



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 7P3N / pdb_00007p3n
EMDB ID : EMD-13181
Title : F1Fo-ATP synthase from *Acinetobacter baumannii* (state 2)
Authors : Demmer, J.K.; Phillips, B.P.; Uhrig, O.L.; Filloux, A.; Allsopp, L.P.; Bublitz, M.; Meier, T.
Deposited on : 2021-07-08
Resolution : 4.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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:

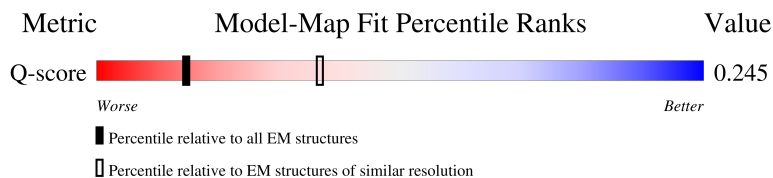
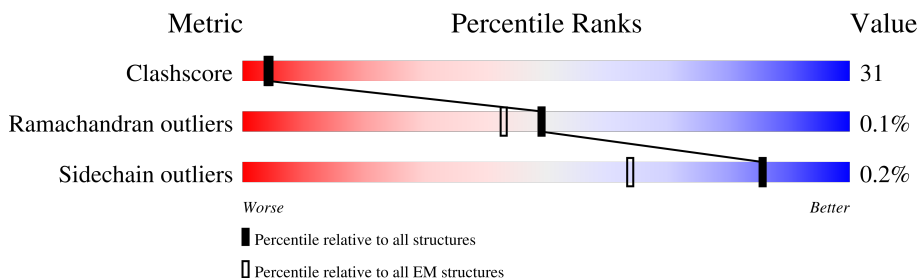
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.60 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.



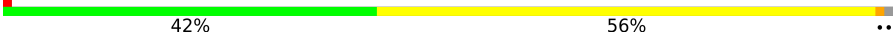
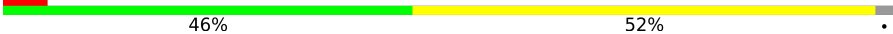
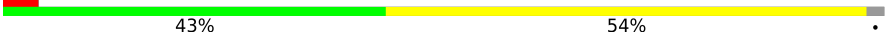
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	A	514	 47% 52%
1	B	514	 46% 54%
1	C	514	 41% 57% ..
2	D	464	 40% 60%

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Mol	Chain	Length	Quality of chain
2	E	464	
2	F	464	
3	G	81	
3	H	81	
3	J	81	
3	K	81	
3	L	81	
3	O	81	
3	P	81	
3	Q	81	
3	R	81	
3	S	81	
4	a	291	
5	b	156	
5	p	156	
6	d	178	
7	e	139	
8	g	289	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ADP	E	601	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 37114 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	512	Total	C	N	O	S	0	0
			3875	2438	665	757	15		
1	B	514	Total	C	N	O	S	0	0
			3892	2448	668	760	16		
1	C	506	Total	C	N	O	S	0	0
			3821	2405	656	745	15		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	464	Total	C	N	O	S	0	0
			3533	2228	603	688	14		
2	E	463	Total	C	N	O	S	0	0
			3525	2223	602	687	13		
2	F	463	Total	C	N	O	S	0	0
			3525	2223	602	687	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	79	Total	C	N	O	S	0	0
			577	388	92	95	2		
3	H	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	J	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	K	79	Total	C	N	O	S	0	0
			577	388	92	95	2		
3	L	79	Total	C	N	O	S	0	0
			577	388	92	95	2		
3	O	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	P	80	Total	C	N	O	S	0	0
			585	393	93	96	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	R	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	S	79	Total	C	N	O	S	0	0
			577	388	92	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	277	Total	C	N	O	S	0	0
			2104	1405	336	350	13		

- Molecule 5 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	145	Total	C	N	O	S	0	0
			1112	688	207	214	3		
5	p	155	Total	C	N	O	S	0	0
			1185	734	220	228	3		

- Molecule 6 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	174	Total	C	N	O	S	0	0
			1347	849	227	270	1		

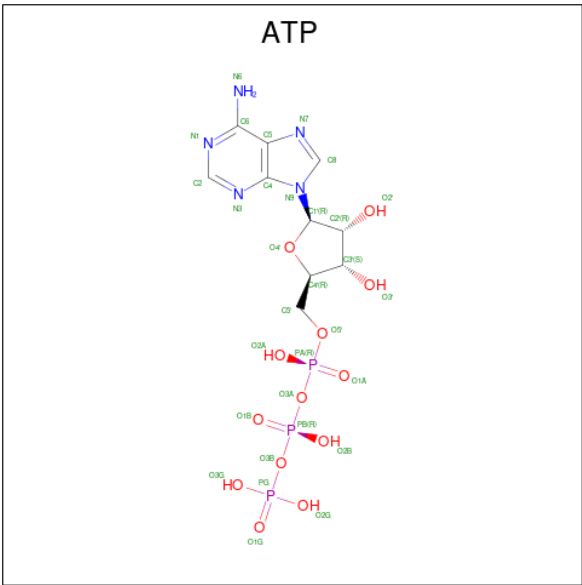
- Molecule 7 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	138	Total	C	N	O	S	0	0
			1010	631	175	201	3		

- Molecule 8 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	288	Total	C	N	O	S	0	0
			2243	1411	400	420	12		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

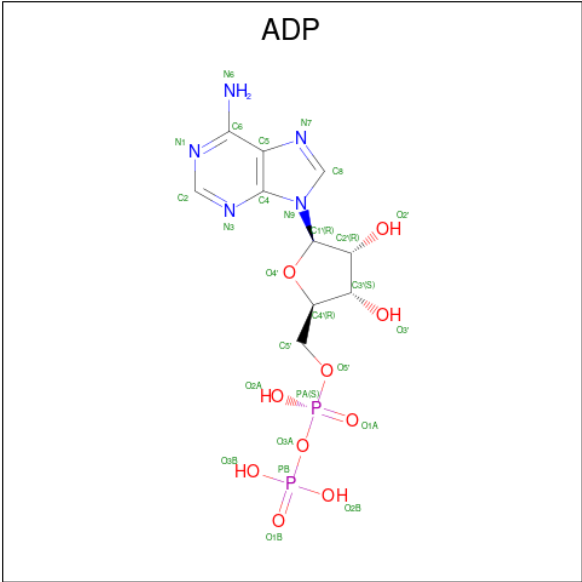


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

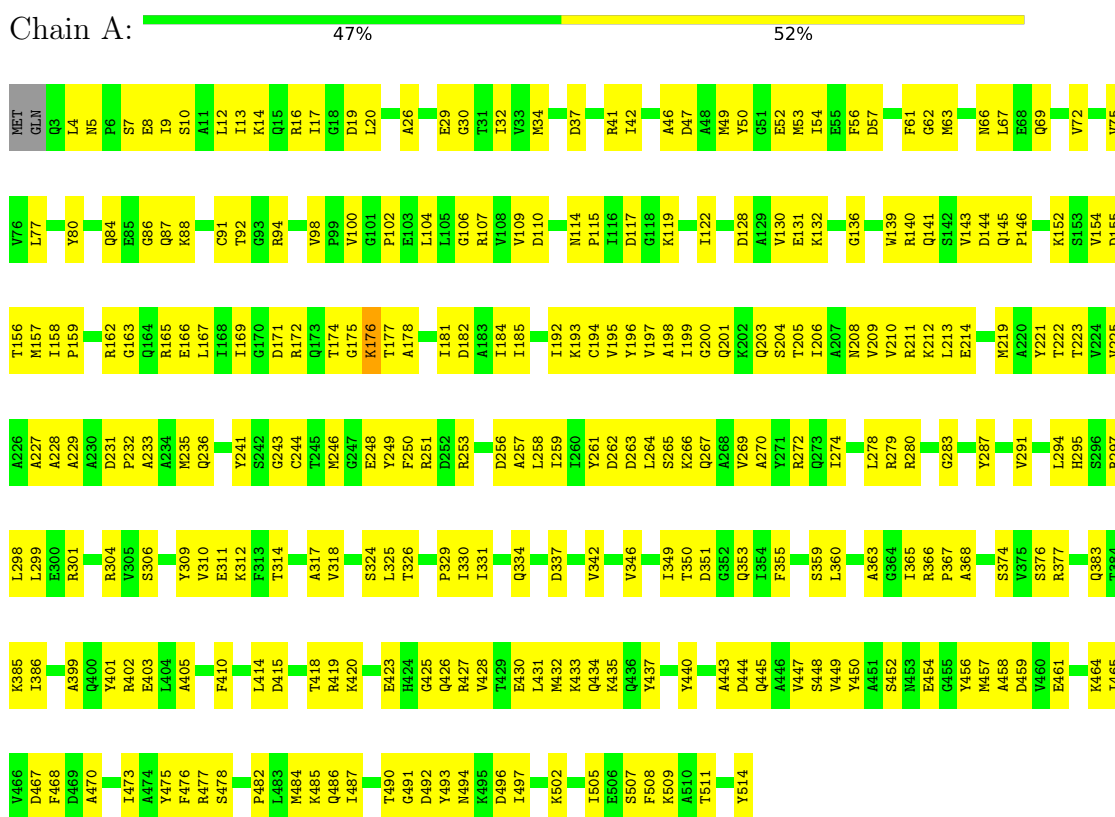


Mol	Chain	Residues	Atoms					AltConf
11	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

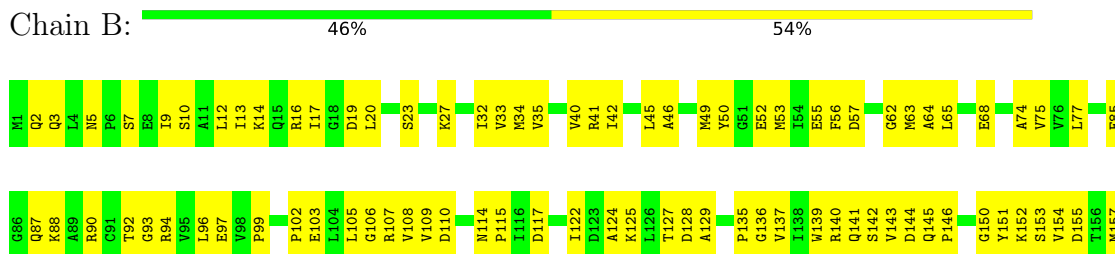
3 Residue-property plots

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.

