)	0	100	100
6	I	36/42 (86%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	N	196/199 (98%)	196 (100%)	0	100	100
8	P	36/48 (75%)	36 (100%)	0	100	100
9	R	65/82 (79%)	64 (98%)	1 (2%)	65	87
10	S	64/85 (75%)	64 (100%)	0	100	100
11	T	34/58 (59%)	33 (97%)	1 (3%)	42	73
12	Q	51/68 (75%)	51 (100%)	0	100	100
13	A	387/412 (94%)	386 (100%)	1 (0%)	92	97
13	B	397/412 (96%)	395 (100%)	2 (0%)	88	95
13	C	400/412 (97%)	400 (100%)	0	100	100
14	D	355/388 (92%)	355 (100%)	0	100	100
14	E	374/388 (96%)	374 (100%)	0	100	100
14	F	379/388 (98%)	379 (100%)	0	100	100
15	G	228/229 (100%)	228 (100%)	0	100	100
16	O	162/165 (98%)	161 (99%)	1 (1%)	86	95
All	All	4030/4316 (93%)	4022 (100%)	8 (0%)	93	98

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

Mol	Chain	Res	Type
16	O	77	ARG
13	B	164	ARG
13	A	164	ARG
11	T	36	ARG
13	B	8	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
13	A	163	GLN
14	E	37	ASN
13	A	379	GLN
13	B	208	GLN
14	E	419	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
17	ATP	B	601	18	26,33,33	2.28	7 (26%)	31,52,52	1.65	6 (19%)
19	ADP	F	501	18	24,29,29	2.35	7 (29%)	29,45,45	1.60	5 (17%)
17	ATP	A	601	18	26,33,33	2.26	6 (23%)	31,52,52	1.72	7 (22%)
19	ADP	D	501	-	24,29,29	0.68	0	29,45,45	0.93	2 (6%)
17	ATP	C	601	18	26,33,33	2.25	7 (26%)	31,52,52	1.54	5 (16%)

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
17	ATP	B	601	18	-	6/18/38/38	0/3/3/3
19	ADP	F	501	18	-	6/12/32/32	0/3/3/3
17	ATP	A	601	18	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	D	501	-	-	4/12/32/32	0/3/3/3
17	ATP	C	601	18	-	2/18/38/38	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	601	ATP	O4'-C1'	7.48	1.51	1.41
17	B	601	ATP	O4'-C1'	7.26	1.51	1.41
17	C	601	ATP	O4'-C1'	7.13	1.51	1.41
19	F	501	ADP	O4'-C1'	6.32	1.49	1.41
17	A	601	ATP	C2'-C1'	-4.98	1.46	1.53

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	601	ATP	N3-C2-N1	-4.21	122.10	128.68
19	F	501	ADP	N3-C2-N1	-4.14	122.20	128.68
17	B	601	ATP	C3'-C2'-C1'	4.11	107.16	100.98
19	F	501	ADP	C3'-C2'-C1'	3.98	106.97	100.98
17	C	601	ATP	N3-C2-N1	-3.92	122.55	128.68

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	C	601	ATP	PB-O3B-PG-O3G
17	B	601	ATP	C5'-O5'-PA-O1A
17	B	601	ATP	O4'-C4'-C5'-O5'
19	F	501	ADP	PA-O3A-PB-O3B
19	F	501	ADP	C5'-O5'-PA-O1A

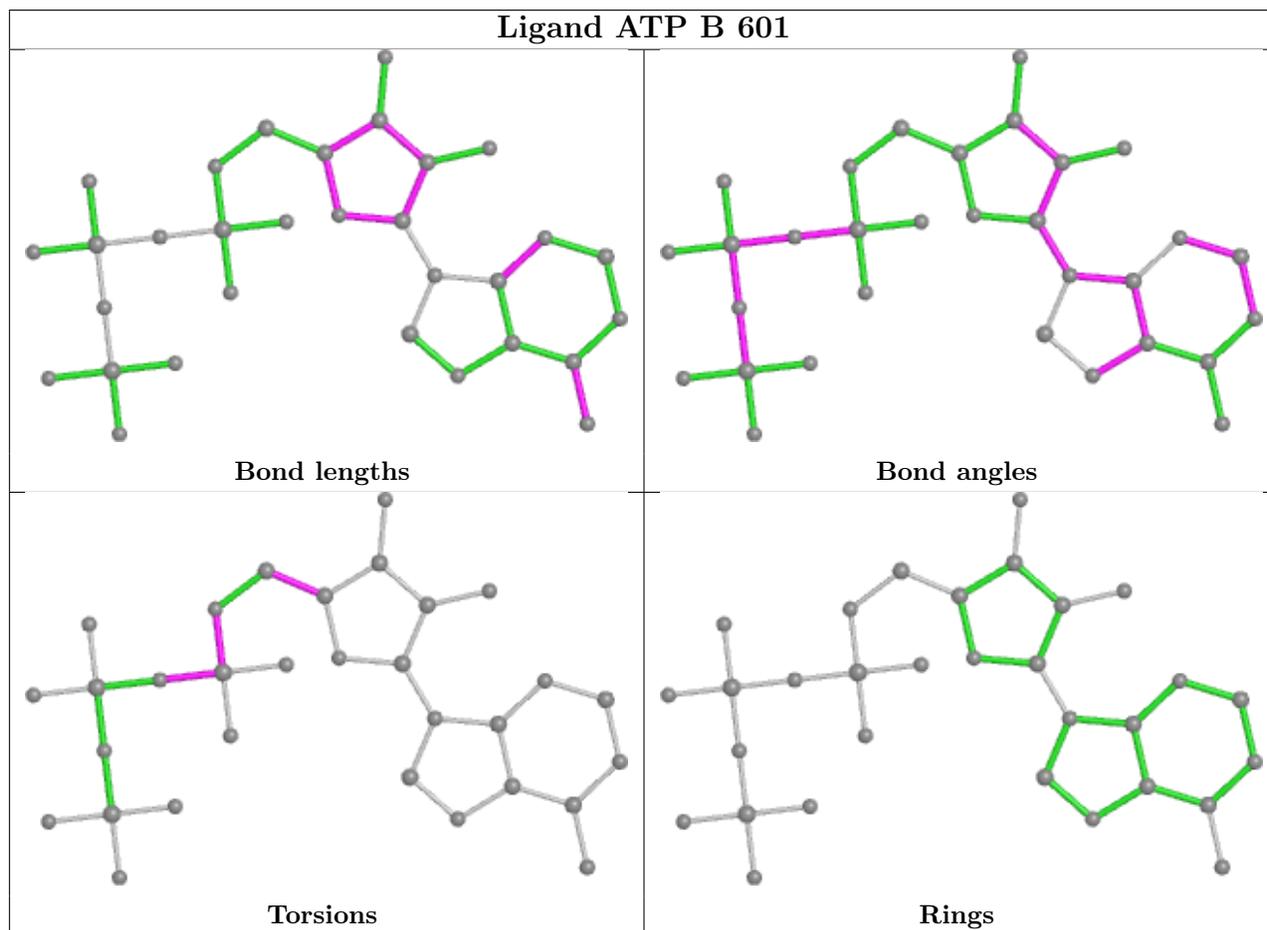
There are no ring outliers.

