wwPDB EM Validation Summary Report (i)

Nov 10, 2024 – 12:24 am GMT

PDB ID	:	6QUM
EMDB ID	:	EMD-4640
Title	:	Thermus thermophilus V/A-type ATPase/synthase, rotational state 1
Authors	:	Zhou, L.; Sazanov, L.
Deposited on	:	2019-02-27
Resolution	:	3.25 Å(reported)
Based on initial models	:	5Y5X, 5Y5Y

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

|		
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.0%
Sidechain outliers		1.0%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
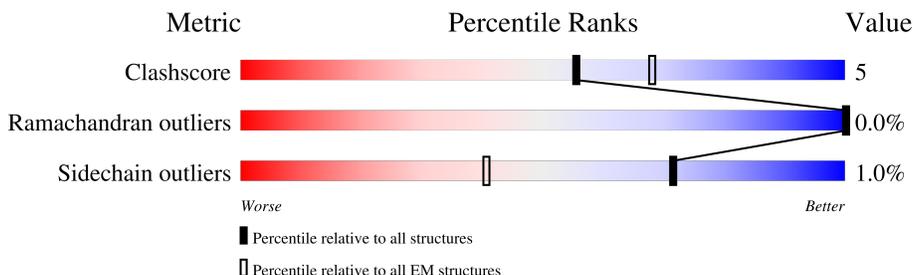
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	87% 13%
1	B	578	90% 10%
1	C	578	85% 15%
2	D	478	87% 12% •
2	E	478	83% 14% •
2	F	478	85% 14% •
3	G	223	7% 81% 12% 7%
4	H	104	8% 90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	103	13% 86% 13%
5	K	103	89% 7%
6	J	188	7% 82% 16%
6	L	188	82% 17%
7	M	323	8% 80% 18%
8	N	652	5% 82% 17%
9	O	74	88% 9%
9	P	74	89% 9%
9	Q	74	86% 14%
9	R	74	85% 12%
9	S	74	85% 11%
9	T	74	88% 9%
9	U	74	84% 15%
9	V	74	82% 16%
9	W	74	7% 82% 16%
9	X	74	82% 15%
9	Y	74	78% 20%
9	Z	74	88% 9%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 44900 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	578	Total	C	N	O	S	0	0
			4477	2857	763	835	22		
1	B	578	Total	C	N	O	S	0	0
			4477	2857	763	835	22		
1	C	578	Total	C	N	O	S	0	0
			4477	2857	763	835	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	470	Total	C	N	O	S	0	0
			3682	2334	636	702	10		
2	E	469	Total	C	N	O	S	0	0
			3682	2336	635	701	10		
2	F	470	Total	C	N	O	S	0	0
			3686	2338	636	702	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	207	Total	C	N	O	S	0	0
			1628	1026	304	296	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	104	Total	C	N	O	S	0	0
			792	501	136	152	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	103	Total 808	C 501	N 150	O 156	S 1	0	0
5	K	99	Total 788	C 489	N 146	O 152	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	186	Total 1437	C 894	N 270	O 273	0	0
6	L	187	Total 1441	C 896	N 271	O 274	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	320	Total 2514	C 1599	N 460	O 451	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	649	Total 4858	C 3176	N 835	O 838	S 9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	73	Total 508	C 331	N 88	O 88	S 1	0	0
9	P	73	Total 508	C 331	N 88	O 88	S 1	0	0
9	Q	74	Total 514	C 334	N 89	O 90	S 1	0	0
9	R	73	Total 508	C 331	N 88	O 88	S 1	0	0
9	S	73	Total 508	C 331	N 88	O 88	S 1	0	0
9	T	73	Total 508	C 331	N 88	O 88	S 1	0	0
9	U	73	Total 508	C 331	N 88	O 88	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	73	Total	C	N	O	S	0	0
			508	331	88	88	1		
9	W	73	Total	C	N	O	S	0	0
			508	331	88	88	1		
9	X	72	Total	C	N	O	S	0	0
			504	329	87	87	1		
9	Y	73	Total	C	N	O	S	0	0
			508	331	88	88	1		
9	Z	73	Total	C	N	O	S	0	0
			508	331	88	88	1		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
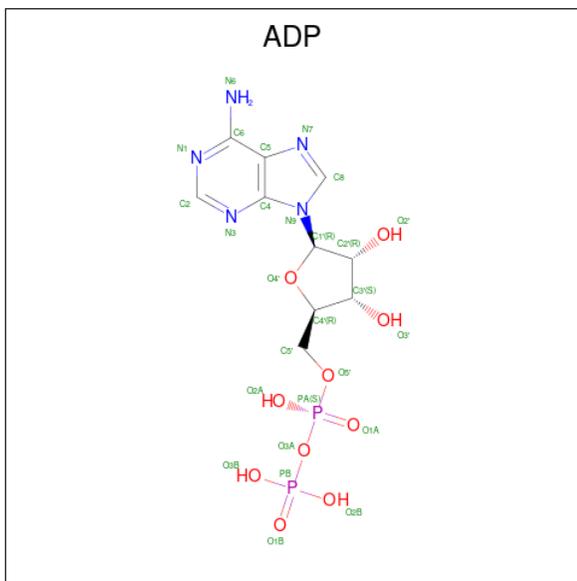
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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: V-type ATP synthase alpha chain
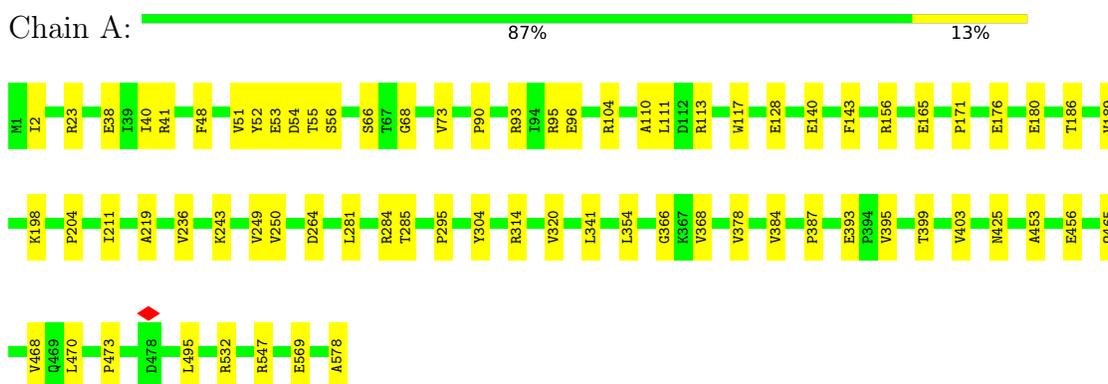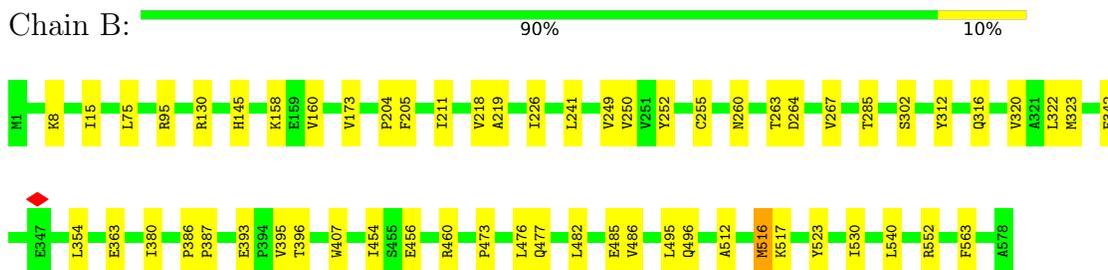
Chain A:

• Molecule 1: V-type ATP synthase alpha chain

Chain B:

• Molecule 1: V-type ATP synthase alpha chain

Chain C:

• Molecule 2: V-type ATP synthase beta chain
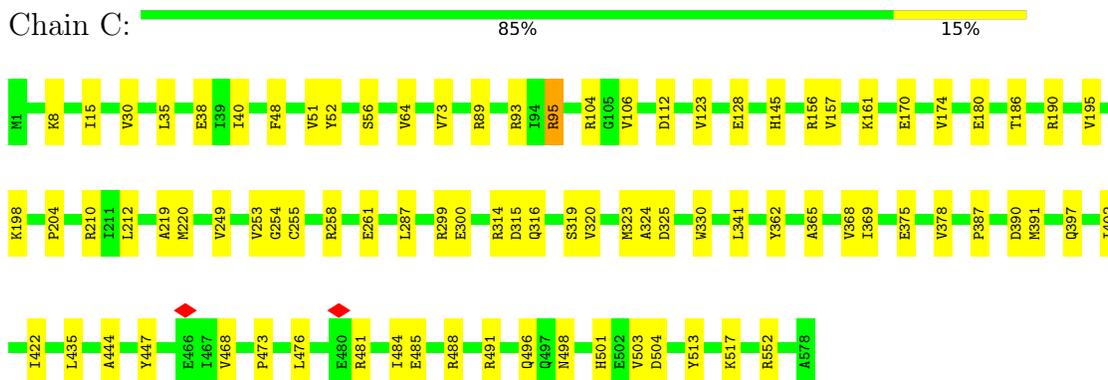
Chain D:
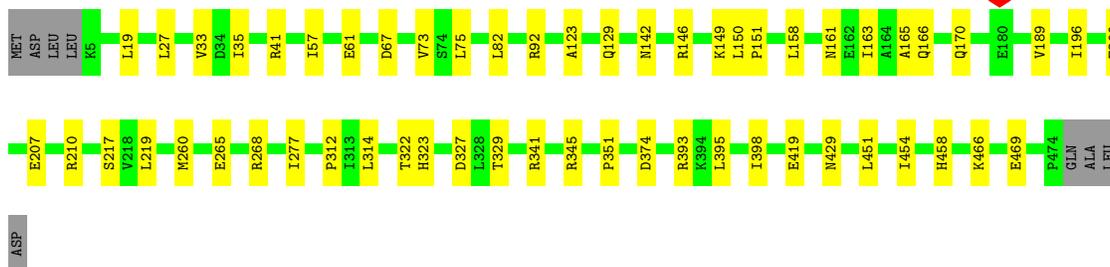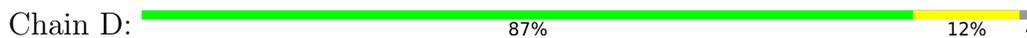
• Molecule 2: V-type ATP synthase beta chain
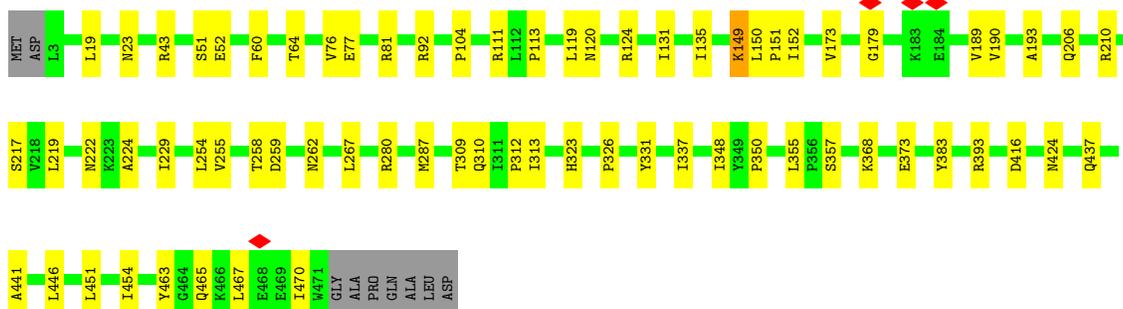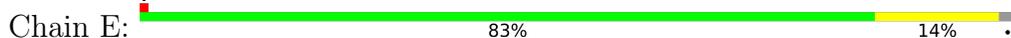
Chain E:

• Molecule 2: V-type ATP synthase beta chain

Chain F:
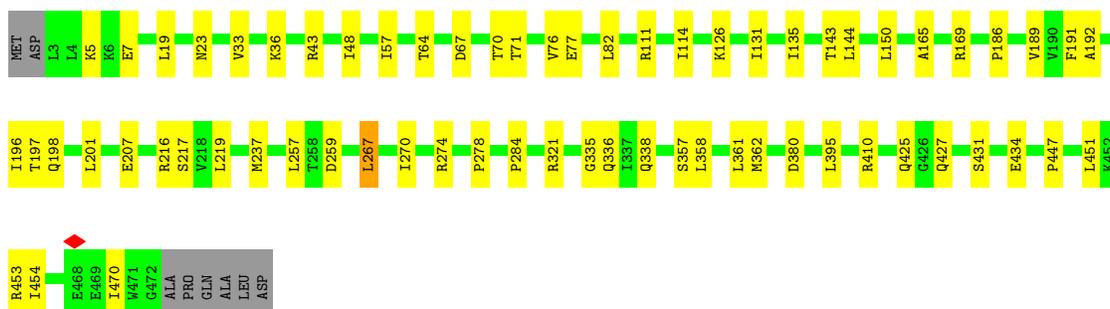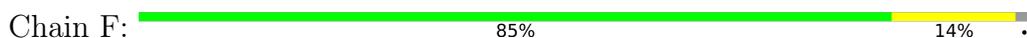
• Molecule 3: V-type ATP synthase subunit D

Chain G:
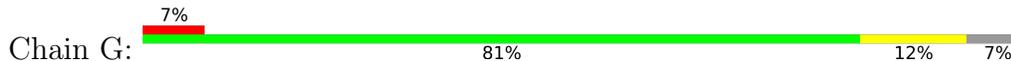
• Molecule 4: V-type ATP synthase subunit F
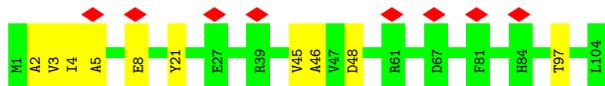
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)
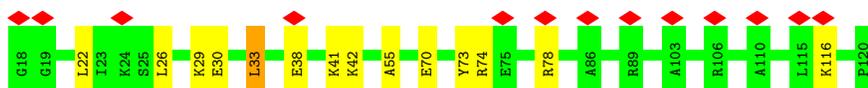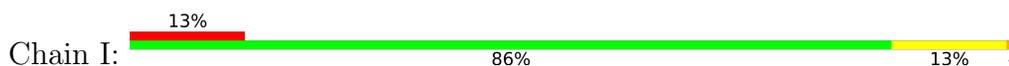
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)


