wwPDB EM Validation Summary Report

May 19, 2024 – 02:12 am BST

PDB ID	:	6TDY
EMDB ID	:	EMD-10471
Title	:	Cryo-EM structure of Euglena gracilis mitochondrial ATP synthase, OSCP/F1/c-ring in rotational state 1
Authors	:	Muhleip, A.; Amunts, A.
Deposited on	:	2019-11-10
Resolution	:	3.04 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

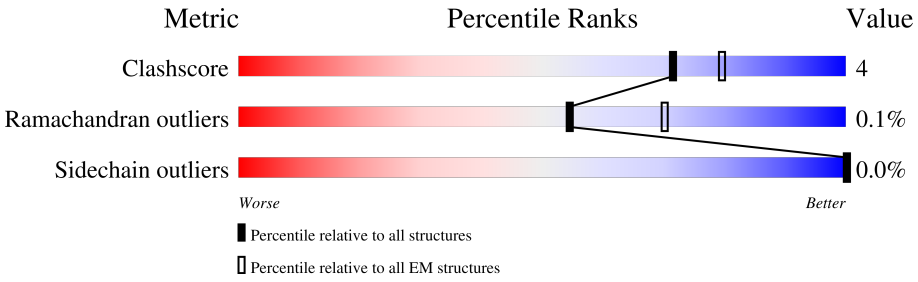
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.04 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 <=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	561	86% 8% 6%
1	B	561	85% 9% 6%
1	C	561	83% 11% 6%
2	D	494	89% 9%
2	E	494	91% 7%
2	F	494	88% 10%
3	G	306	90% 9%
4	H	176	9% 84% 7% 9%

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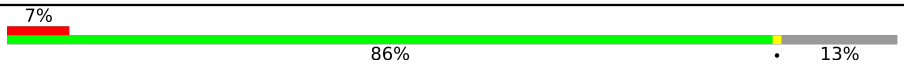
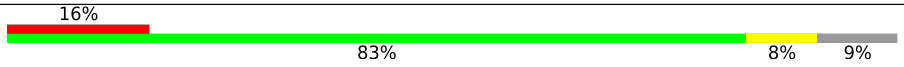
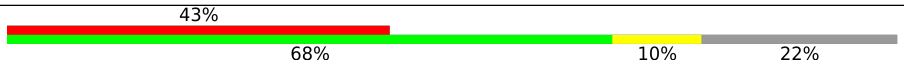
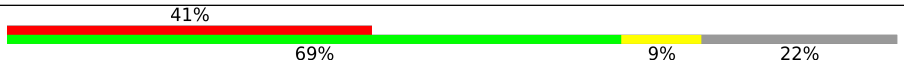
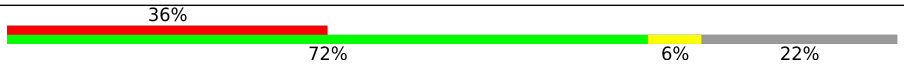
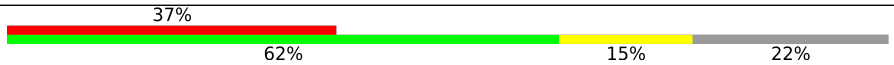
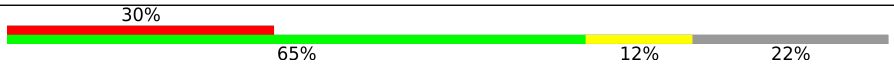
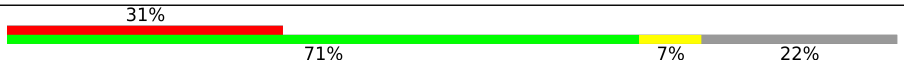
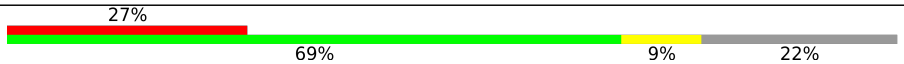
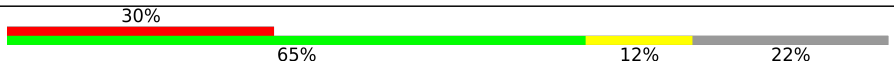
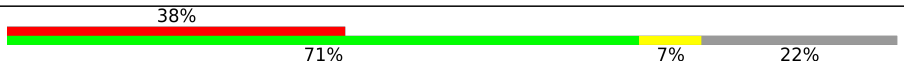
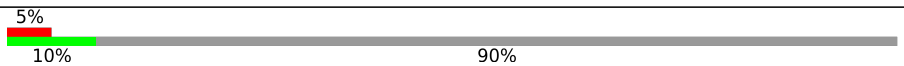
Mol	Chain	Length	Quality of chain
5	I	76	
6	J	192	
6	K	192	
6	L	192	
7	M	267	
8	N	103	
9	O	104	
9	P	104	
9	Q	104	
9	R	104	
9	S	104	
9	T	104	
9	U	104	
9	V	104	
9	W	104	
9	X	104	
10	h	476	
11	c	169	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 81811 atoms, of which 41207 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	526	Total	C	H	N	O	S	0	0
			8292	2611	4197	700	766	18		
1	B	526	Total	C	H	N	O	S	0	0
			8292	2611	4197	700	766	18		
1	C	529	Total	C	H	N	O	S	0	0
			8336	2625	4219	703	771	18		

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called p18.

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

- Molecule 7 is a protein called oligomycin sensitivity conferring protein (OSCP).