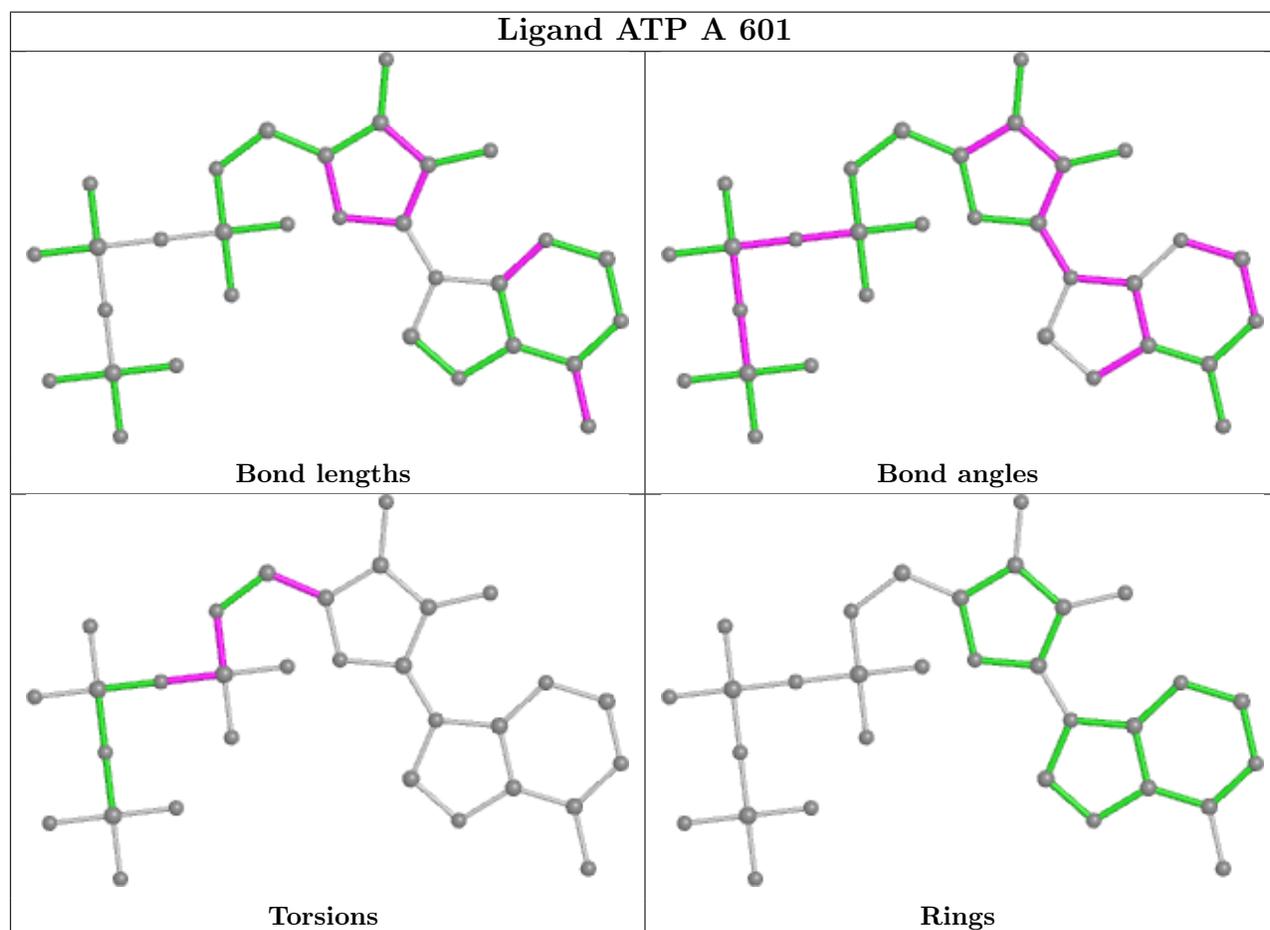
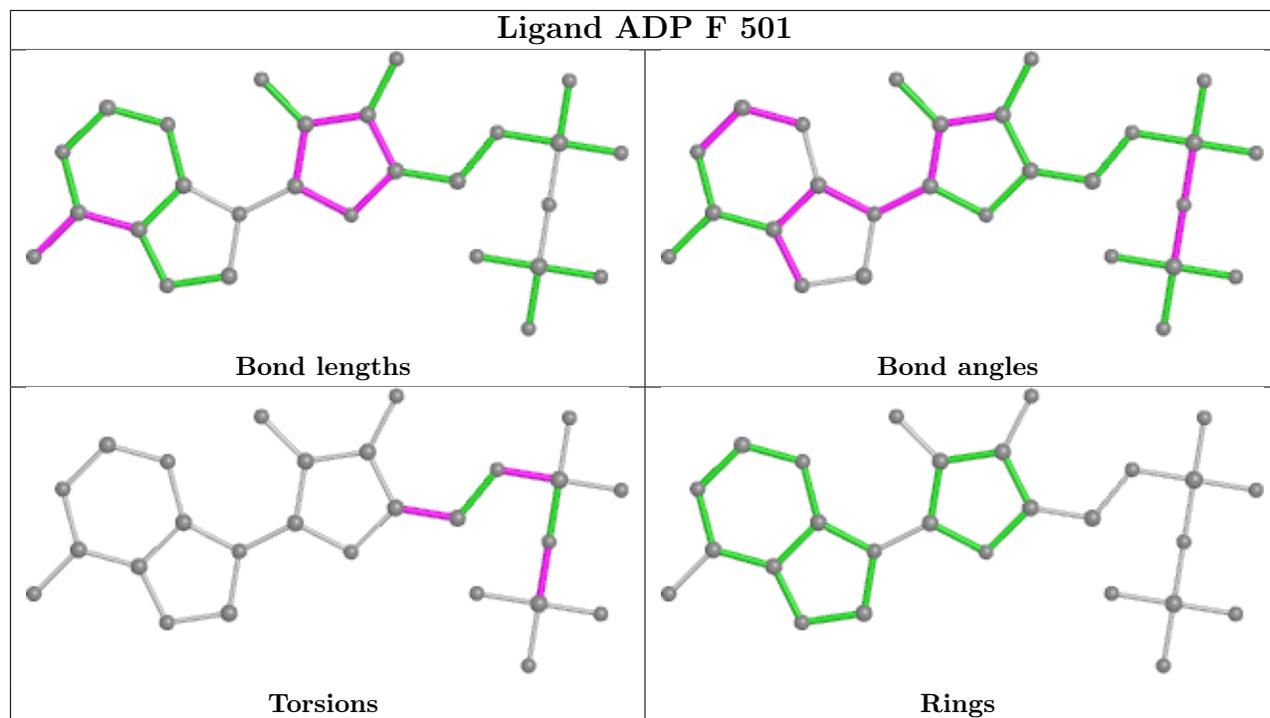
4 monomers are involved in 8 short contacts:

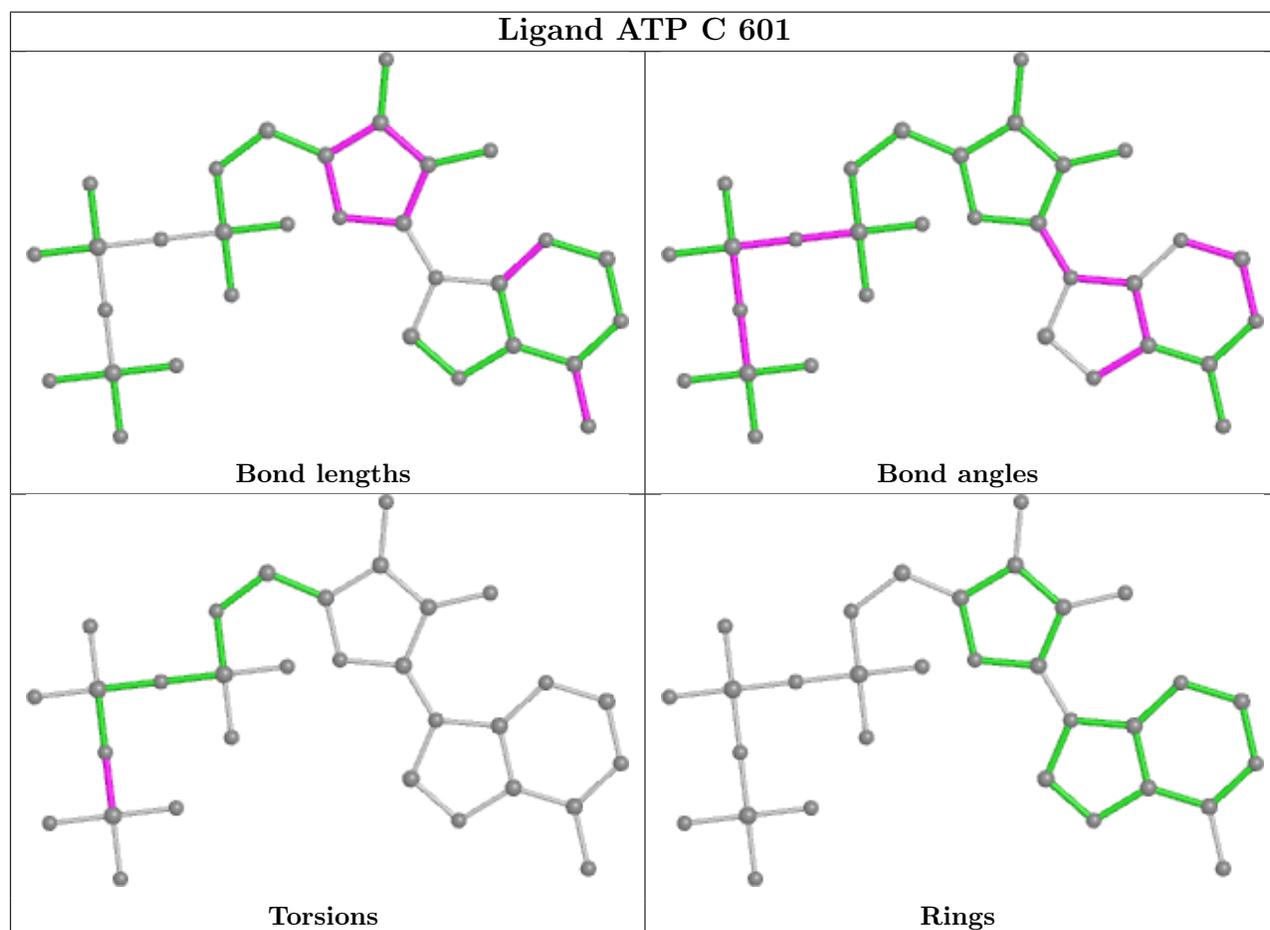
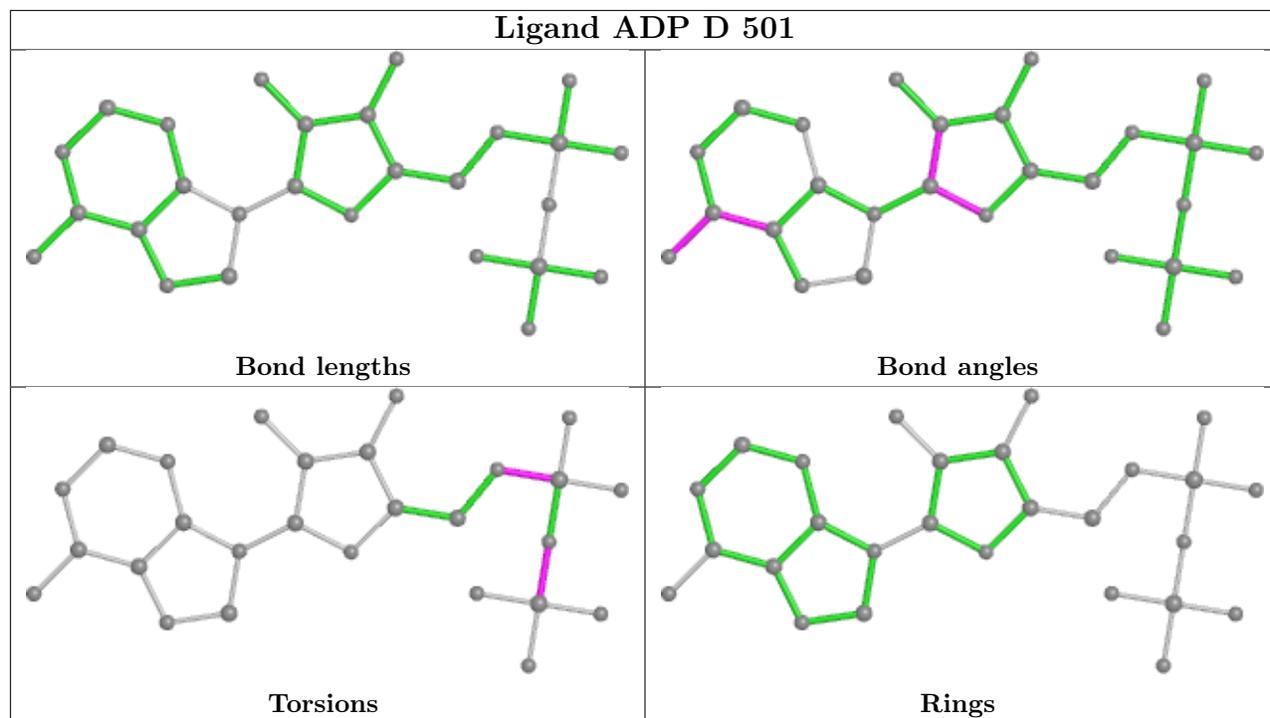
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	601	ATP	1	0
19	F	501	ADP	1	0
17	A	601	ATP	1	0
19	D	501	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