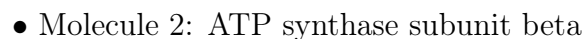
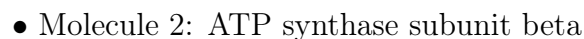
• Molecule 1: ATP synthase subunit alpha

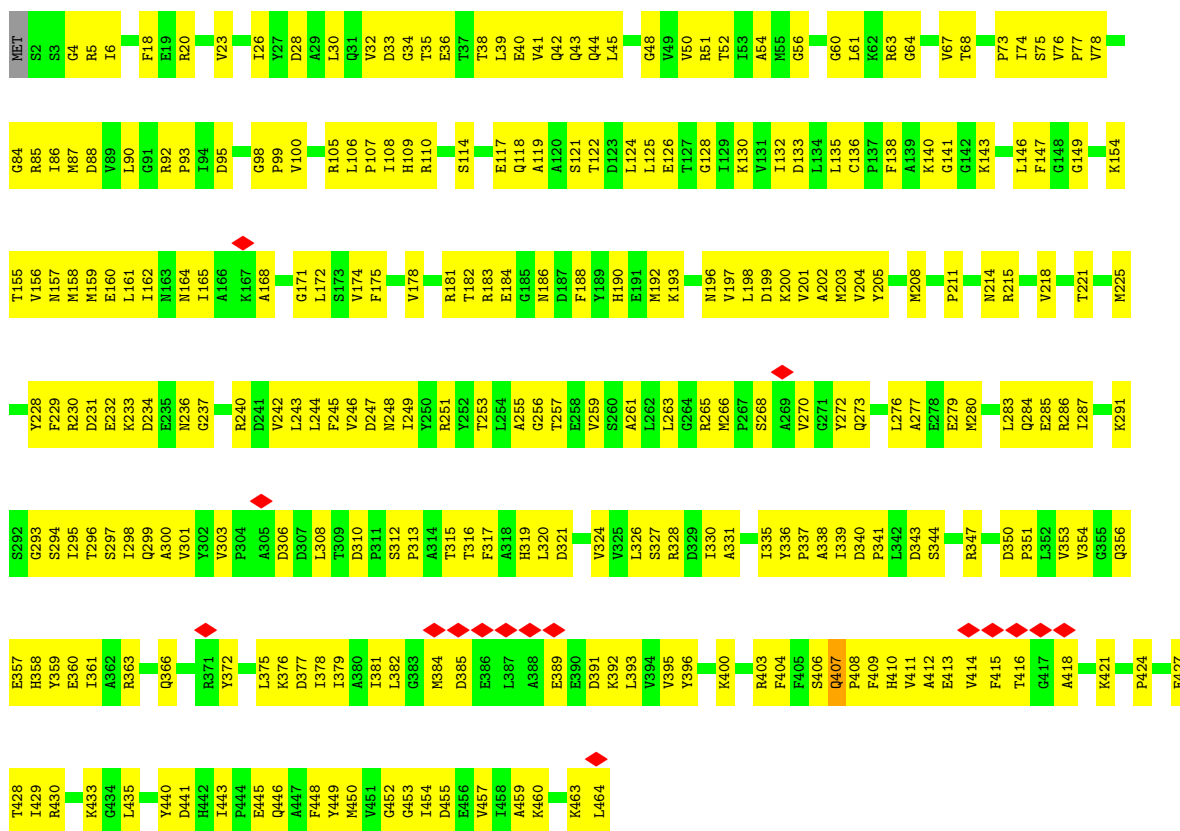


• Molecule 1: ATP synthase subunit alpha

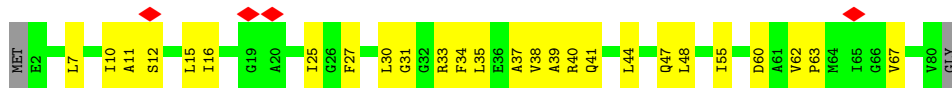




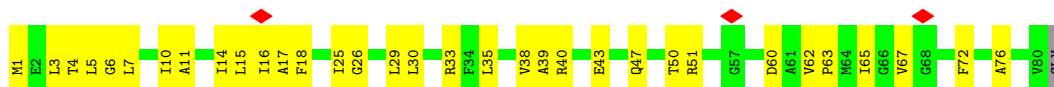




• Molecule 3: ATP synthase subunit c



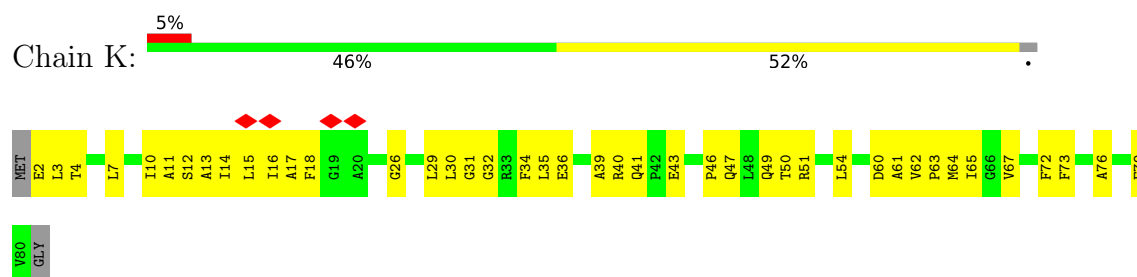
• Molecule 3: ATP synthase subunit c



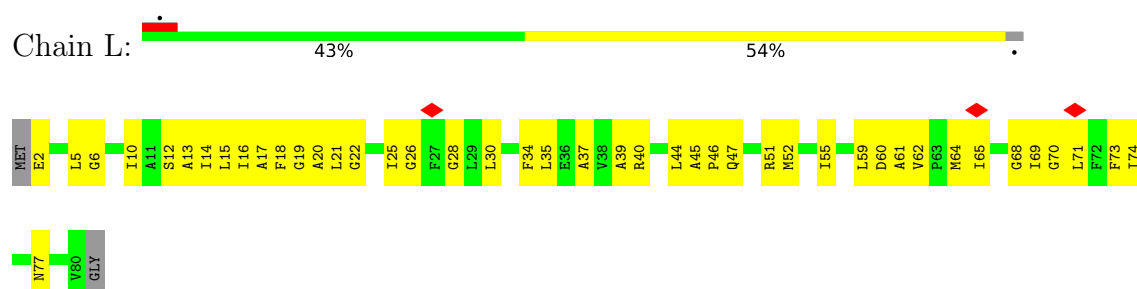
• Molecule 3: ATP synthase subunit c



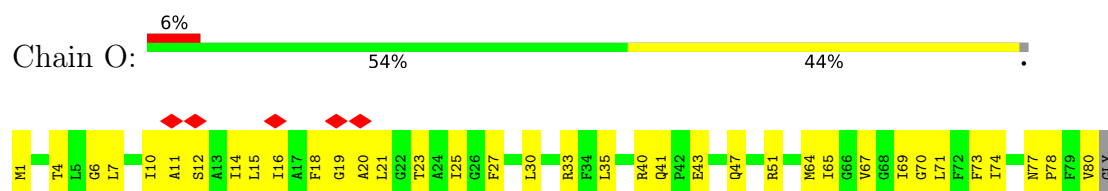
• Molecule 3: ATP synthase subunit c



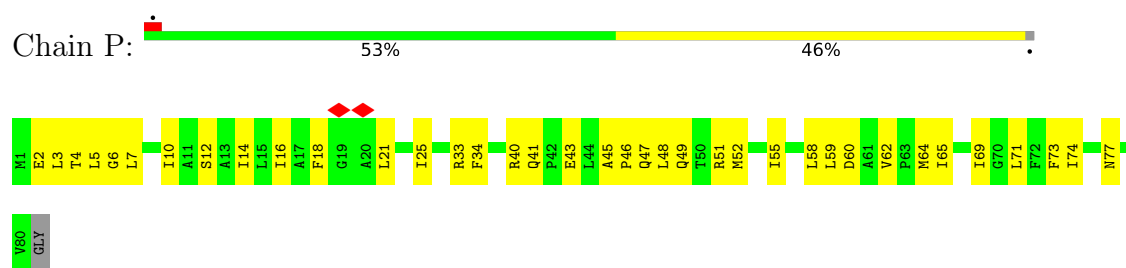
• Molecule 3: ATP synthase subunit c



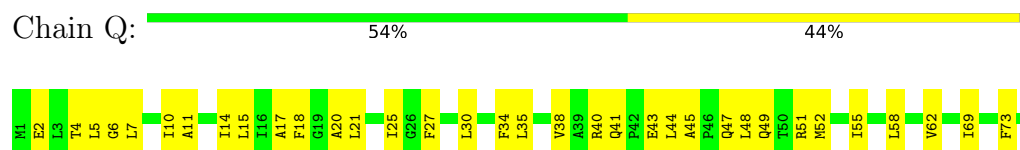
• Molecule 3: ATP synthase subunit c



• Molecule 3: ATP synthase subunit c

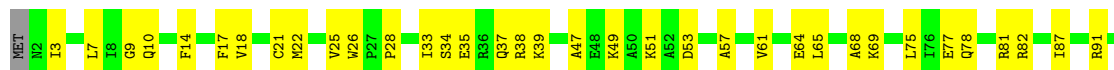


• Molecule 3: ATP synthase subunit c



• Molecule 3: ATP synthase subunit c

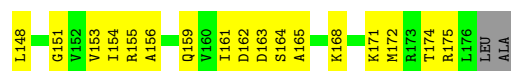
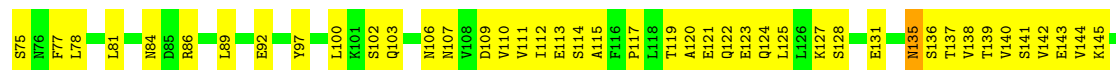






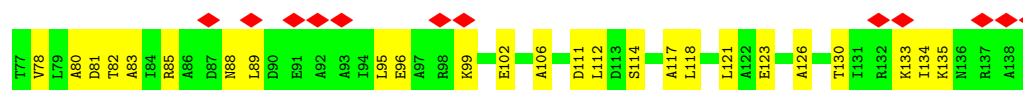
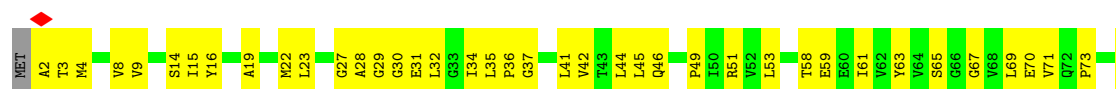
• Molecule 6: ATP synthase subunit delta

Chain d: 41% 56% ..



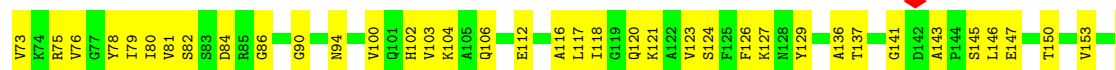
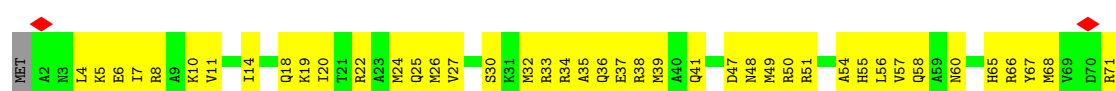
• Molecule 7: ATP synthase epsilon chain

Chain e: 9% 53% 47% .



• Molecule 8: ATP synthase gamma chain

Chain g: 47% 52%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26147	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	85000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0381	Depositor
Map size (Å)	382.5, 382.5, 382.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/3932	0.47	0/5321
1	B	0.27	0/3949	0.50	1/5343 (0.0%)
1	C	0.26	0/3877	0.45	0/5246
2	D	0.26	0/3590	0.46	0/4864
2	E	0.25	0/3582	0.47	1/4854 (0.0%)
2	F	0.24	0/3582	0.47	0/4854
3	G	0.17	0/588	0.38	0/798
3	H	0.22	0/596	0.43	0/808
3	J	0.25	0/596	0.60	2/808 (0.2%)
3	K	0.23	0/588	0.53	0/798
3	L	0.22	0/588	0.46	0/798
3	O	0.20	0/596	0.45	0/808
3	P	0.19	0/596	0.39	0/808
3	Q	0.22	0/596	0.48	0/808
3	R	0.22	0/596	0.46	0/808
3	S	0.20	0/588	0.45	0/798
4	a	0.22	0/2162	0.52	0/2953
5	b	0.45	0/1121	0.91	6/1508 (0.4%)
5	p	0.21	0/1194	0.45	0/1608
6	d	0.27	0/1364	0.49	0/1854
7	e	0.19	0/1018	0.44	0/1383
8	g	0.23	0/2273	0.46	0/3062
All	All	0.26	0/37572	0.49	10/50890 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	57	ALA	N-CA-C	10.30	122.09	111.07
5	b	51	LYS	N-CA-C	9.17	120.88	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	57	ALA	CA-C-N	7.79	131.05	120.38
5	b	57	ALA	C-N-CA	7.79	131.05	120.38
1	B	513	THR	CB-CA-C	6.01	119.92	111.86

There are no chirality outliers.

There are no planarity outliers.

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	A	3875	0	3906	253	0
1	B	3892	0	3926	305	0
1	C	3821	0	3858	319	0
2	D	3533	0	3567	260	0
2	E	3525	0	3555	274	0
2	F	3525	0	3555	239	0
3	G	577	0	614	30	0
3	H	585	0	626	33	0
3	J	585	0	626	59	0
3	K	577	0	614	52	0
3	L	577	0	614	48	0
3	O	585	0	626	40	0
3	P	585	0	626	33	0
3	Q	585	0	626	41	0
3	R	585	0	626	34	0
