



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 06:04 AM JST

PDB ID : 5Y60
EMDB ID : EMD-6813
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, rotational state 3.
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2017-08-10
Resolution : 7.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

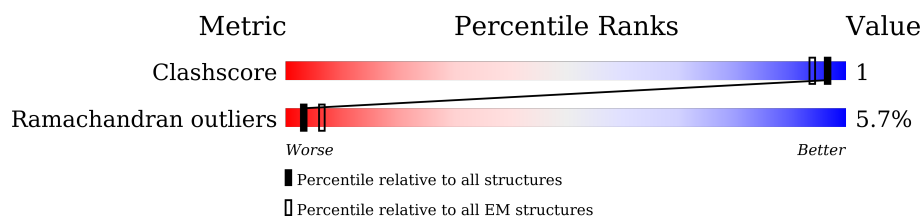
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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

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	578	 91% 9%
1	B	578	 90% 10%
1	C	578	 88% 11% .
2	D	478	 90% 6% .
2	E	478	 85% 11% .
2	F	478	 84% 12% .
3	G	223	 5% 84% 10% 6%
4	H	104	 6% 81% 14% . .
5	I	120	 82% . 17%

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Mol	Chain	Length	Quality of chain
5	K	120	
6	J	188	
6	L	188	
7	M	323	
8	N	652	
9	O	99	
9	P	99	
9	Q	99	
9	R	99	
9	S	99	
9	T	99	
9	U	99	
9	V	99	
9	W	99	
9	X	99	
9	Y	99	
9	Z	99	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23433 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	B	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	C	577	Total	C	N	O	0	0
			2307	1154	577	576		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	459	Total	C	N	O	0	0
			1835	918	459	458		
2	E	459	Total	C	N	O	0	0
			1835	918	459	458		
2	F	459	Total	C	N	O	0	0
			1835	918	459	458		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	210	Total	C	N	O	0	0
			839	420	210	209		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	100	Total	C	N	O	0	0
			399	200	100	99		
5	K	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	185	Total	C	N	O	0	0
			738	370	185	183		
6	L	185	Total	C	N	O	0	0
			738	370	185	183		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	320	Total	C	N	O	0	0
			1279	640	320	319		

- Molecule 8 is a protein called V-type ATP synthase subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	632	Total	C	N	O	0	0
			2526	1264	632	630		

- Molecule 9 is a protein called V-type ATP synthase, subunit K.

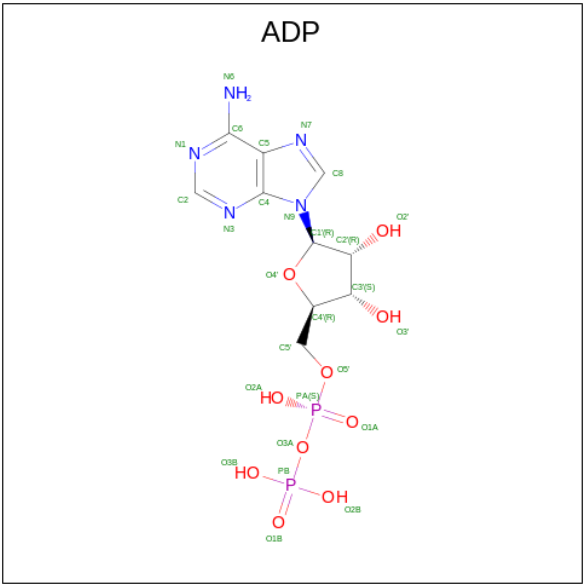
Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	76	Total	C	N	O	0	0
			303	152	76	75		
9	P	76	Total	C	N	O	0	0
			303	152	76	75		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	76	Total	C	N	O	0	0
			303	152	76	75		
9	R	76	Total	C	N	O	0	0
			303	152	76	75		
9	S	76	Total	C	N	O	0	0
			303	152	76	75		
9	T	76	Total	C	N	O	0	0
			303	152	76	75		
9	U	76	Total	C	N	O	0	0
			303	152	76	75		
9	V	76	Total	C	N	O	0	0
			303	152	76	75		
9	W	76	Total	C	N	O	0	0
			303	152	76	75		
9	X	76	Total	C	N	O	0	0
			303	152	76	75		
9	Y	76	Total	C	N	O	0	0
			303	152	76	75		
9	Z	76	Total	C	N	O	0	0
			303	152	76	75		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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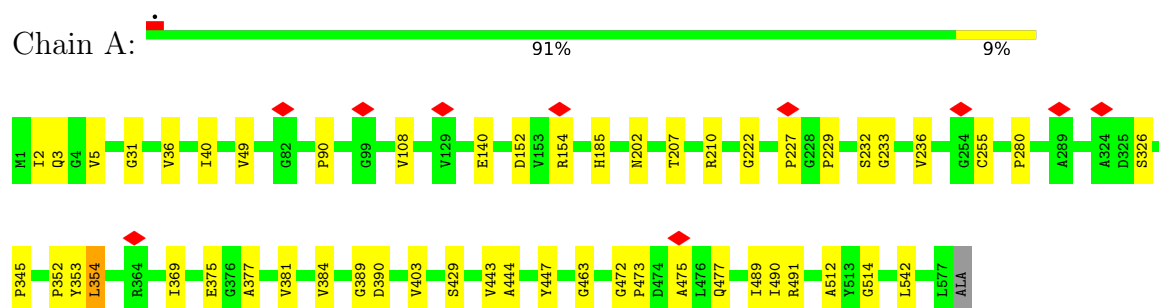
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	B	1	27	10	5	10	2	0

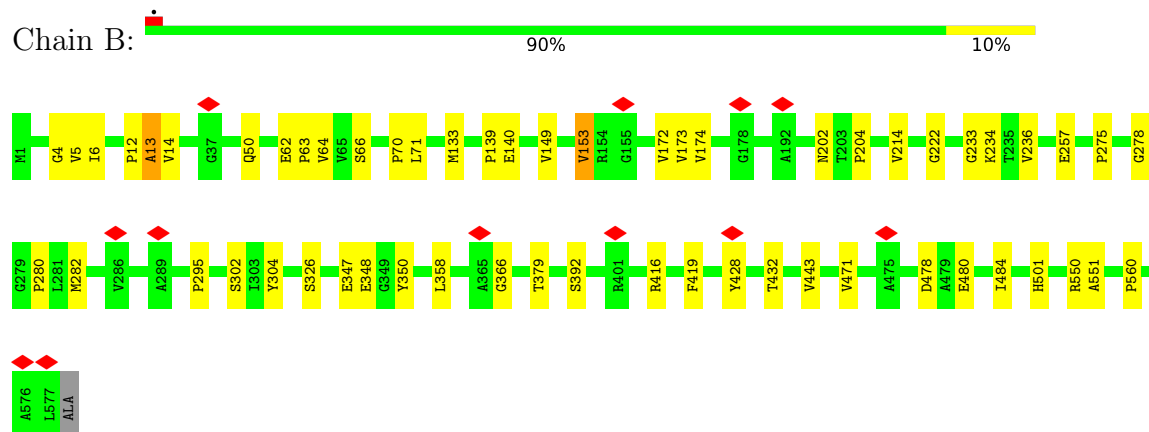
3 Residue-property plots

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.

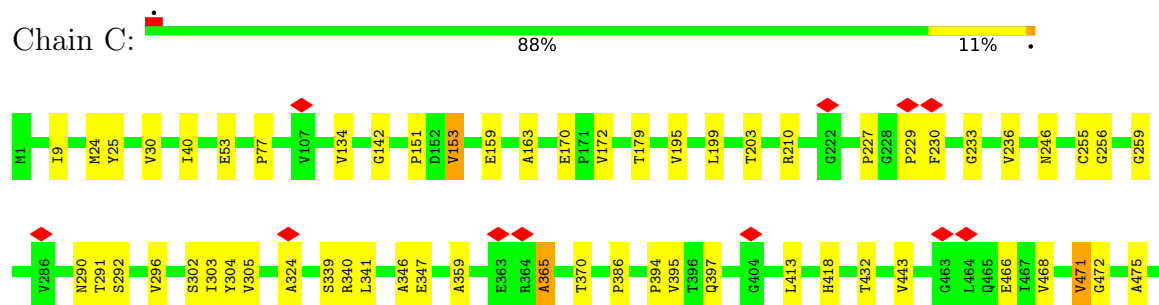
- Molecule 1: V-type ATP synthase alpha chain

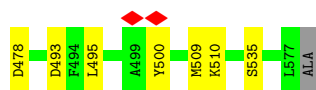


- Molecule 1: V-type ATP synthase alpha chain



- Molecule 1: V-type ATP synthase alpha chain





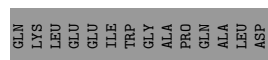
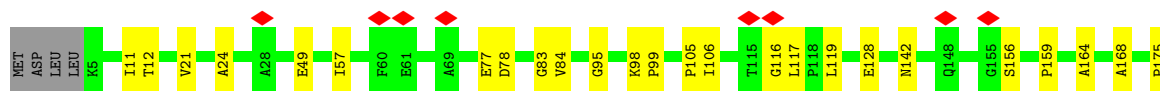
- Molecule 2: V-type ATP synthase beta chain

Chain D: 90% 6% .