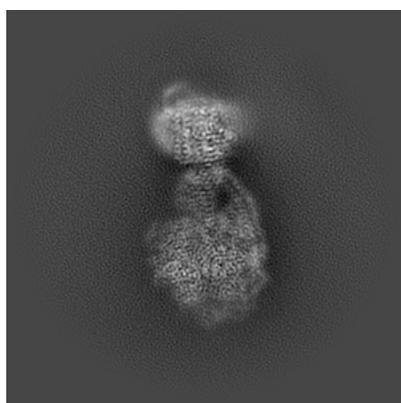
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34581. These allow visual inspection of the internal detail of the map and identification of artifacts.

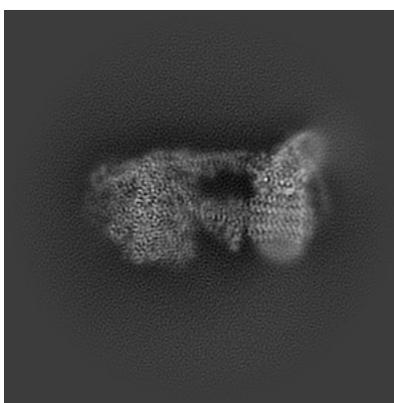
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

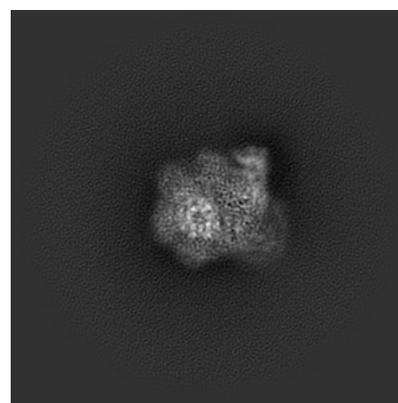
6.1.1 Primary map



X



Y

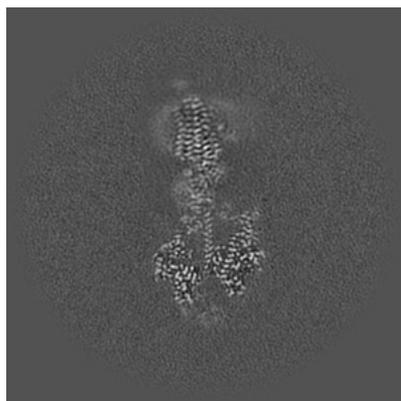


Z

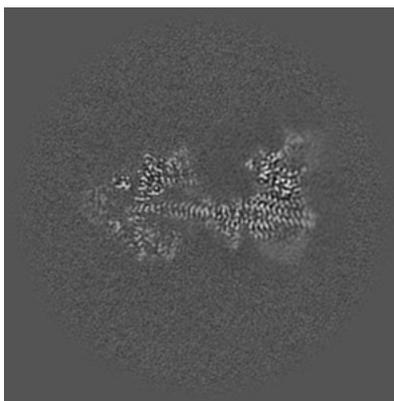
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

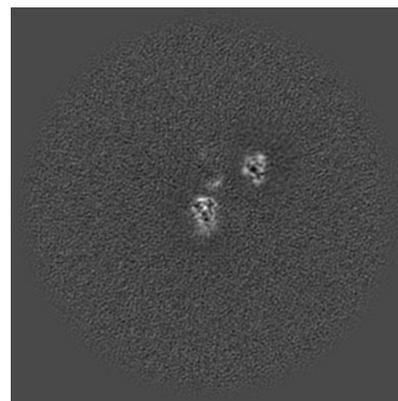
6.2.1 Primary map



X Index: 256



Y Index: 256

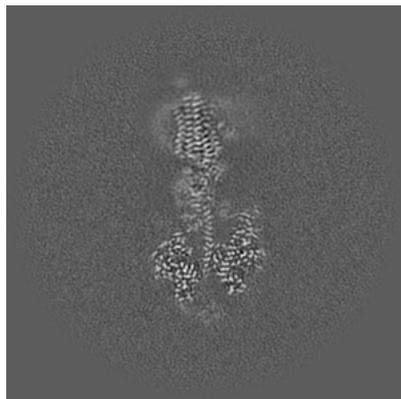


Z Index: 256

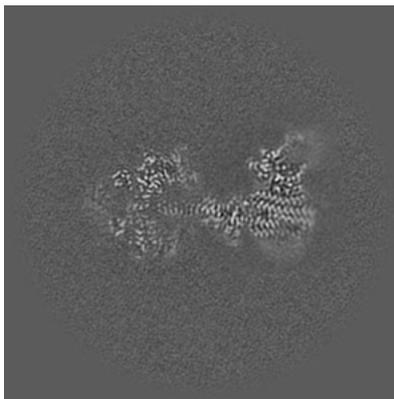
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

