



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 11:42 pm GMT

PDB ID : 6TDZ
EMDB ID : EMD-10472
Title : Cryo-EM structure of *Euglena gracilis* mitochondrial ATP synthase, OSCP/F1/c-ring, rotational state 2
Authors : Muhleip, A.; Amunts, A.
Deposited on : 2019-11-10
Resolution : 3.14 Å(reported)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

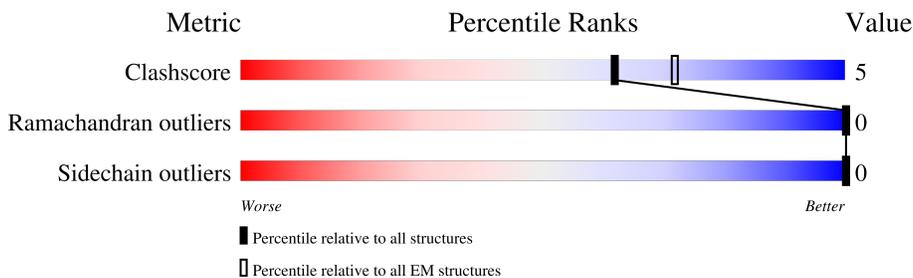
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	267	
2	h	476	
3	c	169	
4	G	306	
5	H	176	
6	I	76	
7	O	104	
7	P	104	

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Mol	Chain	Length	Quality of chain
7	Q	104	
7	R	104	
7	S	104	
7	T	104	
7	U	104	
7	V	104	
7	W	104	
7	X	104	
8	A	561	
8	B	561	
8	C	561	
9	D	494	
9	E	494	
9	F	494	
10	J	192	
10	K	192	
10	L	192	
11	N	103	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 81734 atoms, of which 41166 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 oligomycin sensitivity conferring protein (OSCP).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	M	243	3778	1212	1885	310	370	1	0	0

- Molecule 2 is a protein called subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	h	48	790	250	400	65	74	1	0	0

- Molecule 3 is a protein called subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	c	50	857	273	436	71	76	1	0	0

- Molecule 4 is a protein called subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	G	303	4898	1543	2462	420	459	14	0	0

- Molecule 5 is a protein called subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	H	160	2448	787	1202	207	251	1	0	0

- Molecule 6 is a protein called subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	I	66	1077	346	541	91	98	1	0	0

- Molecule 7 is a protein called subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace	
7	O	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	P	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	Q	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	R	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	S	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	T	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	U	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	V	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	W	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
7	X	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		

- Molecule 8 is a protein called subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace	
8	B	526	Total	C	H	N	O	S	0	0
			8292	2611	4197	700	766	18		
8	C	530	Total	C	H	N	O	S	0	0
			8353	2631	4226	706	772	18		
8	A	527	Total	C	H	N	O	S	0	0
			8302	2614	4202	701	767	18		

- Molecule 9 is a protein called subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
9	E	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		
9	F	487	Total	C	H	N	O	S	0	0
			7408	2318	3730	620	713	27		
9	D	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		

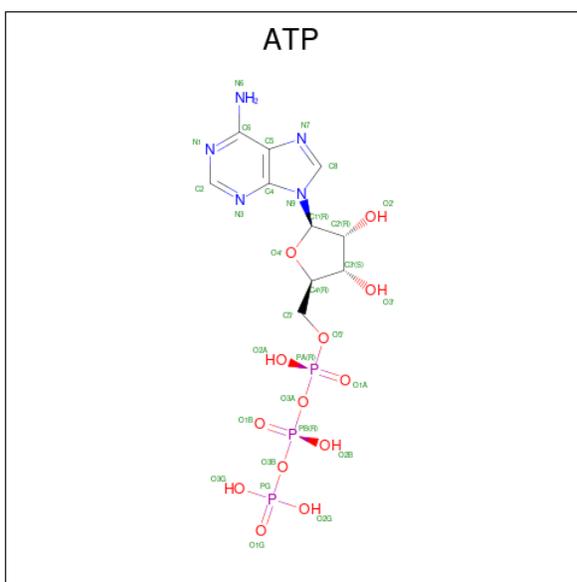
- Molecule 10 is a protein called p18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	K	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
10	L	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
10	J	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		

- Molecule 11 is a protein called inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	N	49	Total	C	H	N	O	S	0	0
			802	247	399	72	82	2		

- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

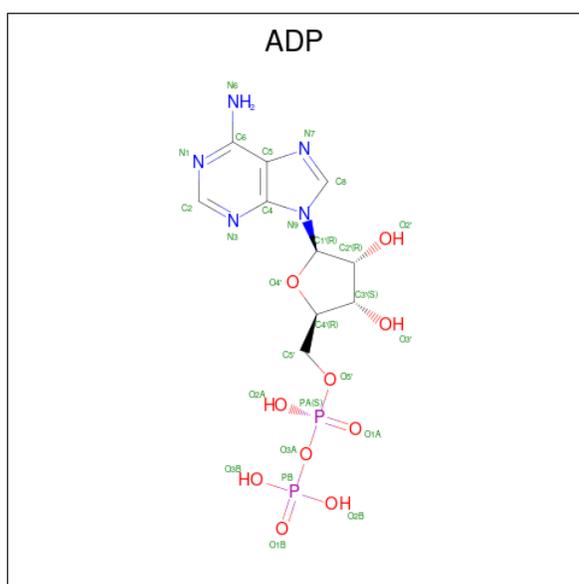


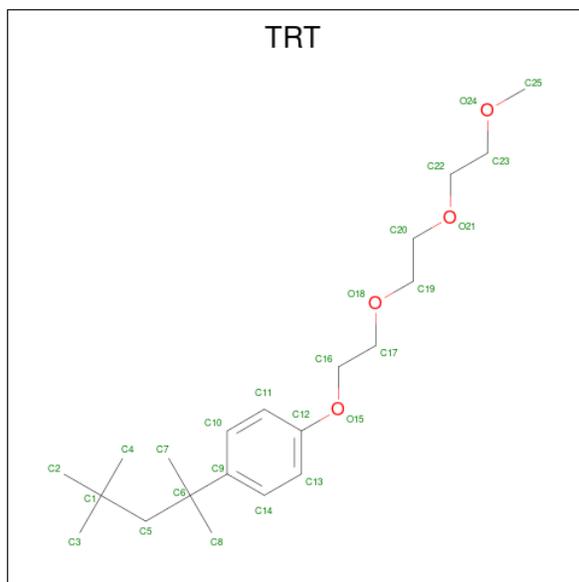
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
12	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
12	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
12	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
12	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



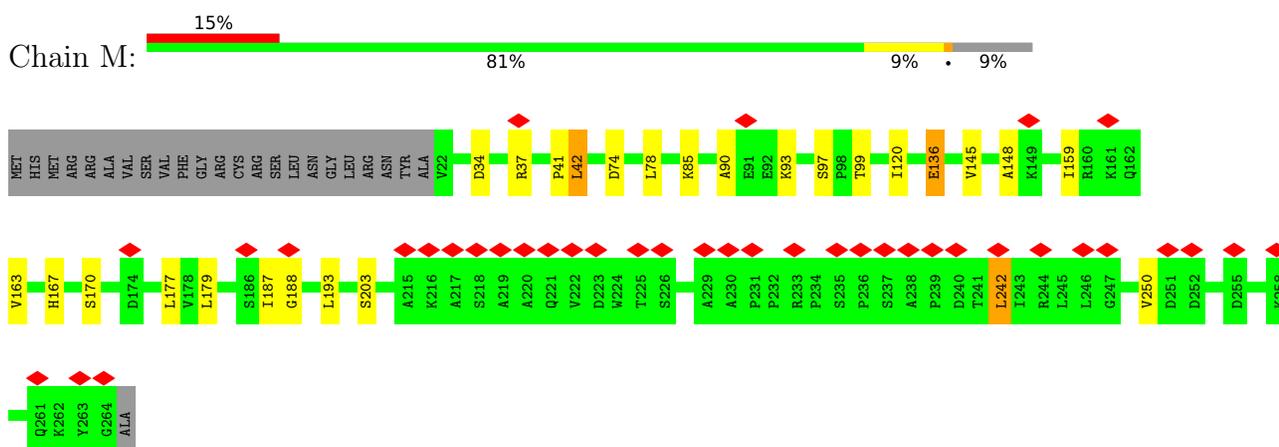


Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
15	F	1	61	21	36	4	0

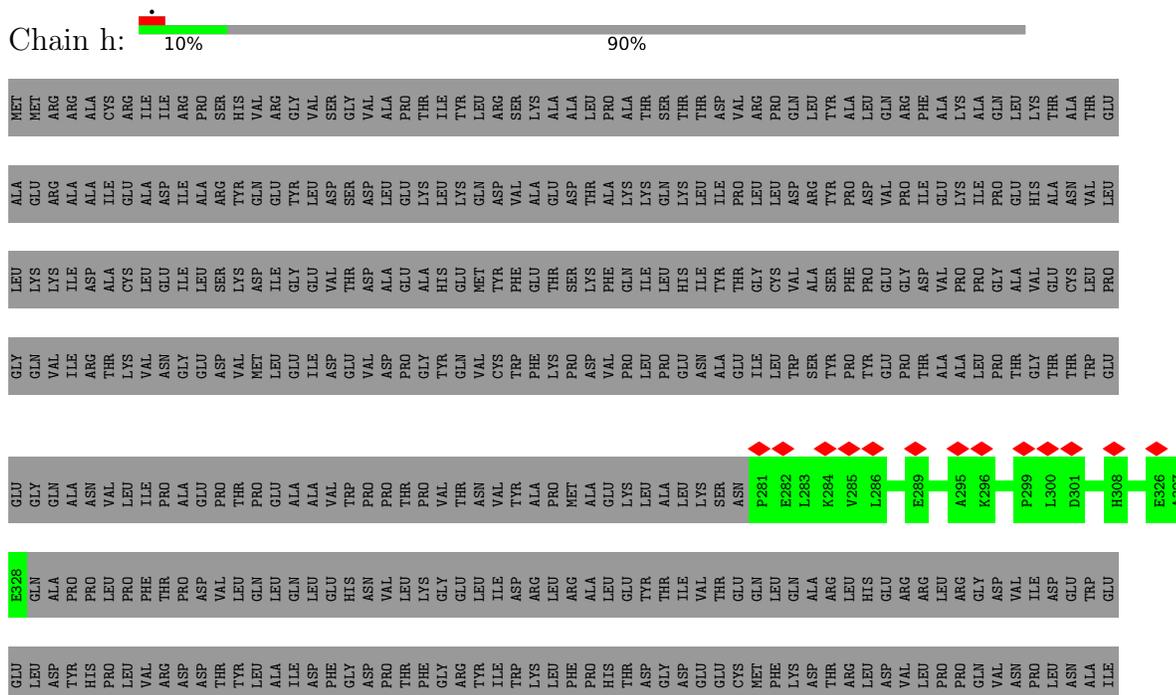
3 Residue-property plots

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: oligomycin sensitivity conferring protein (OSCP)