3	S	577	0	614	31	0
4	a	2104	0	2124	106	0
5	b	1112	0	1124	84	0
5	p	1185	0	1203	69	0
6	d	1347	0	1355	95	0
7	e	1010	0	1048	68	0
8	g	2243	0	2294	142	0
9	A	31	0	12	4	0
9	B	31	0	12	4	0
9	C	31	0	12	8	0
10	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	E	1	0	0	0	0
11	E	27	0	12	20	0
All	All	37114	0	37775	2351	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 31.

The worst 5 of 2351 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)
1:C:361:PHE:CE2	1:C:368:ALA:HB3	1.47	1.45
1:C:361:PHE:CD2	1:C:368:ALA:HB3	1.57	1.38
1:C:361:PHE:HB3	1:C:366:ARG:NH1	1.50	1.25
1:C:179:MET:CE	1:C:356:LEU:HD11	1.68	1.23
1:C:377:ARG:HD2	2:E:183:ARG:NH2	1.55	1.20

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	A	510/514 (99%)	465 (91%)	44 (9%)	1 (0%)	43	77
1	B	512/514 (100%)	474 (93%)	38 (7%)	0	100	100
1	C	504/514 (98%)	467 (93%)	36 (7%)	1 (0%)	43	77
2	D	462/464 (100%)	422 (91%)	40 (9%)	0	100	100
2	E	461/464 (99%)	423 (92%)	36 (8%)	2 (0%)	30	67
2	F	461/464 (99%)	425 (92%)	35 (8%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	77/81 (95%)	71 (92%)	6 (8%)	0	100	100
3	H	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	J	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
3	K	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
3	L	77/81 (95%)	71 (92%)	6 (8%)	0	100	100
3	O	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	P	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
3	Q	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	R	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
3	S	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
4	a	275/291 (94%)	242 (88%)	33 (12%)	0	100	100
5	b	143/156 (92%)	133 (93%)	9 (6%)	1 (1%)	18	55
5	p	153/156 (98%)	152 (99%)	1 (1%)	0	100	100
6	d	172/178 (97%)	159 (92%)	13 (8%)	0	100	100
7	e	136/139 (98%)	126 (93%)	10 (7%)	0	100	100
8	g	286/289 (99%)	269 (94%)	17 (6%)	0	100	100
All	All	4851/4953 (98%)	4484 (92%)	361 (7%)	6 (0%)	49	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	268	SER
5	b	52	ALA
1	A	175	GLY
1	C	178	ALA
2	F	414	VAL

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	A	404/406 (100%)	403 (100%)	1 (0%)	87	85
1	B	406/406 (100%)	406 (100%)	0	100	100
1	C	398/406 (98%)	396 (100%)	2 (0%)	81	81
2	D	379/379 (100%)	379 (100%)	0	100	100
2	E	378/379 (100%)	376 (100%)	2 (0%)	81	81
2	F	378/379 (100%)	377 (100%)	1 (0%)	86	84
3	G	56/57 (98%)	56 (100%)	0	100	100
3	H	57/57 (100%)	57 (100%)	0	100	100
3	J	57/57 (100%)	57 (100%)	0	100	100
3	K	56/57 (98%)	56 (100%)	0	100	100
3	L	56/57 (98%)	56 (100%)	0	100	100
3	O	57/57 (100%)	57 (100%)	0	100	100
3	P	57/57 (100%)	57 (100%)	0	100	100
3	Q	57/57 (100%)	57 (100%)	0	100	100
3	R	57/57 (100%)	57 (100%)	0	100	100
3	S	56/57 (98%)	56 (100%)	0	100	100
4	a	216/246 (88%)	216 (100%)	0	100	100
5	b	106/115 (92%)	105 (99%)	1 (1%)	70	76
5	p	114/115 (99%)	114 (100%)	0	100	100
6	d	146/148 (99%)	145 (99%)	1 (1%)	76	79
7	e	106/107 (99%)	106 (100%)	0	100	100
8	g	235/236 (100%)	235 (100%)	0	100	100
All	All	3832/3892 (98%)	3824 (100%)	8 (0%)	85	85