• Molecule 6: V-type ATP synthase subunit E
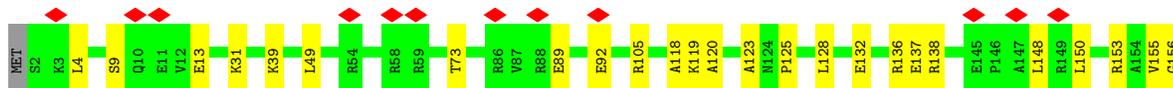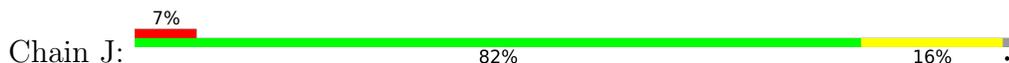
• Molecule 6: V-type ATP synthase subunit E
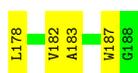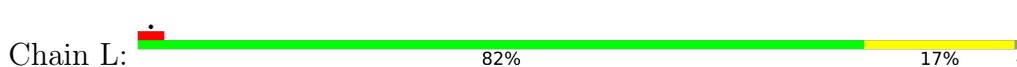
• Molecule 7: V-type ATP synthase subunit C

Chain M:

8%
80% 18%
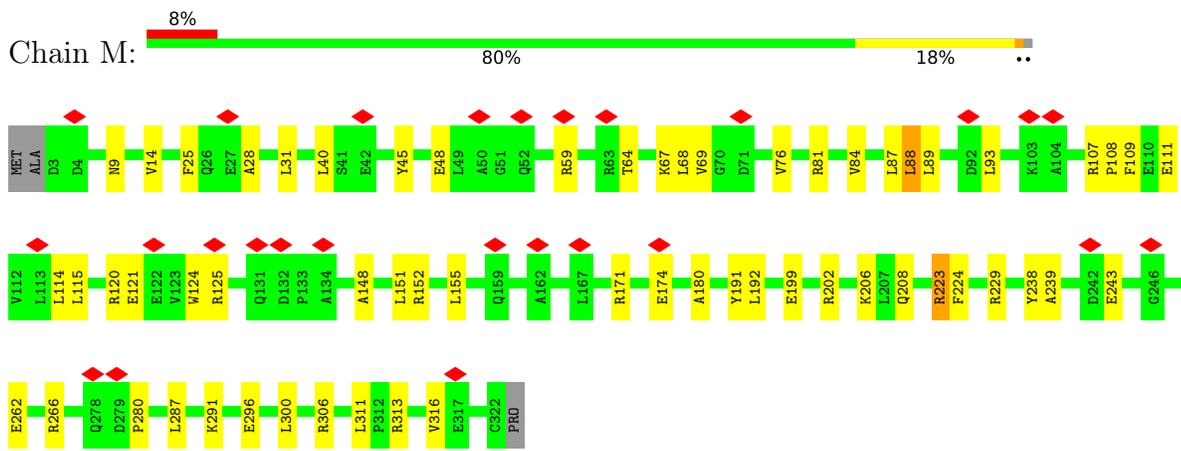
• Molecule 8: V-type ATP synthase subunit I
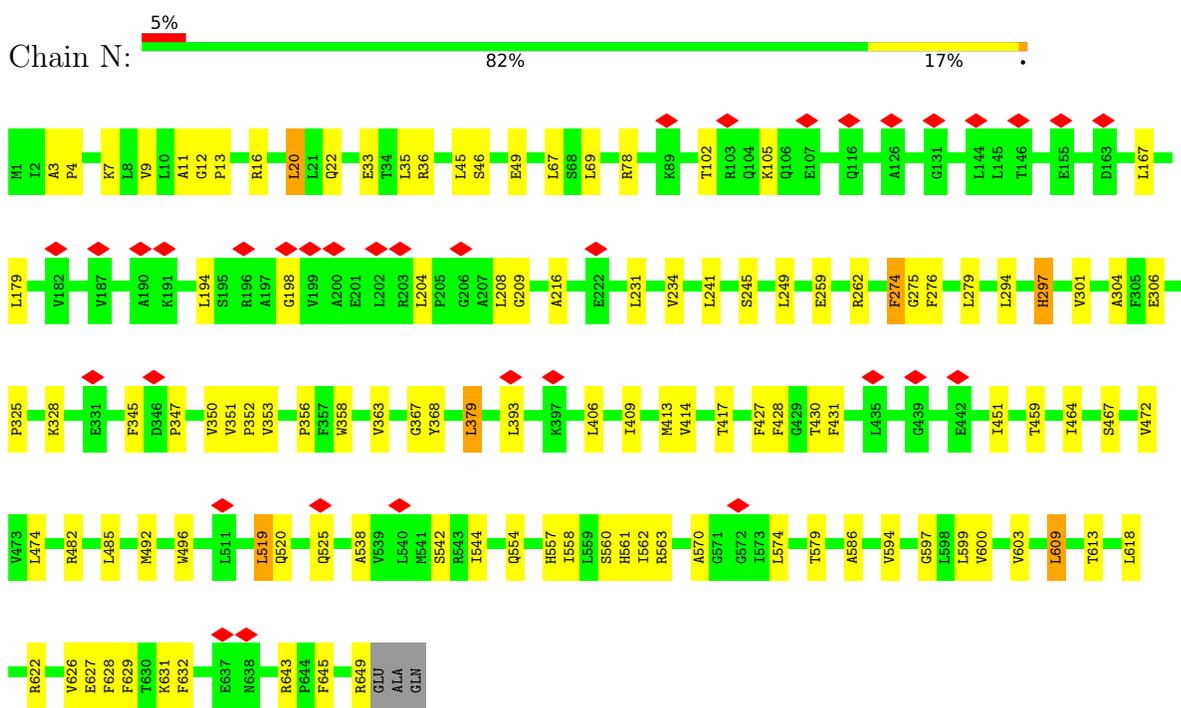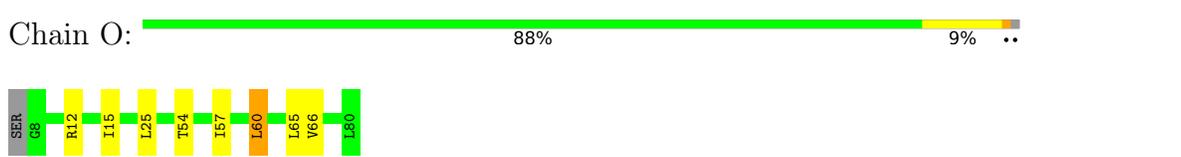
Chain N:

5%
82% 17%

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

Chain O:

88% 9%

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

Chain P:

89% 9%

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

Chain Q:

86%   14%

S7 G13 L14 V23 G24 L25 T30 G31 V32 T54 I57 L65 I72 L80

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

Chain R:

85%   12%

SER G8 G9 L10 G13 G18 V23 G24 L25 A46 E47 D48 N51 L65 V66 G78 R79 L80

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

Chain S:

85%   11%

SER G8 G9 L10 D11 R12 I15 A16 V17 L25 T30 T54 I57 P62 G78 R79 L80

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

Chain T:

88%   9%

SER G8 G9 L10 I15 L25 T54 I57 L65 I72 L76 L80

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

Chain U:

84%   15%

SER G8 G9 L10 I15 V23 G24 L25 T30 E47 T54 I57 L65 V66 I72 L76 N77 G78 R79 L80

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

Chain V:

82%   16%

SER G8 D11 L14 I15 A16 V17 V23 G24 L25 A33 R36 E47 T54 I57 L65 V66 L80

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

Chain W:

7%

82%   16%

SER G8 G9 L10 G13 L14 I15 M19 L25 G31 A39 E47 S50 G53 T54 I57 V66 G78 R79 L80

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

Chain X:
82% 15%

SER GLY G9 G13 L14 V17 L25 R36 E47 G53 T54 I57 E63 L71 I72 N77 G78 R79 L80

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

Chain Y:
78% 20%

SER G8 G9 L10 G13 L14 I15 V23 G24 L25 T30 A33 Q34 A35 E47 G53 I57 L61 P62 L65 I72 A73 F74 L80

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

Chain Z:
88% 9%

SER G8 G9 L10 V23 G24 L25 T30 A35 L60 L61 P62 L65 L80
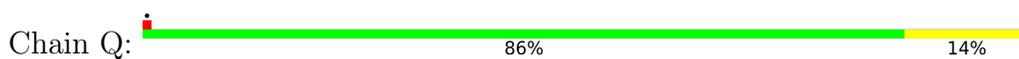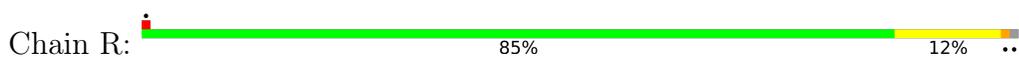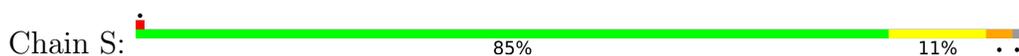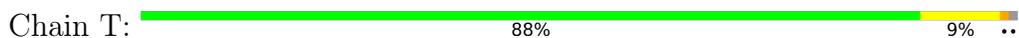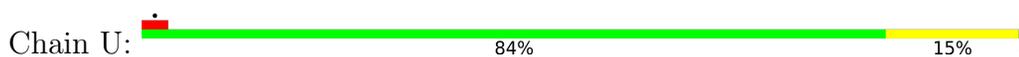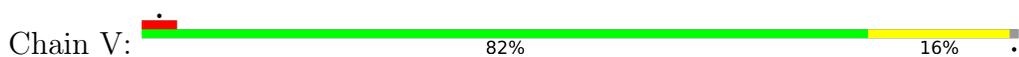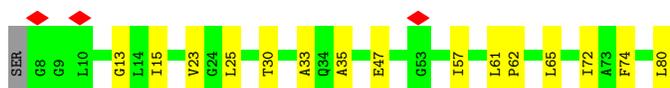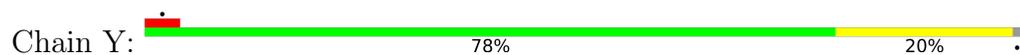
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39429	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1780	Depositor
Magnification	129032	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.296	Depositor
Minimum map value	-0.177	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	146.475, 146.475, 250.63501	wwPDB
Map dimensions	231, 135, 135	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	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

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	0.41	0/4573	0.59	1/6205 (0.0%)
1	B	0.40	0/4573	0.60	2/6205 (0.0%)
1	C	0.41	0/4573	0.59	3/6205 (0.0%)
2	D	0.40	0/3752	0.61	3/5081 (0.1%)
2	E	0.39	0/3751	0.63	3/5079 (0.1%)
2	F	0.41	0/3755	0.65	4/5084 (0.1%)
3	G	0.32	0/1648	0.56	0/2217
4	H	0.31	0/803	0.64	0/1084
5	I	0.33	0/810	0.58	0/1078
5	K	0.28	0/790	0.57	1/1052 (0.1%)
6	J	0.29	0/1451	0.54	0/1959
6	L	0.30	0/1455	0.61	0/1964
7	M	0.30	0/2553	0.66	3/3447 (0.1%)
8	N	0.33	0/4977	0.70	7/6780 (0.1%)
9	O	0.37	0/512	0.71	1/692 (0.1%)
9	P	0.33	0/512	0.66	0/692
9	Q	0.36	0/518	0.66	0/700
9	R	0.33	0/512	0.70	1/692 (0.1%)
9	S	0.34	0/512	0.69	1/692 (0.1%)
9	T	0.33	0/512	0.67	0/692
9	U	0.34	0/512	0.63	0/692
9	V	0.32	0/512	0.64	0/692
9	W	0.36	0/512	0.68	0/692
9	X	0.35	0/508	0.66	0/687
9	Y	0.38	0/512	0.66	0/692
9	Z	0.38	0/512	0.68	0/692
All	All	0.37	0/45610	0.63	30/61747 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
8	N	0	3
All	All	0	4

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	231	LEU	CA-CB-CG	8.07	133.85	115.30
7	M	114	LEU	CA-CB-CG	7.97	133.63	115.30
9	S	10	LEU	CA-CB-CG	6.75	130.82	115.30
2	F	150	LEU	CA-CB-CG	6.60	130.48	115.30
8	N	609	LEU	CA-CB-CG	6.55	130.36	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	179	GLY	Peptide
8	N	297	HIS	Peptide
8	N	301	VAL	Peptide
8	N	36	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4477	0	4495	40	0
1	B	4477	0	4496	33	0
1	C	4477	0	4496	51	0
2	D	3682	0	3707	33	0
2	E	3682	0	3714	38	0
2	F	3686	0	3717	35	0
3	G	1628	0	1707	22	0
4	H	792	0	803	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	808	0	852	10	0
5	K	788	0	832	5	0
6	J	1437	0	1489	18	0
6	L	1441	0	1492	25	0
7	M	2514	0	2587	36	0
8	N	4858	0	4778	60	0
9	O	508	0	547	5	0
9	P	508	0	547	5	0
9	Q	514	0	552	7	0
9	R	508	0	547	9	0
9	S	508	0	547	8	0
9	T	508	0	547	6	0
9	U	508	0	547	8	0
9	V	508	0	547	10	0
9	W	508	0	547	8	0
9	X	504	0	544	10	0
9	Y	508	0	547	13	0
9	Z	508	0	547	7	0
10	A	1	0	0	0	0
11	A	54	0	24	3	0
All	All	44900	0	45755	436	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 5.

The worst 5 of 436 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:40:ILE:O	1:C:48:PHE:HB3	1.77	0.83
7:M:151:LEU:O	7:M:155:LEU:HB2	1.81	0.81
2:F:36:LYS:O	2:F:71:THR:HA	1.84	0.77
6:L:36:GLU:O	6:L:39:LYS:O	2.10	0.70
8:N:542:SER:HB3	8:N:544:ILE:HG22	1.75	0.68

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	576/578 (100%)	543 (94%)	33 (6%)	0	100	100
1	B	576/578 (100%)	528 (92%)	47 (8%)	1 (0%)	44	71
1	C	576/578 (100%)	535 (93%)	41 (7%)	0	100	100
2	D	468/478 (98%)	439 (94%)	29 (6%)	0	100	100
2	E	467/478 (98%)	429 (92%)	38 (8%)	0	100	100
2	F	468/478 (98%)	439 (94%)	29 (6%)	0	100	100
3	G	205/223 (92%)	198 (97%)	7 (3%)	0	100	100
4	H	102/104 (98%)	89 (87%)	13 (13%)	0	100	100
5	I	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
5	K	97/103 (94%)	96 (99%)	1 (1%)	0	100	100
6	J	184/188 (98%)	178 (97%)	6 (3%)	0	100	100
6	L	185/188 (98%)	177 (96%)	7 (4%)	1 (0%)	25	56
7	M	318/323 (98%)	295 (93%)	23 (7%)	0	100	100
8	N	647/652 (99%)	573 (89%)	74 (11%)	0	100	100
9	O	71/74 (96%)	70 (99%)	1 (1%)	0	100	100
9	P	71/74 (96%)	67 (94%)	4 (6%)	0	100	100
9	Q	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
9	R	71/74 (96%)	68 (96%)	3 (4%)	0	100	100
9	S	71/74 (96%)	67 (94%)	4 (6%)	0	100	100
9	T	71/74 (96%)	69 (97%)	2 (3%)	0	100	100
9	U	71/74 (96%)	68 (96%)	3 (4%)	0	100	100
9	V	71/74 (96%)	67 (94%)	4 (6%)	0	100	100
9	W	71/74 (96%)	67 (94%)	4 (6%)	0	100	100
9	X	70/74 (95%)	67 (96%)	3 (4%)	0	100	100
9	Y	71/74 (96%)	65 (92%)	6 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Z	71/74 (96%)	69 (97%)	2 (3%)	0	100	100
All	All	5822/5940 (98%)	5429 (93%)	391 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	40	ALA
1	B	477	GLN