- Molecule 2: subunit d



LEU
ALA
GLN
HIS
THR
ALA
GLN
THR
PRO
LEU
VAL
HIS
ARG
SER
LEU
GLU
LYS
ARG
LEU
TRP
THR
GLU
VAL
ARG
ALA
THR
ALA
VAL
SER
GLU

• Molecule 3: subunit c

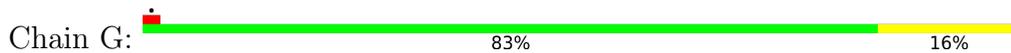


MET PHE ARG GLY PHE ARG PRO VAL LEU LEU ALA ALA ASP ALA V14 G27 D31 Q32 D37 A42 I43 F44 GLY ALA SER TRP LYS LYS ASP LEU LEU ASN TRP LYS PHE ASP SER TYR ALA PRO LYS LEU PRO ALA ALA ARG ASP ARG LYS LYS ASP L78

R90 Y96 ILE LEU ALA CYS LEU PRO GLY VAL LYS ASP VAL ASP LEU THR GLU LYS HIS LEU LEU LEU THR GLY LYS ALA ARG LEU LEU GLU V66 G63 I67 L61 S70 L73 L74 I78 V99 T105 M117 T118 F121 L130 Q140 E147 G166 S169 P178

ALA GLU LYS SER LYS ALA LEU ALA ASP LYS VAL ILE ALA SER PRO

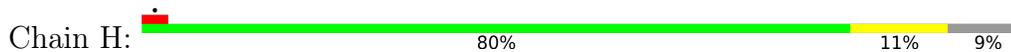
• Molecule 4: subunit gamma



MET PRO G3 G4 G5 Y17 I27 L32 R36 R41 V44 L49 R50 Y51 T52 R53 D57 D62 D63 V66 I67 S70 L73 L74 I78 V99 T105 M117 T118 F121 L130 Q140 E147 G166 S169 P178

E199 E200 G201 S205 K209 G213 Y224 H227 V232 L233 N234 V236 N239 N253 Q254 L255 G256 T259 G260 L261 K274 K295 K296 W305 LYS

• Molecule 5: subunit delta



MET ARG ALA SER ARG THR LEU LEU LEU VAL VAL ARG ARG PHE MET ARG Q17 D18 R29 F30 F31 G39 I43 T52 R53 Q54 D55 E56 T71 G74 E75 M76 G77 Y84 Q87 E99 N116 D117 D122 I123 N124 E155 R158 H176

• Molecule 6: subunit epsilon



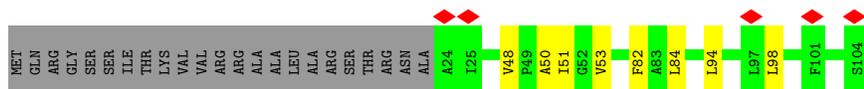
MET S2 R12 E27 N34 S38 L45 Y46 L47 H49 E87 ASN GLN VAL ALA ALA GLN GLN HIS HIS ALA

• Molecule 7: subunit c



MET GLN ARG GLY SER SER ILE THR LYS VAL VAL ARG ARG ALA ALA ARG ARG SER THR ARG ARG ALA A24 Y27 N35 A39 F82 A83 L84 L88 A96 L97 L100 F101 Y102 F103 S104

• Molecule 7: subunit c



• Molecule 7: subunit c



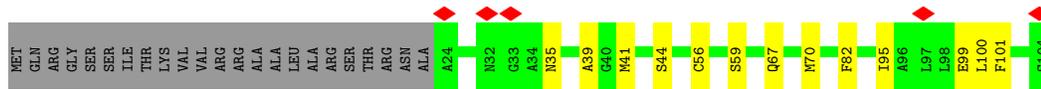
• Molecule 7: subunit c



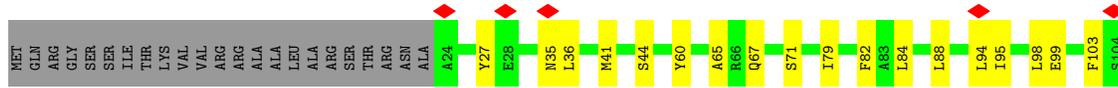
• Molecule 7: subunit c



• Molecule 7: subunit c



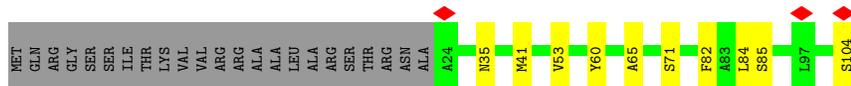
• Molecule 7: subunit c



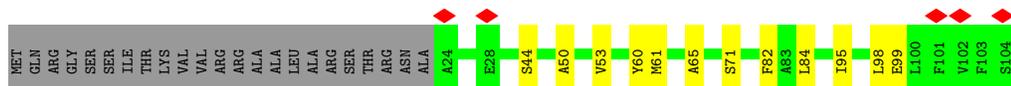
• Molecule 7: subunit c



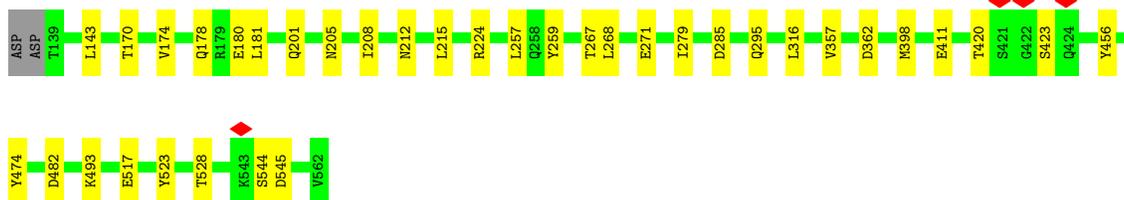
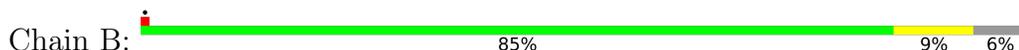
• Molecule 7: subunit c



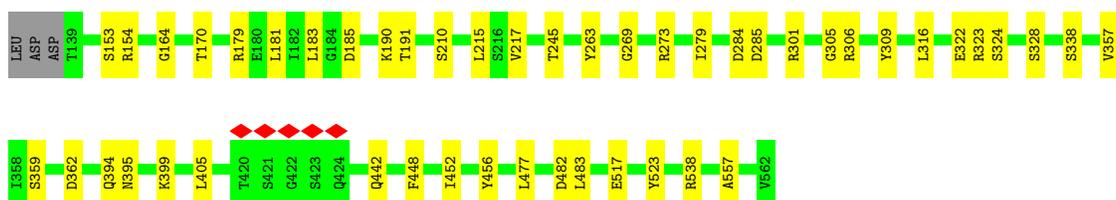
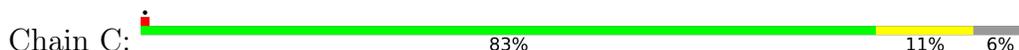
• Molecule 7: subunit c



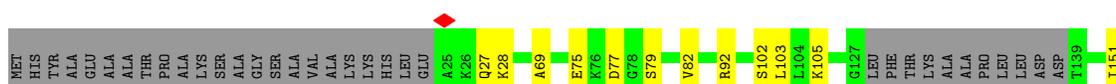
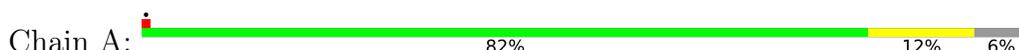
• Molecule 8: subunit alpha

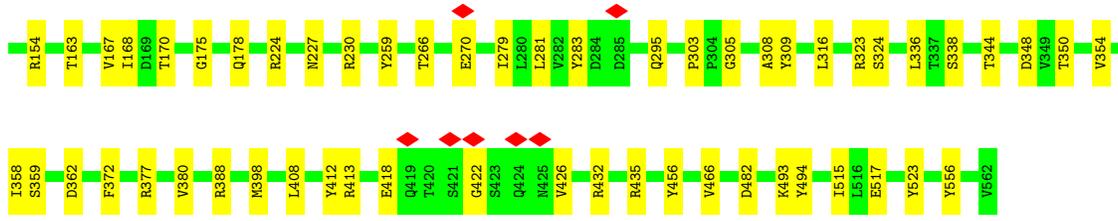


• Molecule 8: subunit alpha

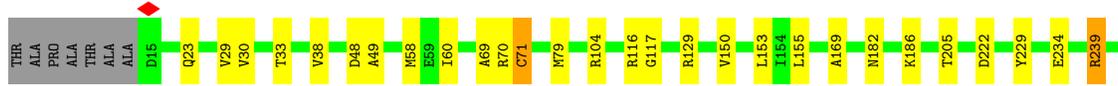
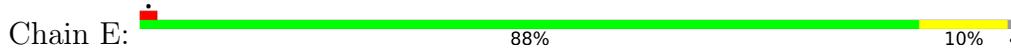


• Molecule 8: subunit alpha





• Molecule 9: subunit beta



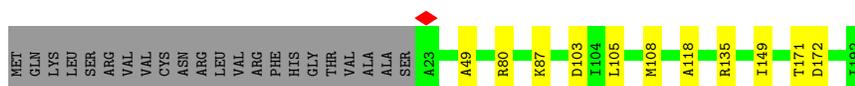
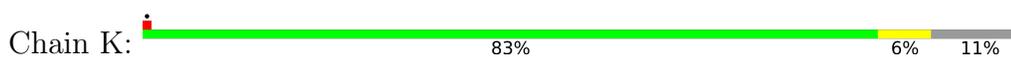
• Molecule 9: subunit beta



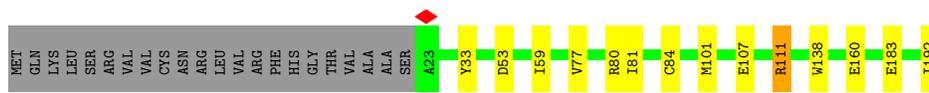
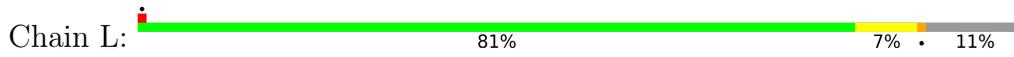
• Molecule 9: subunit beta