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

Mol	Chain	Res	Type
6	d	135	ASN
5	b	65	LEU
2	E	415	PHE
2	E	266	MET
2	F	407	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
6	d	72	GLN
5	p	139	GLN
6	d	76	ASN
8	g	258	GLN
2	E	358	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
11	ADP	E	601	10	28,29,29	1.49	4 (14%)	43,45,45	2.46	9 (20%)
9	ATP	B	601	10	32,33,33	2.08	4 (12%)	48,52,52	1.51	8 (16%)
9	ATP	C	601	10	32,33,33	2.07	4 (12%)	48,52,52	1.50	7 (14%)
9	ATP	A	601	10	32,33,33	2.07	4 (12%)	48,52,52	1.51	8 (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
11	ADP	E	601	10	-	3/16/32/32	0/3/3/3
9	ATP	B	601	10	-	9/22/38/38	0/3/3/3
9	ATP	C	601	10	-	8/22/38/38	0/3/3/3
9	ATP	A	601	10	-	6/22/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	601	ATP	PA-O3A	6.81	1.66	1.59
9	B	601	ATP	PA-O3A	6.80	1.66	1.59
9	C	601	ATP	PB-O3A	6.74	1.66	1.59
9	A	601	ATP	PB-O3A	6.73	1.66	1.59
9	A	601	ATP	PA-O3A	6.73	1.66	1.59

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	601	ADP	C1'-N9-C8	-8.24	108.81	127.09
11	E	601	ADP	C4-N9-C8	6.65	112.72	105.74
11	E	601	ADP	N9-C8-N7	-5.81	105.69	113.94
9	B	601	ATP	C5-C4-N3	-5.39	119.29	126.72
9	C	601	ATP	C5-C4-N3	-5.37	119.33	126.72

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

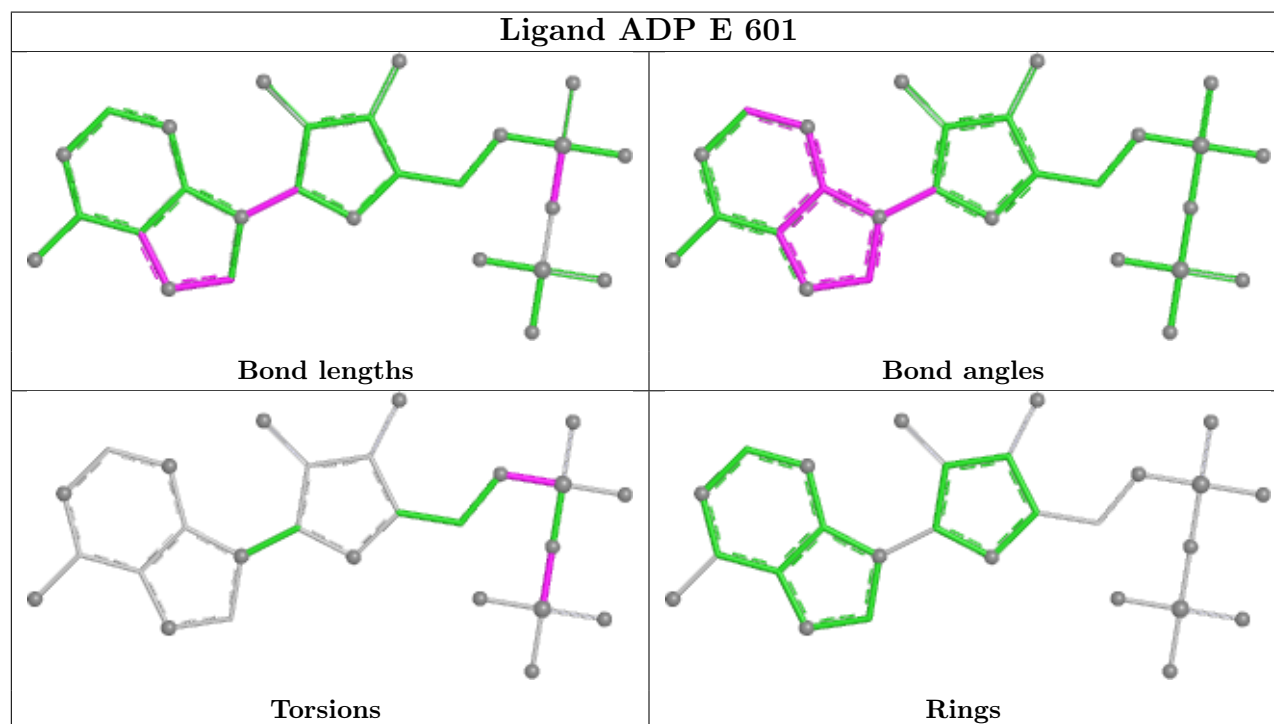
Mol	Chain	Res	Type	Atoms
9	A	601	ATP	PB-O3B-PG-O2G
9	A	601	ATP	PB-O3B-PG-O3G
9	A	601	ATP	C5'-O5'-PA-O2A
9	A	601	ATP	C5'-O5'-PA-O3A
9	B	601	ATP	PB-O3B-PG-O2G

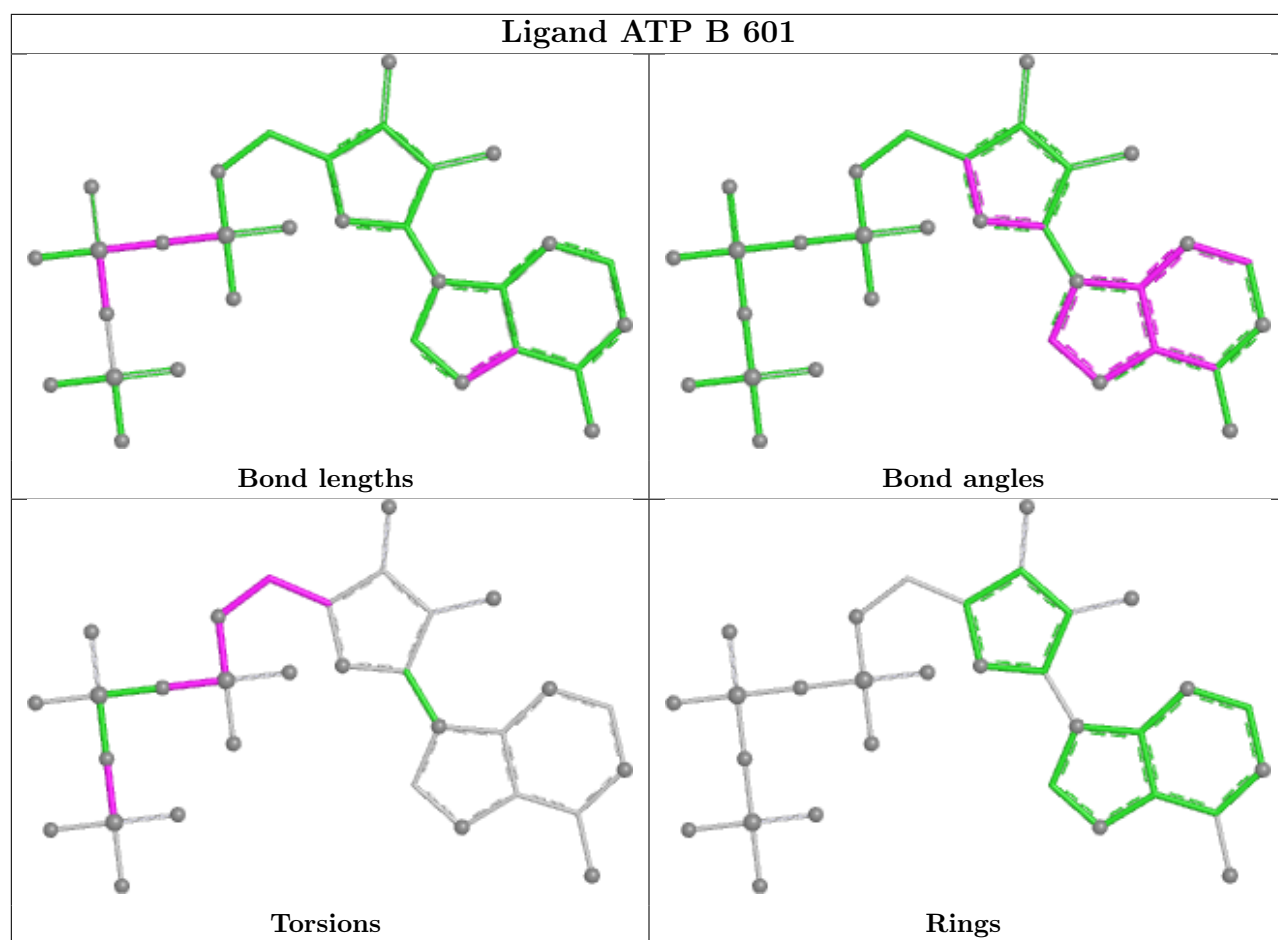
There are no ring outliers.

