



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 05:50 AM JST

PDB ID : 5Y5X
EMDB ID : EMD-6810
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, rotational state 1
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2017-08-10
Resolution : 5.00 Å(reported)

This is a Full wwPDB EM Validation 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

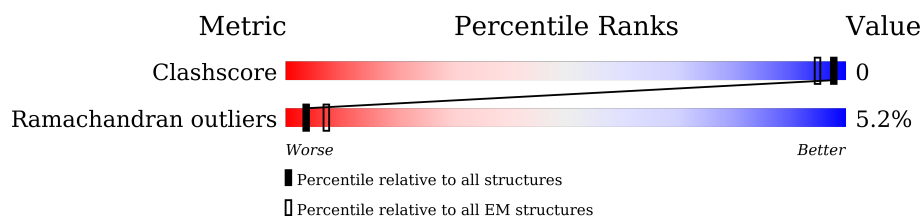
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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	
1	B	578	
1	C	578	
2	D	478	
2	E	478	
2	F	478	
3	G	223	
4	H	104	
5	I	120	

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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.

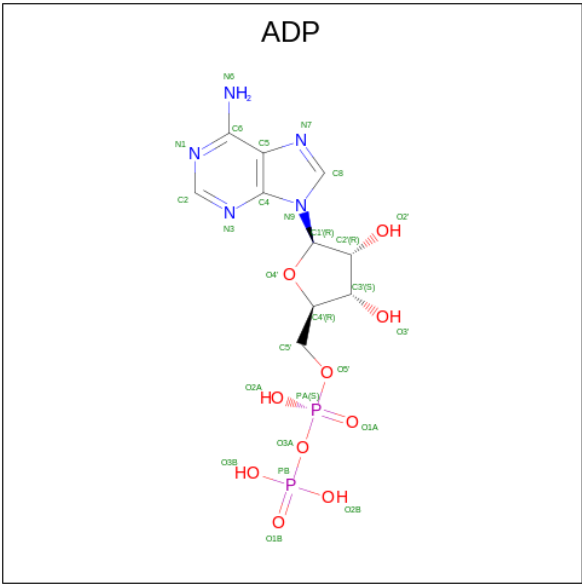
Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	76	Total	C	N	O	0	0
			303	152	76	75		
9	P	76	Total	C	N	O	0	0
			303	152	76	75		

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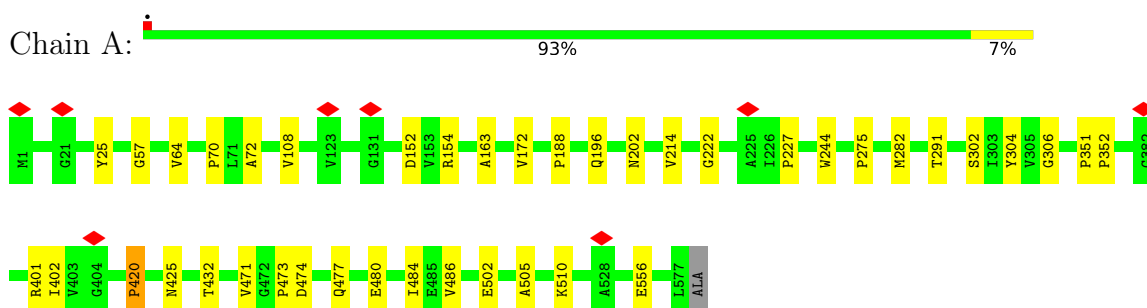
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	C	1	27	10	5	10	2	0

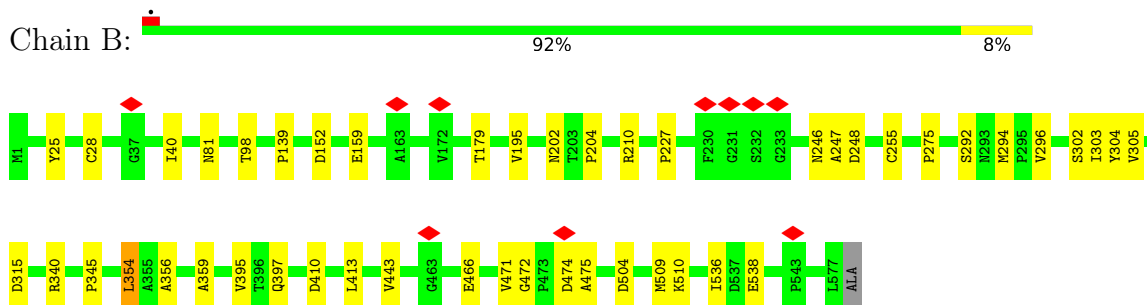
3 Residue-property plots

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.

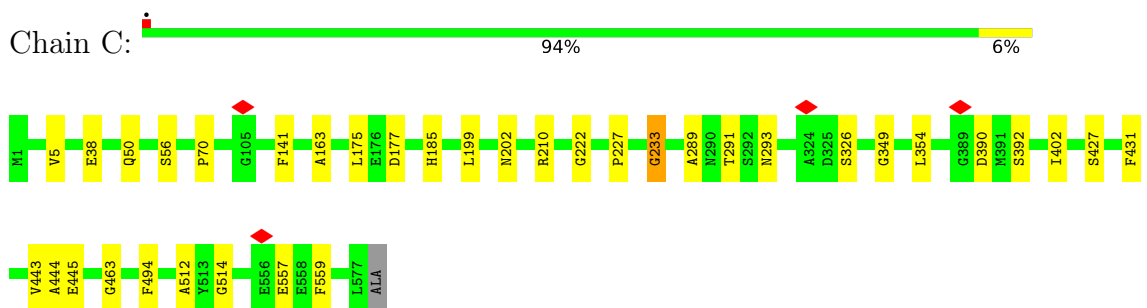
- Molecule 1: V-type ATP synthase alpha chain



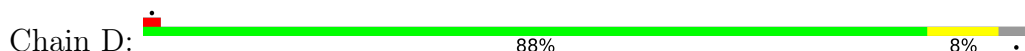
- Molecule 1: V-type ATP synthase alpha chain

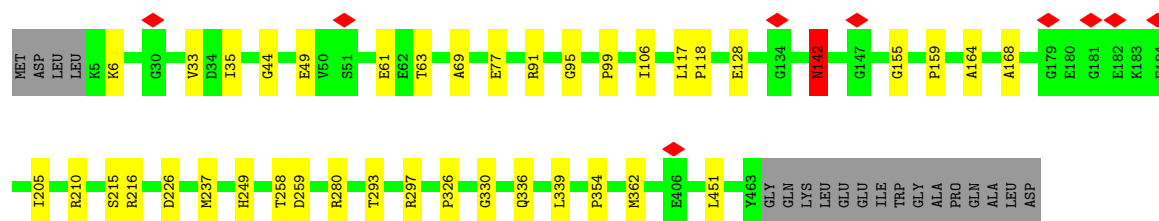


- Molecule 1: V-type ATP synthase alpha chain

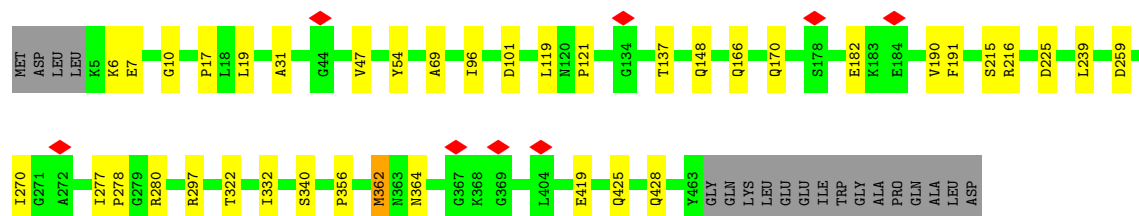
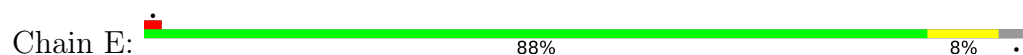


- Molecule 2: V-type ATP synthase beta chain

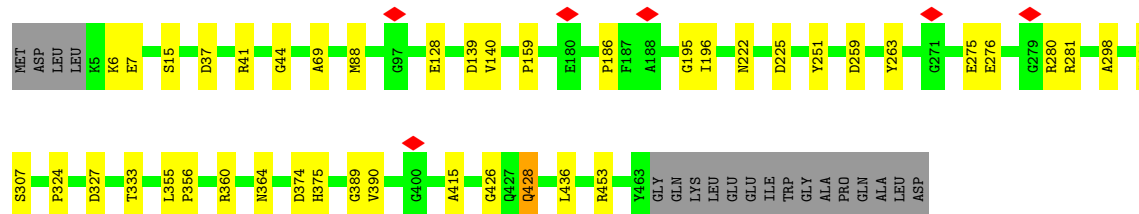
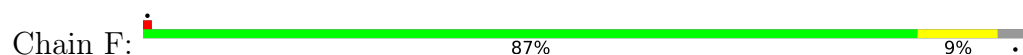




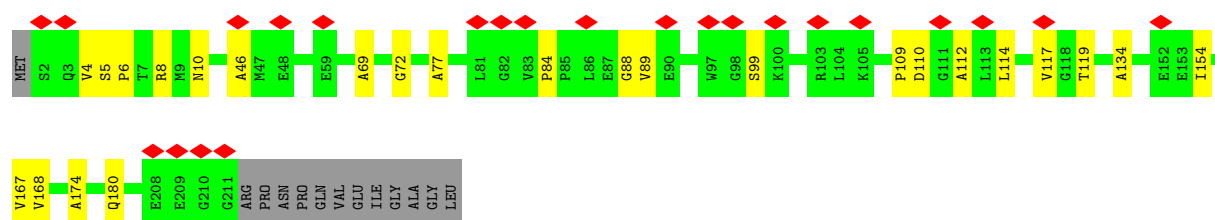
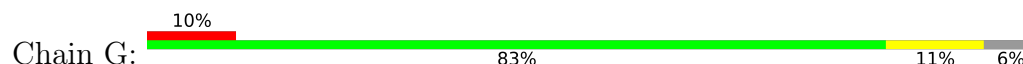
• Molecule 2: V-type ATP synthase beta chain