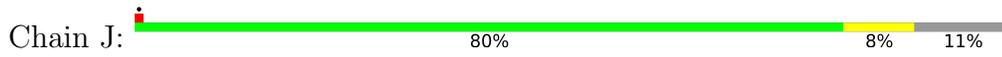
• Molecule 10: p18



• Molecule 10: p18



• Molecule 10: p18



• Molecule 11: inhibitor of F1 (IF1)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122085	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 ($e^-/\text{\AA}^2$)	36.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.246	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TRT, ATP, 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	M	0.44	1/1933 (0.1%)	0.59	2/2623 (0.1%)
2	h	0.43	0/396	0.66	0/535
3	c	0.38	0/427	0.52	0/576
4	G	0.42	0/2476	0.57	1/3337 (0.0%)
5	H	0.39	0/1270	0.55	0/1720
6	I	0.34	0/549	0.51	0/744
7	O	0.35	0/590	0.51	0/802
7	P	0.35	0/590	0.54	0/802
7	Q	0.32	0/590	0.52	0/802
7	R	0.44	0/590	0.55	0/802
7	S	0.38	0/590	0.49	0/802
7	T	0.37	0/590	0.49	0/802
7	U	0.37	0/590	0.49	0/802
7	V	0.36	0/590	0.48	0/802
7	W	0.34	0/590	0.51	0/802
7	X	0.34	0/590	0.50	0/802
8	A	0.50	0/4169	0.56	0/5642
8	B	0.46	0/4164	0.55	1/5635 (0.0%)
8	C	0.50	0/4197	0.55	0/5680
9	D	0.49	0/3732	0.54	0/5056
9	E	0.45	1/3732 (0.0%)	0.54	1/5056 (0.0%)
9	F	0.45	0/3732	0.54	0/5056
10	J	0.40	0/1328	0.47	0/1792
10	K	0.36	0/1328	0.44	0/1792
10	L	0.44	0/1328	0.57	3/1792 (0.2%)
11	N	0.31	0/408	0.49	0/547
All	All	0.44	2/41069 (0.0%)	0.54	8/55603 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	136	GLU	CG-CD	-6.14	1.42	1.51
9	E	71	CYS	CB-SG	-5.33	1.73	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	111	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	M	42	LEU	CA-CB-CG	6.97	131.33	115.30
4	G	49	LEU	CA-CB-CG	6.54	130.33	115.30
10	L	111	ARG	NE-CZ-NH1	-6.49	117.05	120.30
10	L	111	ARG	CD-NE-CZ	6.27	132.38	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1893	1885	1885	16	0
2	h	390	400	400	0	0
3	c	421	436	436	0	0
4	G	2436	2462	2462	41	0
5	H	1246	1202	1202	16	0
6	I	536	541	541	8	0
7	O	580	605	605	8	0
7	P	580	605	605	6	0
7	Q	580	605	605	8	0
7	R	580	605	605	15	0
7	S	580	605	605	13	0
7	T	580	605	605	10	0
7	U	580	605	605	14	0
7	V	580	605	605	12	0
7	W	580	605	605	8	0
7	X	580	605	605	10	0
8	A	4100	4202	4202	45	0
8	B	4095	4197	4197	32	0
8	C	4127	4226	4226	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	3678	3729	3729	35	0
9	E	3678	3729	3729	37	0
9	F	3678	3730	3730	34	0
10	J	1302	1294	1294	12	0
10	K	1302	1294	1294	8	0
10	L	1302	1294	1294	10	0
11	N	403	399	399	3	0
12	A	31	12	12	0	0
12	B	31	12	12	0	0
12	C	31	12	12	0	0
12	D	31	12	12	1	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
14	E	27	12	12	0	0
15	F	25	36	36	2	0
All	All	40568	41166	41166	358	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 358 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)
4:G:213:GLY:O	7:Q:66:ARG:NH2	2.16	0.79
10:J:59:ILE:HD11	10:J:77:VAL:HG21	1.63	0.78
4:G:296:LYS:NZ	8:A:77:ASP:OD2	2.17	0.77
8:A:435:ARG:NH2	8:A:466:VAL:O	2.18	0.76
4:G:53:ARG:NH2	5:H:31:PHE:O	2.20	0.75

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	241/267 (90%)	233 (97%)	8 (3%)	0	100	100
2	h	46/476 (10%)	45 (98%)	1 (2%)	0	100	100
3	c	46/169 (27%)	46 (100%)	0	0	100	100
4	G	301/306 (98%)	293 (97%)	8 (3%)	0	100	100
5	H	158/176 (90%)	149 (94%)	9 (6%)	0	100	100
6	I	64/76 (84%)	61 (95%)	3 (5%)	0	100	100
7	O	79/104 (76%)	79 (100%)	0	0	100	100
7	P	79/104 (76%)	76 (96%)	3 (4%)	0	100	100
7	Q	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
7	R	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
7	S	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
7	T	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
7	U	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
7	V	79/104 (76%)	74 (94%)	5 (6%)	0	100	100
7	W	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
7	X	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
8	A	523/561 (93%)	497 (95%)	26 (5%)	0	100	100
8	B	522/561 (93%)	495 (95%)	27 (5%)	0	100	100
8	C	526/561 (94%)	508 (97%)	18 (3%)	0	100	100
9	D	485/494 (98%)	467 (96%)	18 (4%)	0	100	100
9	E	485/494 (98%)	465 (96%)	20 (4%)	0	100	100
9	F	485/494 (98%)	465 (96%)	20 (4%)	0	100	100
10	J	168/192 (88%)	165 (98%)	3 (2%)	0	100	100
10	K	168/192 (88%)	163 (97%)	5 (3%)	0	100	100
10	L	168/192 (88%)	167 (99%)	1 (1%)	0	100	100
11	N	47/103 (46%)	45 (96%)	2 (4%)	0	100	100
All	All	5223/6354 (82%)	5035 (96%)	188 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	202/221 (91%)	202 (100%)	0	100	100
2	h	43/414 (10%)	43 (100%)	0	100	100
3	c	48/137 (35%)	48 (100%)	0	100	100
4	G	261/264 (99%)	261 (100%)	0	100	100
5	H	131/146 (90%)	131 (100%)	0	100	100
6	I	58/66 (88%)	58 (100%)	0	100	100
7	O	58/76 (76%)	58 (100%)	0	100	100
7	P	58/76 (76%)	58 (100%)	0	100	100
7	Q	58/76 (76%)	58 (100%)	0	100	100
7	R	58/76 (76%)	58 (100%)	0	100	100
7	S	58/76 (76%)	58 (100%)	0	100	100
7	T	58/76 (76%)	58 (100%)	0	100	100
7	U	58/76 (76%)	58 (100%)	0	100	100
7	V	58/76 (76%)	58 (100%)	0	100	100
7	W	58/76 (76%)	58 (100%)	0	100	100
7	X	58/76 (76%)	58 (100%)	0	100	100
8	A	450/474 (95%)	450 (100%)	0	100	100
8	B	450/474 (95%)	450 (100%)	0	100	100
8	C	453/474 (96%)	453 (100%)	0	100	100
9	D	397/400 (99%)	397 (100%)	0	100	100
9	E	397/400 (99%)	397 (100%)	0	100	100
9	F	397/400 (99%)	397 (100%)	0	100	100
10	J	132/151 (87%)	132 (100%)	0	100	100
10	K	132/151 (87%)	132 (100%)	0	100	100
10	L	132/151 (87%)	132 (100%)	0	100	100
11	N	44/87 (51%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4307/5170 (83%)	4307 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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
12	ATP	D	601	13	26,33,33	0.95	1 (3%)	31,52,52	1.57	5 (16%)
12	ATP	A	601	13	26,33,33	0.87	0	31,52,52	1.45	5 (16%)
12	ATP	B	601	13	26,33,33	0.87	0	31,52,52	1.46	4 (12%)
14	ADP	E	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.50	4 (13%)
15	TRT	F	600	-	25,25,25	0.65	0	33,33,33	0.90	1 (3%)
12	ATP	C	601	13	26,33,33	0.85	0	31,52,52	1.52	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ATP	D	601	13	-	1/18/38/38	0/3/3/3
12	ATP	A	601	13	-	2/18/38/38	0/3/3/3
12	ATP	B	601	13	-	0/18/38/38	0/3/3/3
14	ADP	E	601	-	-	1/12/32/32	0/3/3/3
15	TRT	F	600	-	-	3/23/23/23	0/1/1/1
12	ATP	C	601	13	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	601	ATP	C2'-C1'	-2.47	1.50	1.53
14	E	601	ADP	C5-C4	2.11	1.46	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	601	ATP	N3-C2-N1	-3.94	122.51	128.68
14	E	601	ADP	N3-C2-N1	-3.74	122.83	128.68
12	A	601	ATP	N3-C2-N1	-3.71	122.88	128.68
12	B	601	ATP	N3-C2-N1	-3.67	122.94	128.68
12	C	601	ATP	PB-O3B-PG	-3.67	120.23	132.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	E	601	ADP	C5'-O5'-PA-O1A
15	F	600	TRT	O15-C16-C17-O18
15	F	600	TRT	C1-C5-C6-C9
15	F	600	TRT	O21-C22-C23-O24
12	C	601	ATP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