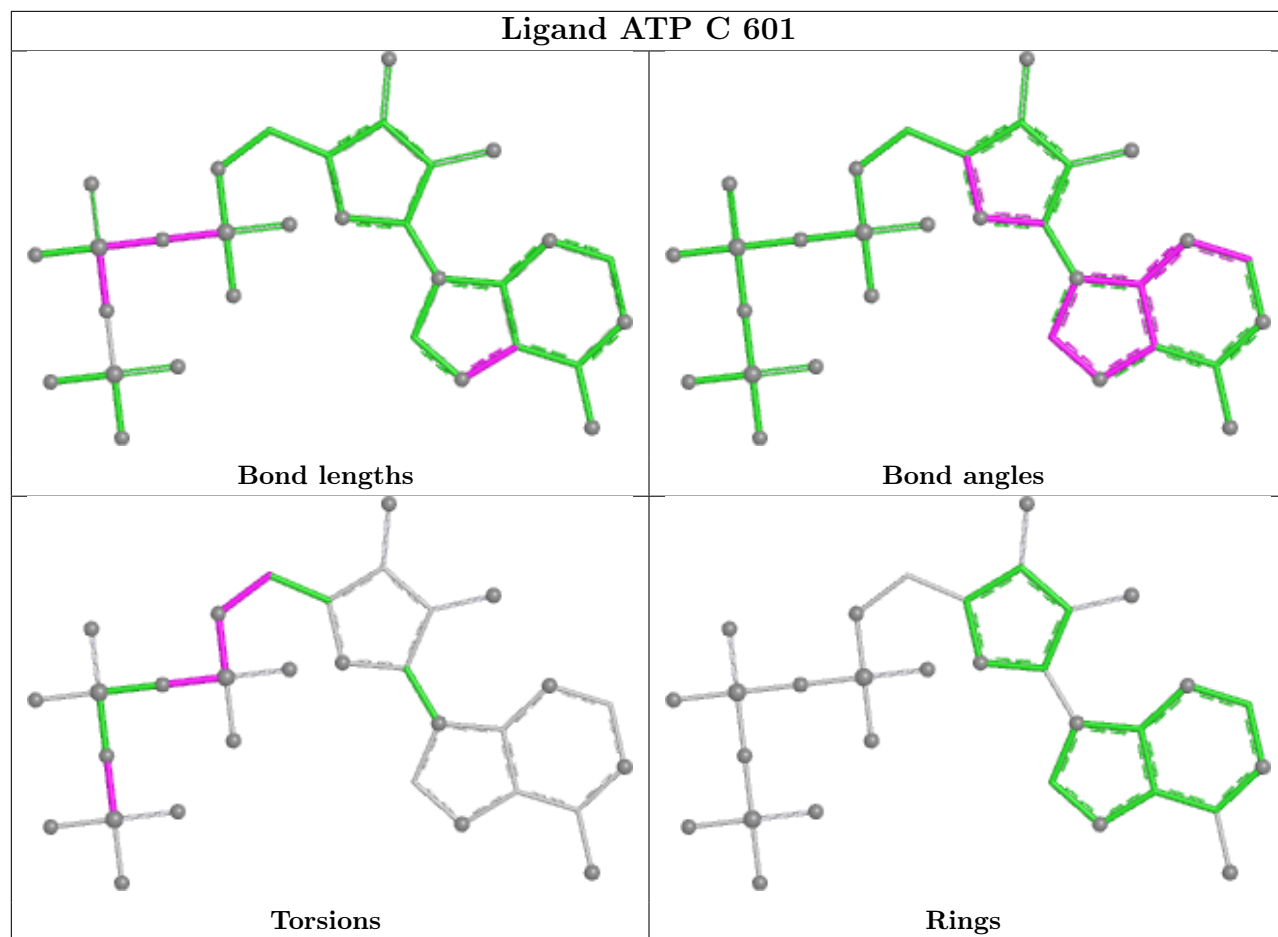
4 monomers are involved in 36 short contacts:

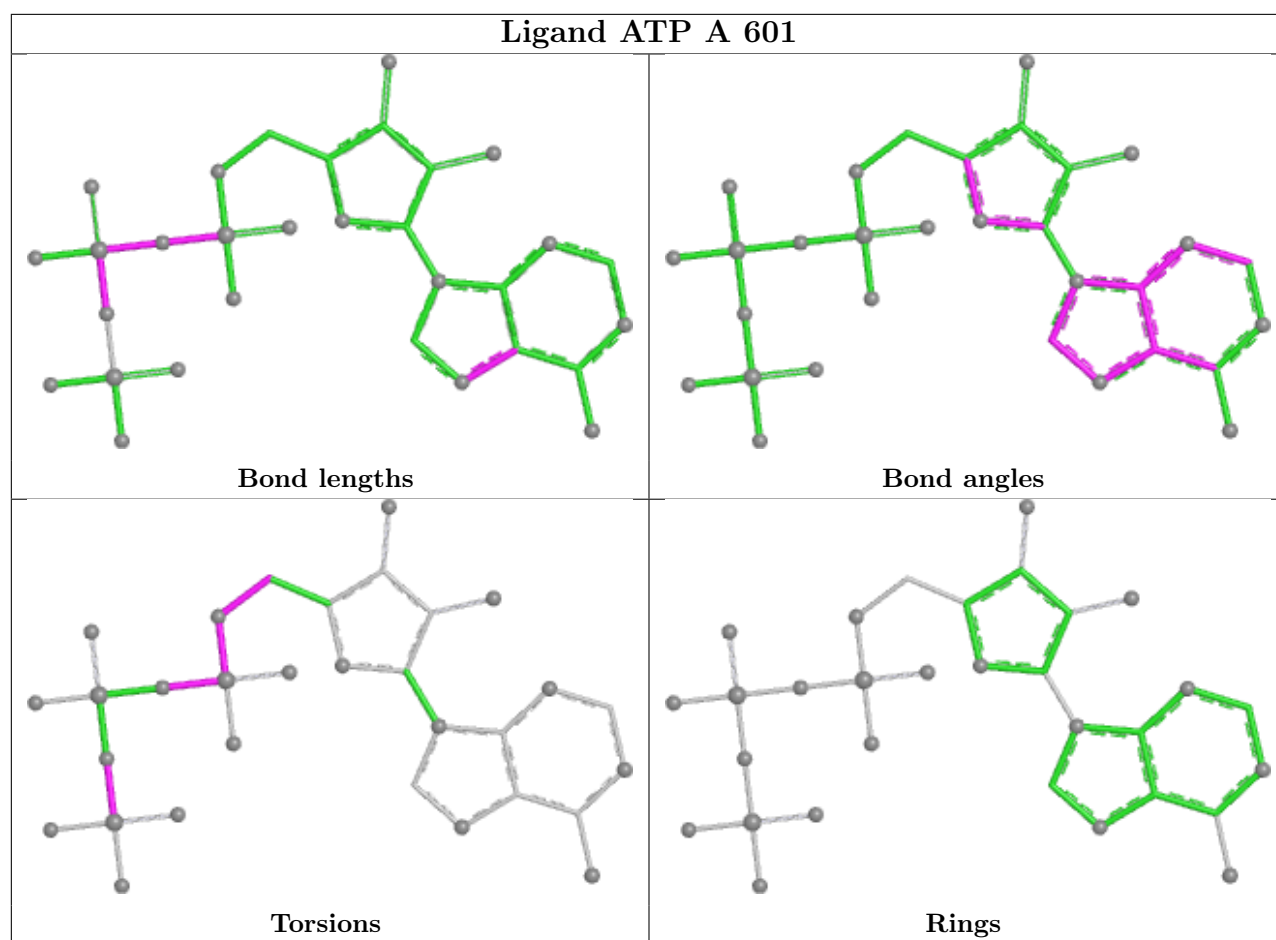
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	601	ADP	20	0
9	B	601	ATP	4	0
9	C	601	ATP	8	0
9	A	601	ATP	4	0

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.

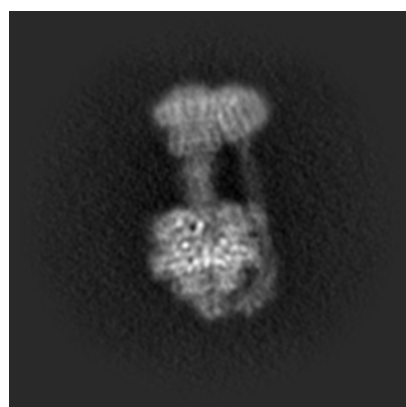
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13181. These allow visual inspection of the internal detail of the map and identification of artifacts.