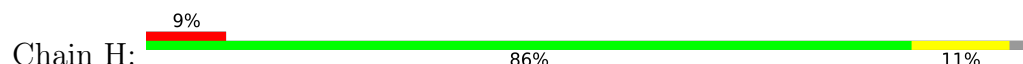
• Molecule 2: V-type ATP synthase beta chain



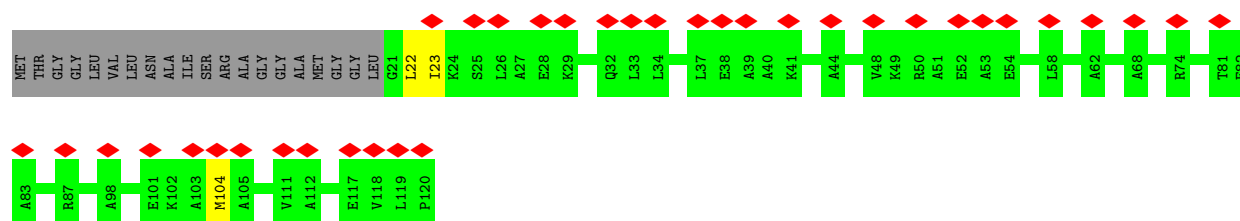
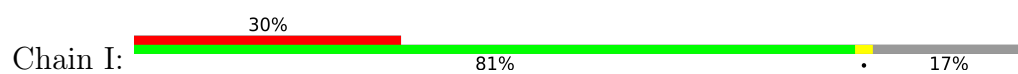
• Molecule 3: V-type ATP synthase subunit D



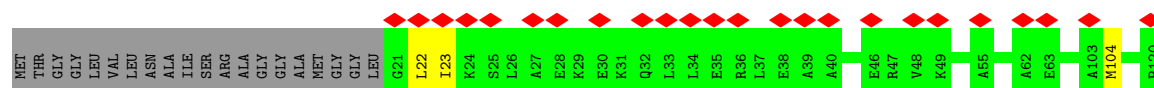
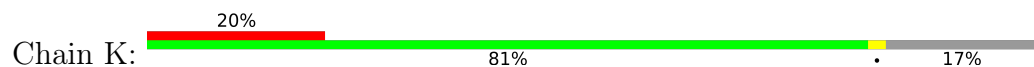
• Molecule 4: V-type ATP synthase subunit F



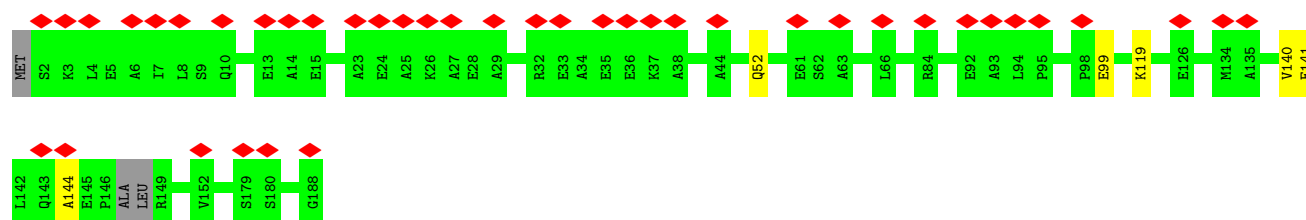
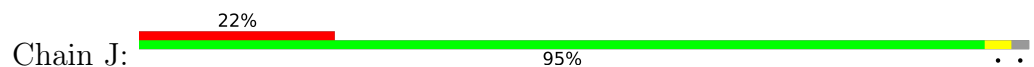
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)



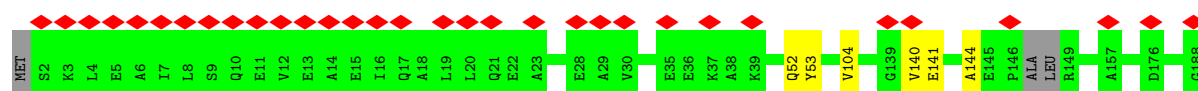
- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)



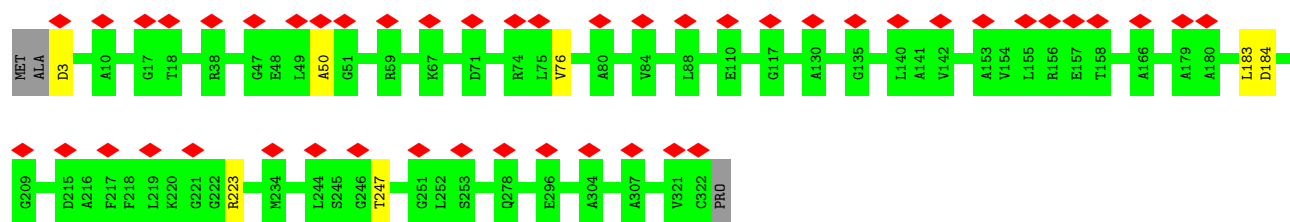
- Molecule 6: V-type ATP synthase subunit E



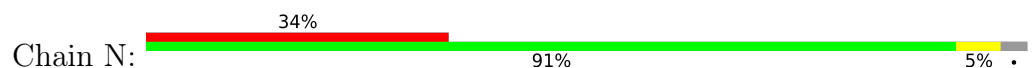
- Molecule 6: V-type ATP synthase subunit E

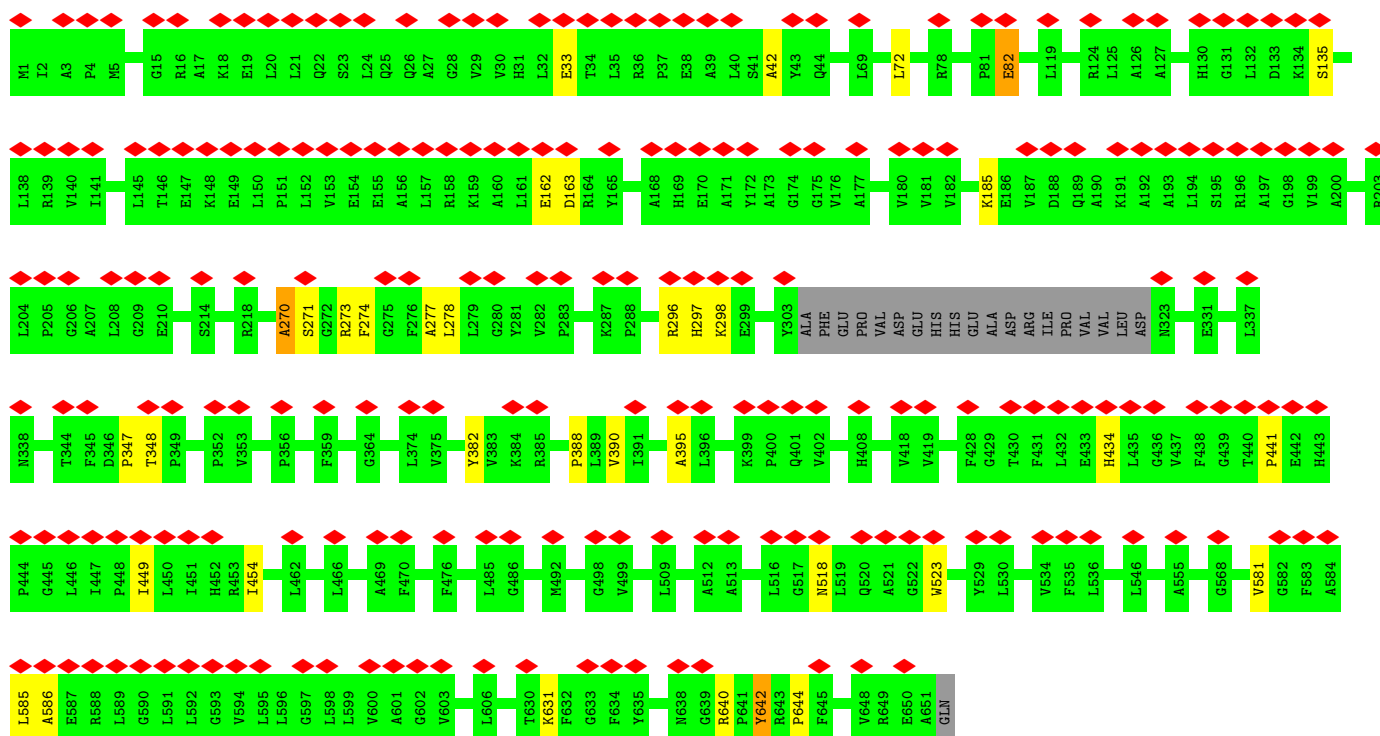


- Molecule 7: V-type ATP synthase subunit C

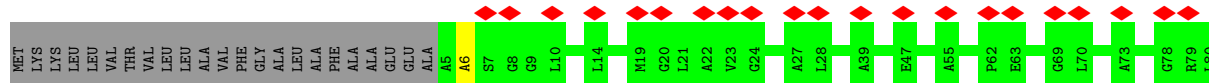
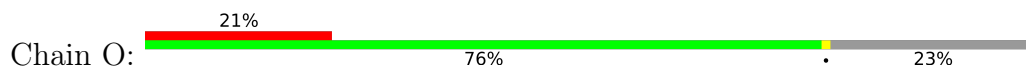


- Molecule 8: V-type ATP synthase subunit I

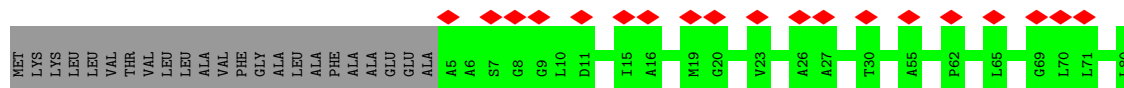
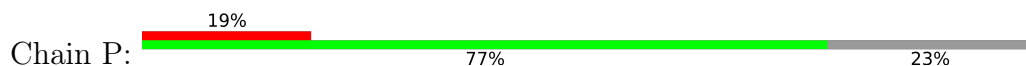