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	468/468 (100%)	465 (99%)	3 (1%)	84	89
1	B	468/468 (100%)	466 (100%)	2 (0%)	89	92
1	C	468/468 (100%)	467 (100%)	1 (0%)	92	95
2	D	394/401 (98%)	393 (100%)	1 (0%)	91	94
2	E	395/401 (98%)	393 (100%)	2 (0%)	86	90
2	F	395/401 (98%)	393 (100%)	2 (0%)	86	90
3	G	165/176 (94%)	164 (99%)	1 (1%)	84	89
4	H	80/80 (100%)	80 (100%)	0	100	100
5	I	76/76 (100%)	73 (96%)	3 (4%)	27	53
5	K	75/76 (99%)	75 (100%)	0	100	100
6	J	140/141 (99%)	138 (99%)	2 (1%)	62	77
6	L	140/141 (99%)	140 (100%)	0	100	100
7	M	254/256 (99%)	249 (98%)	5 (2%)	50	70
8	N	453/520 (87%)	446 (98%)	7 (2%)	60	75
9	O	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	P	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	Q	48/48 (100%)	46 (96%)	2 (4%)	25	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	R	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	S	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	T	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	U	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	V	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	W	47/48 (98%)	45 (96%)	2 (4%)	25	51
9	X	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	Y	47/48 (98%)	46 (98%)	1 (2%)	48	69
9	Z	47/48 (98%)	45 (96%)	2 (4%)	25	51
All	All	4536/4649 (98%)	4492 (99%)	44 (1%)	71	82

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	N	649	ARG
9	T	25	LEU
9	O	25	LEU
9	Q	30	THR
9	V	25	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	252	HIS
3	G	68	GLN
2	E	344	HIS
3	G	180	GLN
2	F	23	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	A	603	-	24,29,29	0.91	1 (4%)	29,45,45	1.33	4 (13%)
11	ADP	A	602	10	24,29,29	1.05	1 (4%)	29,45,45	1.46	2 (6%)

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	A	603	-	-	5/12/32/32	0/3/3/3
11	ADP	A	602	10	-	1/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	602	ADP	C5-C4	2.63	1.47	1.40
11	A	603	ADP	C5-C4	2.26	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	602	ADP	PA-O3A-PB	-4.82	116.29	132.83
11	A	603	ADP	N3-C2-N1	-3.33	123.48	128.68
11	A	602	ADP	N3-C2-N1	-2.81	124.29	128.68
11	A	603	ADP	C4-C5-N7	-2.73	106.56	109.40
11	A	603	ADP	PA-O3A-PB	-2.49	124.27	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	603	ADP	PB-O3A-PA-O5'
11	A	603	ADP	C5'-O5'-PA-O3A
11	A	603	ADP	O4'-C4'-C5'-O5'
11	A	603	ADP	C3'-C4'-C5'-O5'
11	A	603	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	602	ADP	3	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 then 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.

Ligand ADP A 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 602

Bond lengths

Bond angles

Torsions

Rings
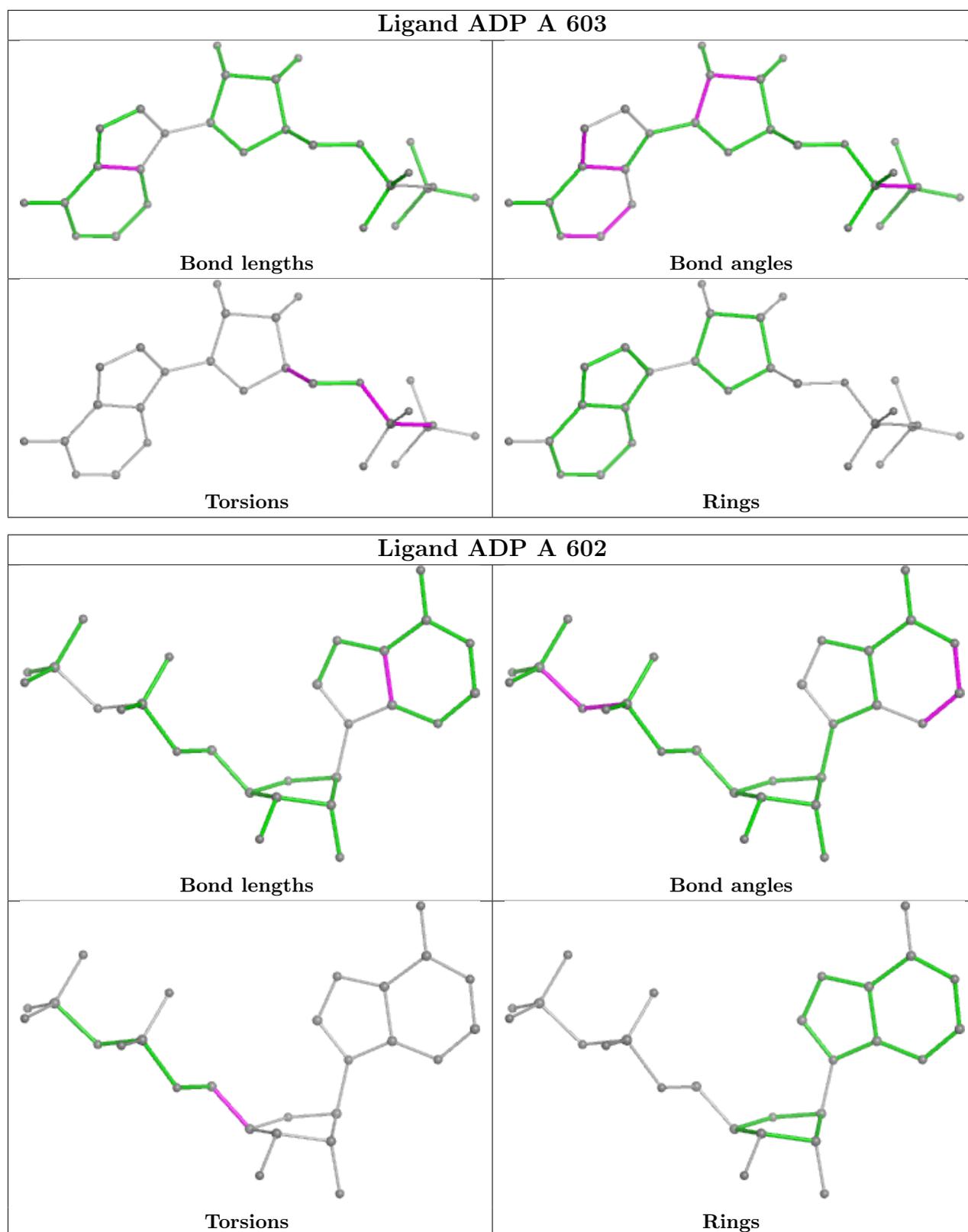
5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-4640. 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 ⓘ