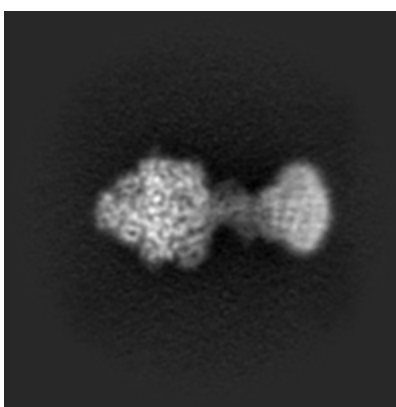
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

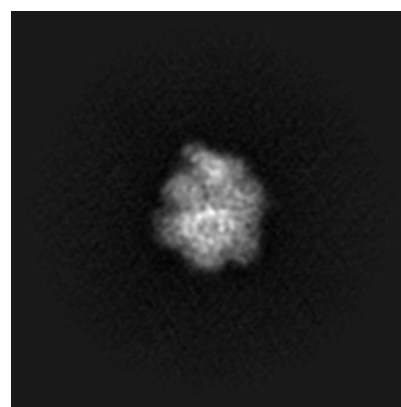
6.1.1 Primary map



X



Y



Z

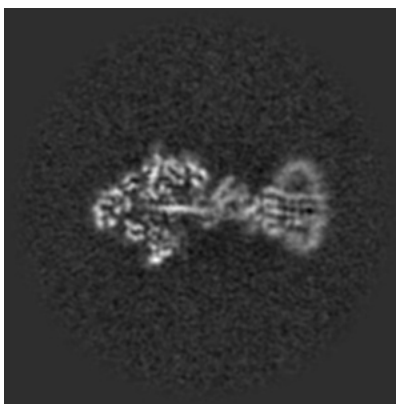
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

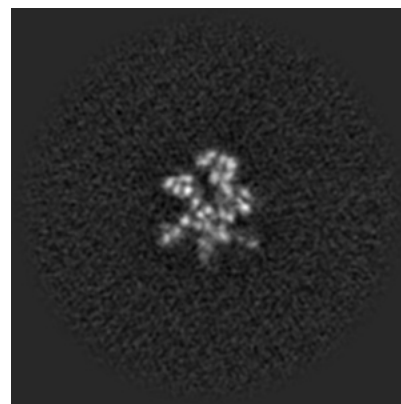
6.2.1 Primary map



X Index: 225



Y Index: 225

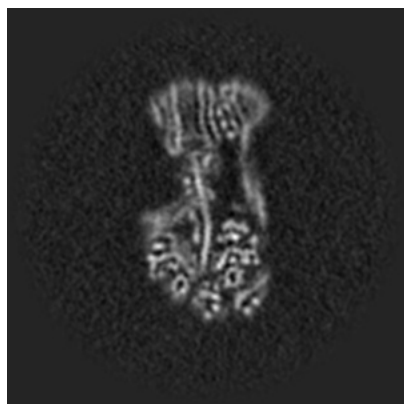


Z Index: 225

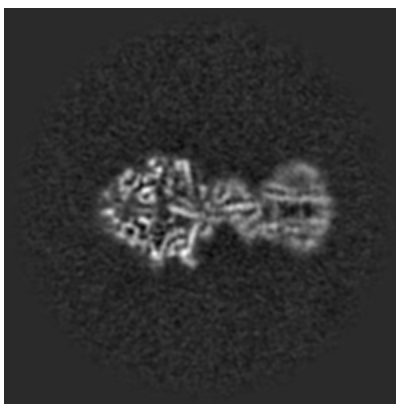
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

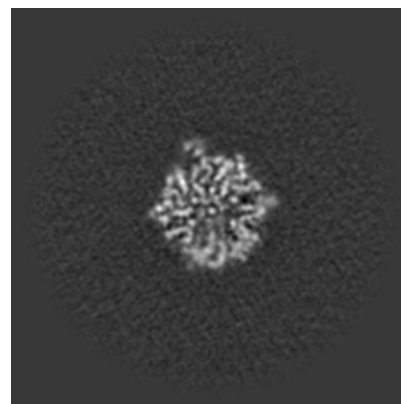
6.3.1 Primary map



X Index: 224



Y Index: 213



Z Index: 171

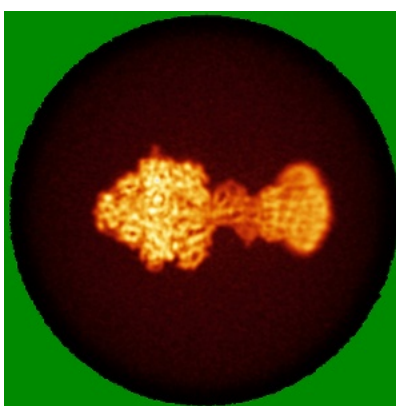
The images above show the largest variance slices of the map in three orthogonal directions.

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

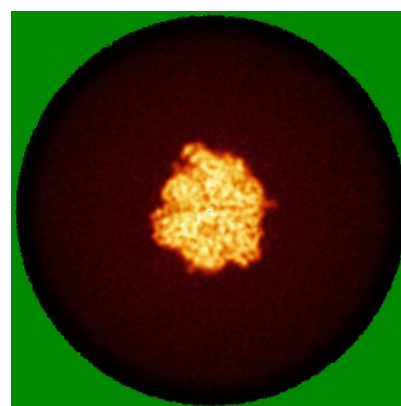
6.4.1 Primary map



X



Y

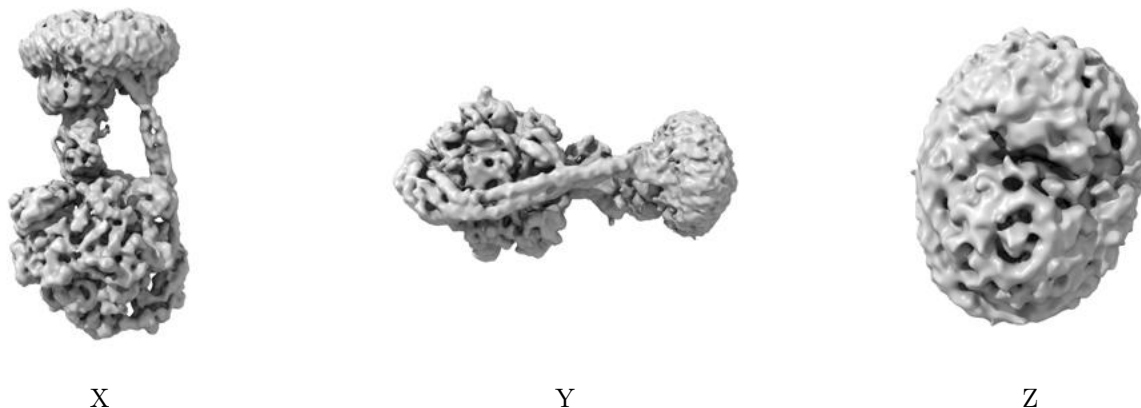


Z

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 0.0381. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

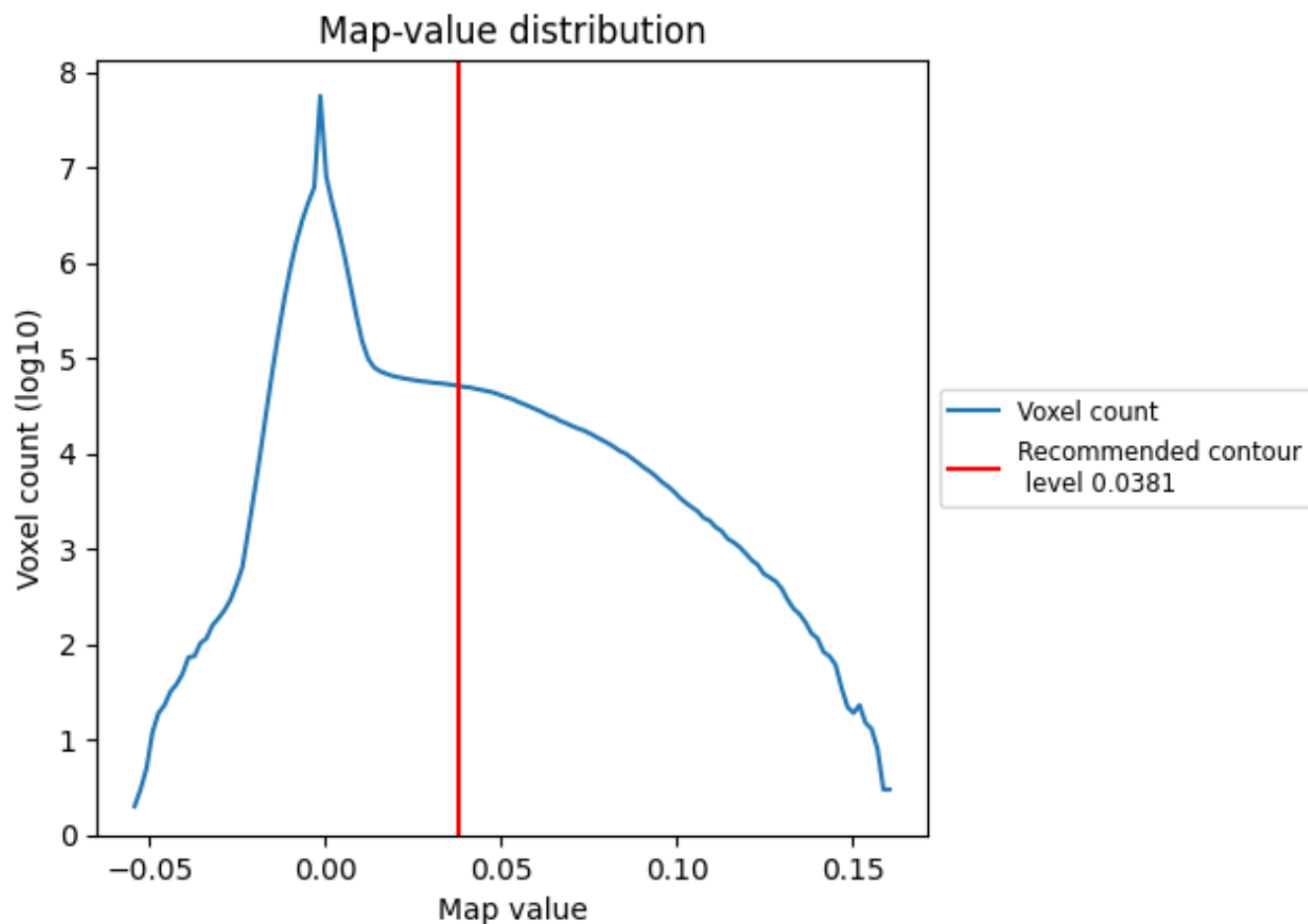
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