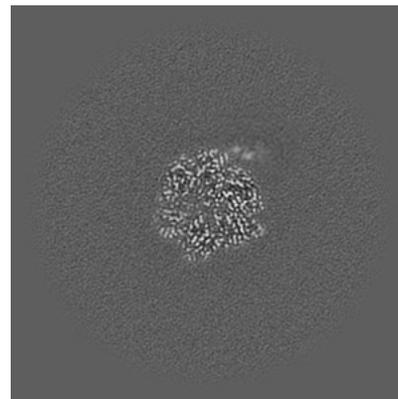
6.3.1 Primary map



X Index: 255



Y Index: 254

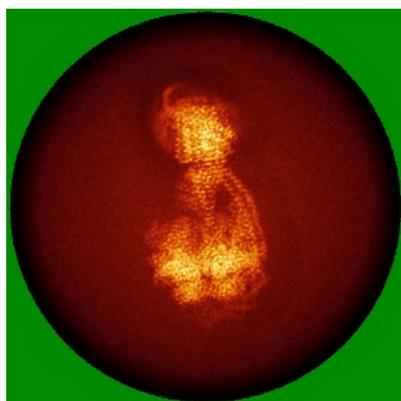


Z Index: 183

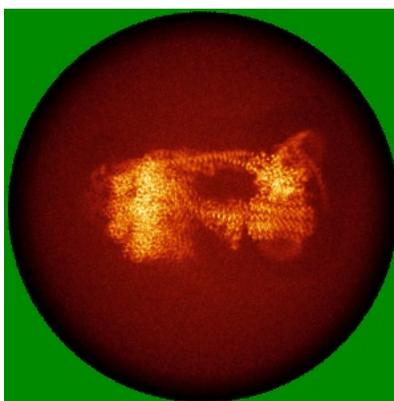
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

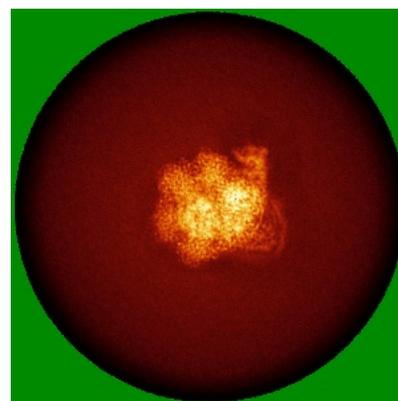
6.4.1 Primary map



X



Y

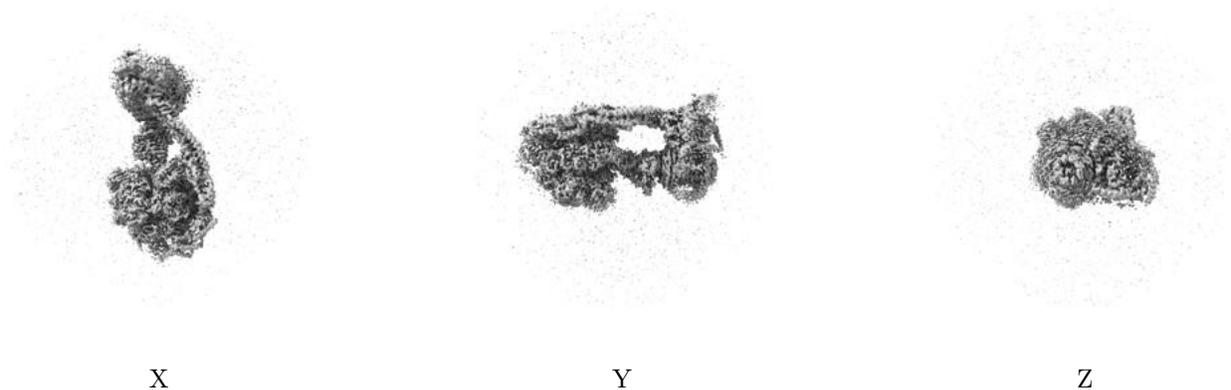


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

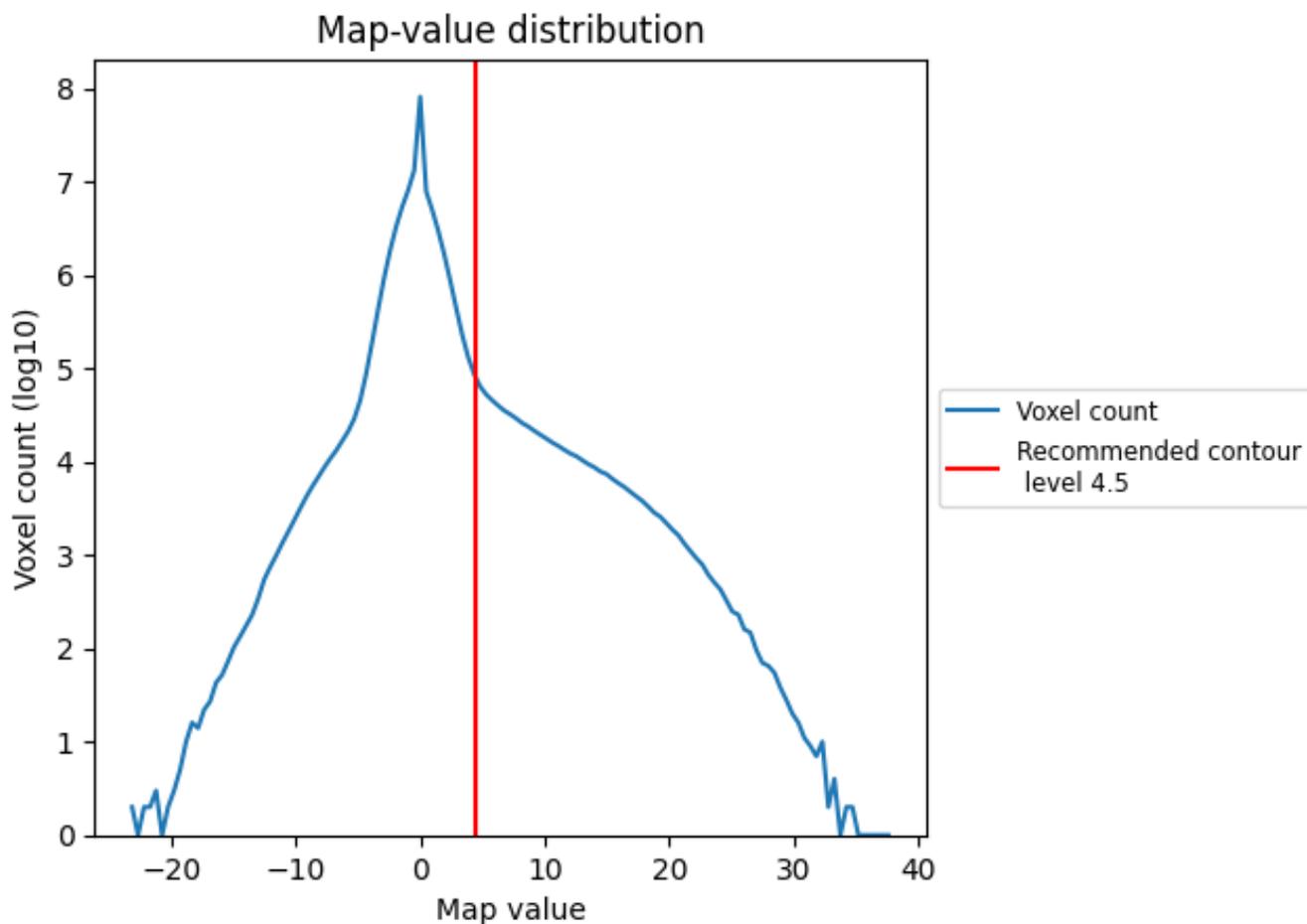
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