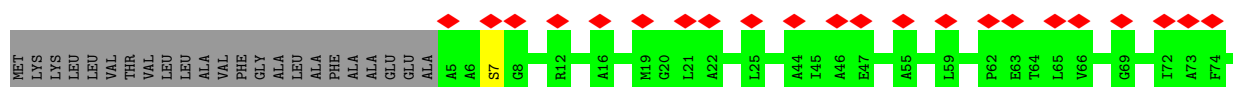
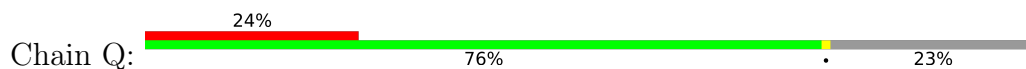
• Molecule 9: V-type ATP synthase, subunit K



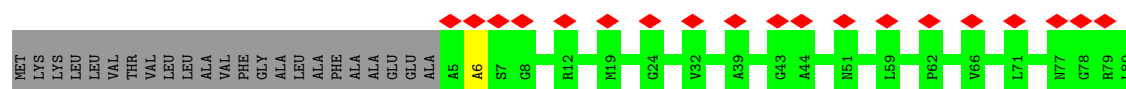
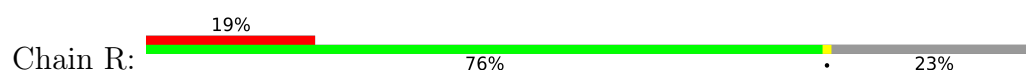
• Molecule 9: V-type ATP synthase, subunit K



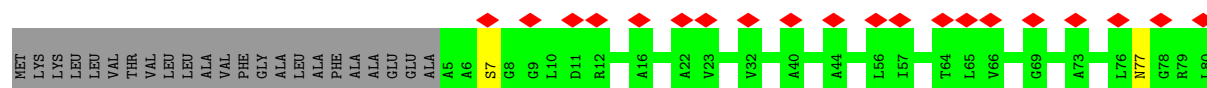
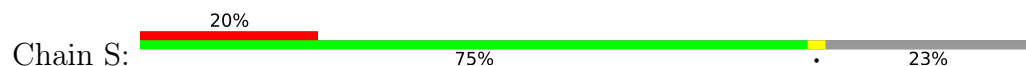
• Molecule 9: V-type ATP synthase, subunit K



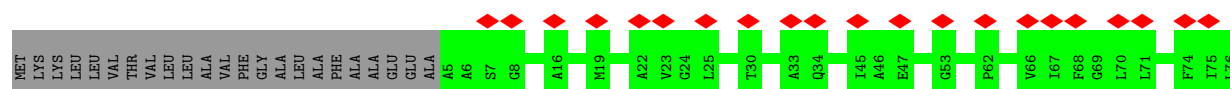
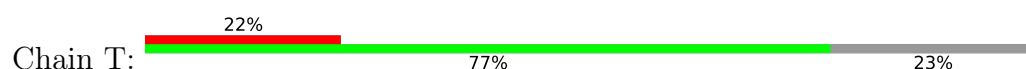
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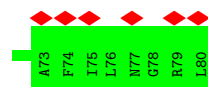
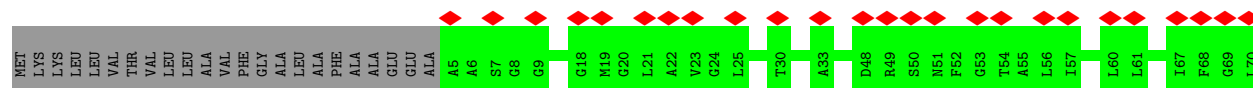
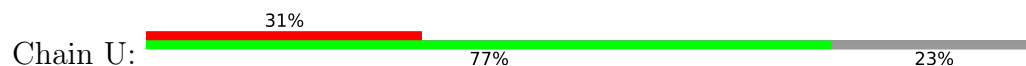
• Molecule 9: V-type ATP synthase, subunit K



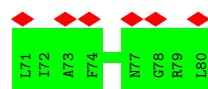
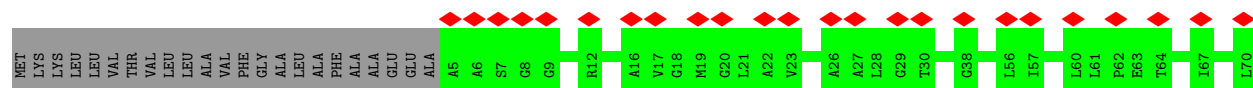
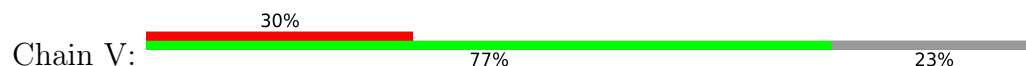
• Molecule 9: V-type ATP synthase, subunit K



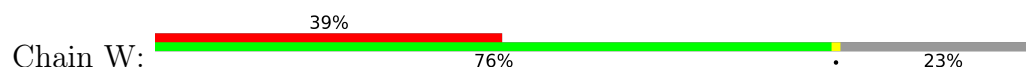
• Molecule 9: V-type ATP synthase, subunit K

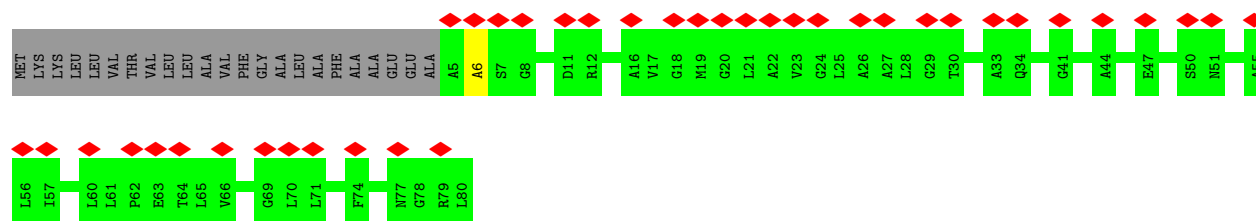


• Molecule 9: V-type ATP synthase, subunit K

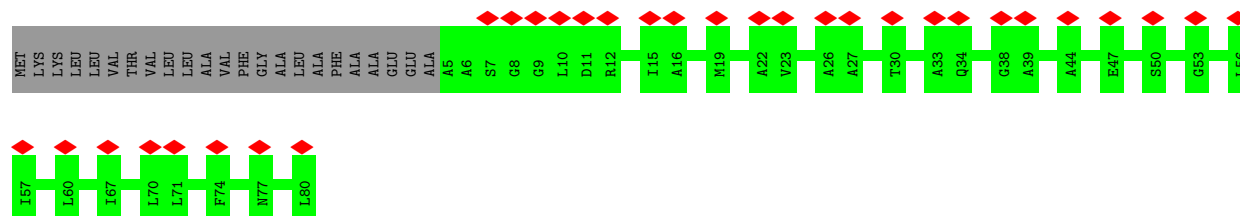
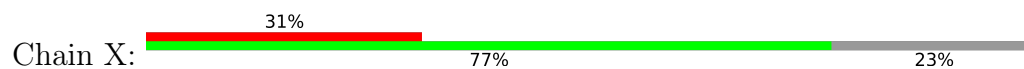


• Molecule 9: V-type ATP synthase, subunit K

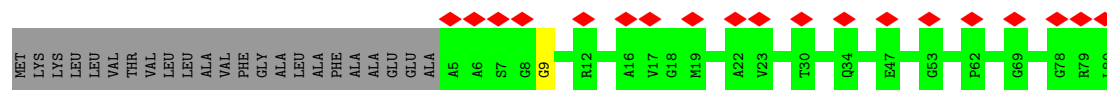
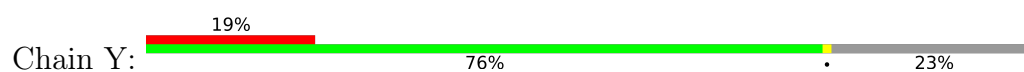




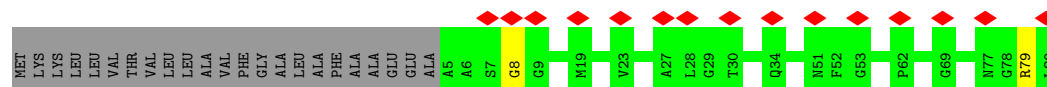
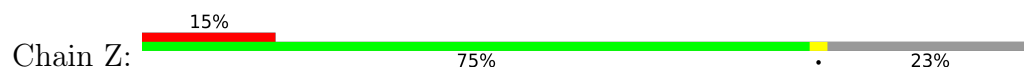
- Molecule 9: V-type ATP synthase, subunit K



- 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	117938	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	0.544	Depositor
Minimum map value	-0.340	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.098	Depositor
Map size (\AA)	330.4, 330.4, 330.4	wwPDB
Map dimensions	236, 236, 236	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	1.44	1/2306 (0.0%)	1.19	5/2881 (0.2%)
1	B	1.36	0/2306	1.19	2/2881 (0.1%)
1	C	1.44	0/2306	1.25	2/2881 (0.1%)
2	D	1.39	0/1834	1.23	5/2291 (0.2%)
2	E	1.44	0/1834	1.25	1/2291 (0.0%)
2	F	1.50	1/1834 (0.1%)	1.24	3/2291 (0.1%)
3	G	1.25	0/838	1.23	3/1046 (0.3%)
4	H	1.25	0/398	1.41	1/496 (0.2%)
5	I	0.90	0/398	0.90	1/496 (0.2%)
5	K	0.89	0/398	0.92	1/496 (0.2%)
6	J	0.95	0/736	0.93	0/917
6	L	1.03	0/736	0.94	1/917 (0.1%)
7	M	1.03	0/1278	0.96	1/1596 (0.1%)
8	N	0.97	0/2524	1.06	3/3152 (0.1%)
9	O	0.95	0/302	0.87	0/376
9	P	0.91	0/302	0.83	0/376
9	Q	0.87	0/302	0.99	0/376
9	R	0.91	0/302	0.86	0/376
9	S	0.96	0/302	0.86	0/376
9	T	0.86	0/302	0.88	0/376
9	U	0.85	0/302	0.89	0/376
9	V	0.90	0/302	0.83	0/376
9	W	0.90	0/302	0.91	0/376
9	X	0.88	0/302	0.91	0/376
9	Y	0.94	0/302	0.92	0/376
9	Z	0.97	0/302	0.94	0/376
All	All	1.24	2/23350 (0.0%)	1.12	29/29144 (0.1%)