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

- Molecule 8 is a protein called inhibitor of F1 (IF1).

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

- Molecule 9 is a protein called ATP synthase subunit c.

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

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	V	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
9	W	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
9	X	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		

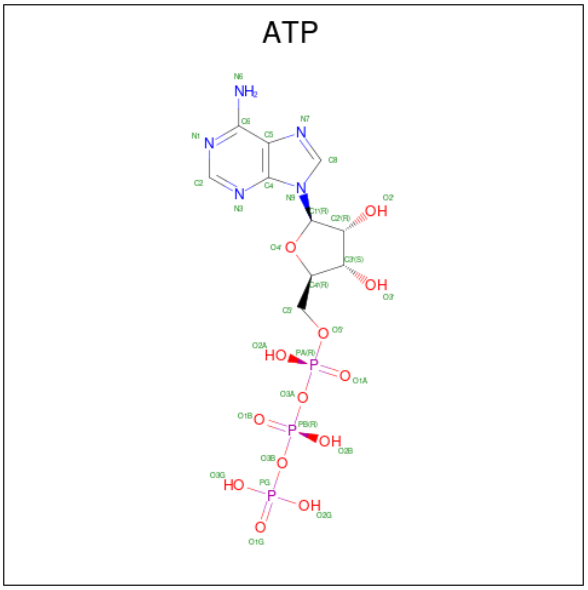
- Molecule 10 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	h	49	Total	C	H	N	O	S	0	0
			807	255	408	67	76	1		

- Molecule 11 is a protein called ATPTB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	c	57	Total	C	H	N	O	S	0	0
			944	300	481	78	83	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
12	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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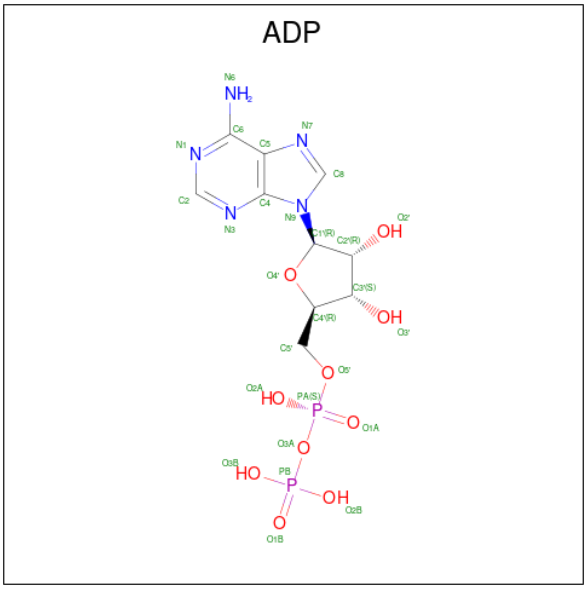
Mol	Chain	Residues	Atoms						AltConf
12	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
12	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
12	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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

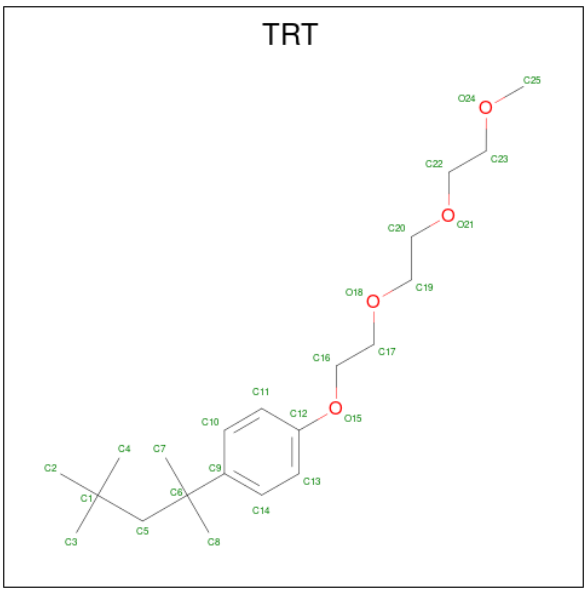
Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Mg	0
			1	1	
13	B	1	Total	Mg	0
			1	1	
13	C	1	Total	Mg	0
			1	1	
13	D	1	Total	Mg	0
			1	1	
13	F	1	Total	Mg	0
			1	1	

- 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
14	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 15 is FRAGMENT OF TRITON X-100 (three-letter code: TRT) (formula: $C_{21}H_{36}O_4$).



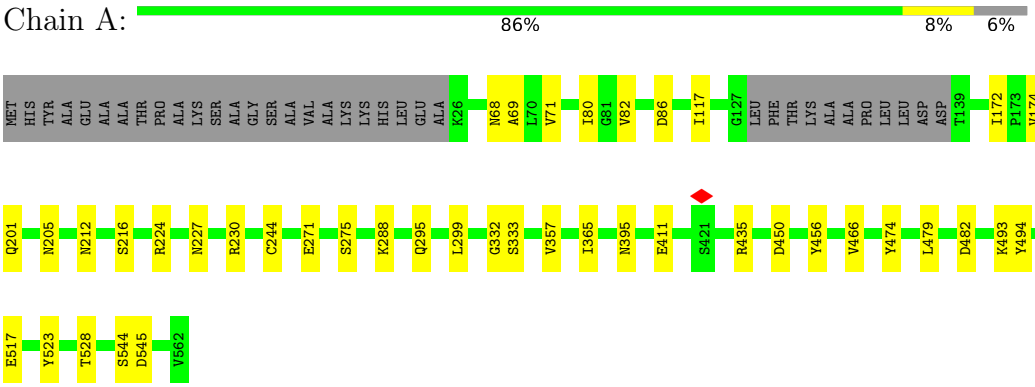
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
15	E	1	61	21	36	4	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