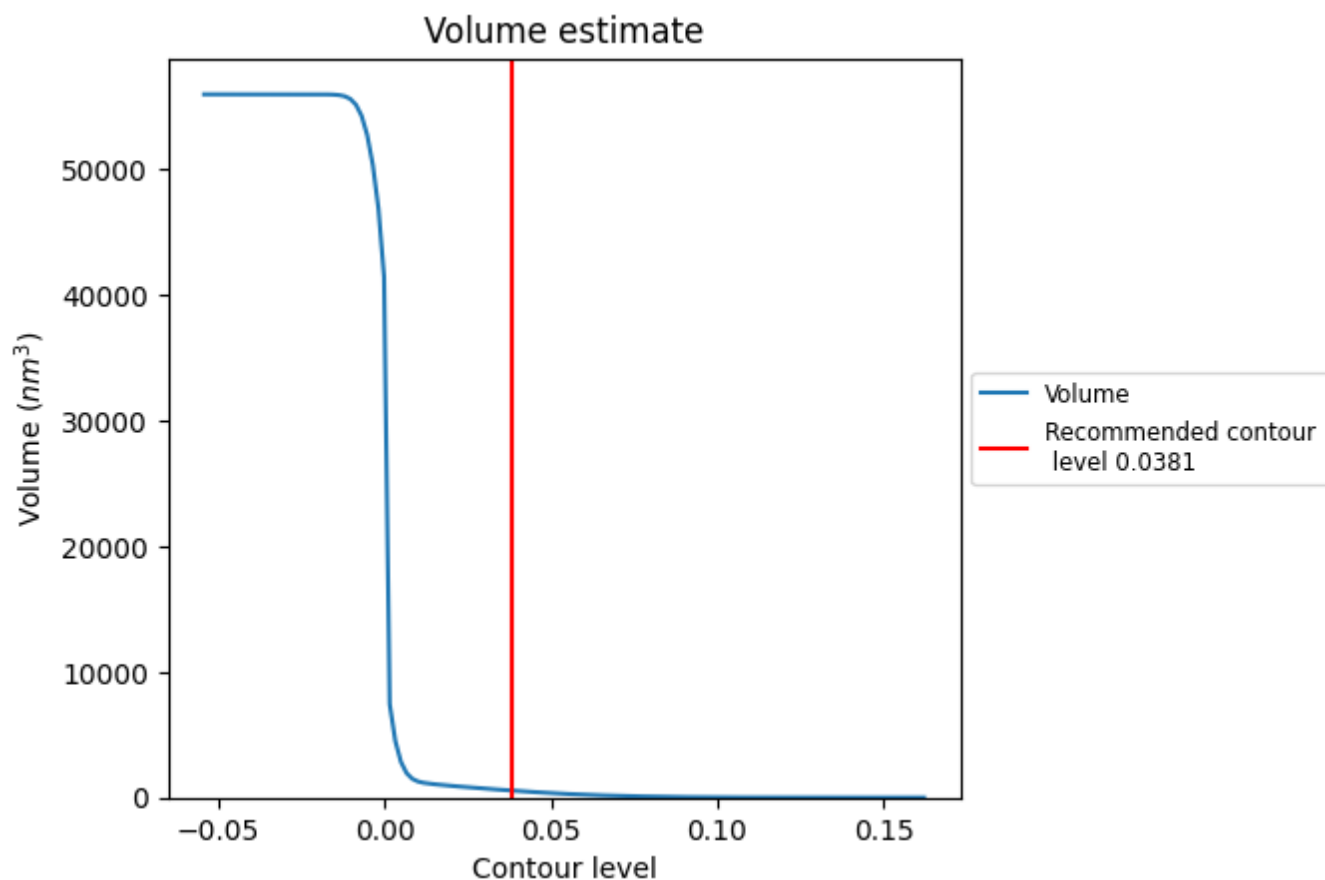
This section contains the results of statistical analysis of the map.

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.

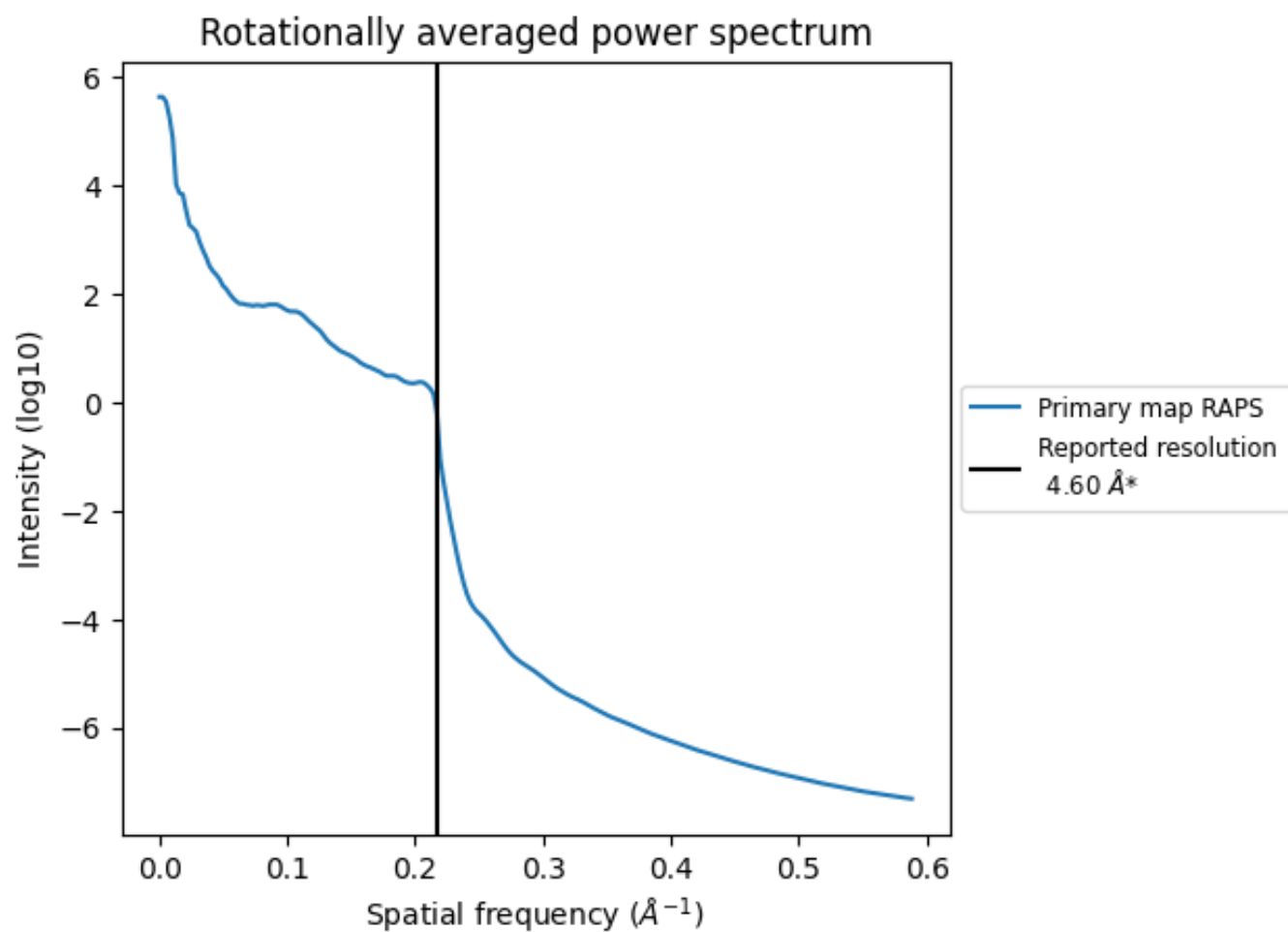
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 559 nm³; this corresponds to an approximate mass of 505 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

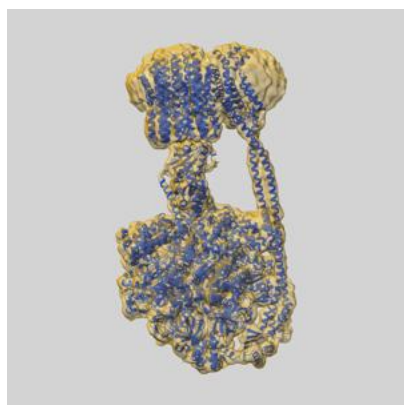
8 Fourier-Shell correlation

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

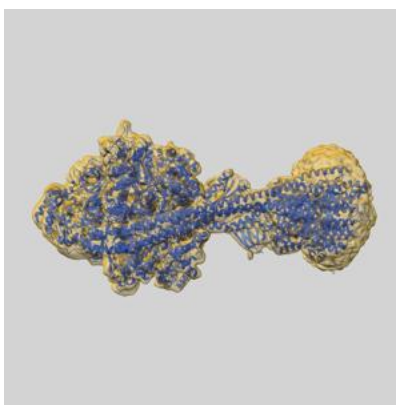
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13181 and PDB model 7P3N. Per-residue inclusion information can be found in section [3](#) on page [8](#).