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	B	0	1
1	C	0	1
2	D	0	2
2	E	0	1
2	F	0	1
7	M	0	2
8	N	0	2
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	GLY	CA-C	-5.75	1.42	1.51
2	F	195	GLY	CA-C	-5.02	1.43	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	PRO	N-CA-C	-7.00	93.90	112.10
1	A	57	GLY	N-CA-C	-6.63	96.53	113.10
1	A	425	ASN	N-CA-C	-6.41	93.70	111.00
2	D	142	ASN	N-CA-C	-6.30	94.00	111.00
1	C	185	HIS	C-N-CA	6.16	137.10	121.70
2	F	374	ASP	N-CA-C	-6.07	94.60	111.00
3	G	77	ALA	C-N-CA	6.01	134.91	122.30
2	F	195	GLY	N-CA-C	-5.99	98.13	113.10
2	F	222	ASN	N-CA-C	-5.81	95.31	111.00
1	A	477	GLN	N-CA-C	-5.65	95.75	111.00
1	A	154	ARG	N-CA-C	-5.64	95.78	111.00
7	M	76	VAL	N-CA-C	-5.56	95.99	111.00
8	N	82	GLU	N-CA-C	-5.54	96.05	111.00
3	G	46	ALA	N-CA-C	5.52	125.91	111.00
6	L	53	TYR	N-CA-C	-5.45	96.30	111.00
5	I	22	LEU	C-N-CA	5.40	135.20	121.70
2	D	258	THR	C-N-CA	5.39	135.18	121.70
1	C	233	GLY	N-CA-C	5.37	126.53	113.10
4	H	72	LEU	N-CA-C	-5.37	96.50	111.00
1	B	410	ASP	C-N-CA	5.35	135.08	121.70
5	K	22	LEU	C-N-CA	5.26	134.86	121.70
2	D	339	LEU	N-CA-C	-5.25	96.81	111.00
3	G	72	GLY	N-CA-C	-5.24	100.00	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	451	LEU	N-CA-C	-5.19	97.00	111.00
2	D	155	GLY	N-CA-C	-5.14	100.24	113.10
2	E	19	LEU	C-N-CA	5.13	134.54	121.70
8	N	270	ALA	C-N-CA	5.11	134.47	121.70
8	N	33	GLU	C-N-CA	5.11	134.47	121.70
1	B	354	LEU	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	204	PRO	Mainchain
1	C	199	LEU	Mainchain
2	D	142	ASN	Mainchain
2	D	6	LYS	Peptide
2	E	6	LYS	Peptide
2	F	6	LYS	Peptide
7	M	183	LEU	Peptide
7	M	3	ASP	Peptide
8	N	642	TYR	Peptide,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	0	0
1	B	2307	0	654	1	0
1	C	2307	0	654	3	0
2	D	1835	0	512	3	0
2	E	1835	0	512	2	0
2	F	1835	0	512	2	0
3	G	839	0	230	1	0
4	H	399	0	119	0	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	1279	0	357	0	0
8	N	2526	0	709	0	0
9	O	303	0	102	0	0
9	P	303	0	102	0	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	0	0
9	Y	303	0	102	0	0
9	Z	303	0	102	0	0
10	A	27	0	12	0	0
10	C	27	0	12	0	0
All	All	23433	0	6745	12	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 0.

All (12) 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)
2:D:35:ILE:H	2:D:44:GLY:H	1.54	0.56
2:F:251:TYR:H	2:F:306:GLY:HA2	1.72	0.54
1:C:38:GLU:H	1:C:50:GLN:H	1.60	0.49
3:G:8:ARG:C	3:G:10:ASN:H	2.16	0.49
2:F:426:GLY:C	2:F:428:GLN:H	2.17	0.47
1:C:557:GLU:C	1:C:559:PHE:H	2.19	0.45
2:E:31:ALA:H	2:E:47:VAL:H	1.65	0.44
1:B:536:ILE:C	1:B:538:GLU:H	2.22	0.43
1:C:175:LEU:C	1:C:177:ASP:H	2.22	0.43
2:D:33:VAL:O	2:D:44:GLY:HA2	2.17	0.43
2:D:35:ILE:H	2:D:44:GLY:N	2.15	0.43
2:E:362:MET:C	2:E:364:ASN:H	2.22	0.42

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%)	452 (79%)	87 (15%)	36 (6%)	1	18
1	B	575/578 (100%)	431 (75%)	101 (18%)	43 (8%)	1	15
1	C	575/578 (100%)	451 (78%)	96 (17%)	28 (5%)	2	22
2	D	457/478 (96%)	342 (75%)	83 (18%)	32 (7%)	1	16
2	E	457/478 (96%)	332 (73%)	91 (20%)	34 (7%)	1	15
2	F	457/478 (96%)	347 (76%)	74 (16%)	36 (8%)	1	14
3	G	208/223 (93%)	151 (73%)	37 (18%)	20 (10%)	0	10
4	H	98/104 (94%)	74 (76%)	14 (14%)	10 (10%)	0	9
5	I	98/120 (82%)	93 (95%)	3 (3%)	2 (2%)	7	39
5	K	98/120 (82%)	96 (98%)	0	2 (2%)	7	39
6	J	181/188 (96%)	157 (87%)	18 (10%)	6 (3%)	4	29
6	L	181/188 (96%)	162 (90%)	14 (8%)	5 (3%)	5	32
7	M	318/323 (98%)	296 (93%)	18 (6%)	4 (1%)	12	48
8	N	628/652 (96%)	555 (88%)	38 (6%)	35 (6%)	2	20
9	O	74/99 (75%)	71 (96%)	2 (3%)	1 (1%)	11	46
9	P	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	Q	74/99 (75%)	71 (96%)	2 (3%)	1 (1%)	11	46
9	R	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	11	46
9	S	74/99 (75%)	70 (95%)	2 (3%)	2 (3%)	5	33
9	T	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
9	U	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
9	V	74/99 (75%)	74 (100%)	0	0	100	100
9	W	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	11	46
9	X	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	Y	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Z	74/99 (75%)	70 (95%)	2 (3%)	2 (3%)	5	33
All	All	5794/6274 (92%)	4797 (83%)	695 (12%)	302 (5%)	4	21

All (302) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	227	PRO
1	A	401	ARG
1	A	471	VAL
1	A	480	GLU
1	B	152	ASP
1	B	159	GLU
1	B	202	ASN
1	B	227	PRO
1	B	303	ILE
1	B	304	TYR
1	B	305	VAL
1	B	356	ALA
1	B	466	GLU
1	C	70	PRO
1	C	202	ASN
1	C	227	PRO
1	C	233	GLY
1	C	291	THR
1	C	293	ASN
1	C	392	SER
1	C	427	SER
1	C	444	ALA
2	D	49	GLU
2	D	63	THR
2	D	215	SER
2	D	216	ARG
2	D	354	PRO
2	E	7	GLU
2	E	17	PRO
2	E	137	THR
2	E	148	GLN
2	E	215	SER
2	E	216	ARG
2	E	278	PRO
2	E	280	ARG

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Mol	Chain	Res	Type
2	E	297	ARG
2	E	362	MET
2	E	419	GLU
2	F	88	MET
2	F	139	ASP
2	F	225	ASP
2	F	259	ASP
2	F	276	GLU
2	F	280	ARG
2	F	298	ALA
2	F	324	PRO
2	F	327	ASP
2	F	355	LEU
2	F	356	PRO
2	F	360	ARG
2	F	364	ASN
2	F	428	GLN
3	G	112	ALA
3	G	117	VAL
3	G	134	ALA
4	H	81	PHE
5	I	23	ILE
6	J	99	GLU
6	J	144	ALA
5	K	23	ILE
7	M	184	ASP
8	N	135	SER
8	N	162	GLU
8	N	163	ASP
8	N	185	LYS
8	N	298	LYS
8	N	434	HIS
8	N	441	PRO
9	Q	7	SER
9	R	6	ALA
1	A	64	VAL
1	A	72	ALA
1	A	108	VAL
1	A	163	ALA
1	A	188	PRO
1	A	402	ILE
1	A	474	ASP

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Mol	Chain	Res	Type
1	A	505	ALA
1	B	25	TYR
1	B	28	CYS
1	B	179	THR
1	B	210	ARG
1	B	292	SER
1	B	302	SER
1	B	340	ARG
1	B	397	GLN
1	B	443	VAL
1	B	471	VAL
1	B	472	GLY
1	B	474	ASP
1	C	210	ARG
1	C	222	GLY
1	C	289	ALA
1	C	326	SER
1	C	390	ASP
1	C	445	GLU
1	C	512	ALA
2	D	61	GLU
2	D	91	ARG
2	D	95	GLY
2	D	106	ILE
2	D	210	ARG
2	D	259	ASP
2	D	293	THR
2	D	297	ARG
2	D	330	GLY
2	E	69	ALA
2	E	96	ILE
2	E	119	LEU
2	E	182	GLU
2	E	239	LEU
2	E	259	ASP
2	E	332	ILE
2	E	340	SER
2	E	428	GLN
2	F	7	GLU
2	F	15	SER
2	F	41	ARG
2	F	140	VAL

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Mol	Chain	Res	Type
2	F	281	ARG
2	F	333	THR
2	F	389	GLY
2	F	390	VAL
3	G	4	VAL
3	G	84	PRO
3	G	89	VAL
3	G	99	SER
3	G	119	THR
3	G	168	VAL
3	G	180	GLN
4	H	15	LEU
4	H	69	PRO
4	H	79	GLU
4	H	80	ALA
6	J	119	LYS
6	L	141	GLU
6	L	144	ALA
7	M	50	ALA
8	N	72	LEU
8	N	82	GLU
8	N	277	ALA
8	N	390	VAL
8	N	395	ALA
8	N	454	ILE
9	S	7	SER
9	W	6	ALA
9	Y	9	GLY
1	A	152	ASP
1	A	196	GLN
1	A	202	ASN
1	A	302	SER
1	A	304	TYR
1	A	352	PRO
1	A	432	THR
1	A	556	GLU
1	B	195	VAL
1	B	294	MET
1	B	315	ASP
1	B	354	LEU
1	B	475	ALA
1	B	510	LYS