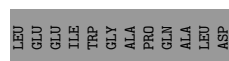
- Molecule 2: V-type ATP synthase beta chain

Chain E: 85% 11% .



- Molecule 2: V-type ATP synthase beta chain

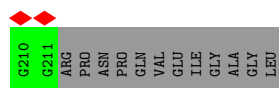
Chain F: 84% 12% .



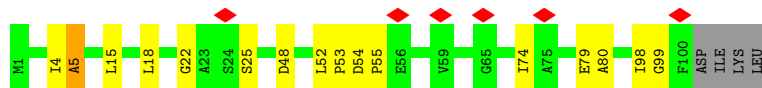
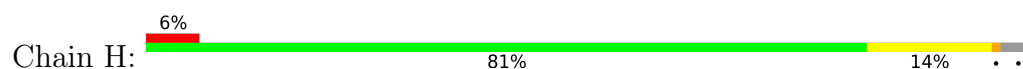
- Molecule 3: V-type ATP synthase subunit D

Chain G: 5% 84% 10% 6%

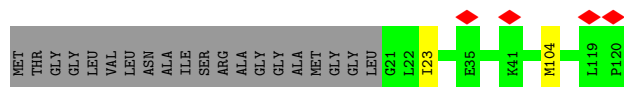
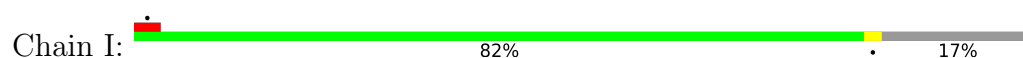




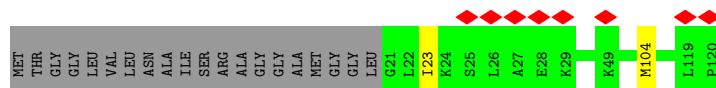
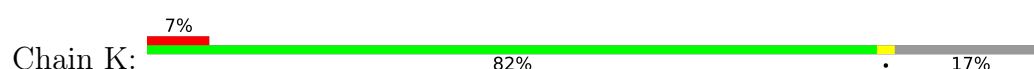
- Molecule 4: V-type ATP synthase subunit F



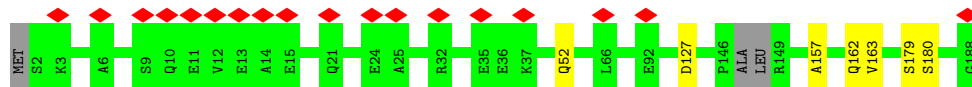
- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)



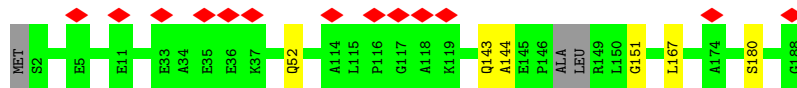
- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)



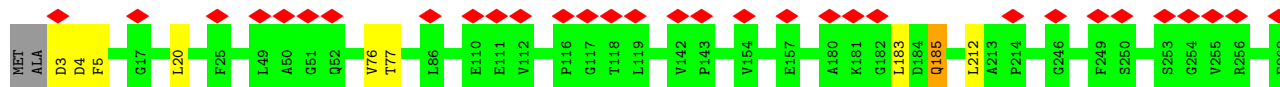
- Molecule 6: V-type ATP synthase subunit E

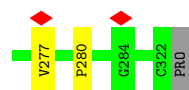


- Molecule 6: V-type ATP synthase subunit E

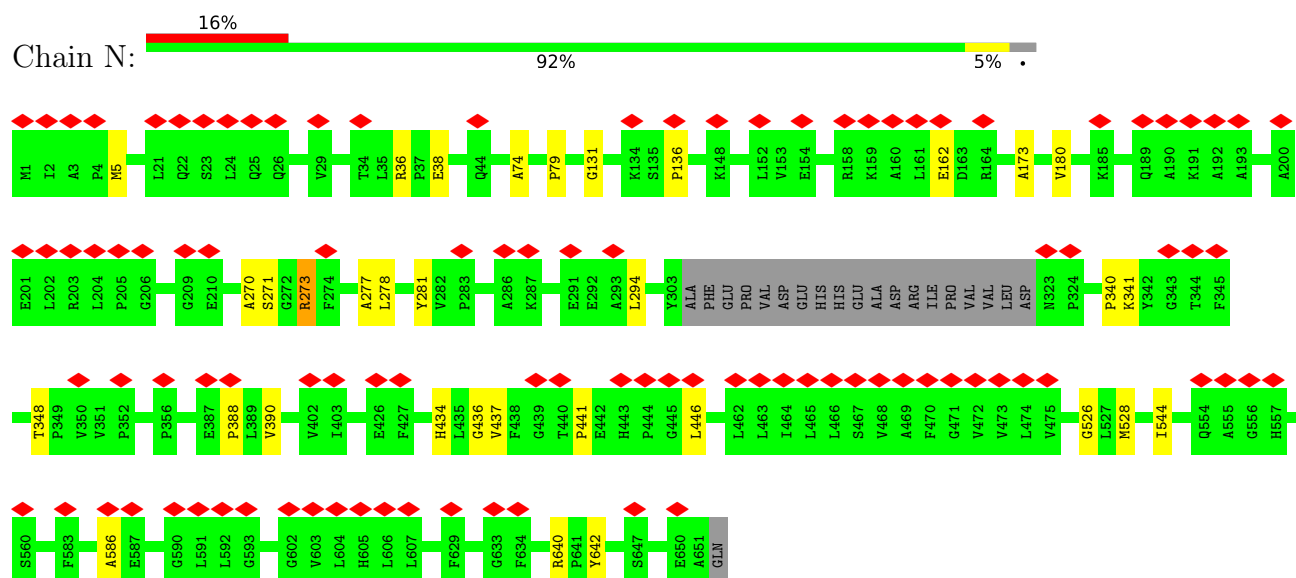


- Molecule 7: V-type ATP synthase subunit C

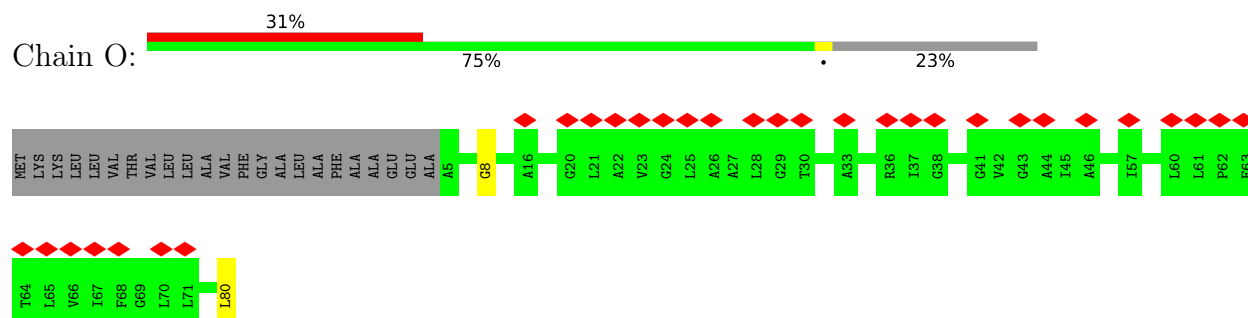




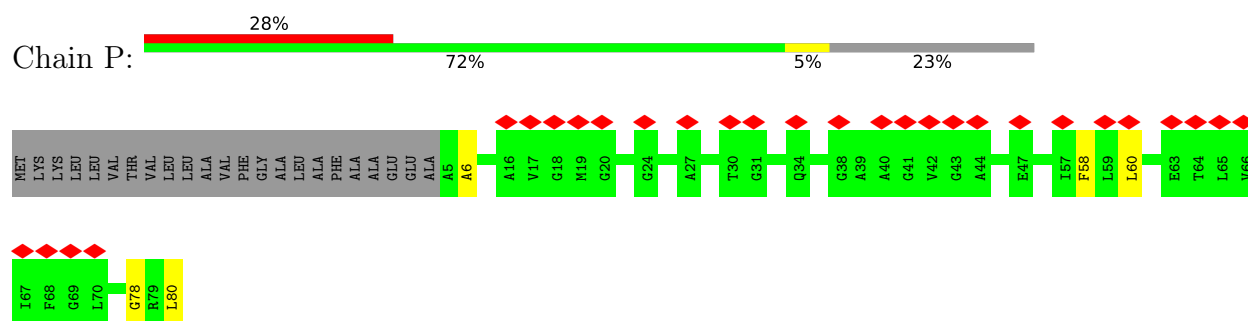
- Molecule 8: V-type ATP synthase subunit I