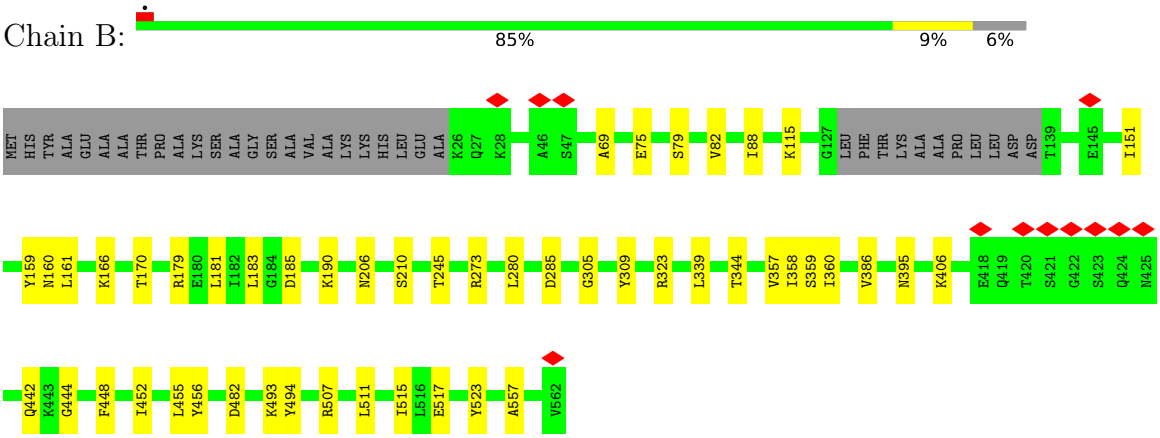
• Molecule 1: ATP synthase subunit alpha

Chain A:



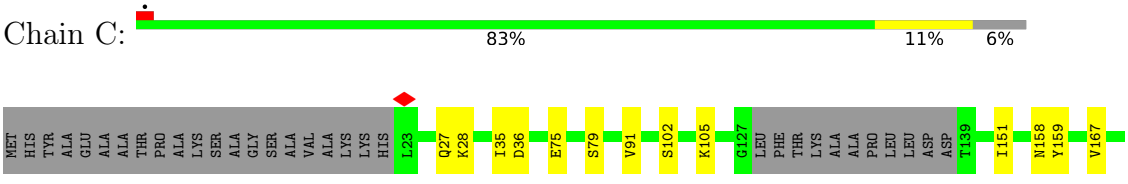
• Molecule 1: ATP synthase subunit alpha

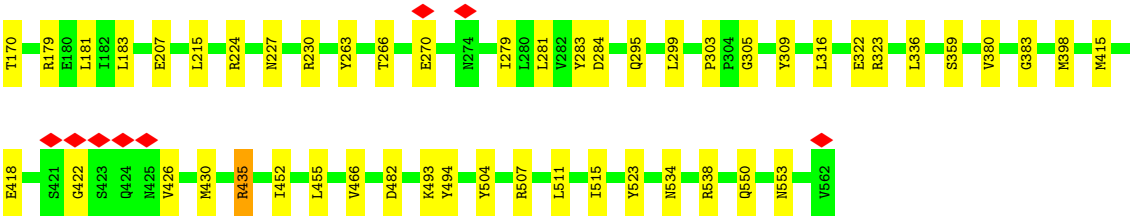
Chain B:



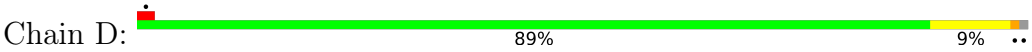
• Molecule 1: ATP synthase subunit alpha

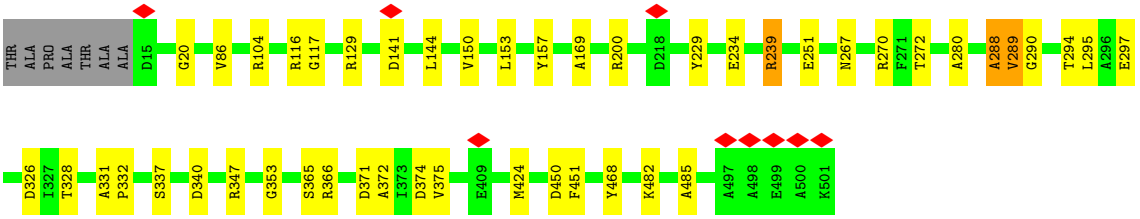
Chain C:



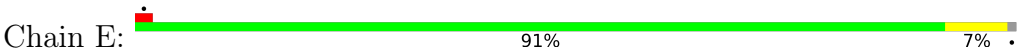


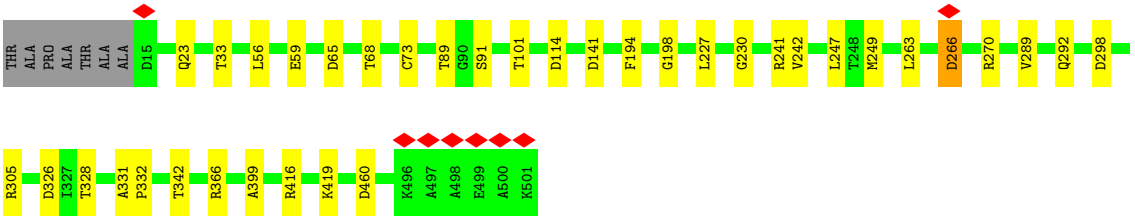
• Molecule 2: ATP synthase subunit beta



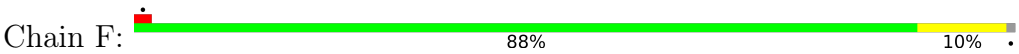


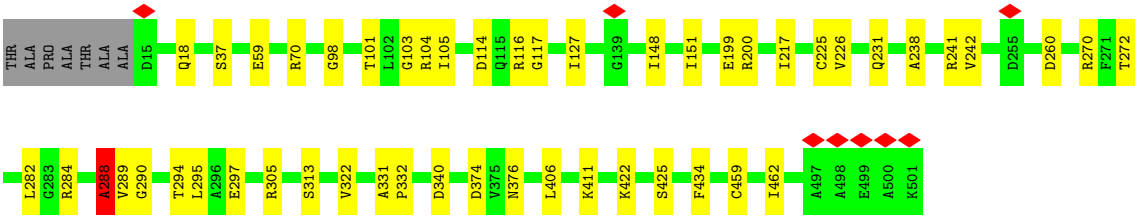
• Molecule 2: ATP synthase subunit beta



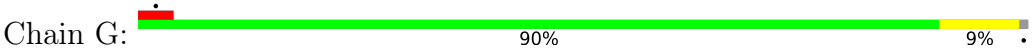


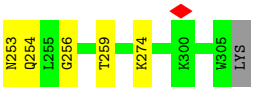
• Molecule 2: ATP synthase subunit beta





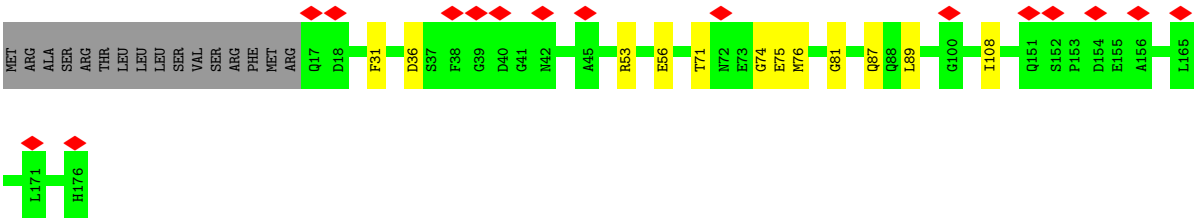
• Molecule 3: ATP synthase subunit gamma





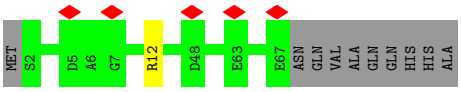
• Molecule 4: ATP synthase subunit delta

Chain H:



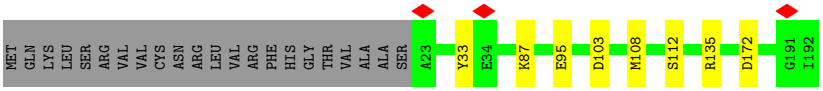
• Molecule 5: ATP synthase subunit epsilon

Chain I:



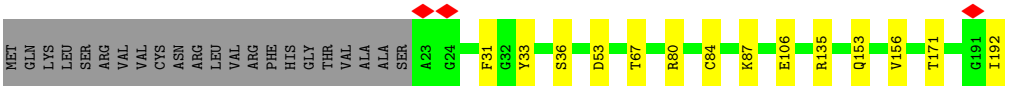
• Molecule 6: p18

Chain J:



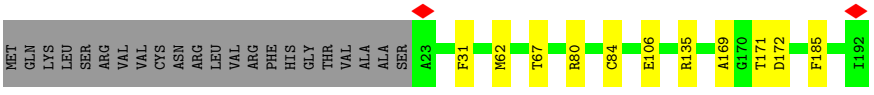
• Molecule 6: p18

Chain K:



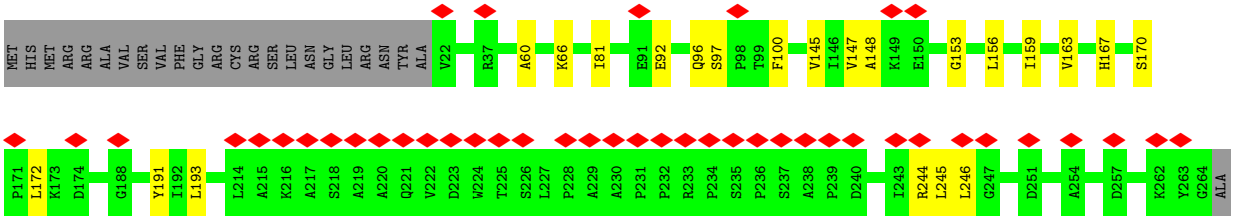
• Molecule 6: p18

Chain L:

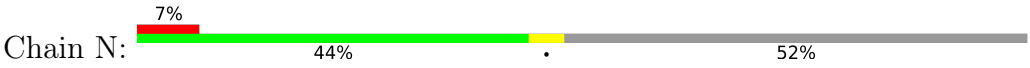


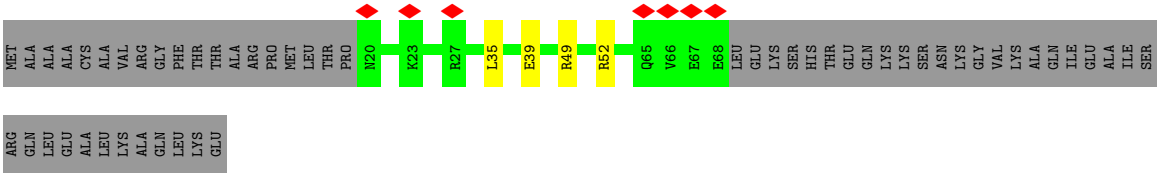
• Molecule 7: oligomycin sensitivity conferring protein (OSCP)

Chain M:

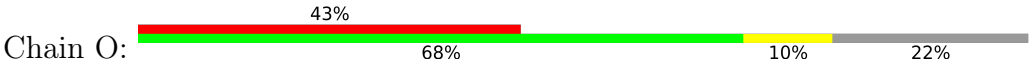


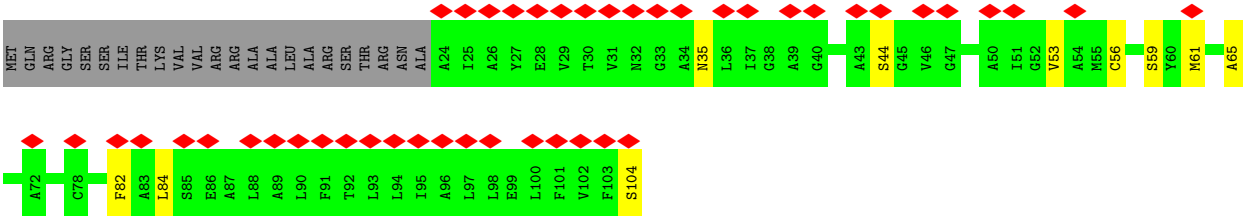
• Molecule 8: inhibitor of F1 (IF1)