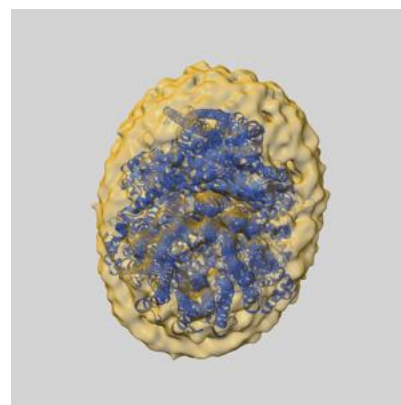
9.1 Map-model overlay [i](#)



X



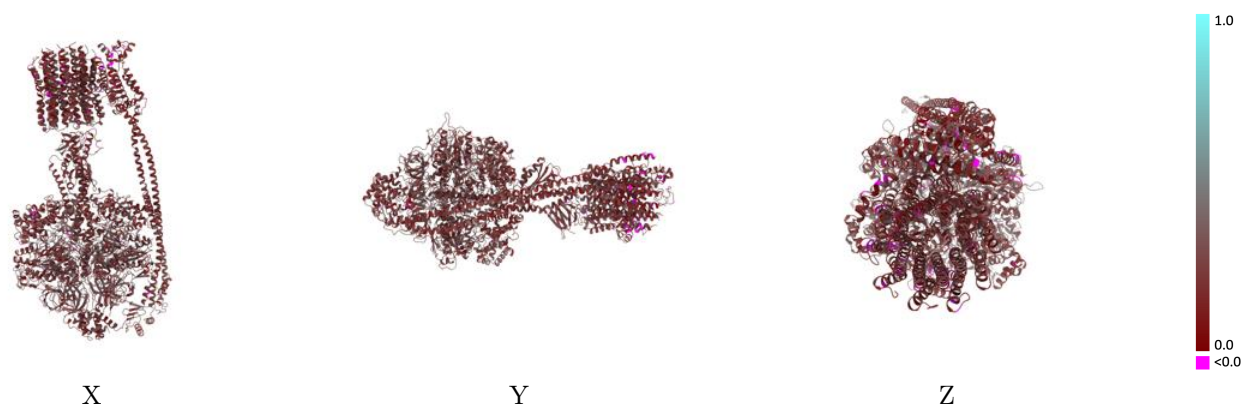
Y



Z

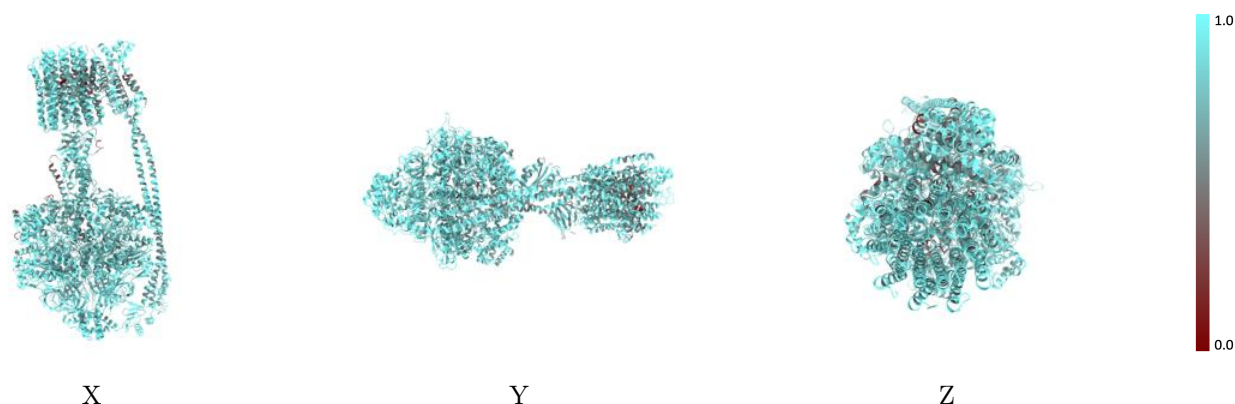
The images above show the 3D surface view of the map at the recommended contour level 0.0381 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



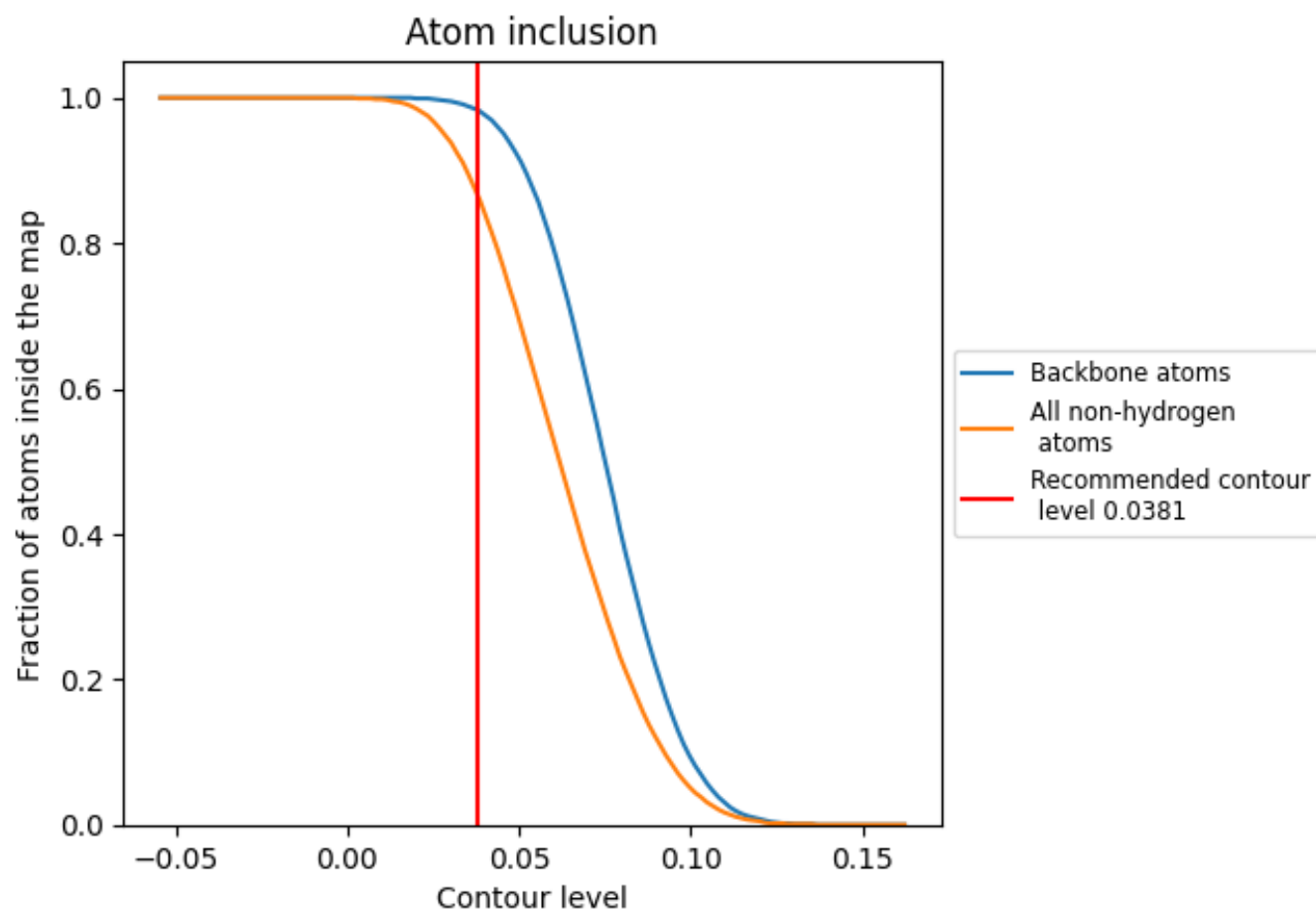
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0381).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 86% 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 (0.0381) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8650	 0.2450
A	 0.9040	 0.2710
B	 0.8970	 0.2680
C	 0.8890	 0.2700
D	 0.8910	 0.2660
E	 0.8740	 0.2700
F	 0.8600	 0.2480
G	 0.8180	 0.2060
H	 0.8140	 0.2280
J	 0.7790	 0.2250
K	 0.7970	 0.1940
L	 0.8130	 0.1910
O	 0.8480	 0.1900
P	 0.8690	 0.1940
Q	 0.8960	 0.1900
R	 0.8890	 0.1950
S	 0.9020	 0.2210
a	 0.7880	 0.1940
b	 0.8240	 0.2130
d	 0.9230	 0.2500
e	 0.7530	 0.2360
g	 0.8260	 0.2260
p	 0.8530	 0.2110