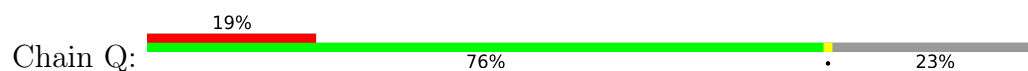
- Molecule 9: V-type ATP synthase, subunit K

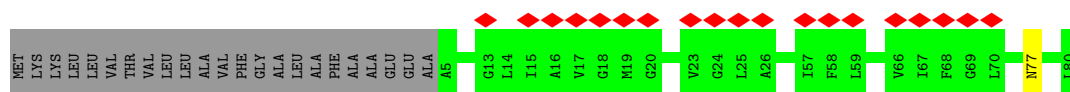


- Molecule 9: V-type ATP synthase, subunit K

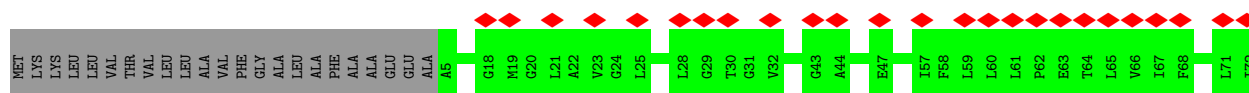
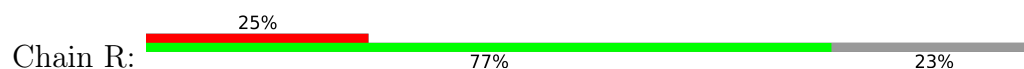


- Molecule 9: V-type ATP synthase, subunit K

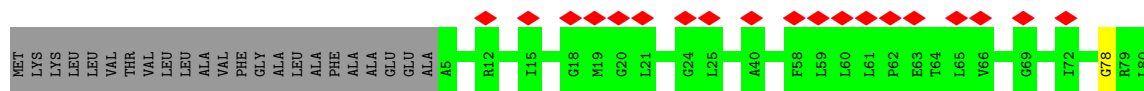
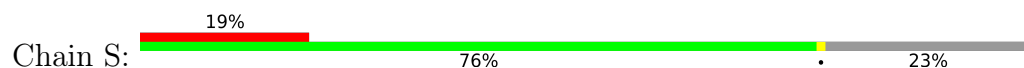




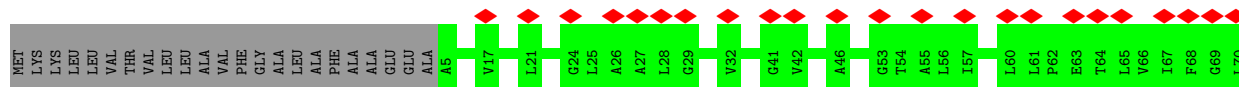
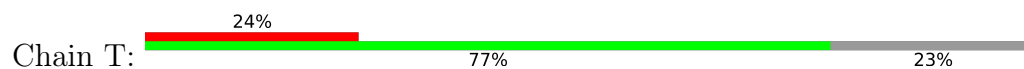
- Molecule 9: V-type ATP synthase, subunit K



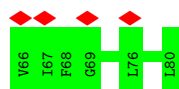
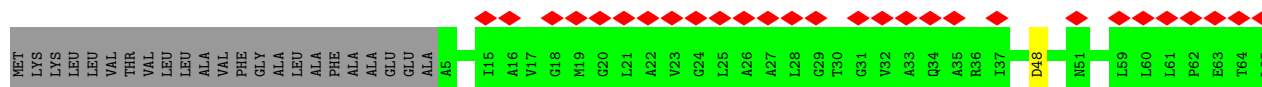
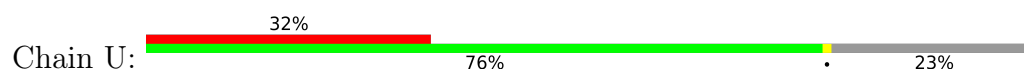
- Molecule 9: V-type ATP synthase, subunit K



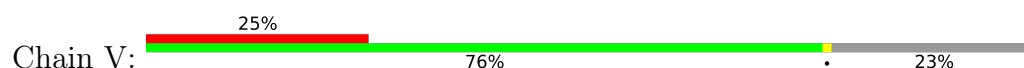
- Molecule 9: V-type ATP synthase, subunit K

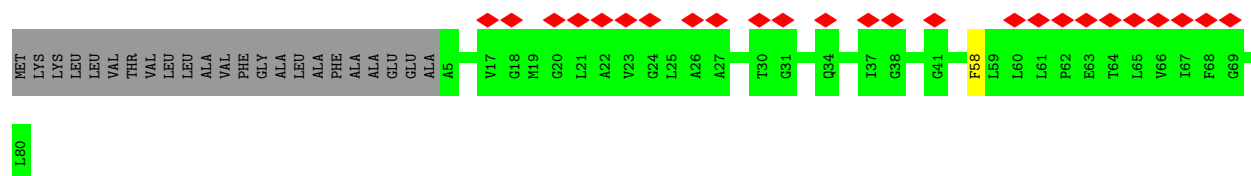


- Molecule 9: V-type ATP synthase, subunit K

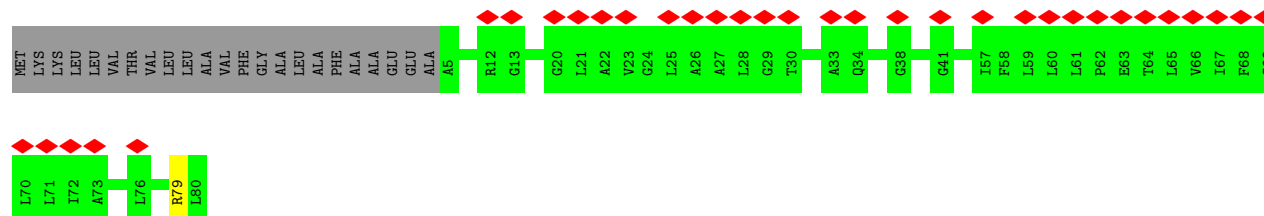
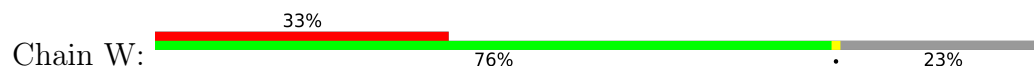


- Molecule 9: V-type ATP synthase, subunit K

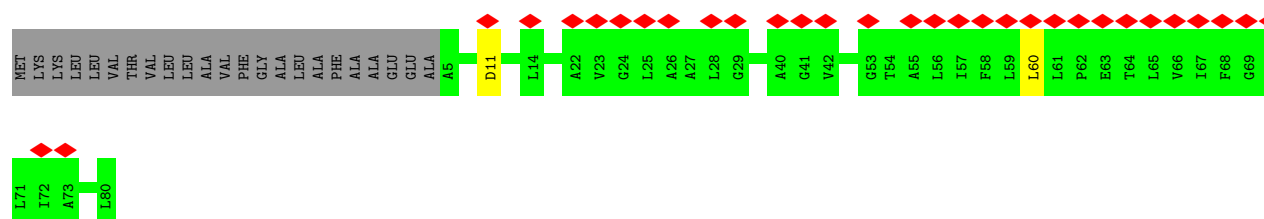
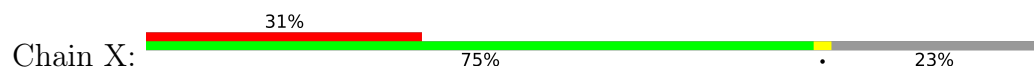




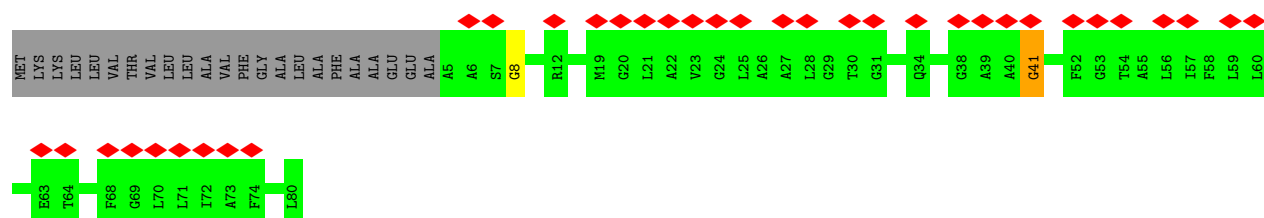
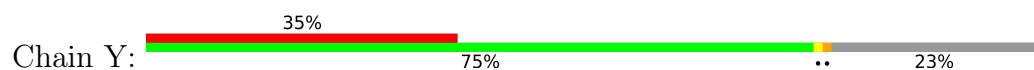
- Molecule 9: V-type ATP synthase, subunit K