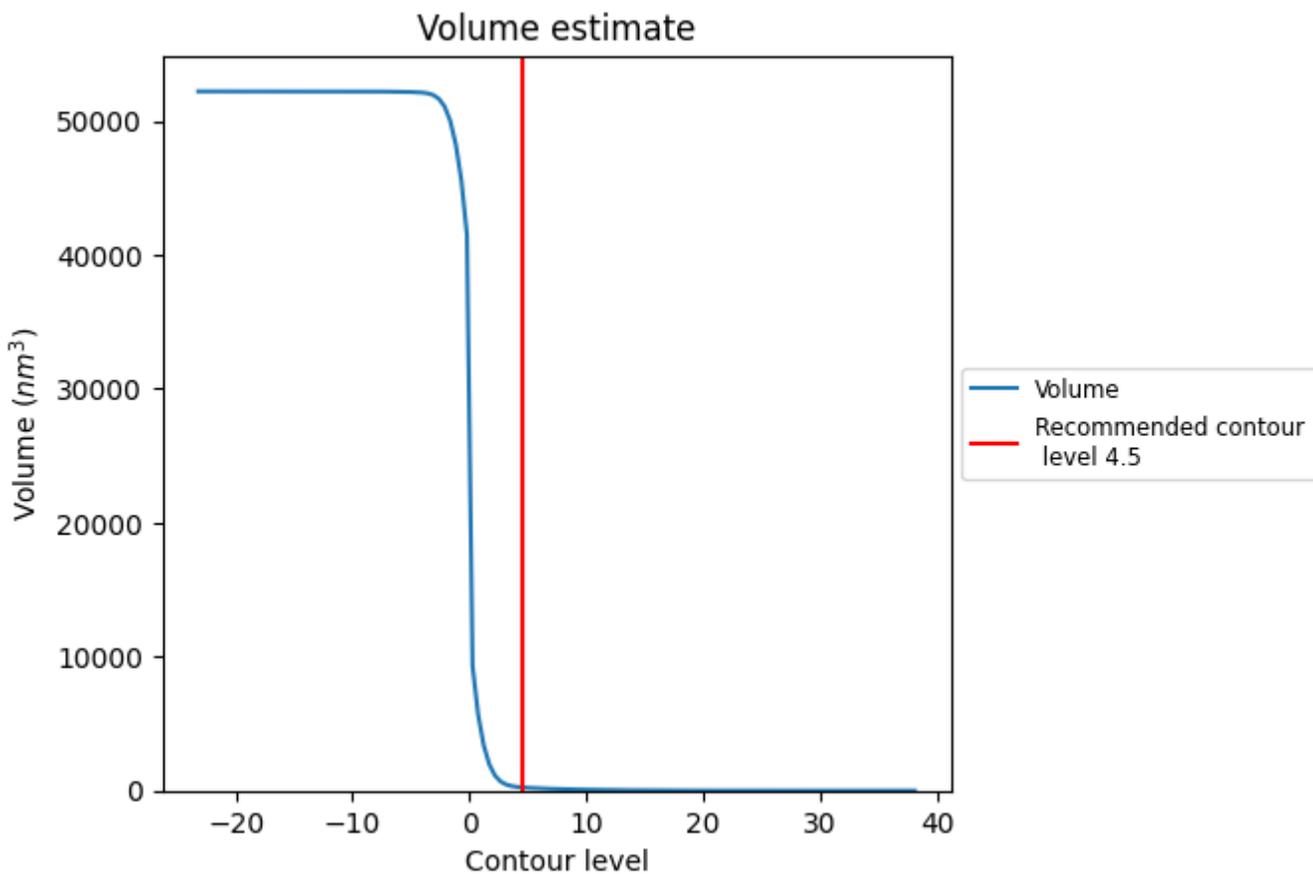
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