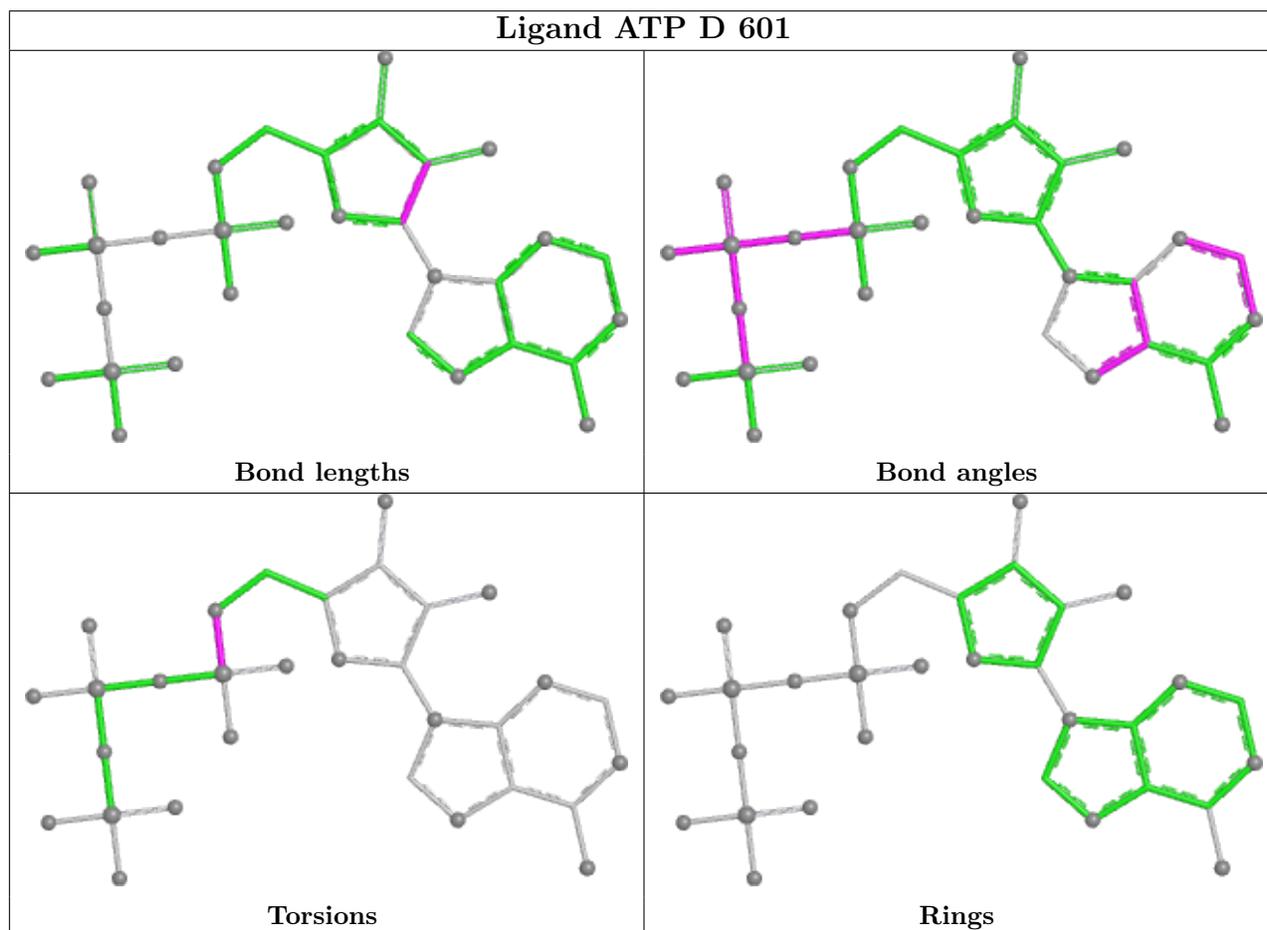
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	601	ATP	1	0

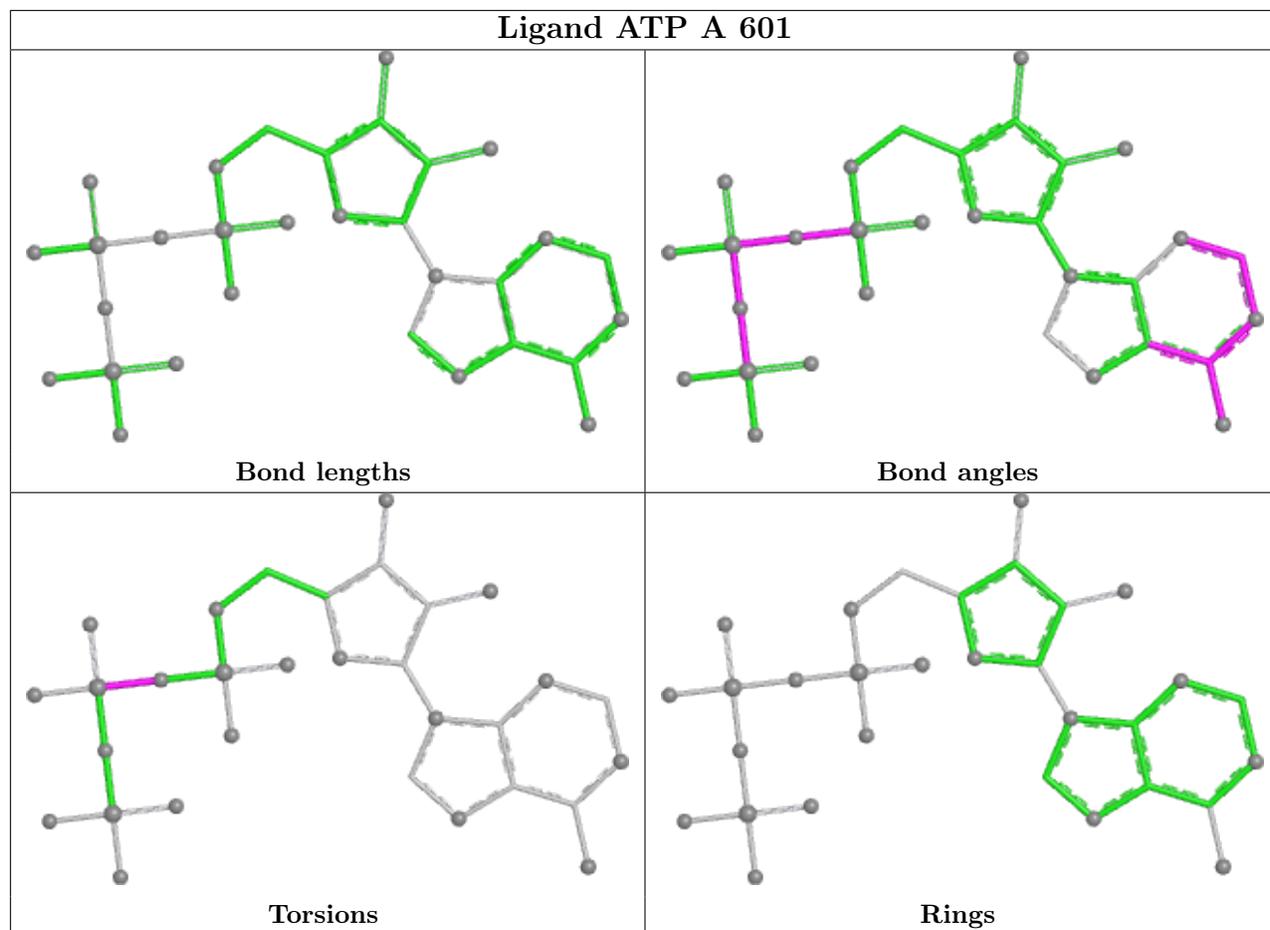
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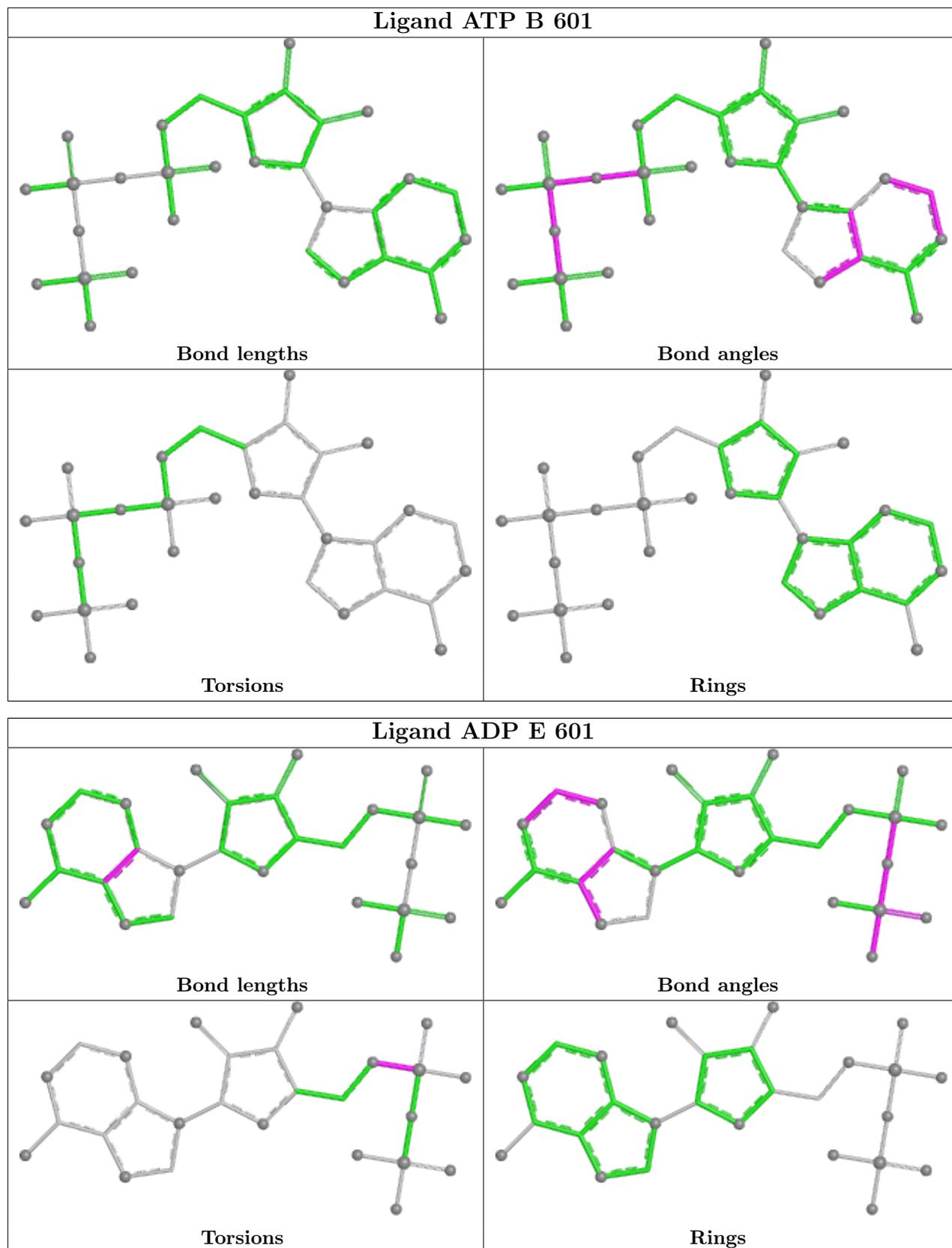
Continued from previous page...