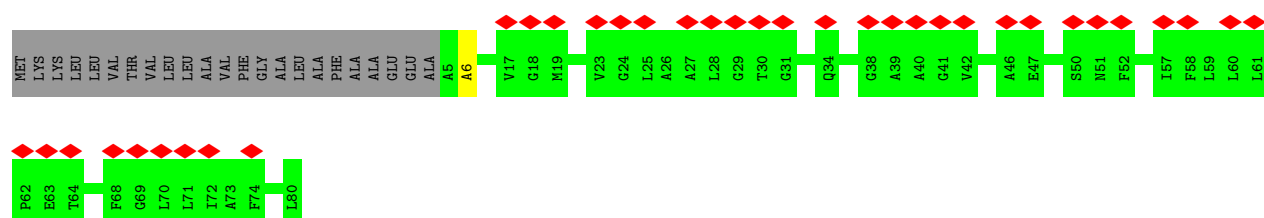
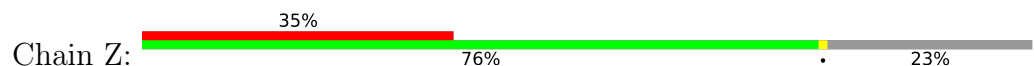
- Molecule 9: V-type ATP synthase, subunit K



- Molecule 9: V-type ATP synthase, subunit K



- Molecule 9: V-type ATP synthase, subunit K



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13851	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 ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	330.4, 330.4, 330.4	wwPDB
Map dimensions	236, 236, 236	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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

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	1.37	0/2306	1.29	9/2881 (0.3%)
1	B	1.37	1/2306 (0.0%)	1.32	10/2881 (0.3%)
1	C	1.34	0/2306	1.29	5/2881 (0.2%)
2	D	1.32	0/1834	1.31	4/2291 (0.2%)
2	E	1.41	0/1834	1.37	13/2291 (0.6%)
2	F	1.42	0/1834	1.36	8/2291 (0.3%)
3	G	1.32	0/838	1.29	1/1046 (0.1%)
4	H	1.24	0/398	1.36	3/496 (0.6%)
5	I	0.97	0/398	1.00	0/496
5	K	1.05	0/398	1.00	0/496
6	J	1.01	0/736	1.04	0/917
6	L	1.10	0/736	1.01	0/917
7	M	1.07	0/1278	1.04	2/1596 (0.1%)
8	N	1.03	0/2524	1.14	3/3152 (0.1%)
9	O	0.86	0/302	1.17	2/376 (0.5%)
9	P	0.89	0/302	1.19	1/376 (0.3%)
9	Q	0.89	0/302	1.03	0/376
9	R	0.86	0/302	1.13	0/376
9	S	0.89	0/302	1.06	1/376 (0.3%)
9	T	0.88	0/302	1.01	0/376
9	U	0.91	0/302	1.08	0/376
9	V	0.93	0/302	1.27	1/376 (0.3%)
9	W	0.85	0/302	1.12	0/376
9	X	0.88	0/302	1.11	1/376 (0.3%)
9	Y	0.85	0/302	1.03	1/376 (0.3%)
9	Z	0.94	0/302	1.12	0/376
All	All	1.22	1/23350 (0.0%)	1.23	65/29144 (0.2%)

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
1	A	0	2
1	B	0	3
1	C	0	1
2	F	0	2
7	M	0	3
9	P	0	1
9	U	0	1
9	Y	0	2
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	GLY	CA-C	-5.40	1.43	1.51

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	HIS	C-N-CA	7.70	140.94	121.70
1	A	232	SER	C-N-CA	7.07	137.14	122.30
1	B	419	PHE	N-CA-C	-6.77	92.72	111.00
1	C	471	VAL	C-N-CA	6.75	136.47	122.30
2	E	12	THR	N-CA-C	-6.61	93.16	111.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	VAL	Mainchain
1	A	49	VAL	Mainchain
1	B	358	LEU	Peptide,Mainchain
1	B	379	THR	Mainchain
1	C	346	ALA	Mainchain

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	2307	0	654	2	0
1	B	2307	0	654	4	0
1	C	2307	0	654	4	0
2	D	1835	0	512	0	0
2	E	1835	0	512	1	0
2	F	1835	0	512	2	0
3	G	839	0	230	1	0
4	H	399	0	119	2	0
5	I	399	0	100	0	0
5	K	399	0	100	0	0
6	J	738	0	192	0	0
6	L	738	0	192	2	0
7	M	1279	0	357	0	0
8	N	2526	0	709	1	0
9	O	303	0	102	0	0
9	P	303	0	102	1	0
9	Q	303	0	102	0	0
9	R	303	0	102	0	0
9	S	303	0	102	0	0
9	T	303	0	102	0	0
9	U	303	0	102	0	0
9	V	303	0	102	0	0
9	W	303	0	102	0	0
9	X	303	0	102	1	0
9	Y	303	0	102	1	0
9	Z	303	0	102	0	0
10	A	27	0	12	0	0
10	B	27	0	12	1	0
All	All	23433	0	6745	20	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 1.

The worst 5 of 20 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:B:6:ILE:H	1:B:62:GLU:H	1.51	0.58
6:L:151:GLY:HA2	6:L:167:LEU:H	1.69	0.57
1:A:352:PRO:C	1:A:354:LEU:H	2.08	0.56
1:C:24:MET:H	2:F:66:LEU:N	2.10	0.50
1:B:236:VAL:H	10:B:600:ADP:PA	2.35	0.49

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	A	575/578 (100%)	462 (80%)	75 (13%)	38 (7%)	1	15
1	B	575/578 (100%)	448 (78%)	86 (15%)	41 (7%)	1	14
1	C	575/578 (100%)	417 (72%)	102 (18%)	56 (10%)	0	10
2	D	457/478 (96%)	355 (78%)	75 (16%)	27 (6%)	1	17
2	E	457/478 (96%)	334 (73%)	84 (18%)	39 (8%)	1	12
2	F	457/478 (96%)	334 (73%)	79 (17%)	44 (10%)	0	10
3	G	208/223 (93%)	149 (72%)	39 (19%)	20 (10%)	0	10
4	H	98/104 (94%)	62 (63%)	24 (24%)	12 (12%)	0	5
5	I	98/120 (82%)	91 (93%)	5 (5%)	2 (2%)	7	38
5	K	98/120 (82%)	94 (96%)	2 (2%)	2 (2%)	7	38
6	J	181/188 (96%)	155 (86%)	19 (10%)	7 (4%)	3	23
6	L	181/188 (96%)	155 (86%)	22 (12%)	4 (2%)	6	35
7	M	318/323 (98%)	299 (94%)	12 (4%)	7 (2%)	6	35
8	N	628/652 (96%)	550 (88%)	49 (8%)	29 (5%)	2	21
9	O	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
9	P	74/99 (75%)	71 (96%)	2 (3%)	1 (1%)	11	46
9	Q	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	11	46
9	R	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	S	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
9	T	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	U	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	V	74/99 (75%)	74 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	11	46
9	X	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
9	Y	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	Z	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	11	46
All	All	5794/6274 (92%)	4770 (82%)	692 (12%)	332 (6%)	3	18

5 of 332 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	THR
1	A	210	ARG
1	A	227	PRO
1	A	229	PRO
1	A	233	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

2 ligands are modelled in this entry.

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
10	ADP	A	600	-	24,29,29	1.10	3 (12%)	29,45,45	1.06	3 (10%)
10	ADP	B	600	-	24,29,29	1.04	1 (4%)	29,45,45	1.22	3 (10%)

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
10	ADP	A	600	-	-	5/12/32/32	0/3/3/3
10	ADP	B	600	-	-	6/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	600	ADP	C2'-C1'	-2.56	1.49	1.53
10	B	600	ADP	C8-N7	-2.54	1.30	1.34
10	A	600	ADP	C8-N7	-2.17	1.30	1.34
10	A	600	ADP	PA-O2A	-2.01	1.45	1.55

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	600	ADP	N6-C6-N1	3.34	125.51	118.57
10	B	600	ADP	PA-O3A-PB	3.01	143.16	132.83
10	A	600	ADP	N6-C6-N1	2.73	124.25	118.57
10	A	600	ADP	C1'-N9-C4	-2.12	122.92	126.64
10	A	600	ADP	C5-C6-N1	-2.08	115.63	120.35

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	600	ADP	C5'-O5'-PA-O3A
10	A	600	ADP	C3'-C4'-C5'-O5'
10	B	600	ADP	C5'-O5'-PA-O2A