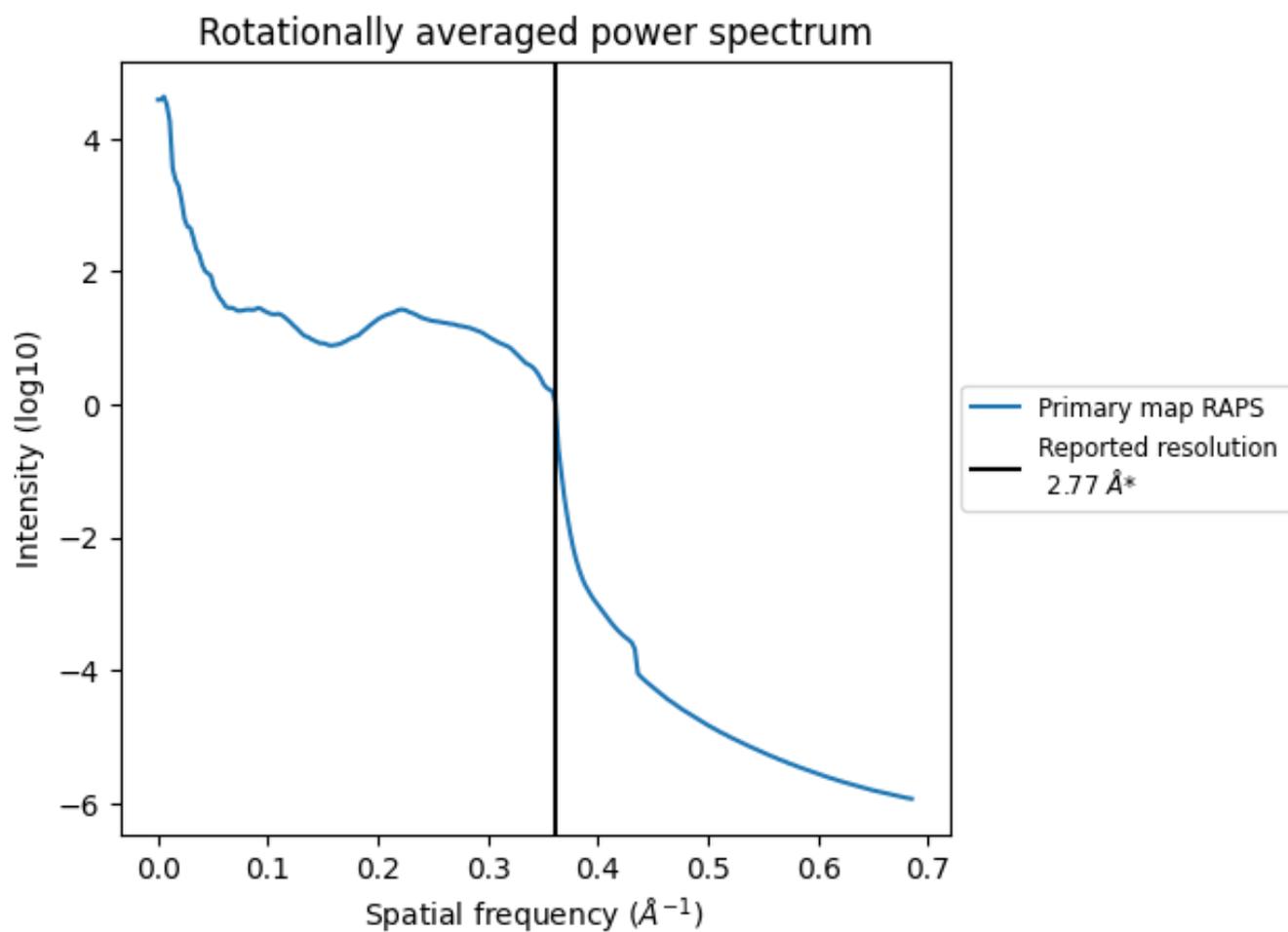
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm³; this corresponds to an approximate mass of 218 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.361\AA^{-1}

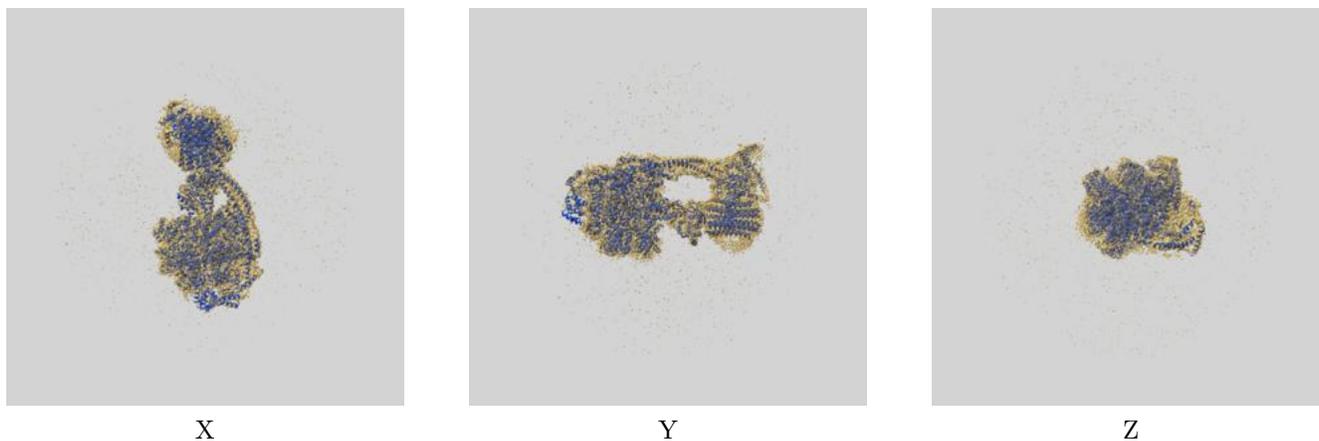
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

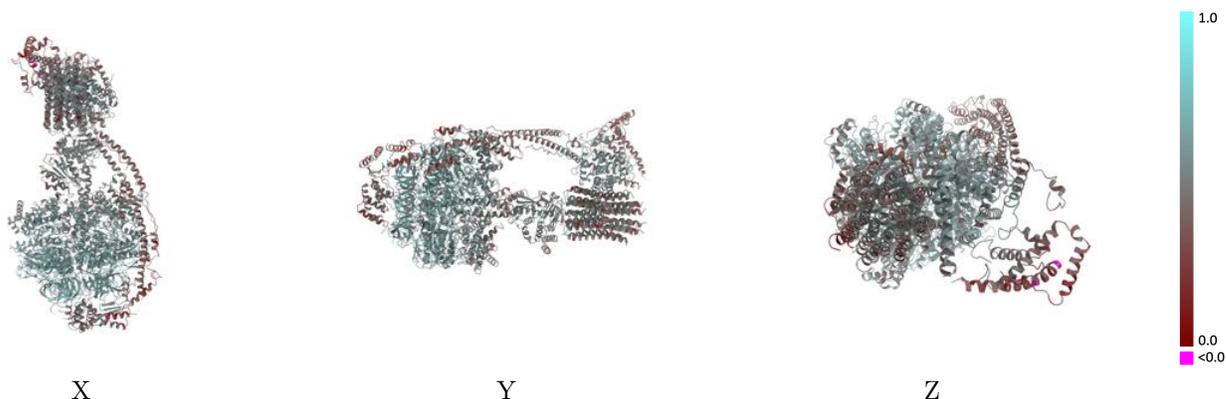
This section contains information regarding the fit between EMDB map EMD-34581 and PDB model 8H9T. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