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Mol	Chain	Res	Type
1	C	56	SER
1	C	354	LEU
1	C	431	PHE
1	C	463	GLY
2	D	69	ALA
2	D	77	GLU
2	D	117	LEU
2	D	159	PRO
2	D	164	ALA
2	D	168	ALA
2	D	249	HIS
2	D	280	ARG
2	D	326	PRO
2	E	10	GLY
2	E	54	TYR
2	E	101	ASP
2	E	121	PRO
2	E	170	GLN
2	F	69	ALA
2	F	275	GLU
2	F	307	SER
2	F	375	HIS
2	F	436	LEU
3	G	6	PRO
3	G	69	ALA
3	G	88	GLY
3	G	114	LEU
3	G	174	ALA
4	H	77	LEU
6	J	141	GLU
5	K	104	MET
8	N	270	ALA
8	N	347	PRO
8	N	518	ASN
8	N	523	TRP
8	N	585	LEU
9	O	6	ALA
9	S	77	ASN
9	Z	79	ARG
1	A	244	TRP
1	A	282	MET
1	A	291	THR

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Mol	Chain	Res	Type
1	A	502	GLU
1	B	247	ALA
1	B	248	ASP
1	B	359	ALA
1	B	395	VAL
1	B	504	ASP
1	C	141	PHE
1	C	494	PHE
2	D	128	GLU
2	D	237	MET
2	D	336	GLN
2	D	362	MET
2	E	166	GLN
2	E	322	THR
2	E	425	GLN
2	F	415	ALA
2	F	453	ARG
4	H	5	ALA
4	H	53	PRO
6	J	52	GLN
6	J	140	VAL
6	L	140	VAL
7	M	223	ARG
8	N	42	ALA
8	N	296	ARG
8	N	297	HIS
8	N	382	TYR
8	N	449	ILE
1	A	275	PRO
1	A	351	PRO
1	A	473	PRO
1	B	81	ASN
1	B	246	ASN
1	B	255	CYS
1	B	345	PRO
1	B	413	LEU
2	D	99	PRO
2	D	142	ASN
2	D	226	ASP
2	E	191	PHE
2	E	225	ASP
2	E	277	ILE

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Mol	Chain	Res	Type
2	F	128	GLU
2	F	186	PRO
2	F	263	TYR
3	G	5	SER
3	G	110	ASP
4	H	33	LEU
4	H	57	ARG
5	I	104	MET
6	L	52	GLN
8	N	274	PHE
8	N	278	LEU
8	N	388	PRO
8	N	586	ALA
8	N	631	LYS
8	N	644	PRO
1	A	25	TYR
1	A	222	GLY
1	A	484	ILE
1	A	510	LYS
1	B	98	THR
1	B	509	MET
1	C	163	ALA
1	C	349	GLY
1	C	443	VAL
2	E	190	VAL
2	F	37	ASP
2	F	196	ILE
8	N	271	SER
8	N	273	ARG
8	N	642	TYR
1	A	214	VAL
1	B	296	VAL
1	C	514	GLY
2	E	270	ILE
3	G	154	ILE
8	N	581	VAL
9	Z	8	GLY
1	A	172	VAL
1	B	40	ILE
1	B	275	PRO
2	F	44	GLY
3	G	167	VAL

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Mol	Chain	Res	Type
1	A	486	VAL
1	C	5	VAL
2	D	118	PRO
2	E	356	PRO
2	F	159	PRO
8	N	348	THR
8	N	640	ARG
1	B	139	PRO
6	L	104	VAL
7	M	247	THR
1	C	402	ILE
2	D	205	ILE
3	G	109	PRO
1	A	420	PRO

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	1.46	3 (12%)	29,45,45	1.18	2 (6%)
10	ADP	C	600	-	24,29,29	1.42	4 (16%)	29,45,45	1.73	7 (24%)

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	-	-	9/12/32/32	0/3/3/3
10	ADP	C	600	-	-	7/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	600	ADP	C8-N7	-3.43	1.28	1.34
10	A	600	ADP	C2'-C1'	-3.30	1.48	1.53
10	C	600	ADP	C8-N7	-3.01	1.29	1.34
10	C	600	ADP	C4-N3	-2.89	1.31	1.35
10	A	600	ADP	C4-N3	-2.78	1.31	1.35
10	C	600	ADP	C2'-C1'	-2.70	1.49	1.53
10	C	600	ADP	O4'-C1'	2.25	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	600	ADP	PA-O3A-PB	5.08	150.27	132.83
10	A	600	ADP	N6-C6-N1	4.23	127.35	118.57
10	C	600	ADP	O4'-C4'-C3'	-3.10	98.98	105.11
10	C	600	ADP	C3'-C2'-C1'	-2.99	96.47	100.98
10	C	600	ADP	N6-C6-N1	2.97	124.73	118.57
10	C	600	ADP	C5-C6-N1	-2.33	115.06	120.35
10	C	600	ADP	O4'-C1'-C2'	-2.30	103.56	106.93
10	A	600	ADP	C5-C6-N1	-2.22	115.32	120.35
10	C	600	ADP	O4'-C4'-C5'	2.10	116.28	109.37

There are no chirality outliers.

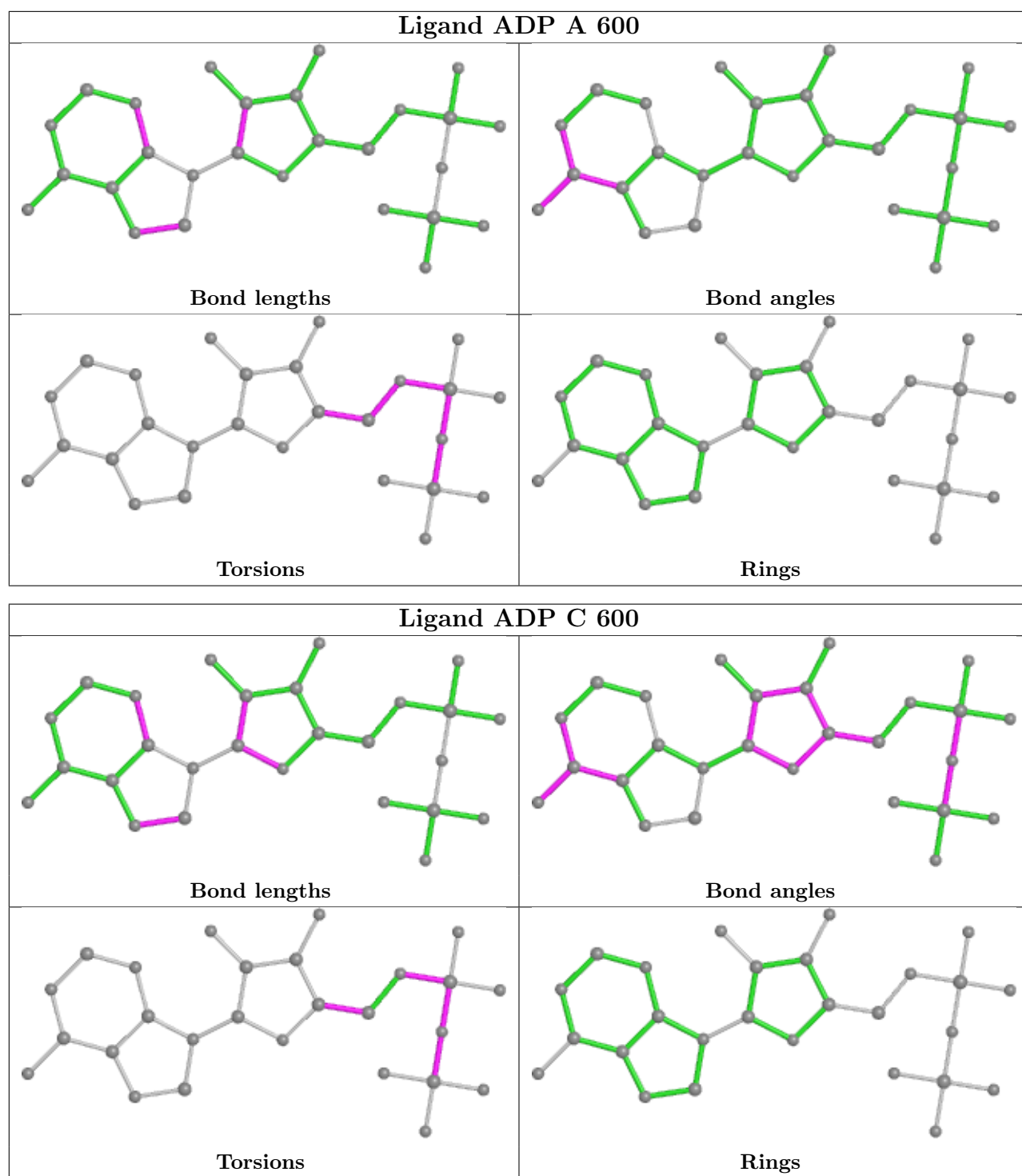
All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	600	ADP	PA-O3A-PB-O2B
10	A	600	ADP	PA-O3A-PB-O3B
10	A	600	ADP	C5'-O5'-PA-O1A
10	C	600	ADP	C5'-O5'-PA-O2A
10	C	600	ADP	C5'-O5'-PA-O3A
10	C	600	ADP	PB-O3A-PA-O1A
10	A	600	ADP	O4'-C4'-C5'-O5'
10	C	600	ADP	PA-O3A-PB-O3B
10	A	600	ADP	PB-O3A-PA-O1A
10	A	600	ADP	C5'-O5'-PA-O2A
10	C	600	ADP	C5'-O5'-PA-O1A
10	A	600	ADP	C3'-C4'-C5'-O5'
10	A	600	ADP	C4'-C5'-O5'-PA
10	C	600	ADP	O4'-C4'-C5'-O5'
10	A	600	ADP	C5'-O5'-PA-O3A
10	C	600	ADP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no chain breaks in this entry.