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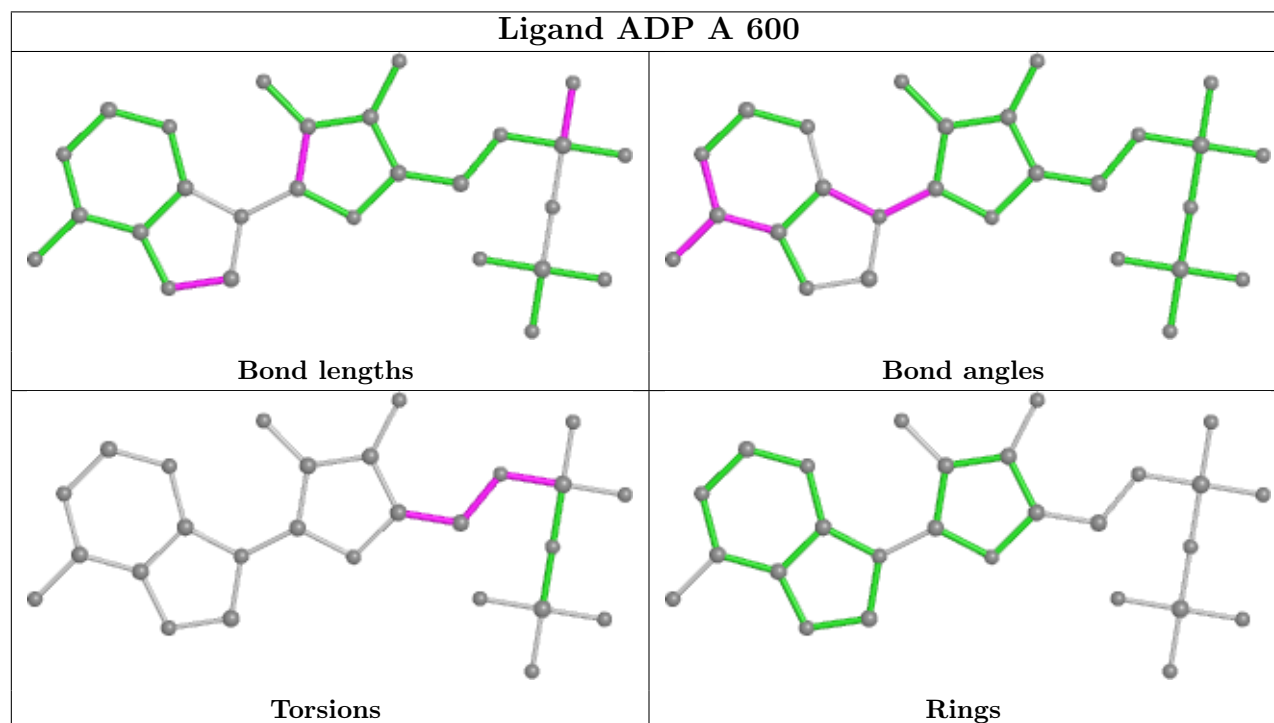
Mol	Chain	Res	Type	Atoms
10	B	600	ADP	C5'-O5'-PA-O3A
10	B	600	ADP	C3'-C4'-C5'-O5'

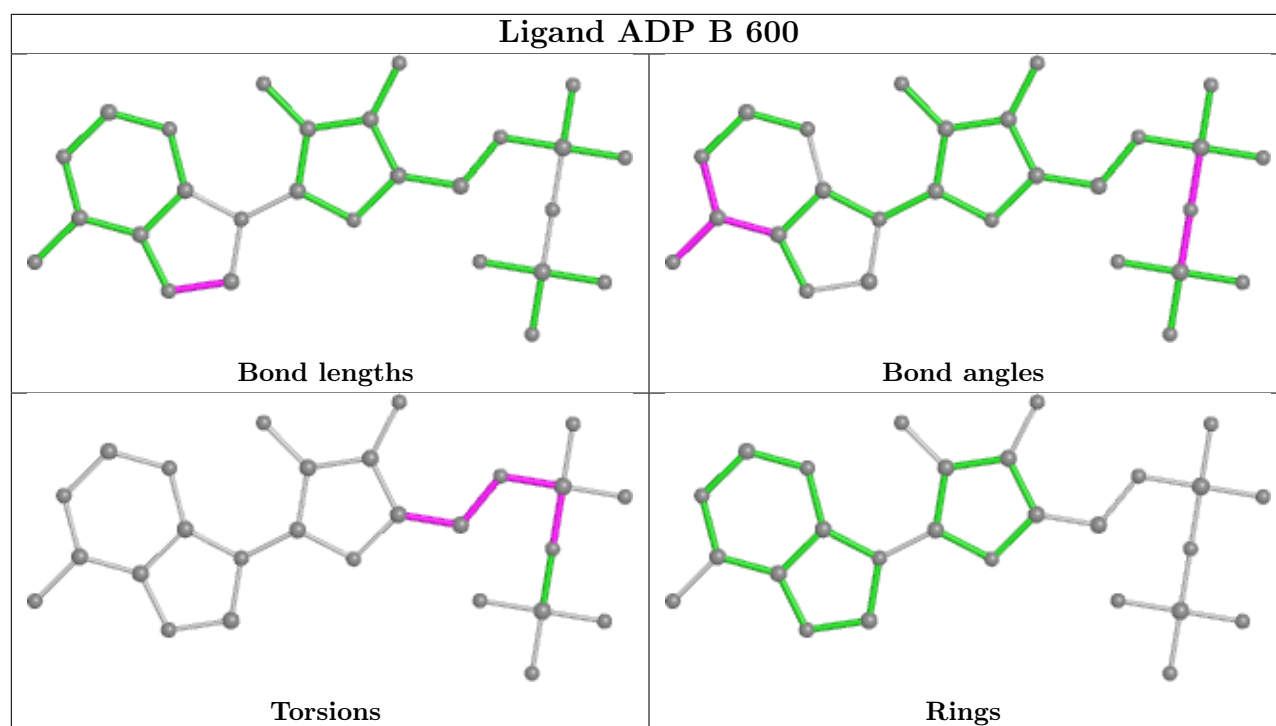
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	600	ADP	1	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.

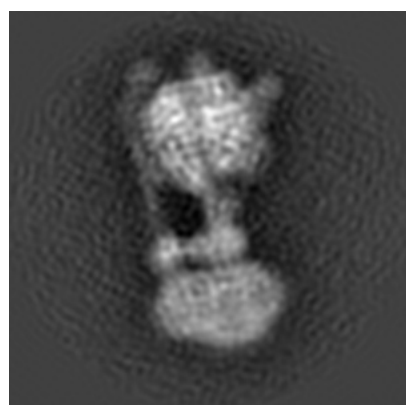
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6813. These allow visual inspection of the internal detail of the map and identification of artifacts.

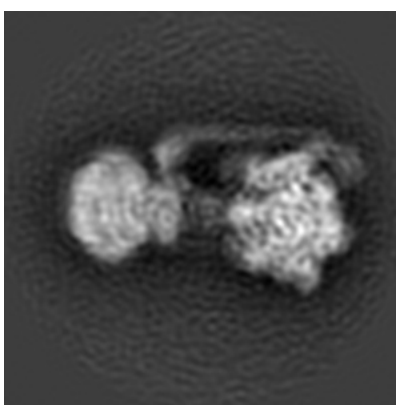
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

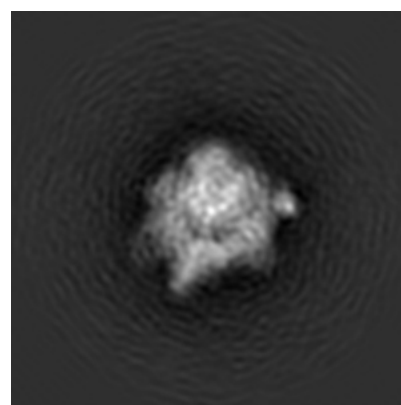
6.1.1 Primary map



X



Y



Z

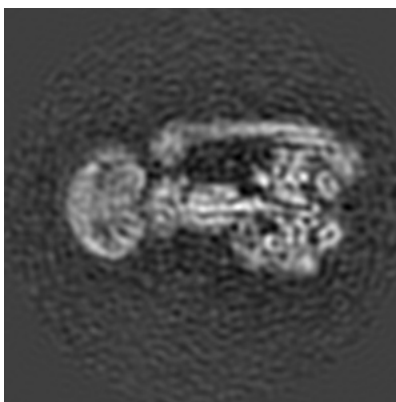
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

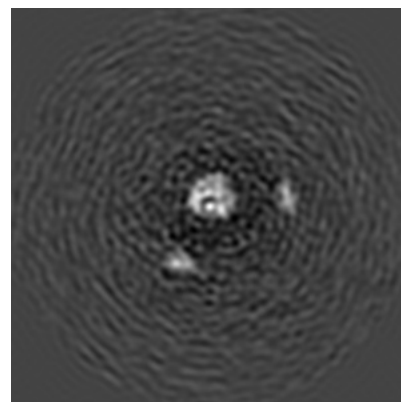
6.2.1 Primary map



X Index: 118



Y Index: 118



Z Index: 118

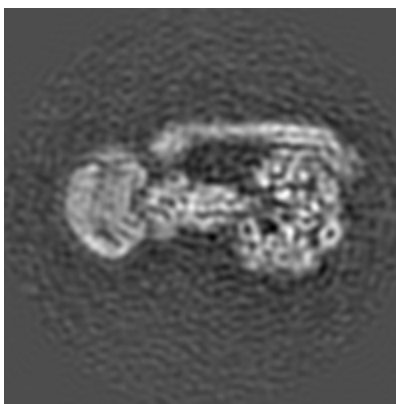
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