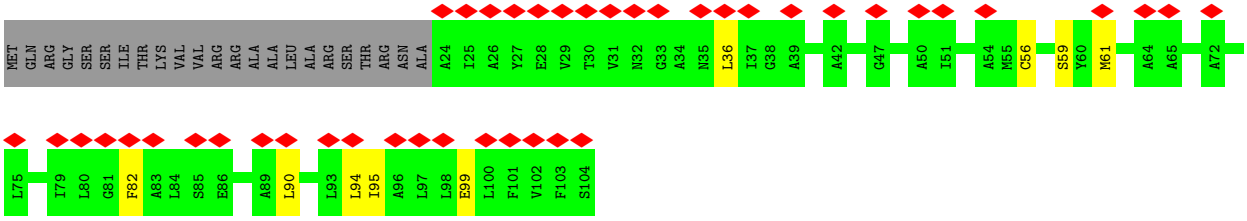


• Molecule 9: ATP synthase subunit c

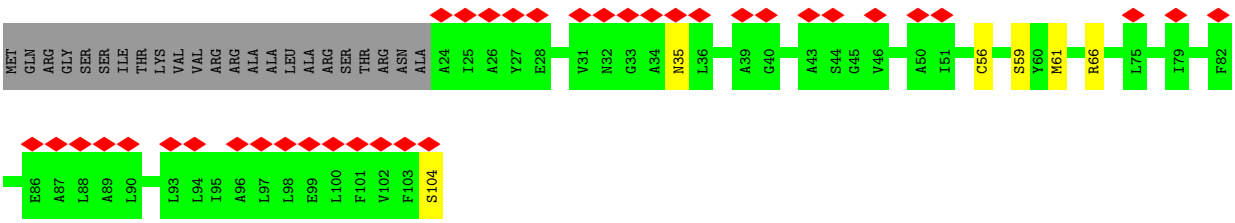




• Molecule 9: ATP synthase subunit c

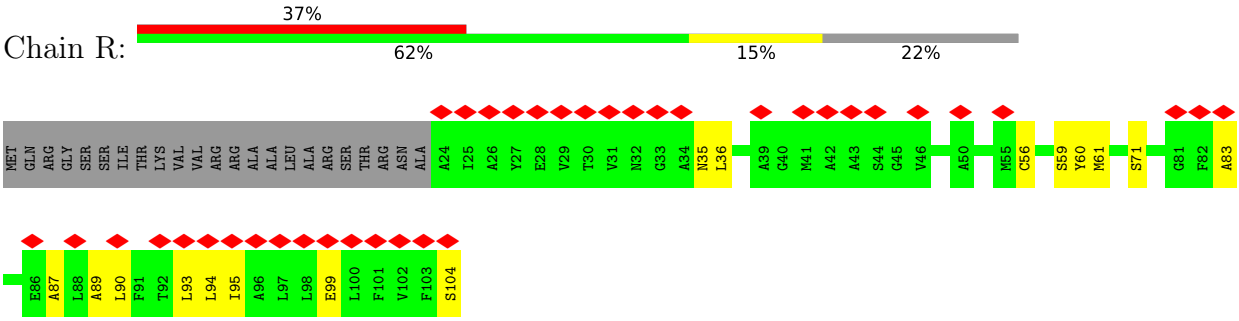


• Molecule 9: ATP synthase subunit c



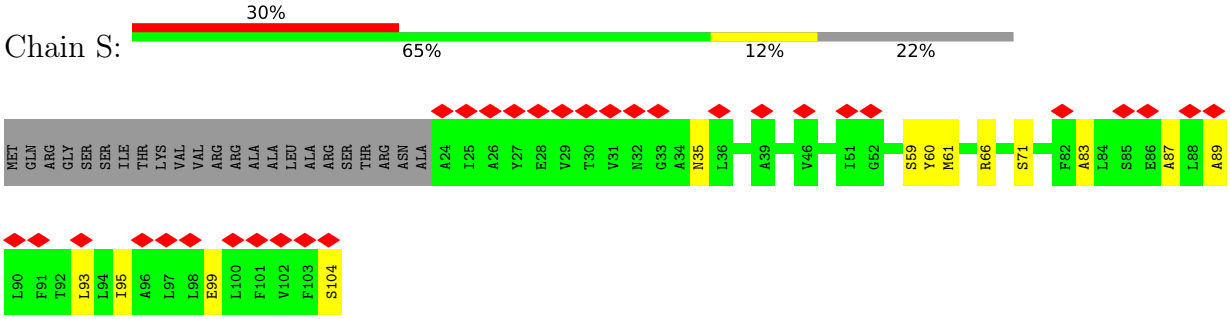
• Molecule 9: ATP synthase subunit c

Chain R:



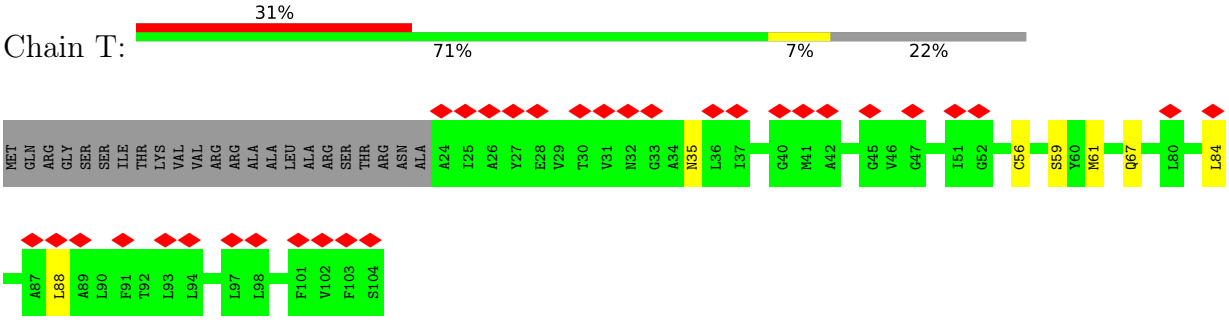
• Molecule 9: ATP synthase subunit c

Chain S:



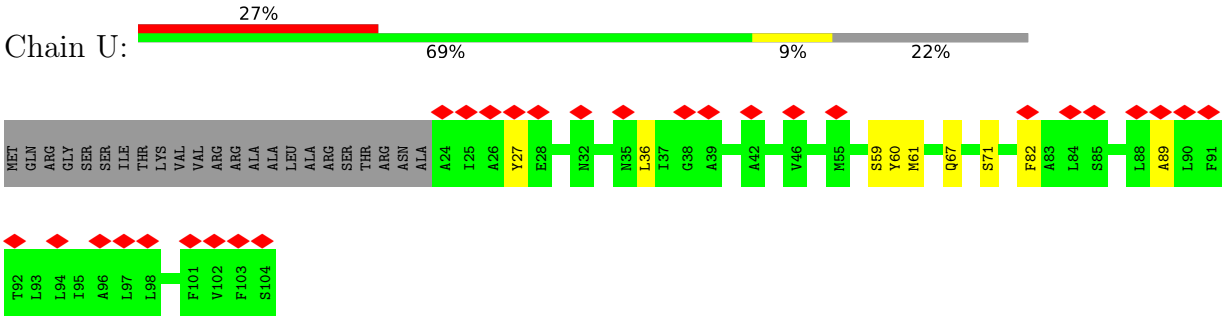
• Molecule 9: ATP synthase subunit c

Chain T:



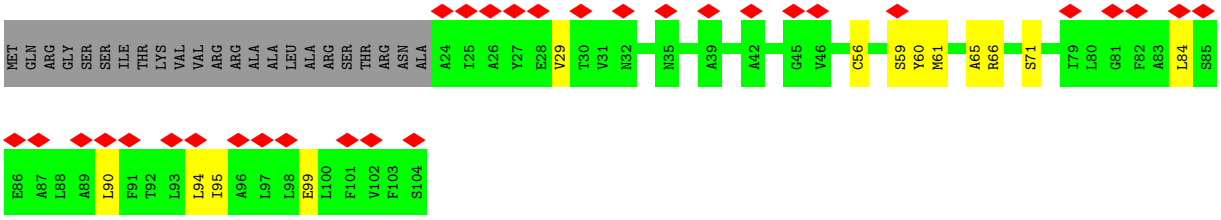
• Molecule 9: ATP synthase subunit c

Chain U:



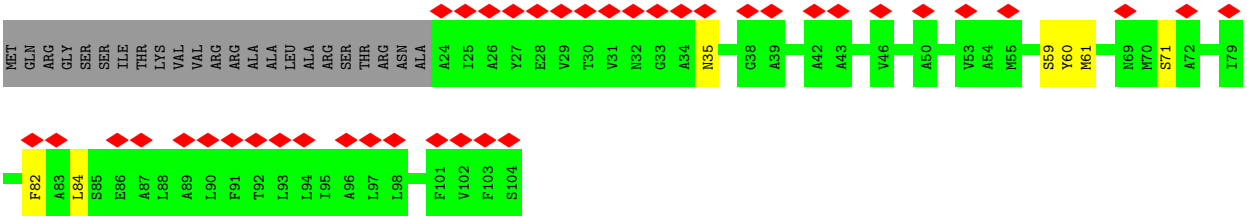
• Molecule 9: ATP synthase subunit c

Chain V:



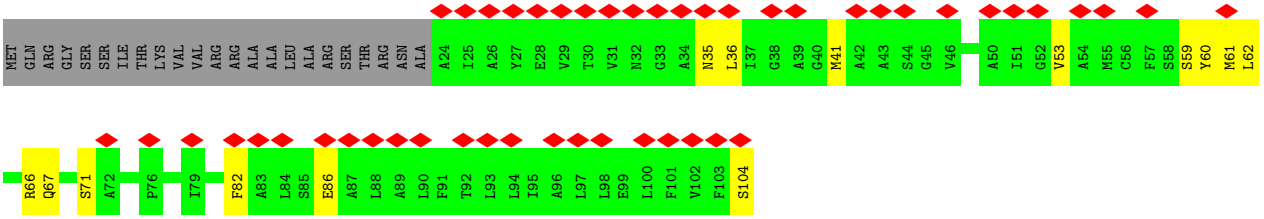
• Molecule 9: ATP synthase subunit c

Chain W:



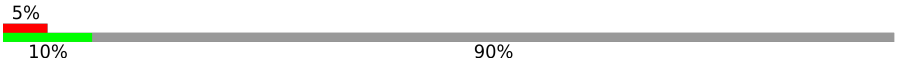
• Molecule 9: ATP synthase subunit c

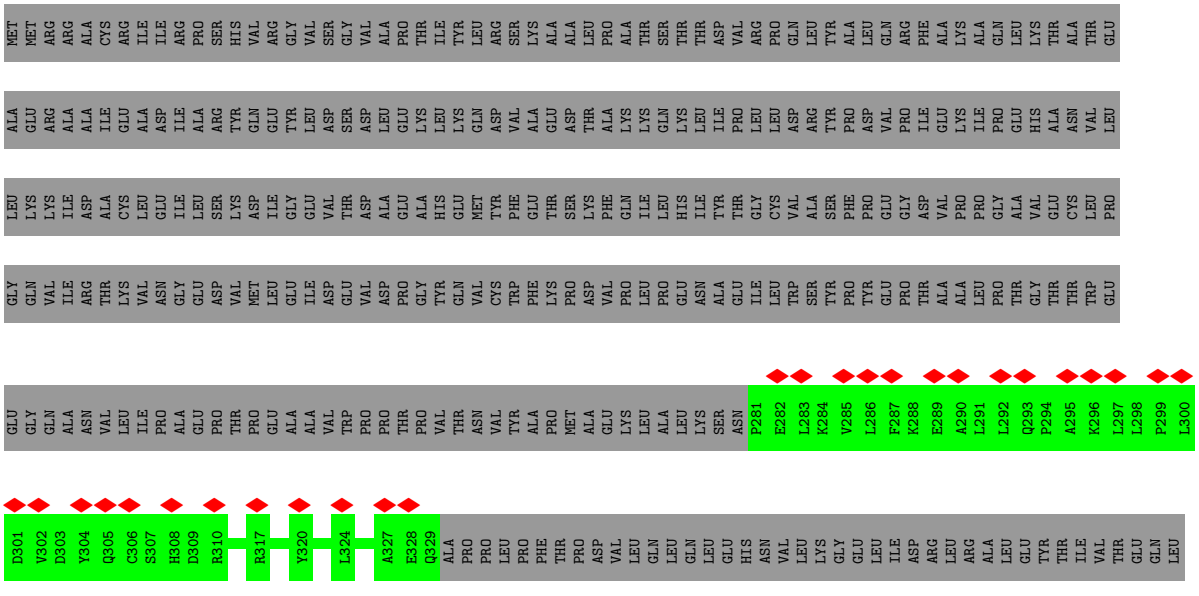
Chain X:

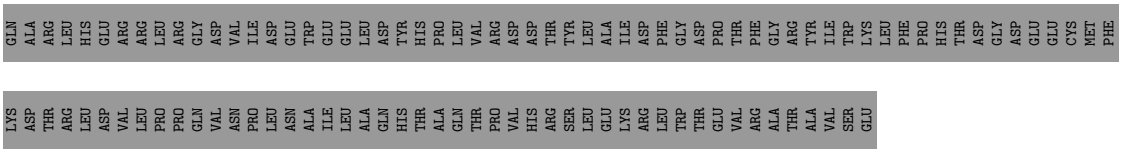


• Molecule 10: ATP synthase subunit d

Chain h:

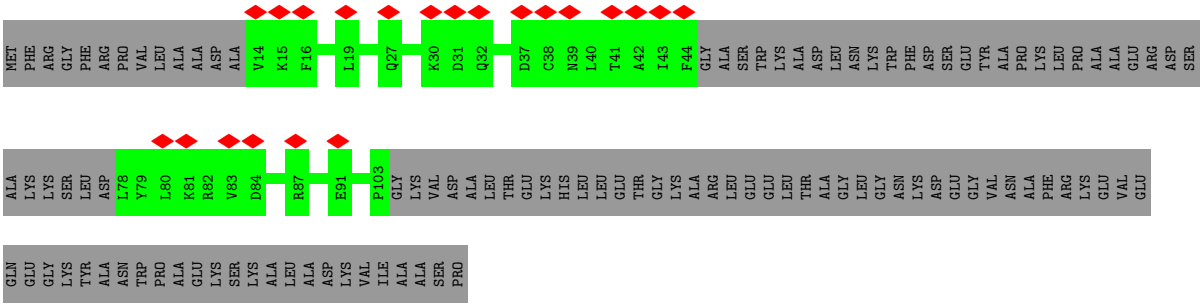






• Molecule 11: ATPTB4

Chain c:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150744	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 ($e^-/Å^2$)	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	0.267	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.001	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, ADP, ATP, TRT