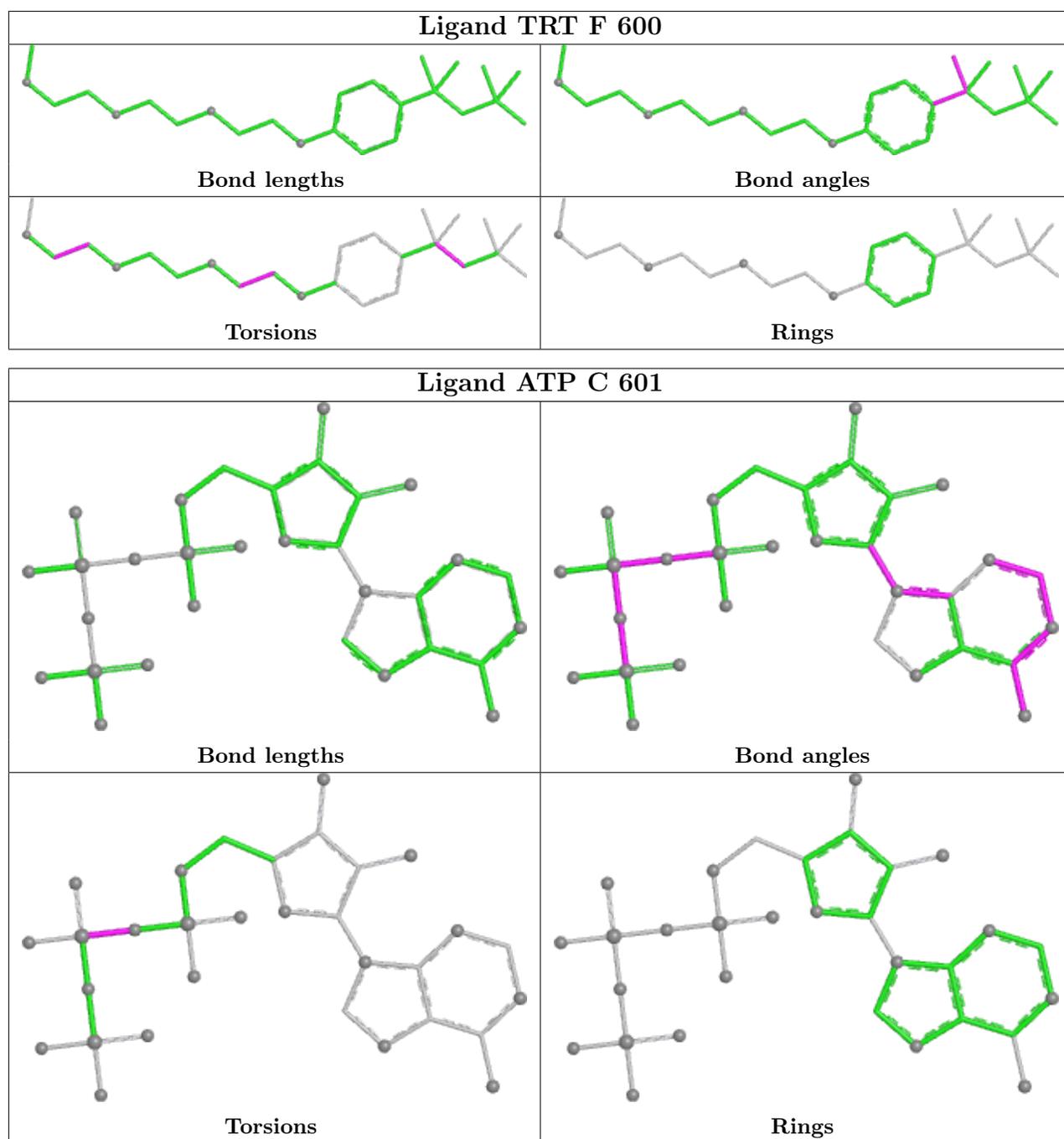
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	600	TRT	2	0

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.

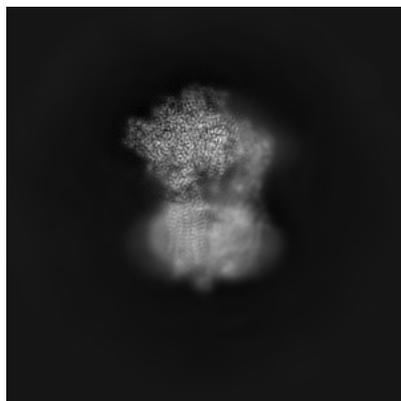
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10472. These allow visual inspection of the internal detail of the map and identification of artifacts.

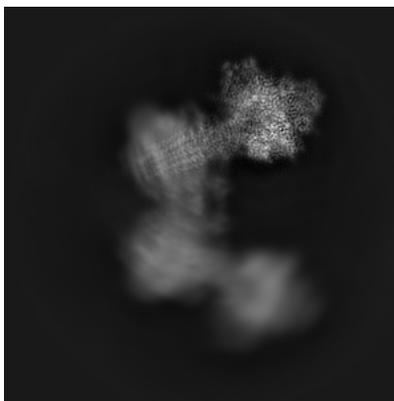
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

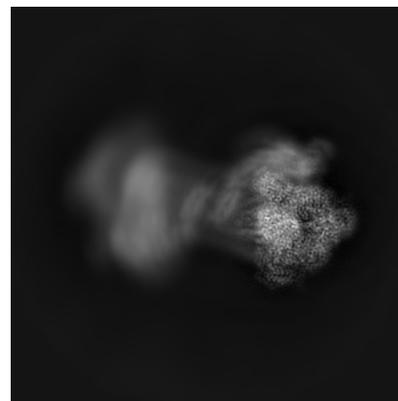
6.1.1 Primary map



X

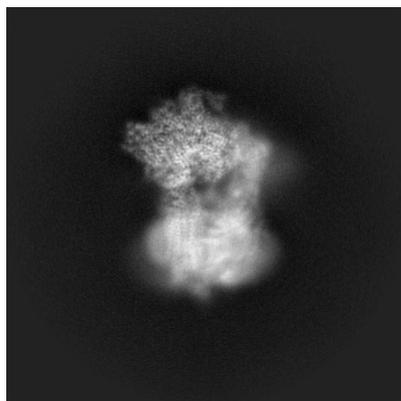


Y

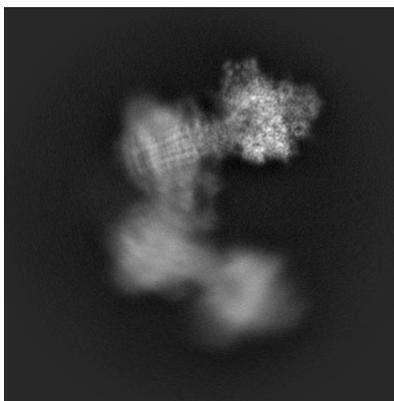


Z

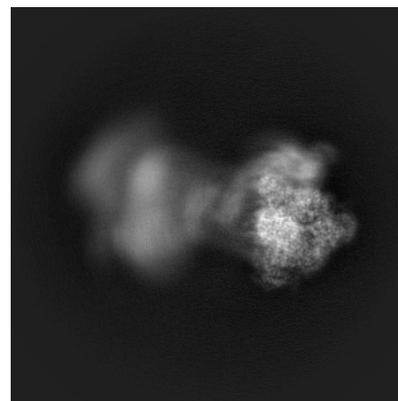
6.1.2 Raw map



X



Y

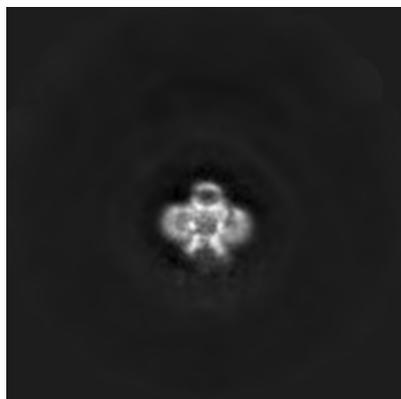


Z

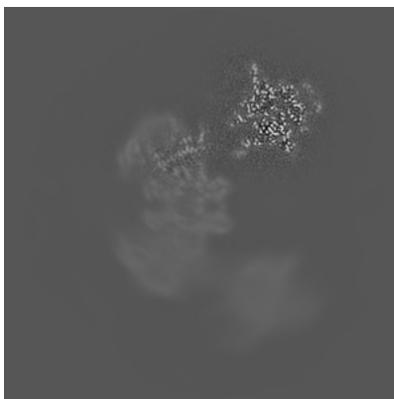
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

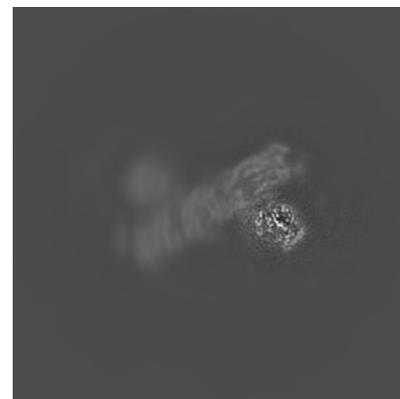
6.2.1 Primary map



X Index: 220

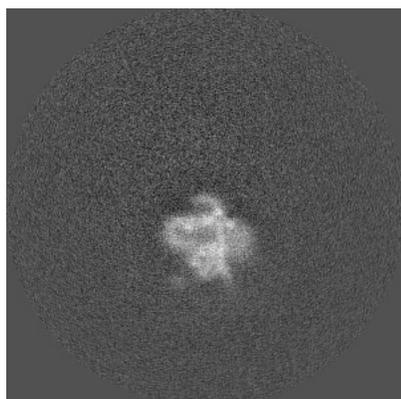


Y Index: 220

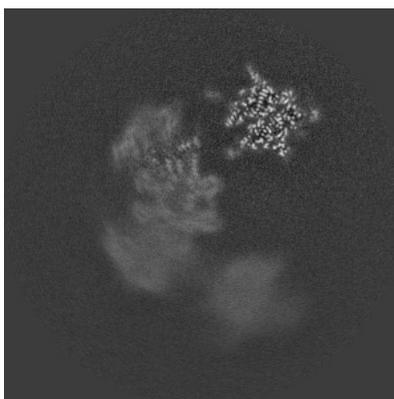


Z Index: 220

6.2.2 Raw map



X Index: 220



Y Index: 220

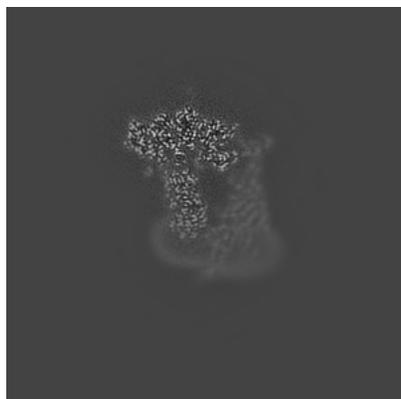


Z Index: 220

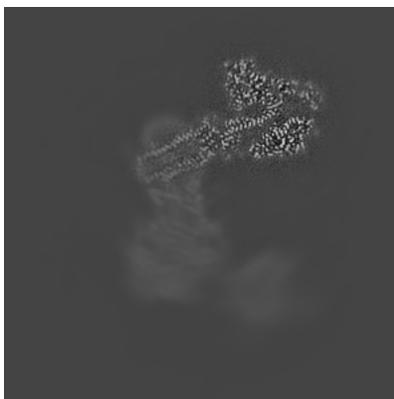
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