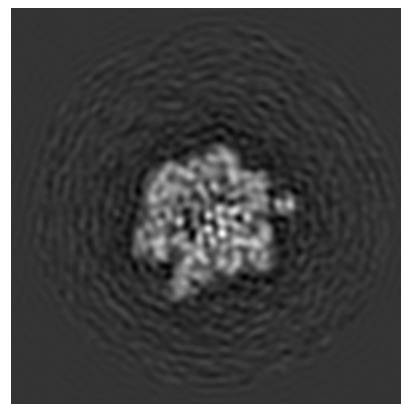
6.3.1 Primary map



X Index: 117



Y Index: 120



Z Index: 171

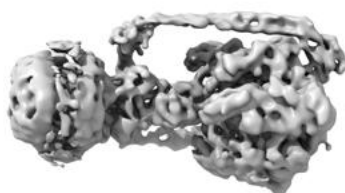
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

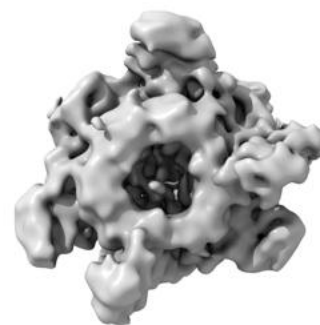
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

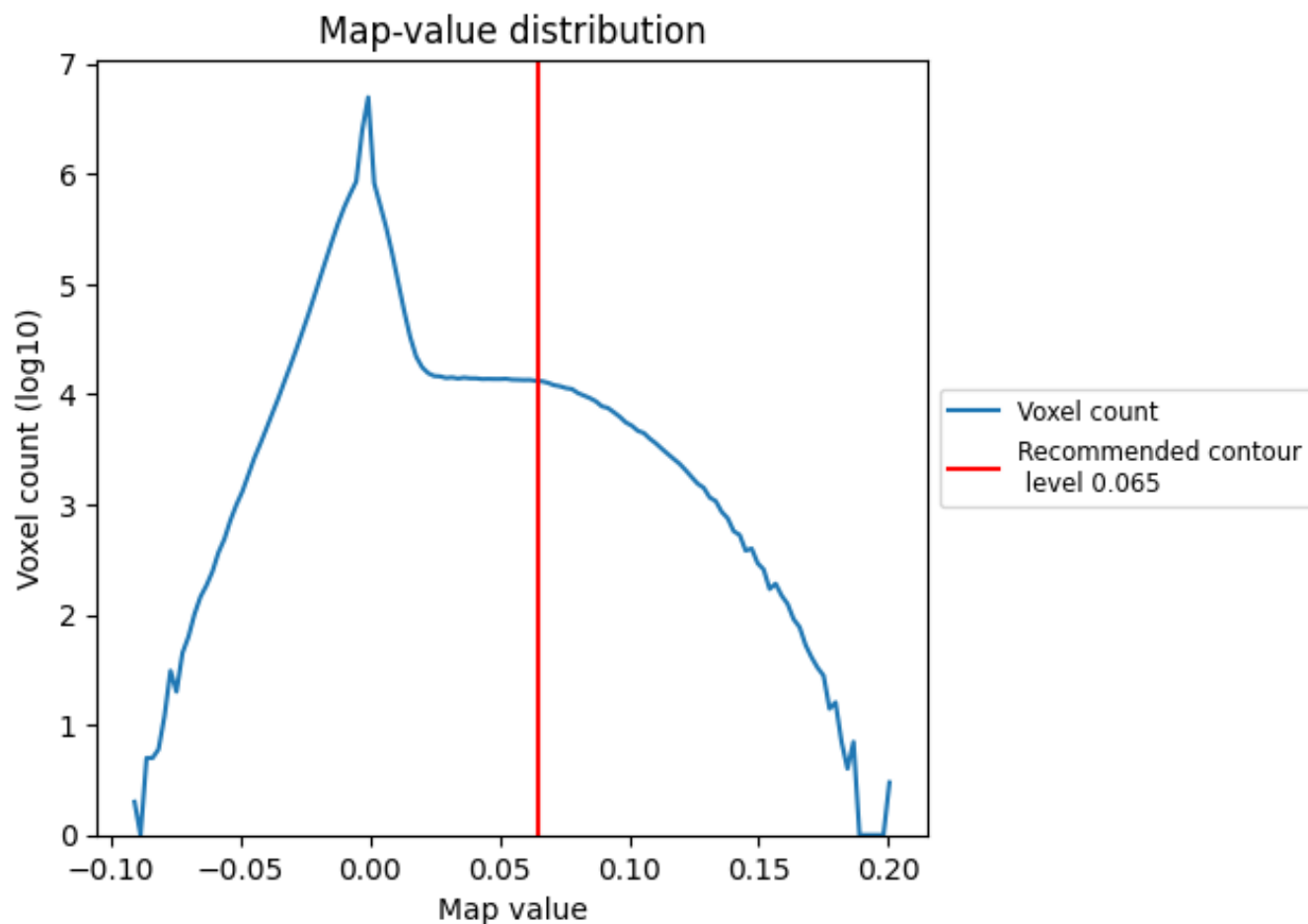
6.5 Mask visualisation

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

7 Map analysis [i](#)

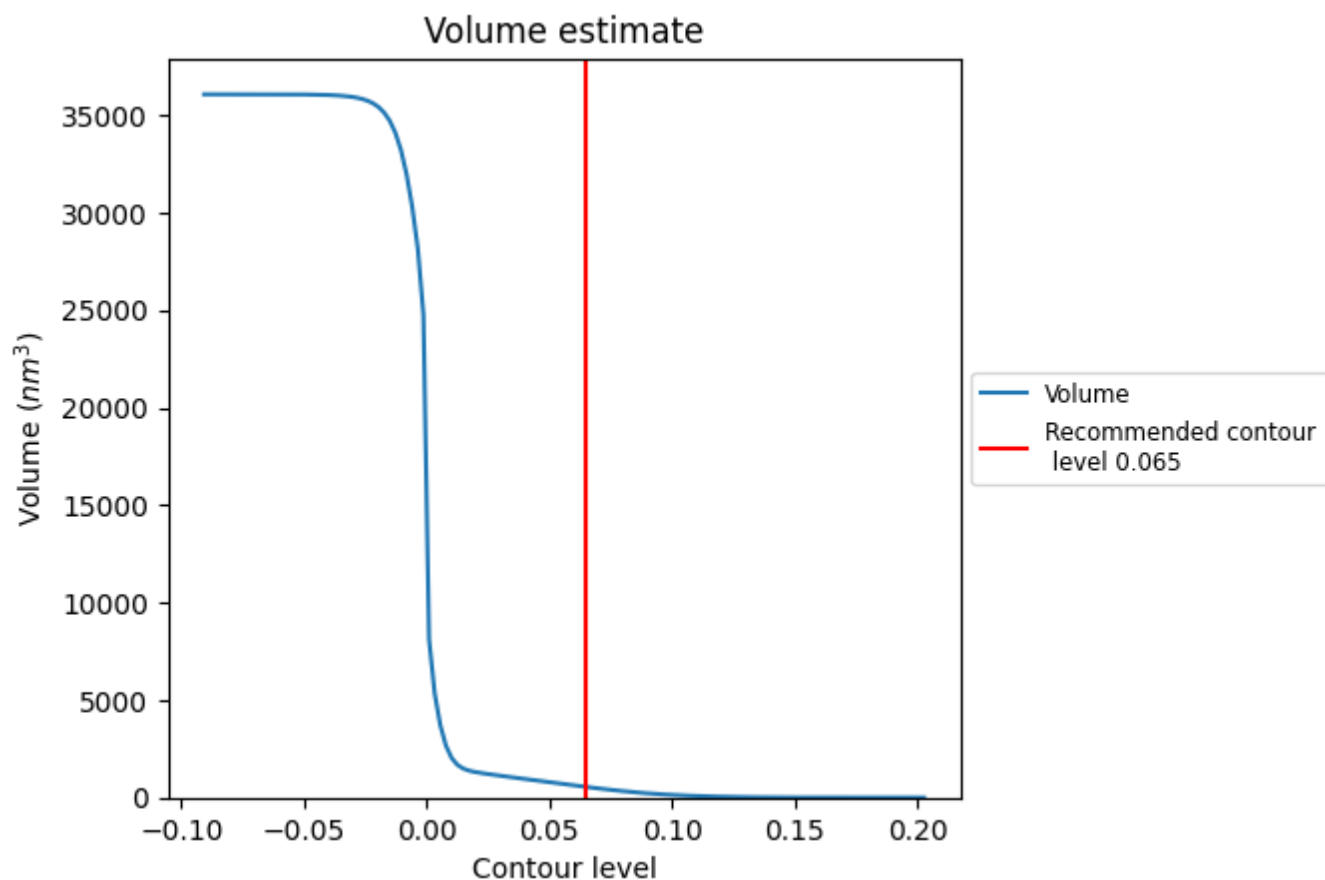
This section contains the results of statistical analysis of the map.