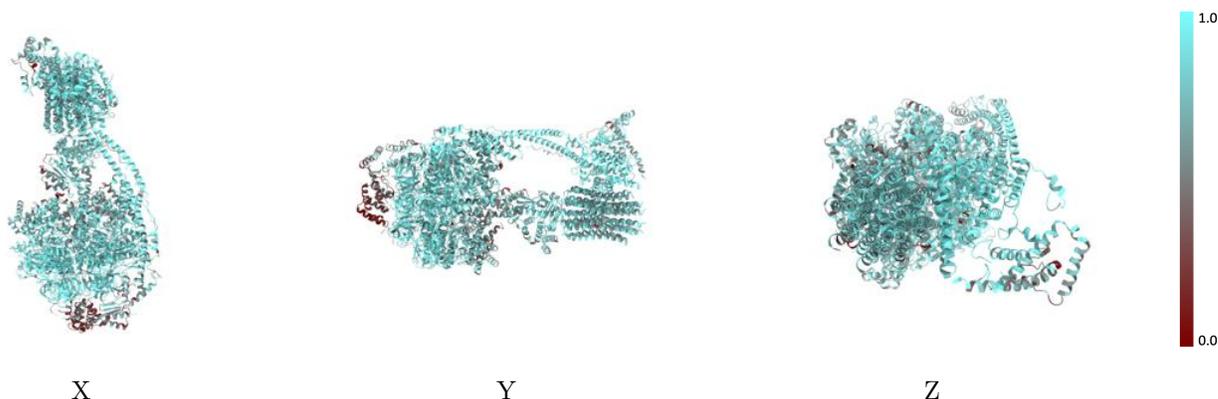
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



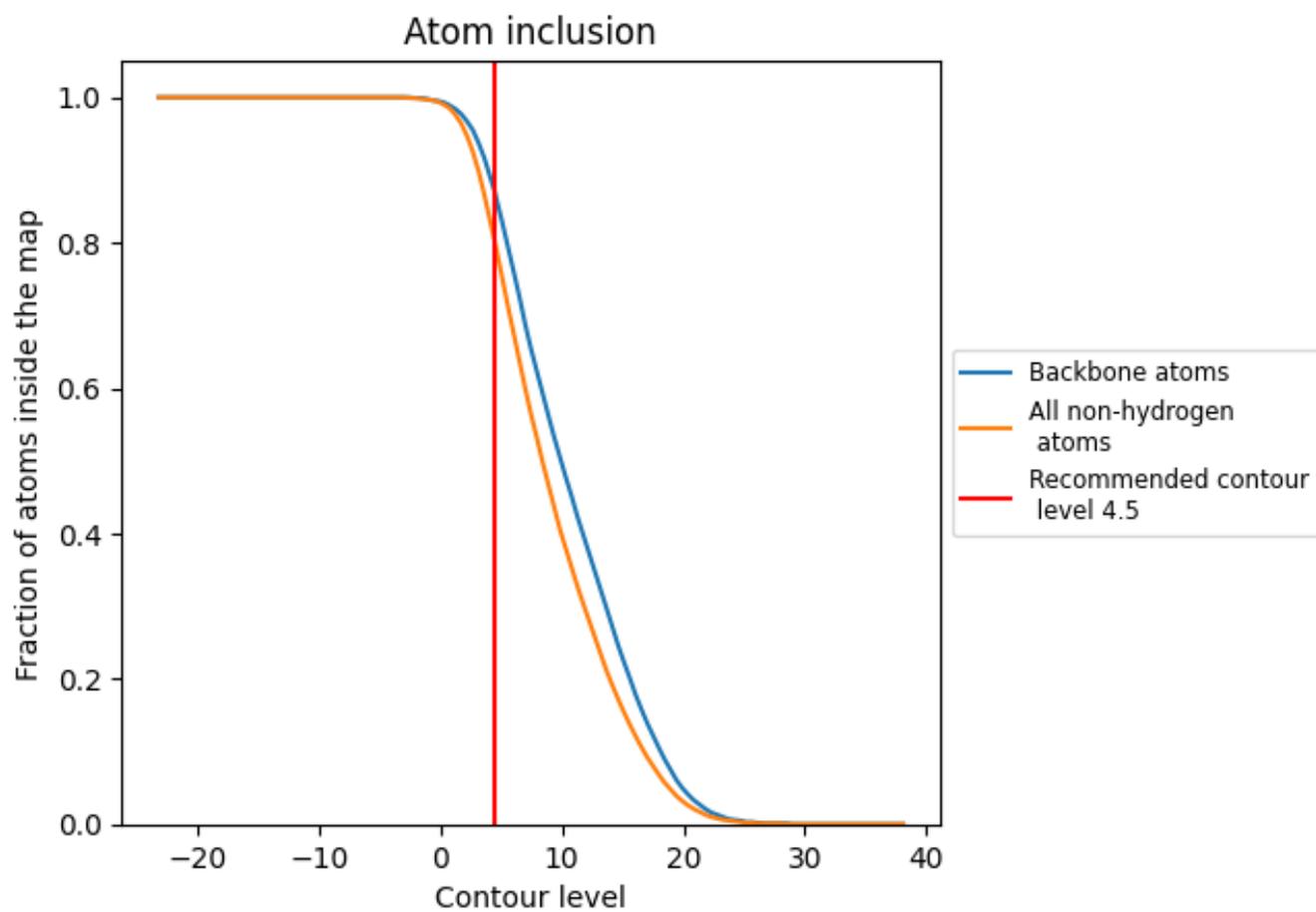
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.5150
1	 0.7770	 0.4370
2	 0.7430	 0.4150
3	 0.7870	 0.4500
4	 0.7530	 0.3830
5	 0.7890	 0.4320
6	 0.7660	 0.4360
7	 0.7740	 0.4390
8	 0.7770	 0.4140
A	 0.8330	 0.5670
B	 0.8620	 0.5840
C	 0.8490	 0.5790
D	 0.7350	 0.5360
E	 0.8480	 0.5750
F	 0.8920	 0.5930
G	 0.7340	 0.4870
H	 0.8000	 0.4700
I	 0.7940	 0.4940
K	 0.8200	 0.4280
L	 0.6970	 0.3150
M	 0.8260	 0.4170
N	 0.8660	 0.5090
O	 0.3610	 0.4210
P	 0.8390	 0.4780
Q	 0.8520	 0.4660
R	 0.8720	 0.4750
S	 0.6700	 0.3460
T	 0.5930	 0.2540