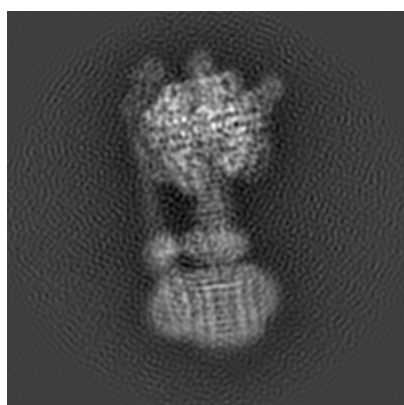
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6810. These allow visual inspection of the internal detail of the map and identification of artifacts.

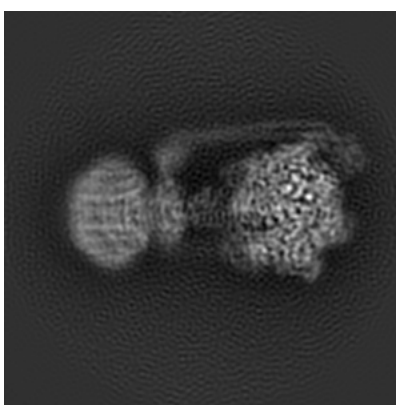
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

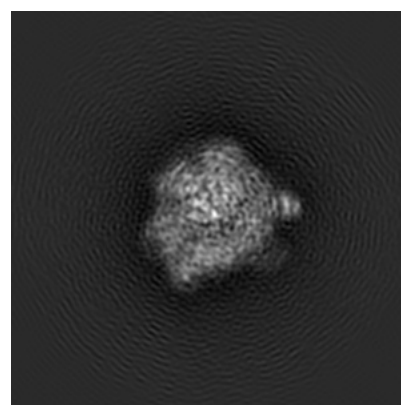
6.1.1 Primary map



X



Y



Z

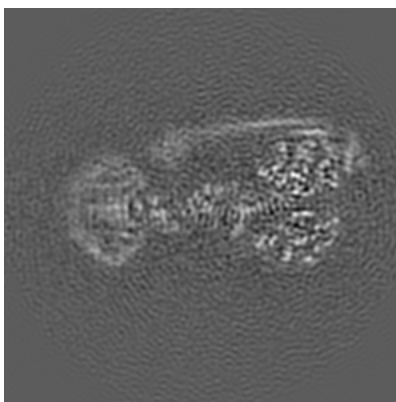
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

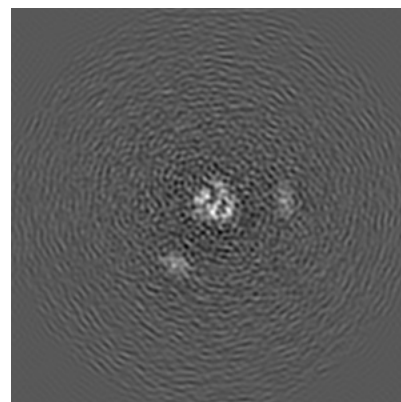
6.2.1 Primary map



X Index: 118



Y Index: 118

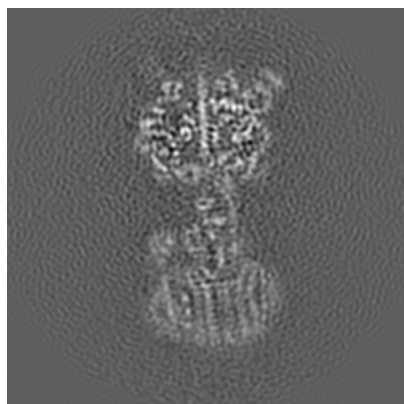


Z Index: 118

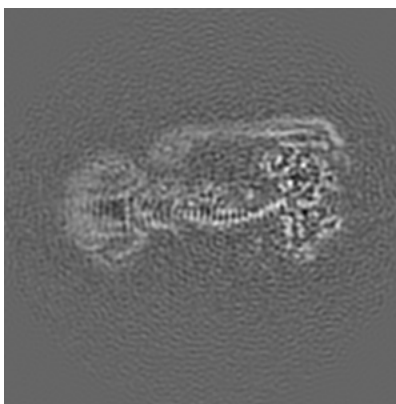
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