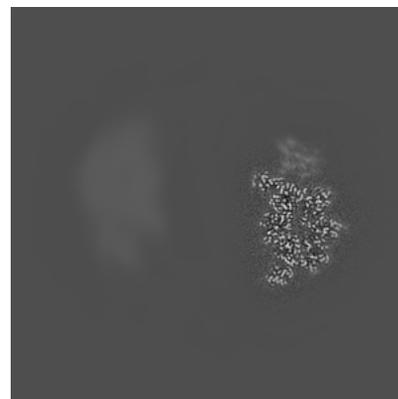
6.3.1 Primary map



X Index: 295

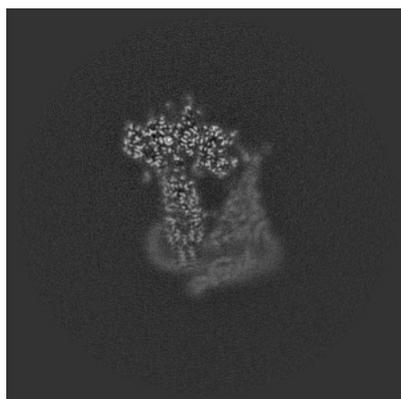


Y Index: 201

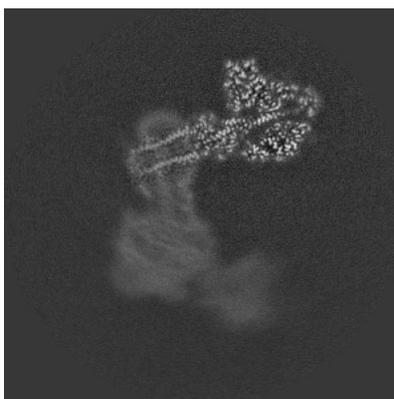


Z Index: 296

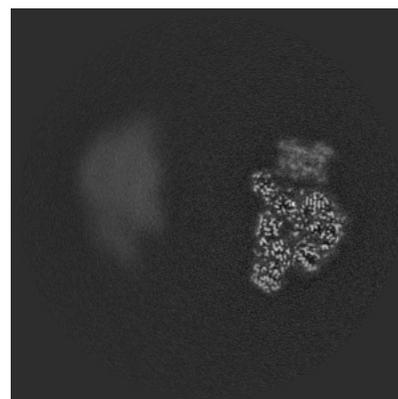
6.3.2 Raw map



X Index: 295



Y Index: 197

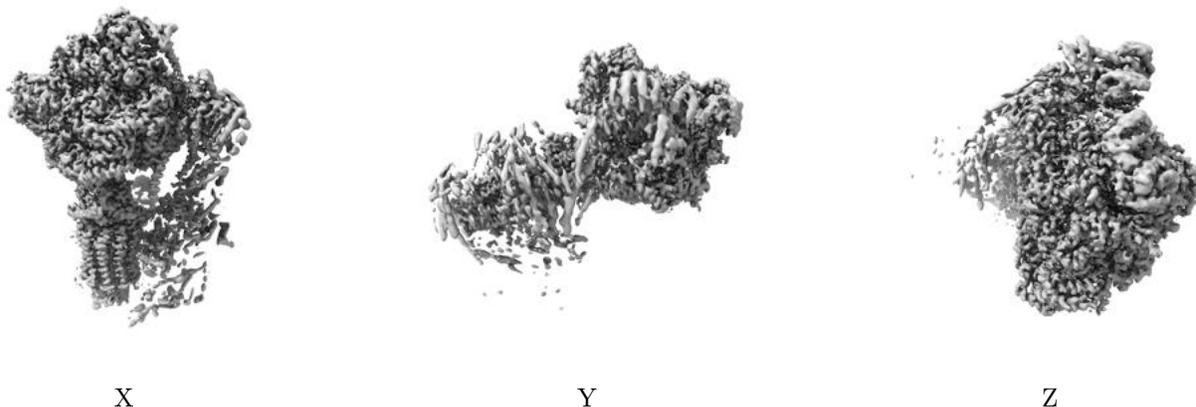


Z Index: 284

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

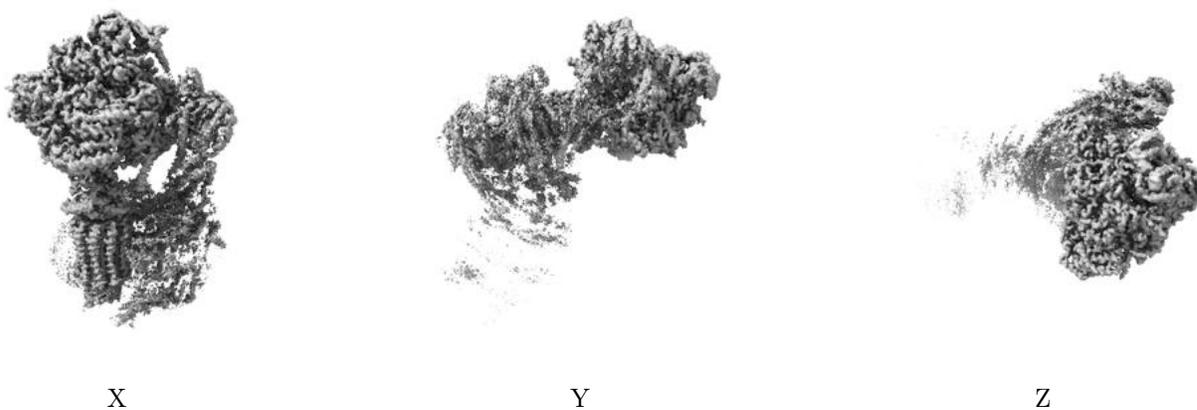
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

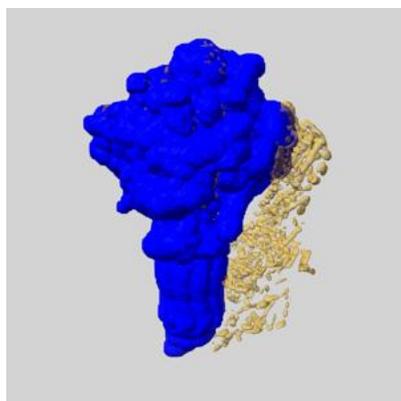
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

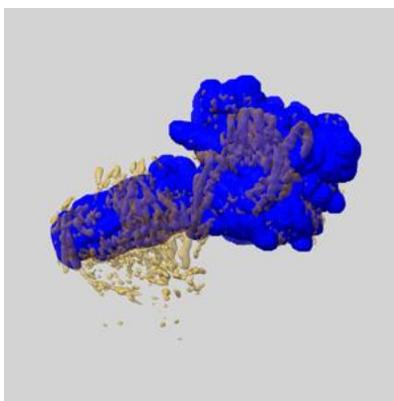
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

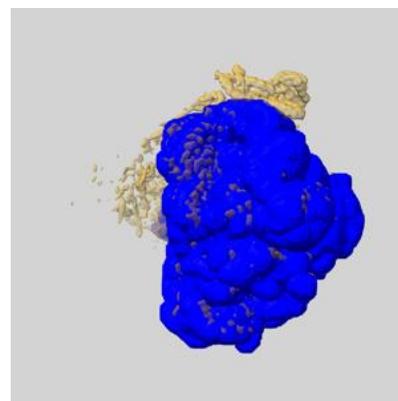
6.5.1 emd_10472_msk_1.map [i](#)