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.

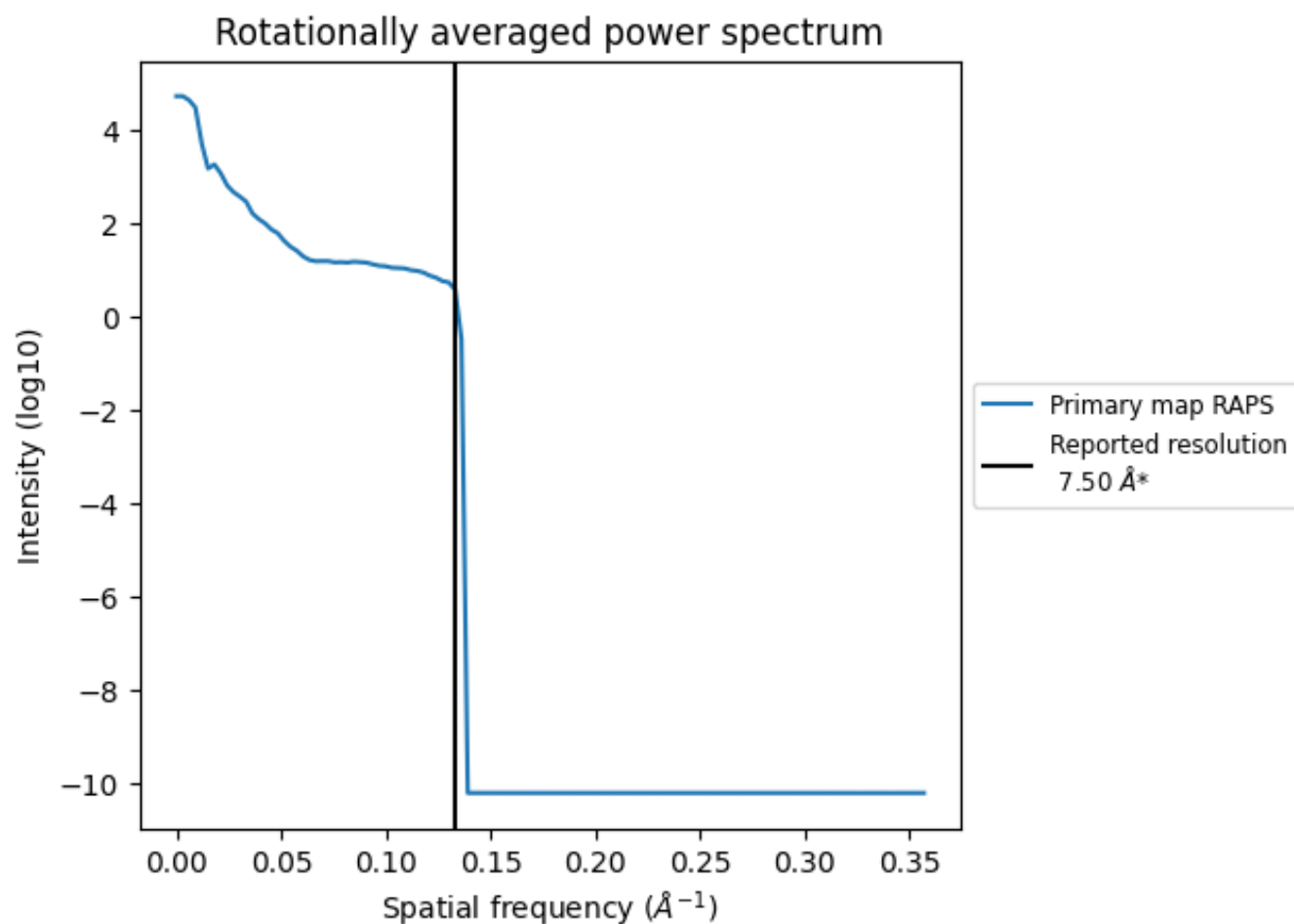
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 545 nm³; this corresponds to an approximate mass of 493 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 ⓘ

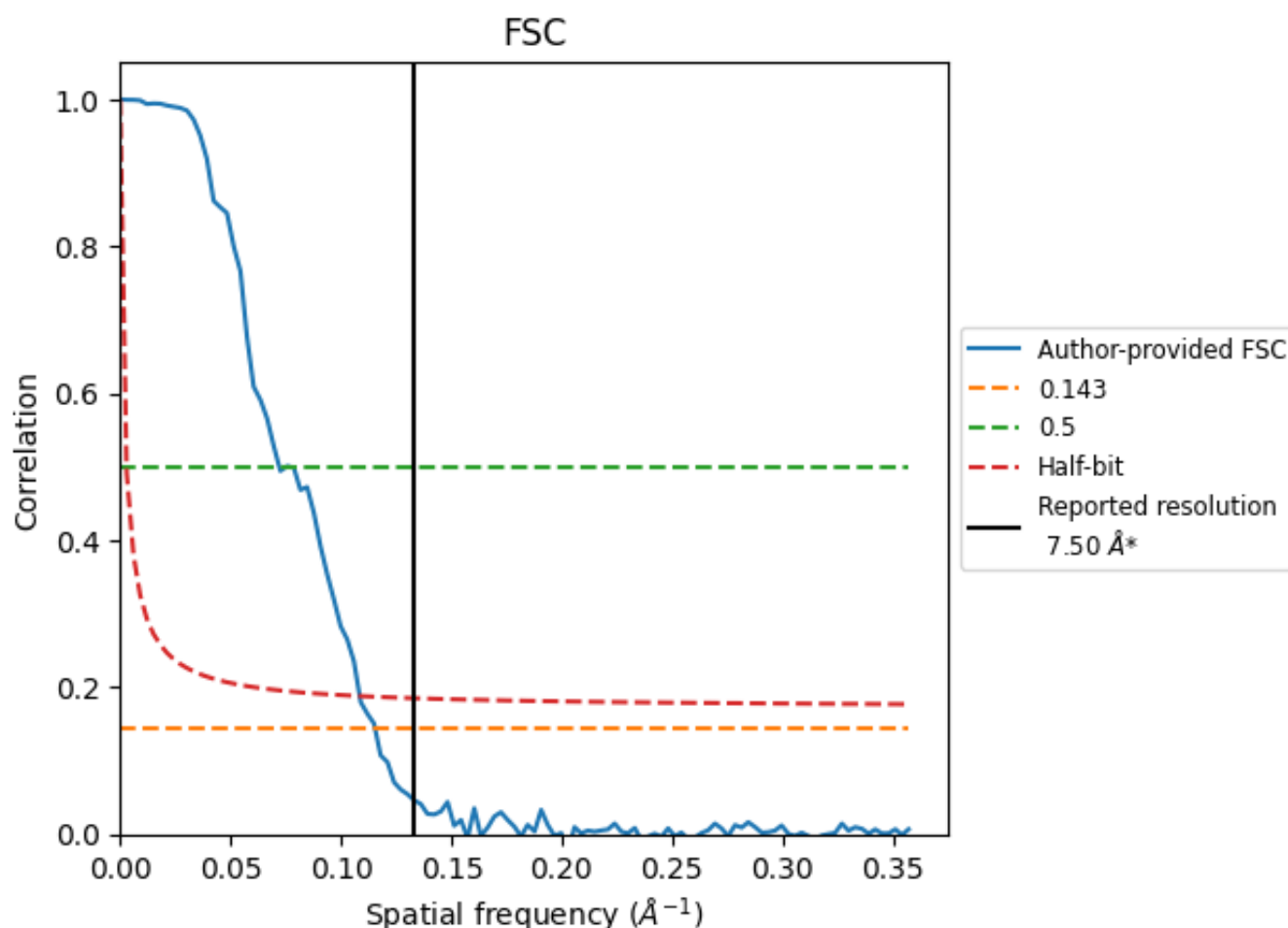


*Reported resolution corresponds to spatial frequency of 0.133 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.133 Å⁻¹

8.2 Resolution estimates [i](#)

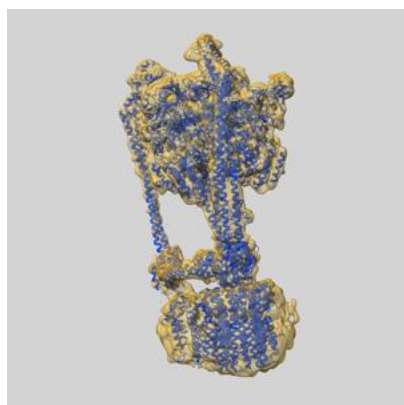
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	8.66	13.87	9.22
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.66 differs from the reported value 7.5 by more than 10 %

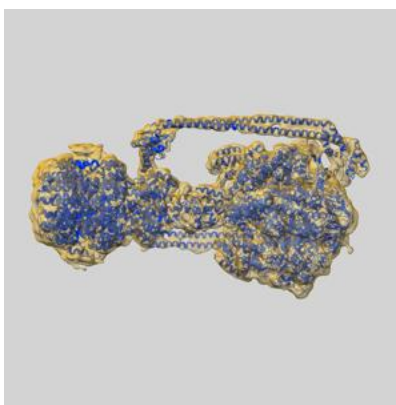
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6813 and PDB model 5Y60. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