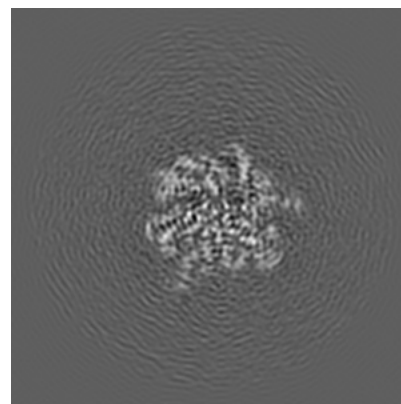
6.3.1 Primary map



X Index: 119



Y Index: 122



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

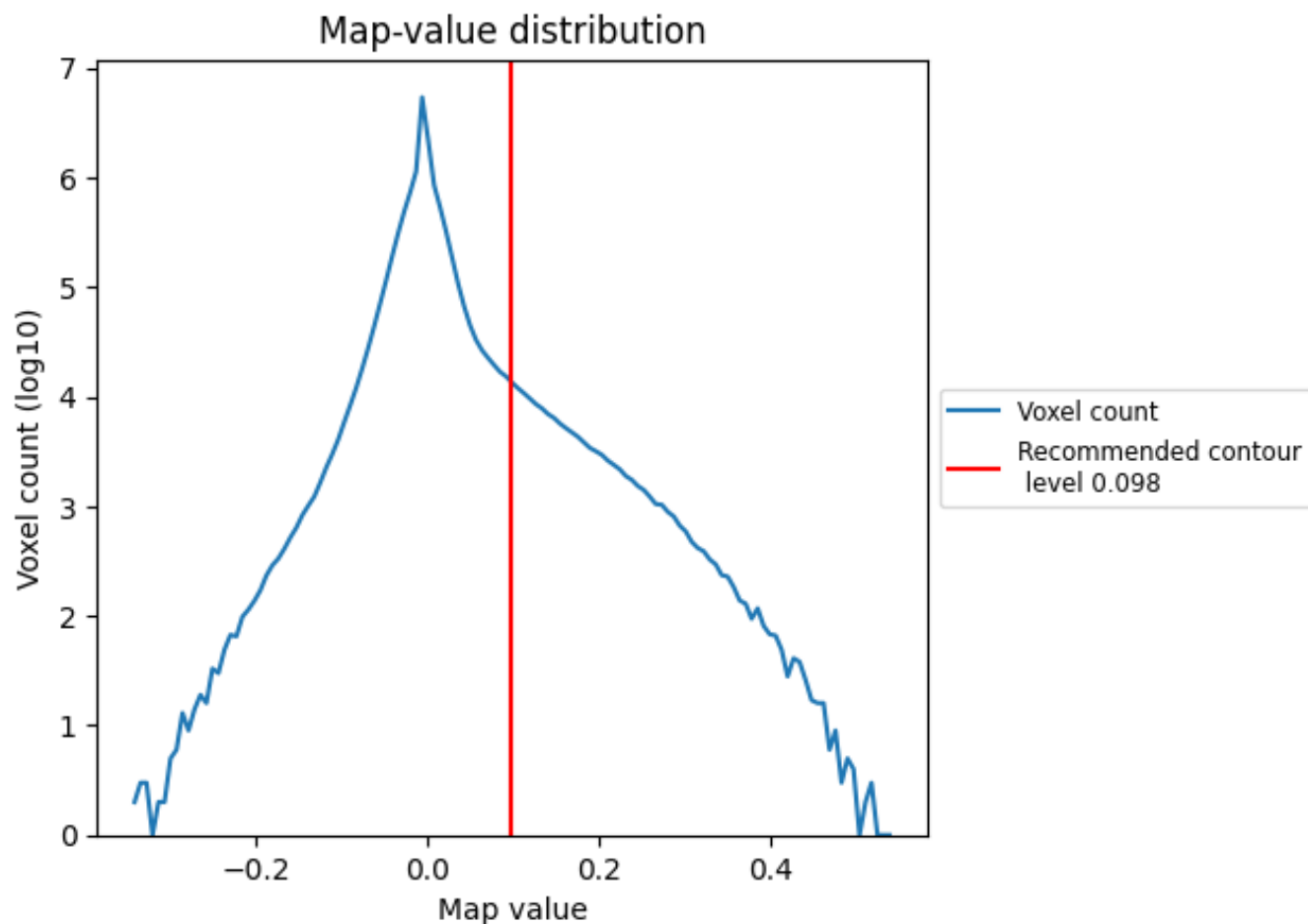
6.5 Mask visualisation

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

7 Map analysis [i](#)

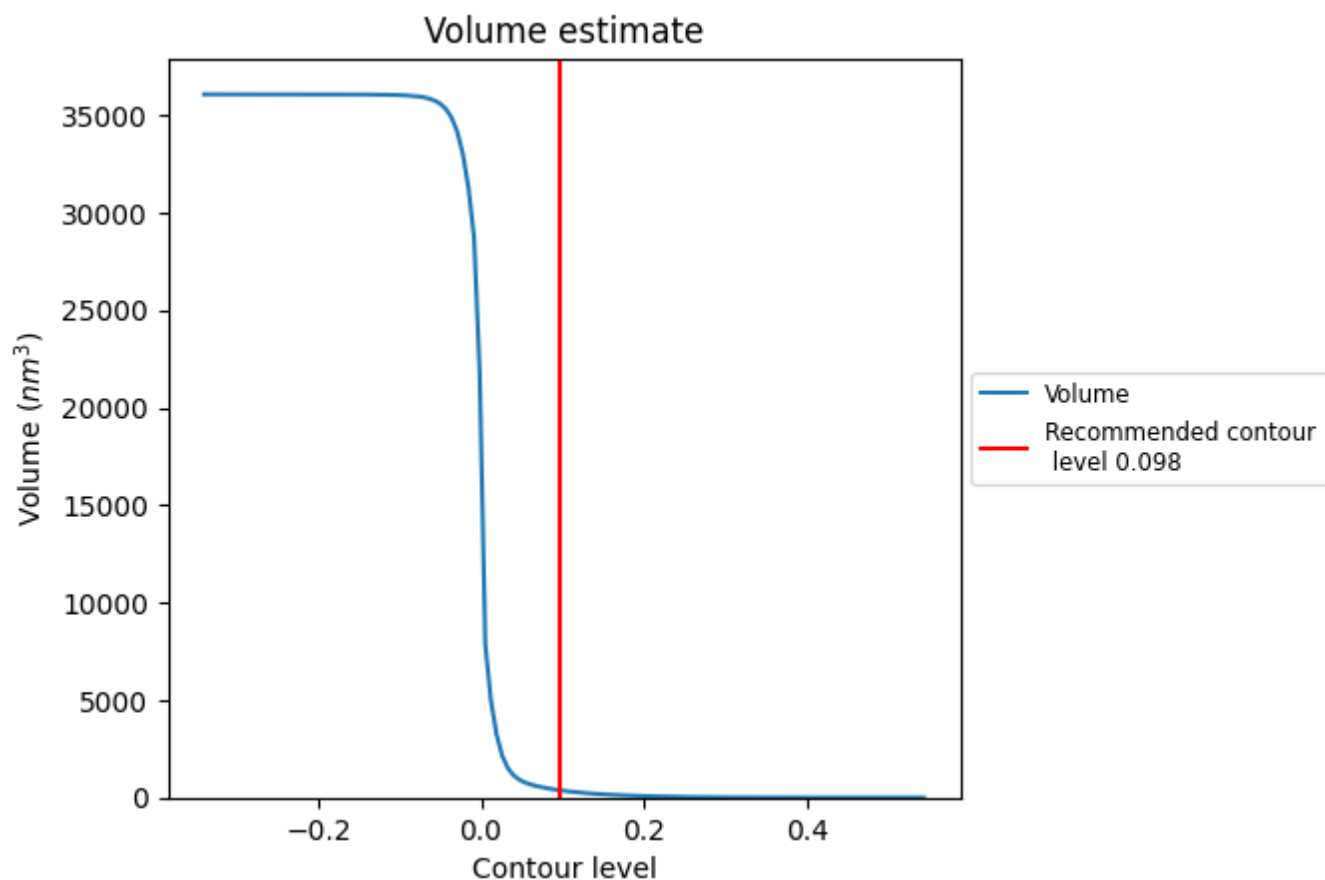
This section contains the results of statistical analysis of the map.

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.

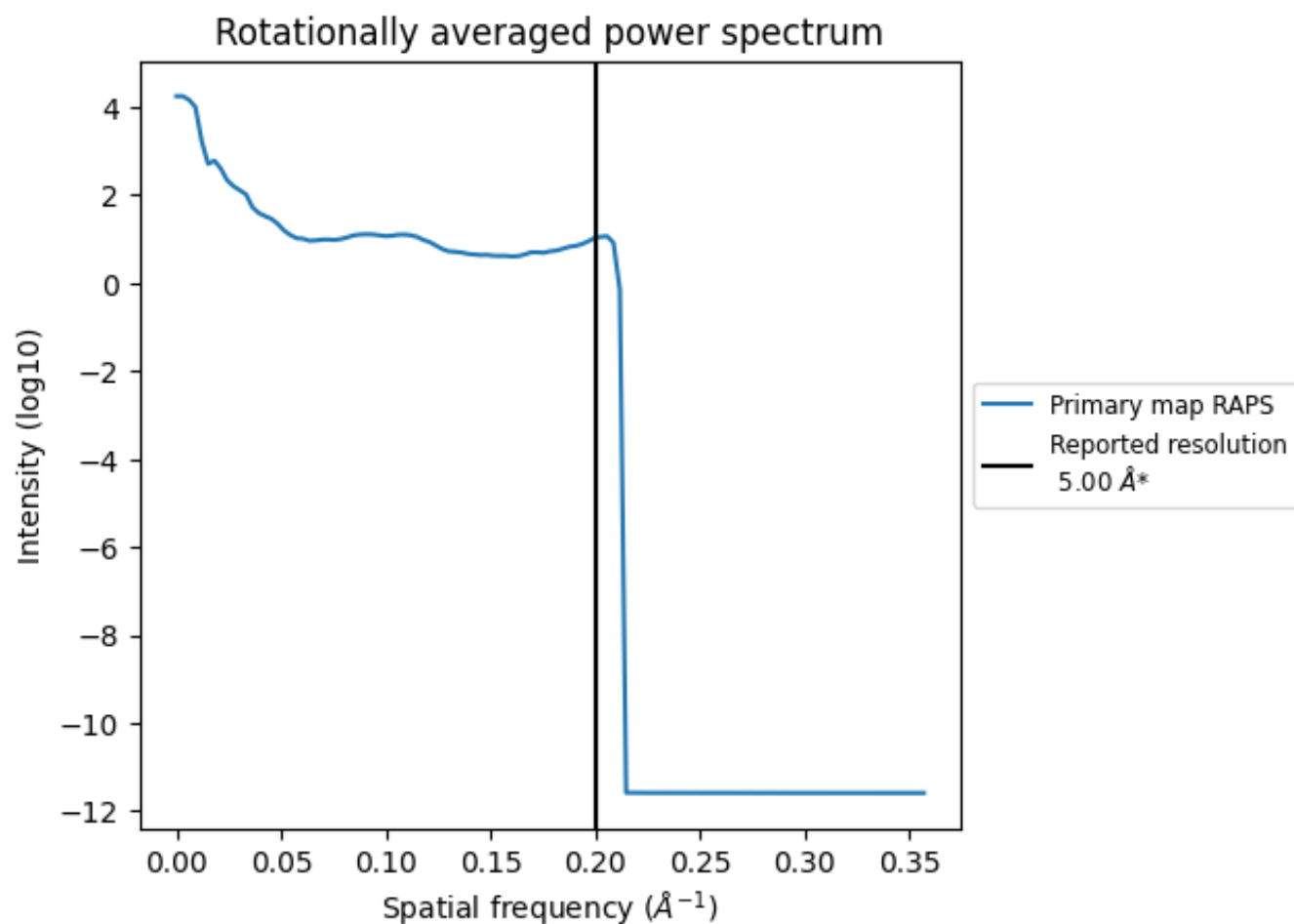
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 367 nm³; this corresponds to an approximate mass of 331 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 ⓘ