X



Y

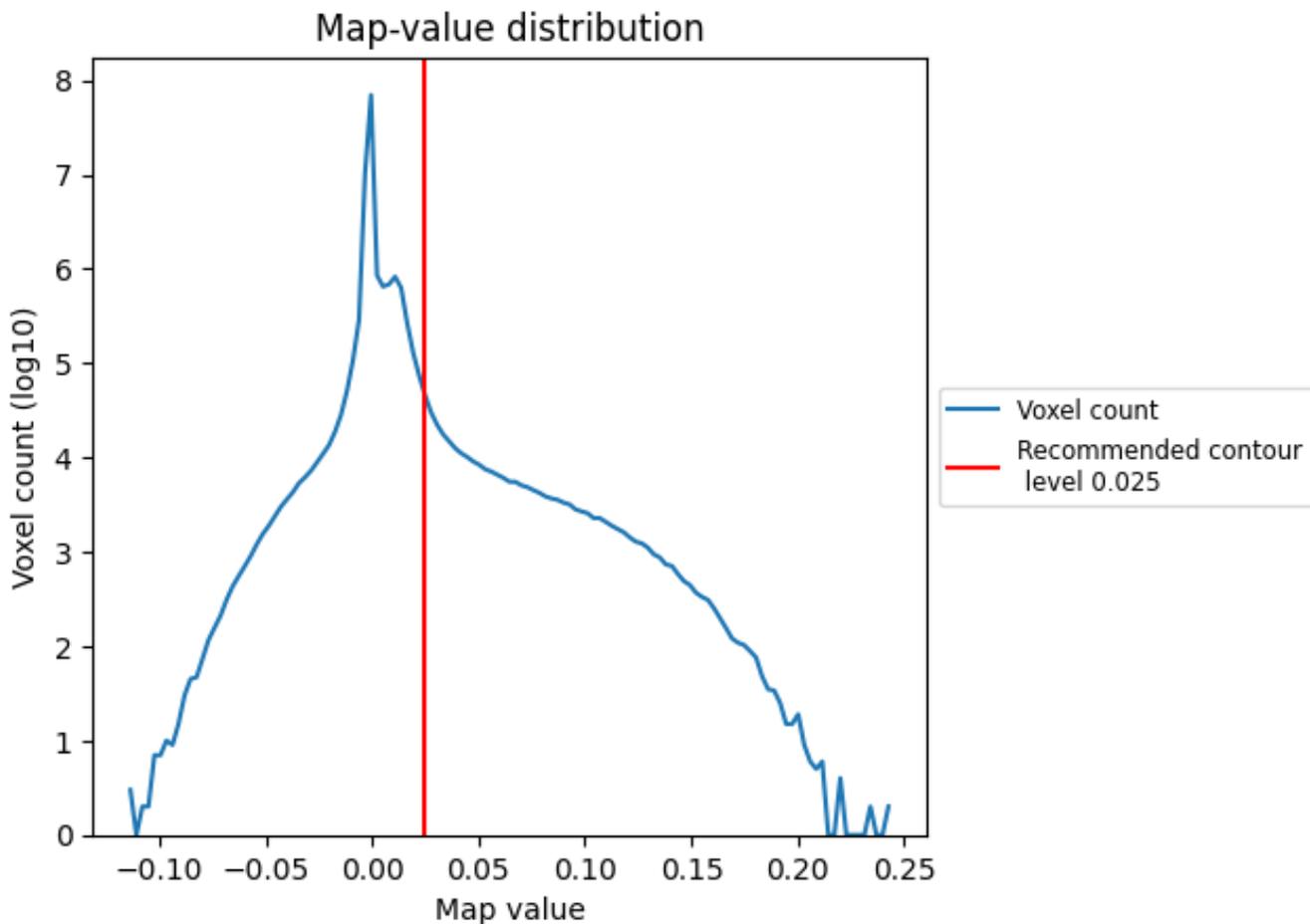


Z

7 Map analysis [i](#)

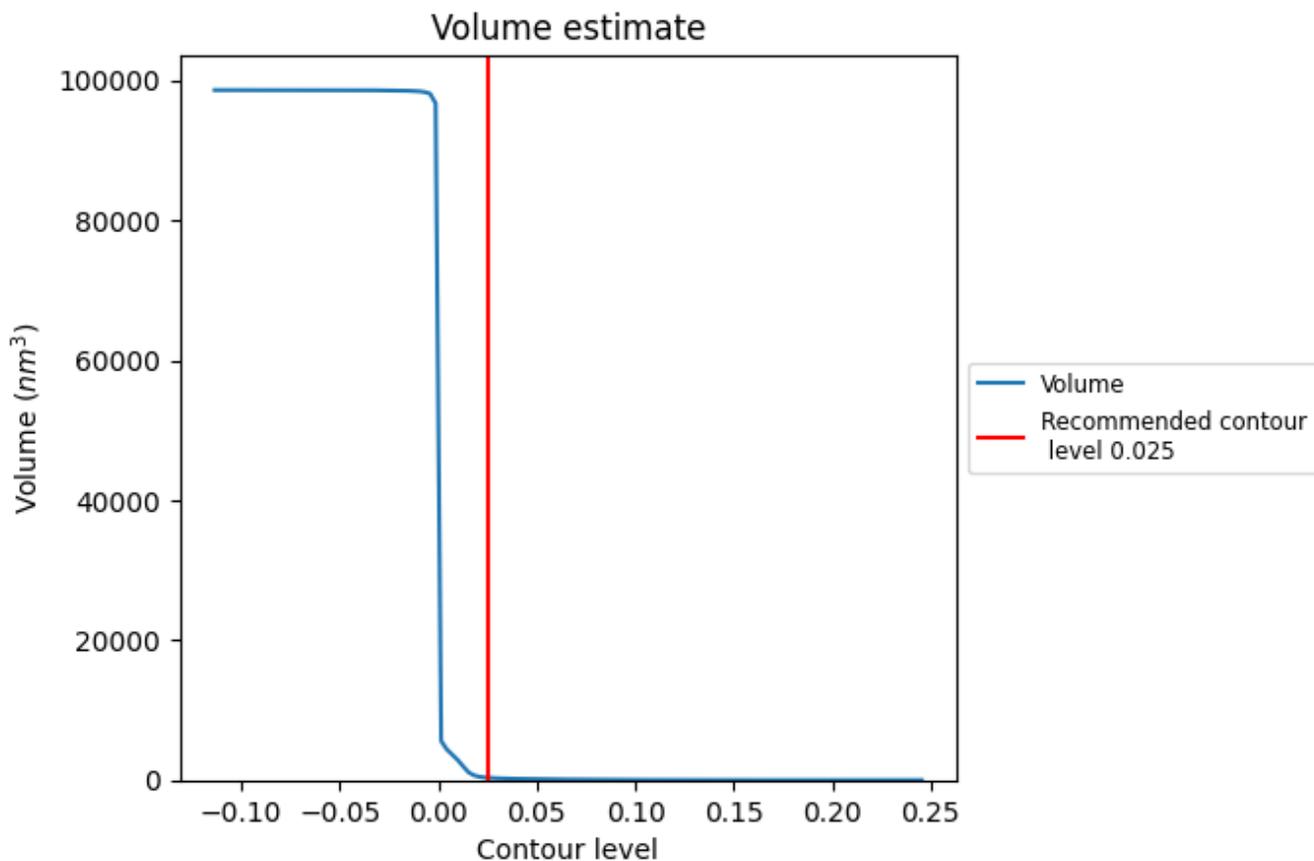
This section contains the results of statistical analysis of the map.

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.

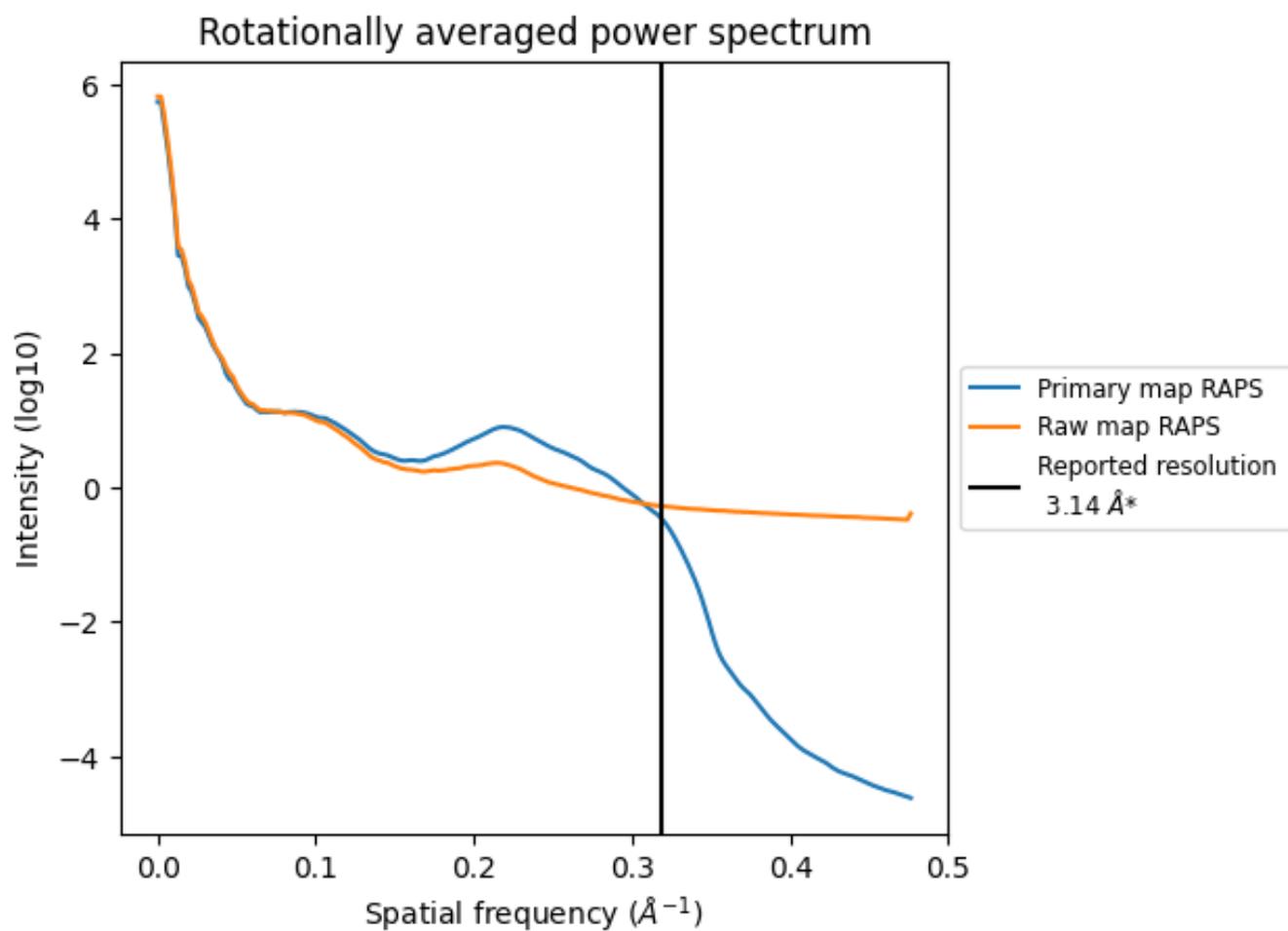
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 337 nm^3 ; this corresponds to an approximate mass of 305 kDa.