6.1.1 Primary map

| X | Y | Z |
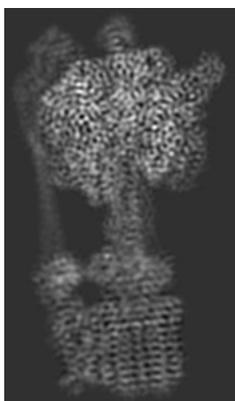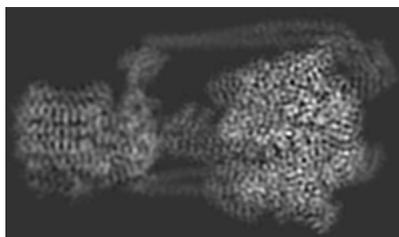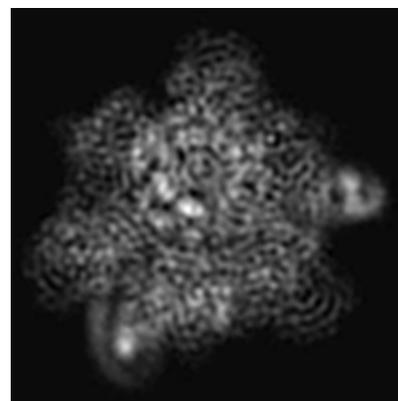
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
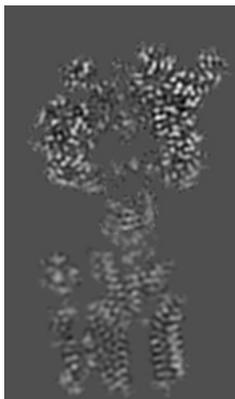
6.2.1 Primary map
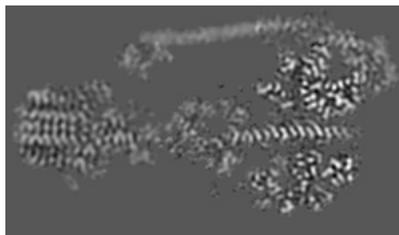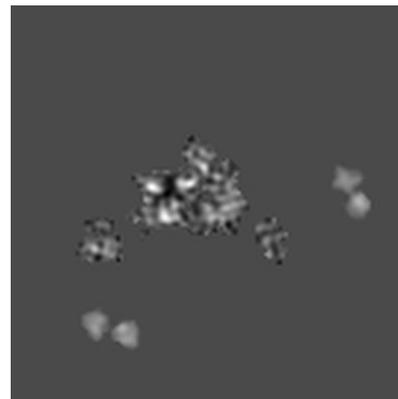
| X Index: 67 | Y Index: 67 | Z Index: 115 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
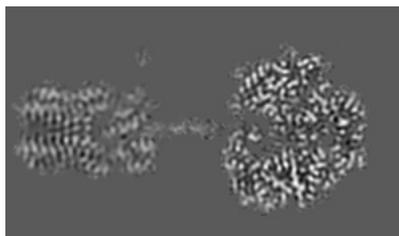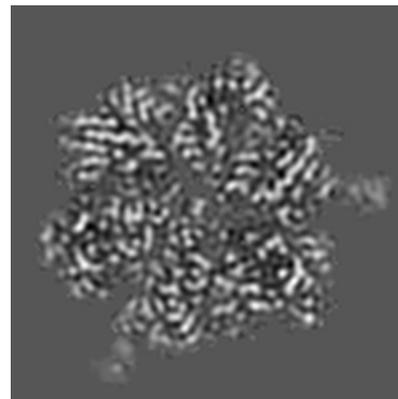
| X Index: 60 | Y Index: 86 | Z Index: 170 |