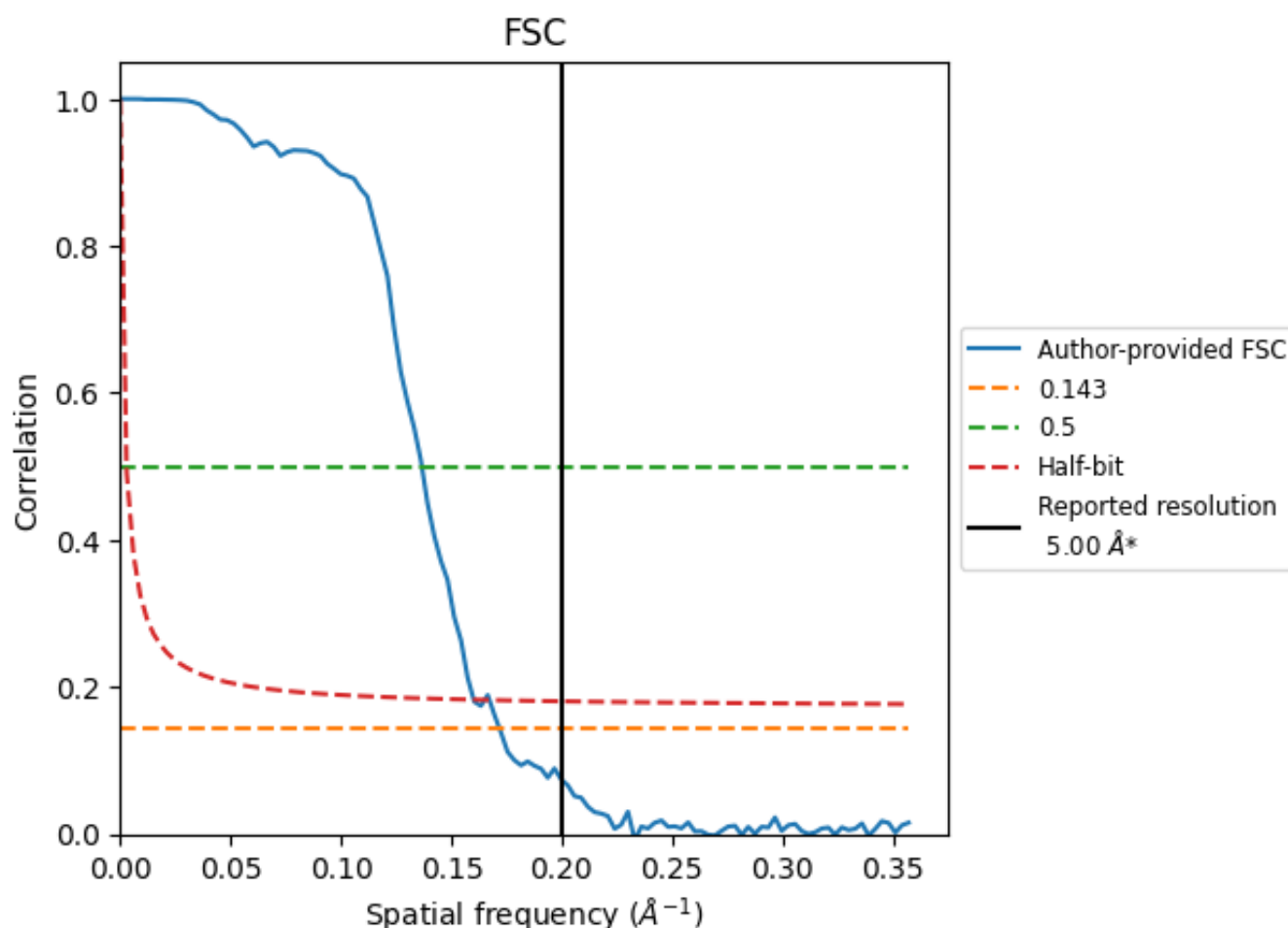


*Reported resolution corresponds to spatial frequency of 0.200 \AA^{-1}

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 0.200 Å⁻¹

8.2 Resolution estimates [i](#)

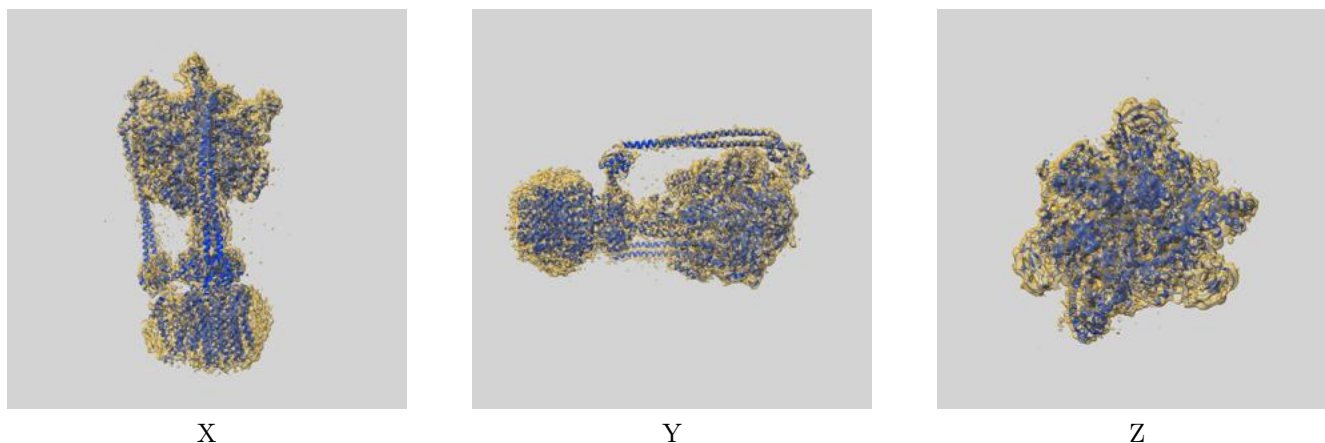
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	5.82	7.32	6.24
Unmasked-calculated*	-	-	-

*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 5.82 differs from the reported value 5.0 by more than 10 %

9 Map-model fit [i](#)

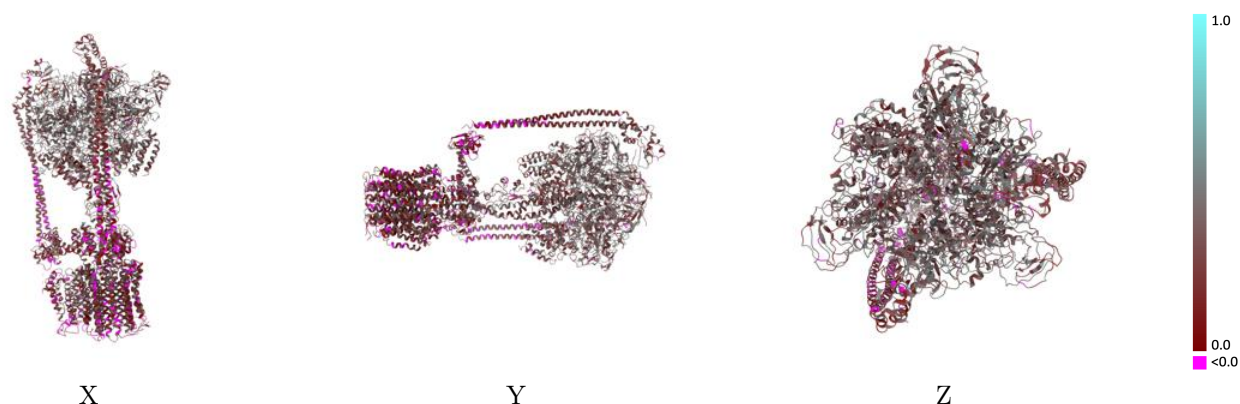
This section contains information regarding the fit between EMDB map EMD-6810 and PDB model 5Y5X. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



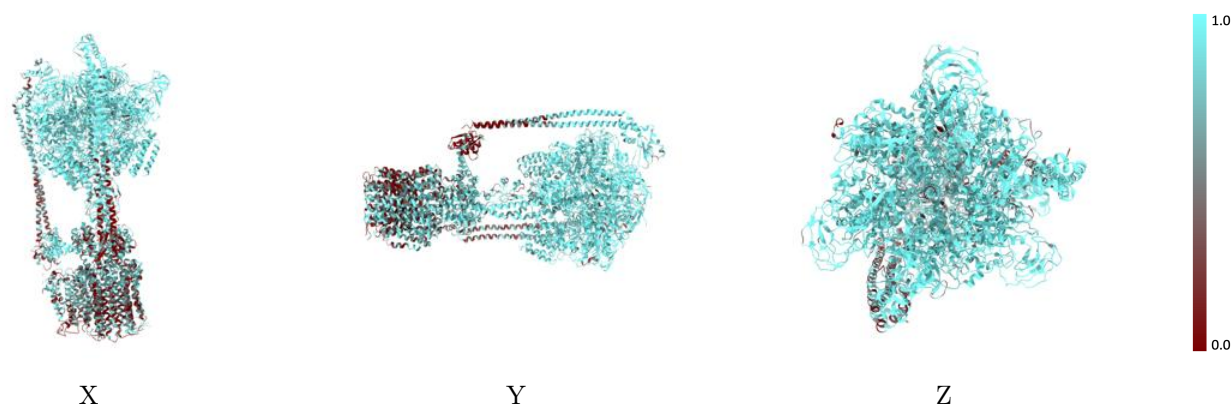
The images above show the 3D surface view of the map at the recommended contour level 0.098 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



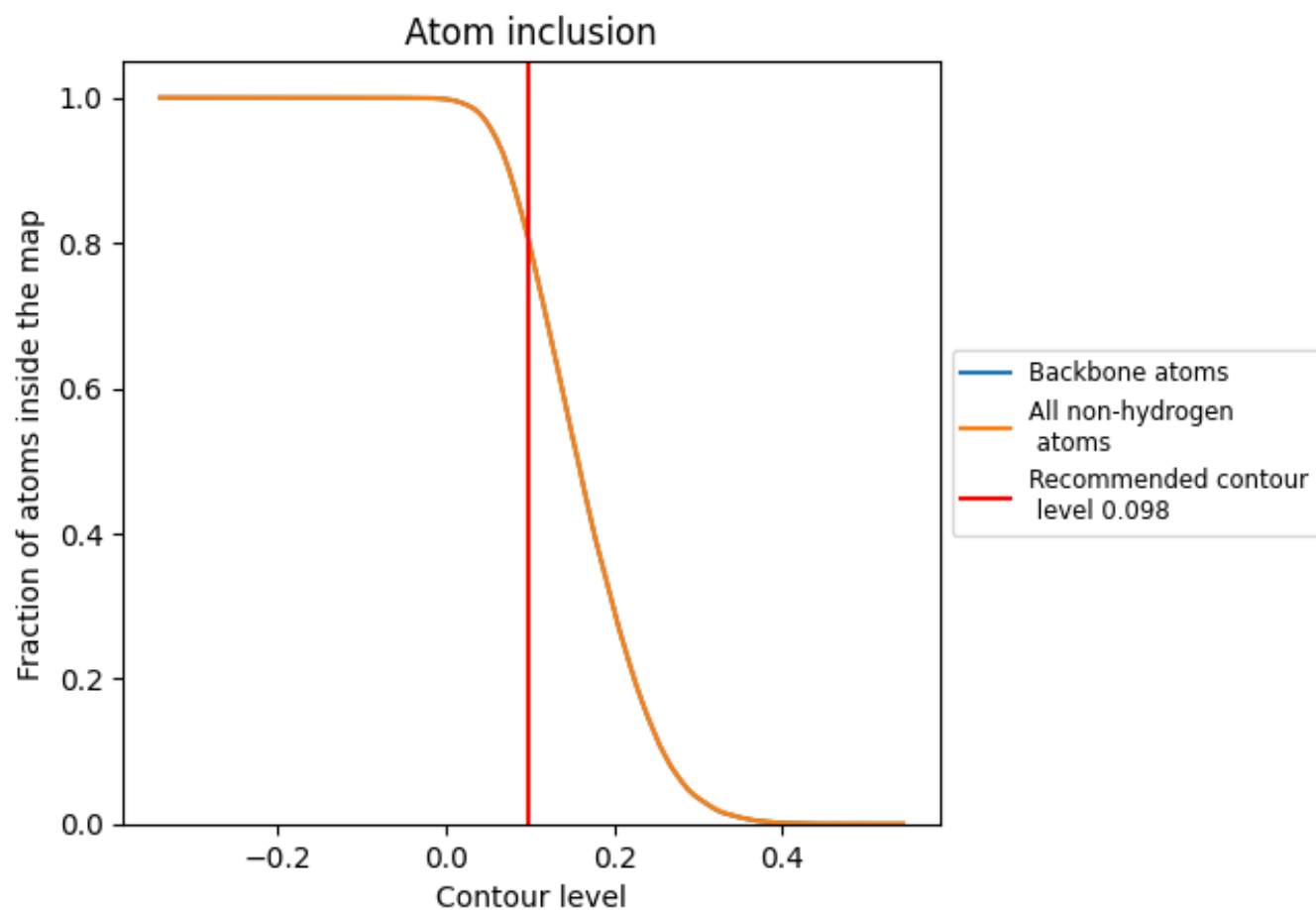
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.098).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.098) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8057	 0.3030
A	 0.9529	 0.3780
B	 0.9410	 0.3630
C	 0.9430	 0.3750
D	 0.9384	 0.3670
E	 0.9531	 0.3850
F	 0.9444	 0.3860
G	 0.8439	 0.3050
H	 0.8246	 0.3170
I	 0.5464	 0.1610
J	 0.7033	 0.2360
K	 0.6867	 0.1820
L	 0.7561	 0.2390
M	 0.7459	 0.2590
N	 0.5614	 0.1760
O	 0.6040	 0.2300
P	 0.6403	 0.2310
Q	 0.5413	 0.2010
R	 0.6337	 0.2440
S	 0.6766	 0.2260
T	 0.5677	 0.1940
U	 0.4884	 0.1870
V	 0.5512	 0.1990
W	 0.4257	 0.2090
X	 0.4752	 0.1880
Y	 0.6469	 0.2270
Z	 0.6865	 0.2400