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

7.3 Rotationally averaged power spectrum i

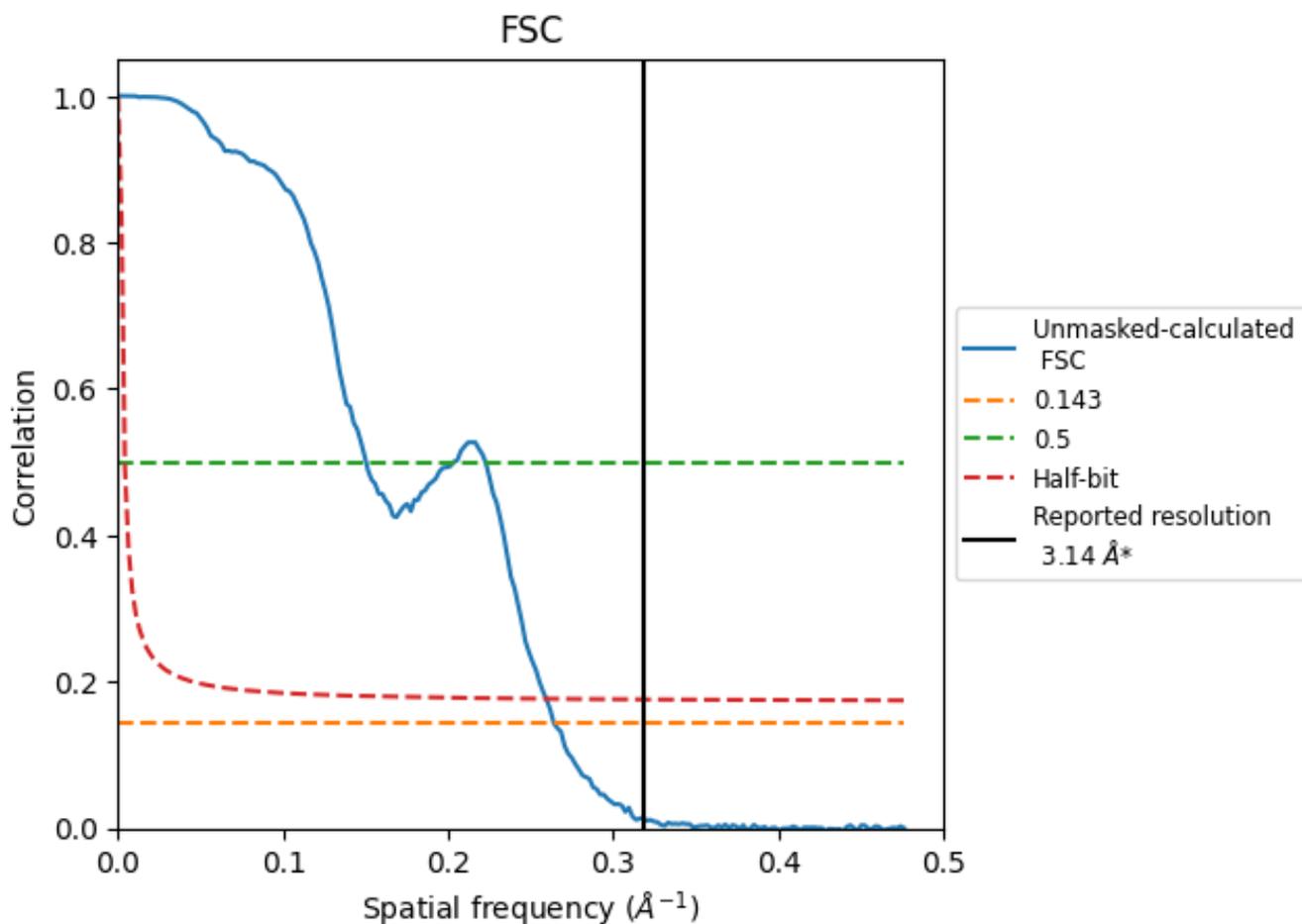


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

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 0.318 Å⁻¹

8.2 Resolution estimates [i](#)

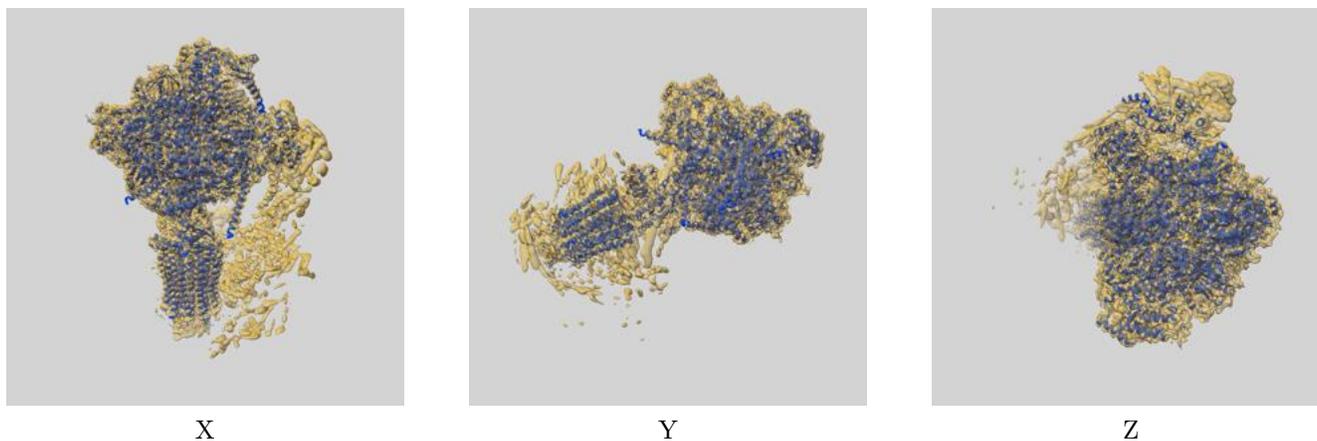
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.79	6.65	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

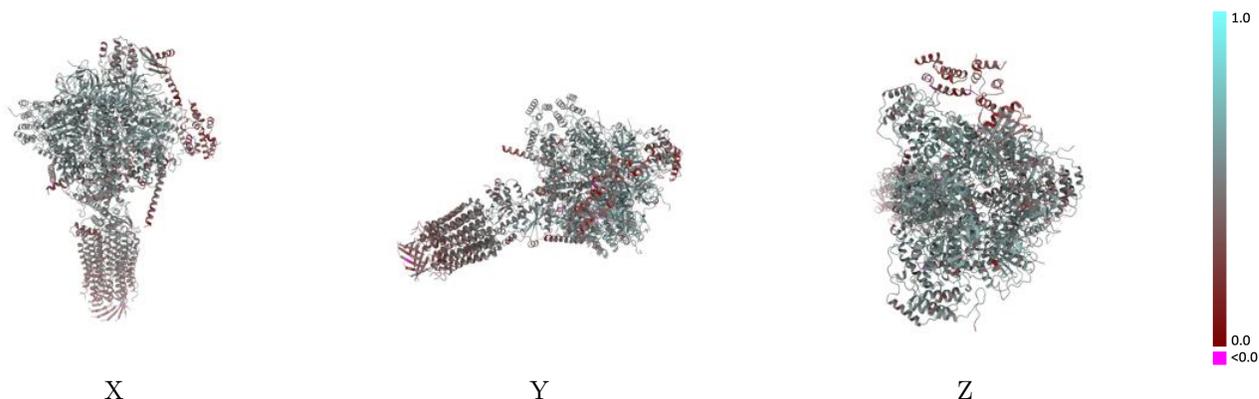
This section contains information regarding the fit between EMDB map EMD-10472 and PDB model 6TDZ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



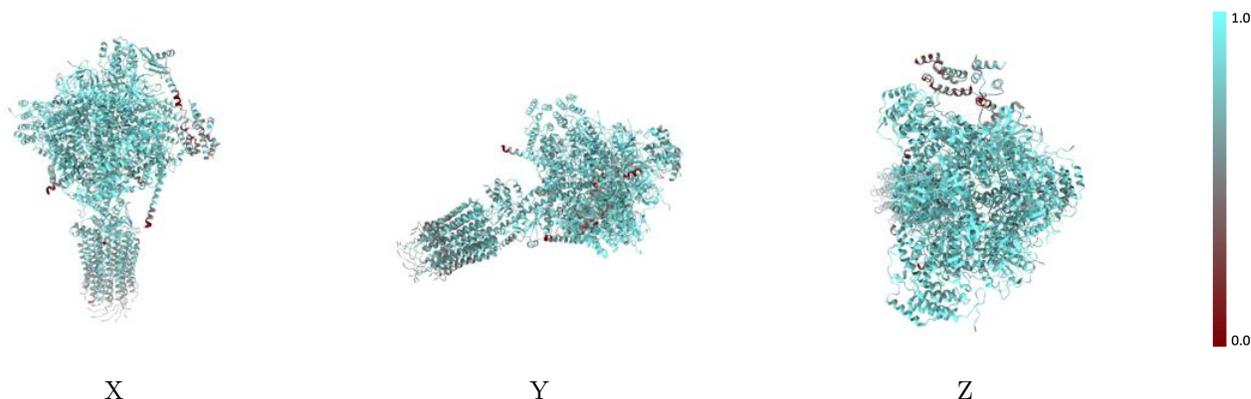
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



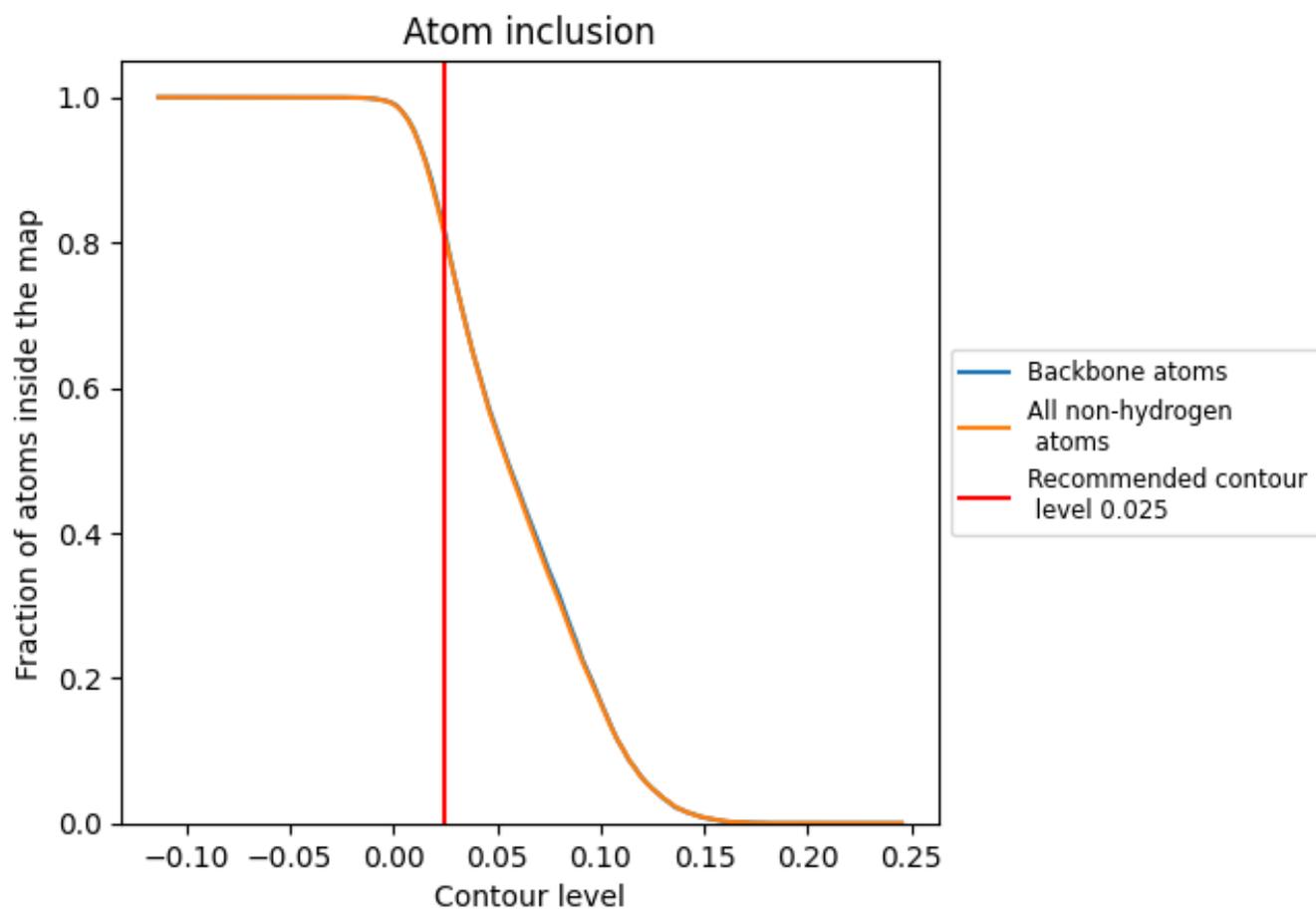
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8059	 0.4820
A	 0.8717	 0.5300
B	 0.8590	 0.5150
C	 0.8723	 0.5350
D	 0.8691	 0.5330
E	 0.8410	 0.5110
F	 0.8466	 0.5140
G	 0.8068	 0.4860
H	 0.7628	 0.4440
I	 0.8199	 0.4750
J	 0.8480	 0.4990
K	 0.8309	 0.4760
L	 0.8441	 0.4980
M	 0.6933	 0.3660
N	 0.6234	 0.4220
O	 0.6748	 0.3800
P	 0.6348	 0.3760
Q	 0.6261	 0.3810
R	 0.6452	 0.3920
S	 0.6557	 0.3890
T	 0.6609	 0.3920
U	 0.6748	 0.3870
V	 0.6678	 0.3940
W	 0.6487	 0.3850
X	 0.6626	 0.3880
c	 0.6350	 0.3100
h	 0.5026	 0.2550