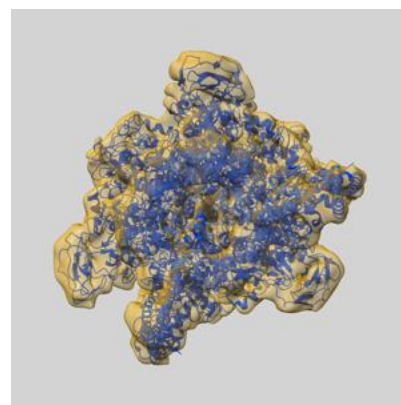
9.1 Map-model overlay [i](#)



X



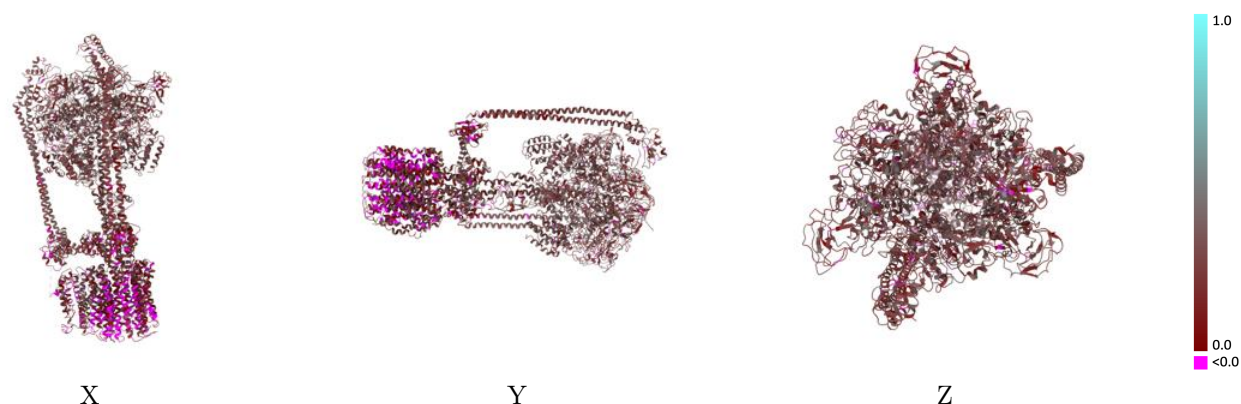
Y



Z

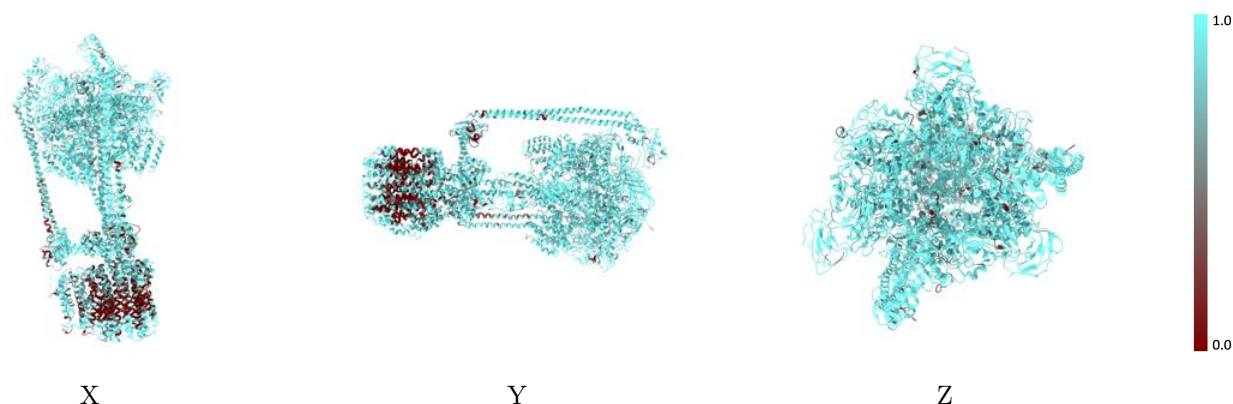
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



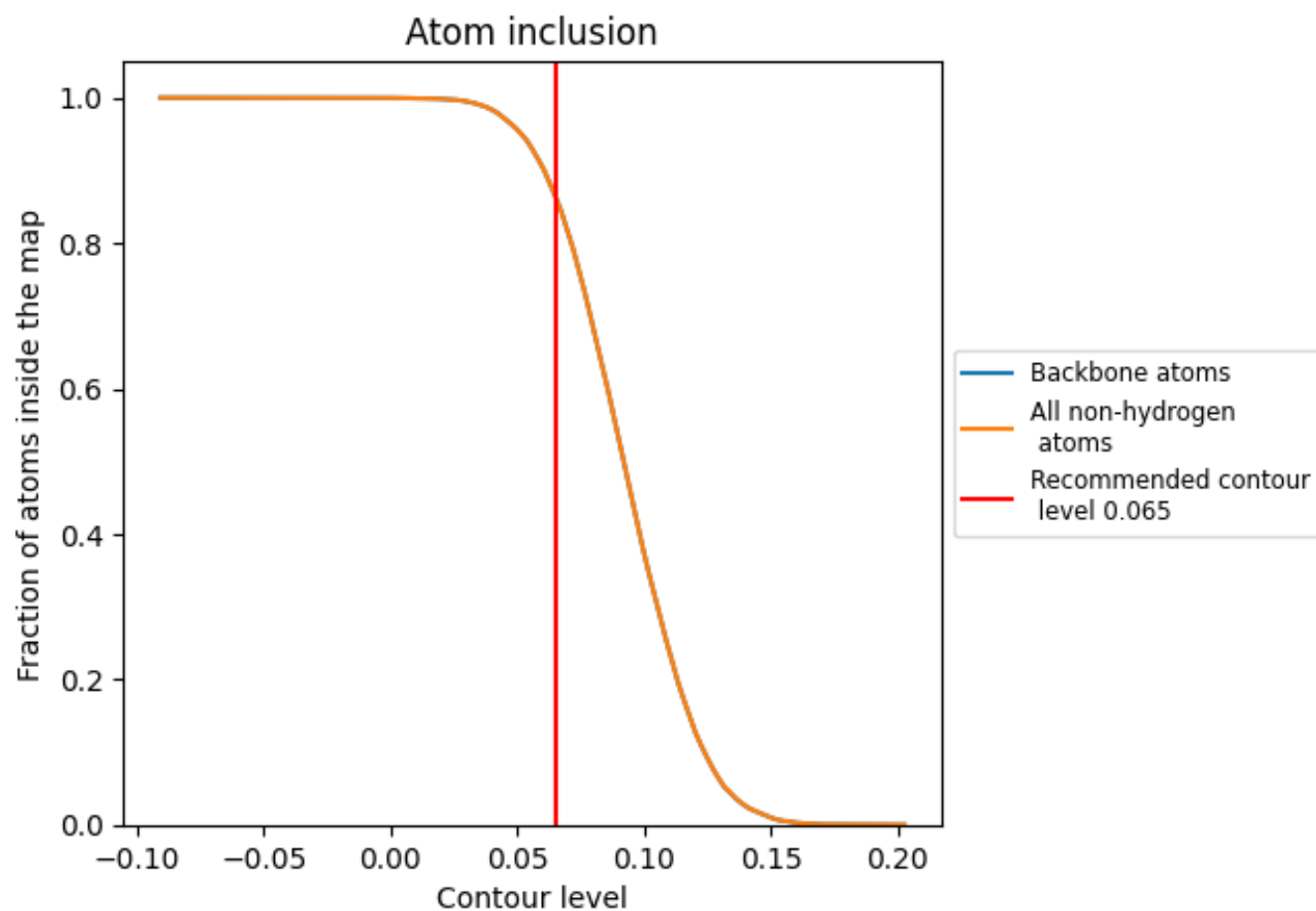
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8642	 0.2320
A	 0.9546	 0.2700
B	 0.9589	 0.2770
C	 0.9558	 0.2780
D	 0.9406	 0.2640
E	 0.9504	 0.2710
F	 0.9657	 0.2860
G	 0.9285	 0.2860
H	 0.8947	 0.2500
I	 0.9273	 0.2490
J	 0.8848	 0.2280
K	 0.9048	 0.2530
L	 0.8862	 0.2340
M	 0.8296	 0.2270
N	 0.7965	 0.1880
O	 0.5050	 0.0790
P	 0.5842	 0.1160
Q	 0.6931	 0.1400
R	 0.5809	 0.1280
S	 0.6799	 0.1360
T	 0.6469	 0.1220
U	 0.5347	 0.0720
V	 0.6007	 0.0510
W	 0.5182	 0.0450
X	 0.5710	 0.1120
Y	 0.4983	 0.0960
Z	 0.4851	 0.1330