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map

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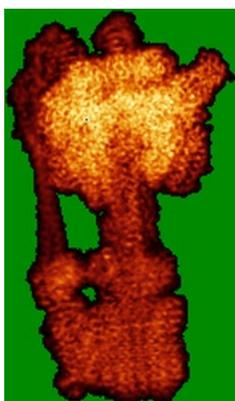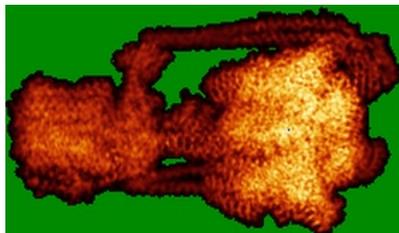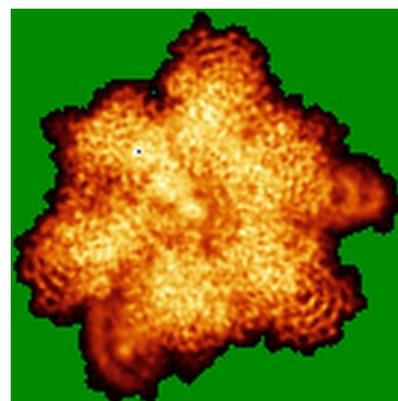
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
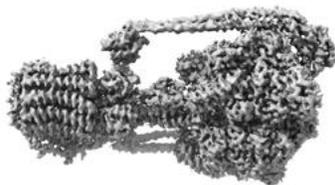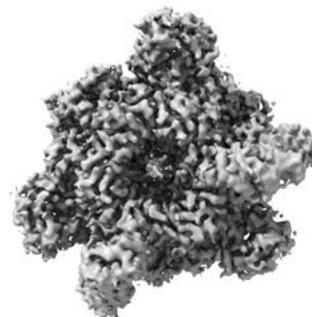
The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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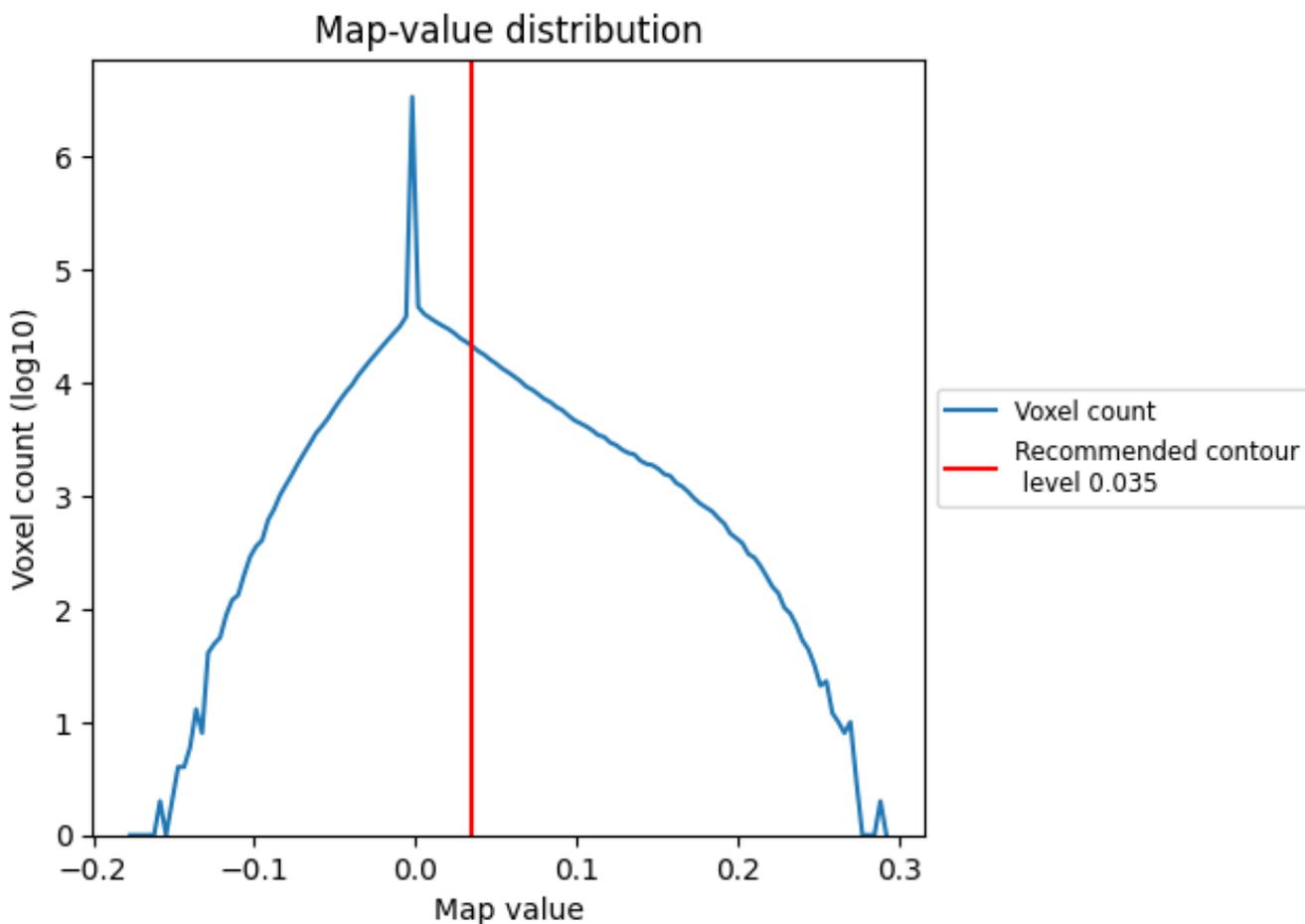
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
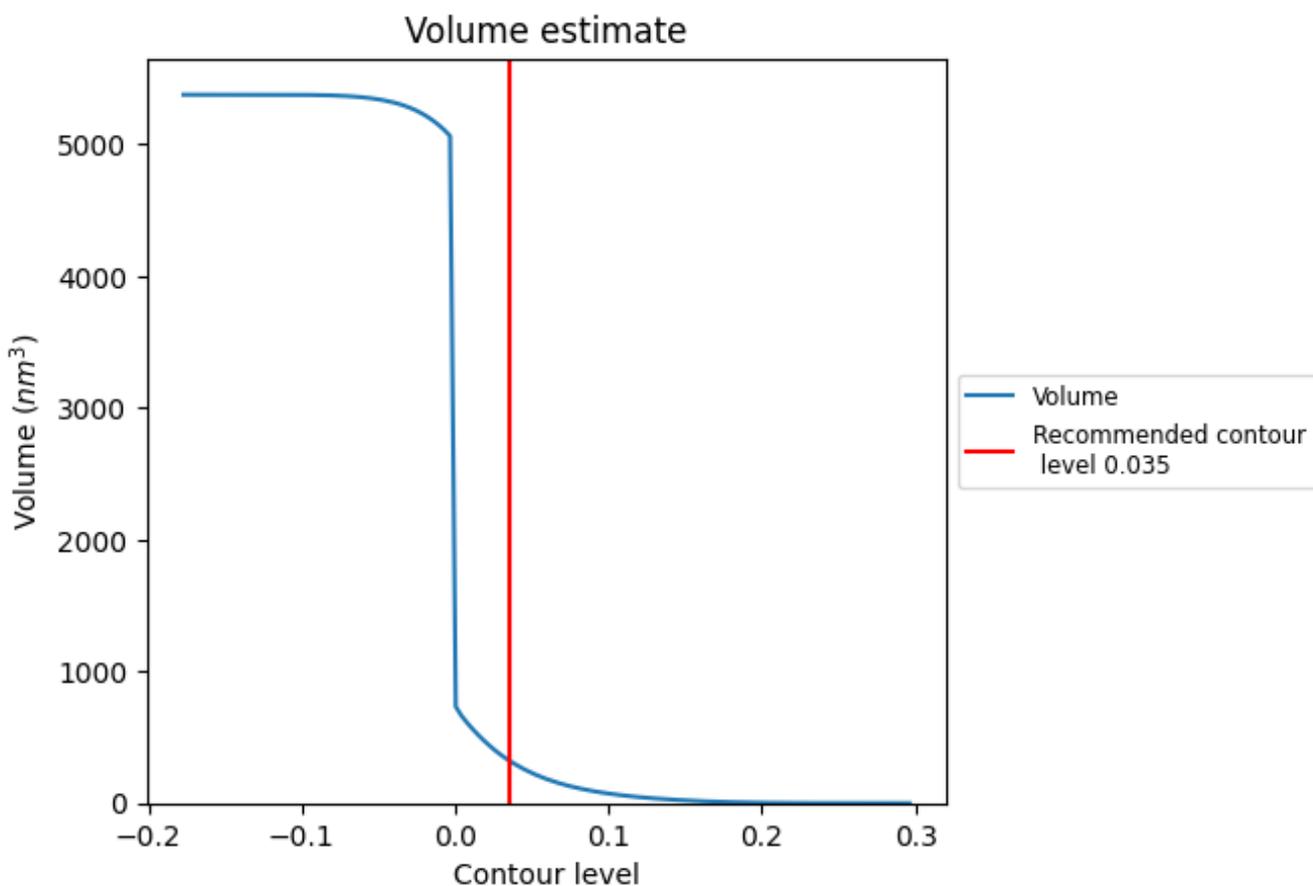
The volume at the recommended contour level is 325 nm^3; this corresponds to an approximate mass of 293 kDa.

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 ⓘ

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-4640 and PDB model 6QUM. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

X   Y   Z
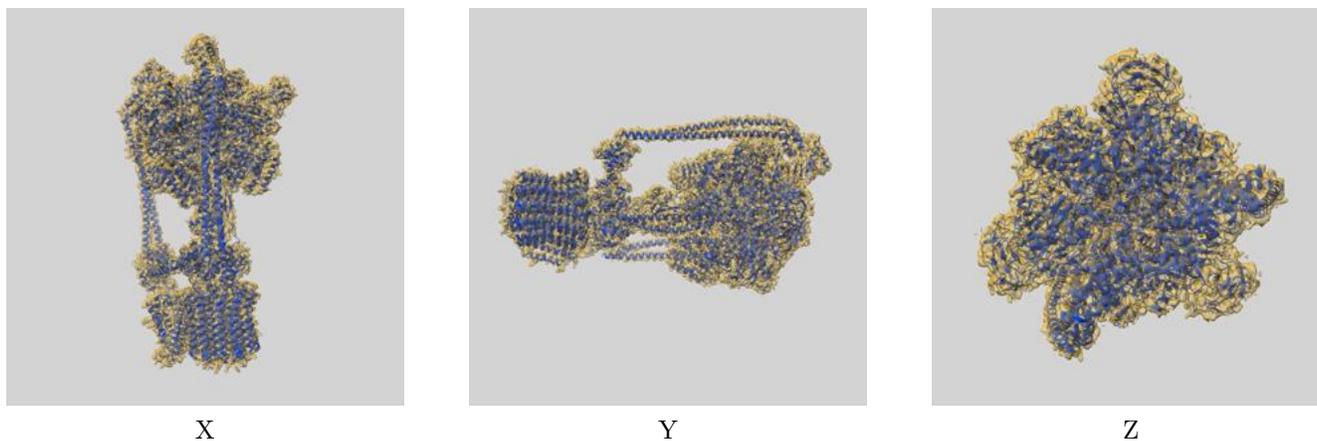
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ
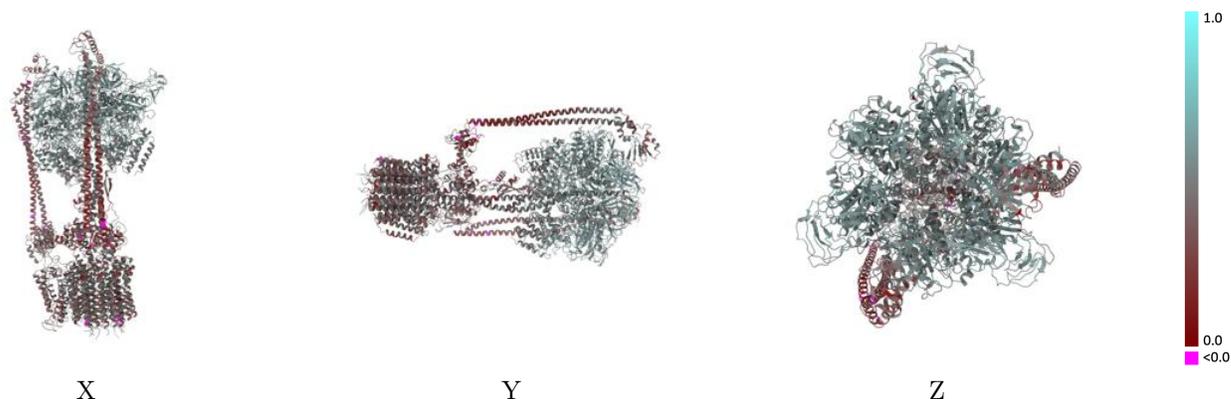
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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   ⓘ
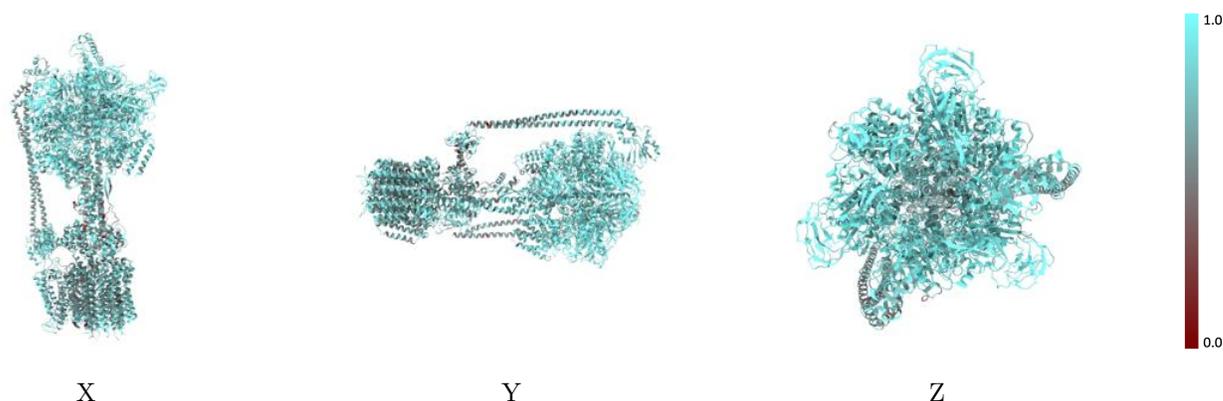
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4   Atom inclusion ⓘ
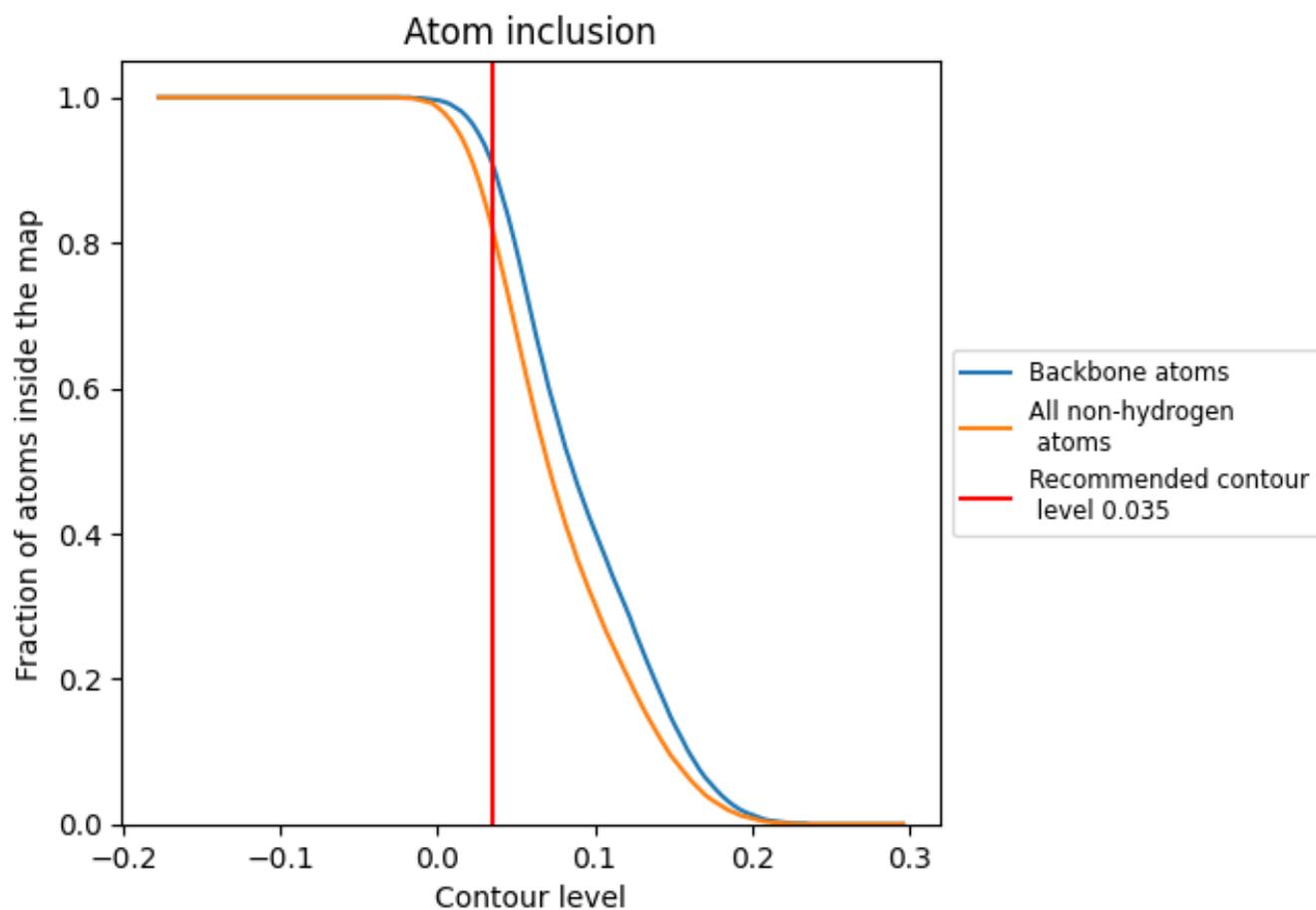
At the recommended contour level, 91% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8190	0.4660
A	0.9010	0.5400
B	0.9040	0.5350
C	0.8970	0.5360
D	0.9070	0.5420
E	0.8750	0.5260
F	0.8950	0.5440
G	0.7590	0.4460
H	0.7120	0.3570
I	0.6170	0.2420
J	0.6880	0.2820
K	0.6690	0.2820
L	0.7410	0.3650
M	0.7150	0.4020
N	0.7630	0.3830
O	0.7040	0.4090
P	0.7200	0.4130
Q	0.7410	0.4200
R	0.7600	0.4170
S	0.7600	0.4170
T	0.7360	0.4040
U	0.7160	0.3950
V	0.7380	0.4050
W	0.6720	0.4080
X	0.6570	0.3990
Y	0.6840	0.4040
Z	0.7140	0.4230

1.0

0.0
<0.0