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	0.50	1/4164 (0.0%)	0.57	1/5635 (0.0%)
1	B	0.48	0/4164	0.56	0/5635
1	C	0.52	0/4186	0.60	1/5665 (0.0%)
2	D	0.47	0/3732	0.58	1/5056 (0.0%)
2	E	0.46	0/3732	0.55	0/5056
2	F	0.51	0/3732	0.58	0/5056
3	G	0.41	0/2476	0.54	0/3337
4	H	0.31	0/1270	0.51	0/1720
5	I	0.31	0/549	0.50	0/744
6	J	0.39	0/1328	0.49	0/1792
6	K	0.39	0/1328	0.49	0/1792
6	L	0.41	0/1328	0.51	0/1792
7	M	0.37	0/1933	0.55	0/2623
8	N	0.36	0/408	0.51	0/547
9	O	0.37	0/590	0.53	0/802
9	P	0.32	0/590	0.50	0/802
9	Q	0.31	0/590	0.50	0/802
9	R	0.31	0/590	0.49	0/802
9	S	0.30	0/590	0.46	0/802
9	T	0.36	0/590	0.52	0/802
9	U	0.35	0/590	0.47	0/802
9	V	0.31	0/590	0.47	0/802
9	W	0.33	0/590	0.52	0/802
9	X	0.31	0/590	0.53	0/802
10	h	0.33	0/405	0.56	0/547
11	c	0.38	0/470	0.55	0/635
All	All	0.44	1/41105 (0.0%)	0.55	3/55652 (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
1	C	0	1
2	E	0	1
2	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	ASN	CB-CG	-5.01	1.39	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	ILE	C-N-CA	7.29	139.93	121.70
2	D	239	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	435	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	284	ASP	Peptide
2	E	266	ASP	Peptide
2	F	288	ALA	Peptide

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	A	4095	4197	4197	27	0
1	B	4095	4197	4197	35	0
1	C	4117	4219	4219	43	0
2	D	3678	3729	3729	32	0
2	E	3678	3730	3730	23	0
2	F	3678	3729	3729	33	0
3	G	2436	2462	2462	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1246	1202	1202	8	0
5	I	536	541	541	2	0
6	J	1302	1294	1294	6	0
6	K	1302	1294	1294	11	0
6	L	1302	1294	1294	9	0
7	M	1893	1885	1885	14	0
8	N	403	399	399	4	0
9	O	580	605	605	9	0
9	P	580	605	605	7	0
9	Q	580	605	605	6	0
9	R	580	605	605	10	0
9	S	580	605	605	9	0
9	T	580	605	605	7	0
9	U	580	605	605	8	0
9	V	580	605	605	10	0
9	W	580	605	605	8	0
9	X	580	605	605	11	0
10	h	399	408	408	0	0
11	c	463	481	481	0	0
12	A	31	12	12	0	0
12	B	31	12	12	0	0
12	C	31	12	12	0	0
12	F	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	F	1	0	0	0	0
14	D	27	12	12	0	0
15	E	25	36	36	2	0
All	All	40604	41207	41207	278	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 4.

The worst 5 of 278 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)
7:M:147:VAL:HG12	7:M:191:TYR:HB3	1.58	0.84
9:W:84:LEU:HD22	9:X:53:VAL:HG11	1.60	0.81
1:C:452:ILE:HG21	1:C:511:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ASN:OD1	1:C:230:ARG:NH2	2.17	0.78
1:A:224:ARG:NH2	2:D:340:ASP:OD1	2.17	0.77

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/561 (93%)	499 (96%)	23 (4%)	0	100	100
1	B	522/561 (93%)	493 (94%)	29 (6%)	0	100	100
1	C	525/561 (94%)	497 (95%)	28 (5%)	0	100	100
2	D	485/494 (98%)	460 (95%)	23 (5%)	2 (0%)	34	69
2	E	485/494 (98%)	458 (94%)	26 (5%)	1 (0%)	47	80
2	F	485/494 (98%)	462 (95%)	21 (4%)	2 (0%)	34	69
3	G	301/306 (98%)	294 (98%)	7 (2%)	0	100	100
4	H	158/176 (90%)	148 (94%)	10 (6%)	0	100	100
5	I	64/76 (84%)	59 (92%)	5 (8%)	0	100	100
6	J	168/192 (88%)	164 (98%)	4 (2%)	0	100	100
6	K	168/192 (88%)	167 (99%)	1 (1%)	0	100	100
6	L	168/192 (88%)	165 (98%)	3 (2%)	0	100	100
7	M	241/267 (90%)	231 (96%)	9 (4%)	1 (0%)	34	69
8	N	47/103 (46%)	46 (98%)	1 (2%)	0	100	100
9	O	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
9	P	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
9	Q	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
9	R	79/104 (76%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	S	79/104 (76%)	76 (96%)	3 (4%)	0	100	100
9	T	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
9	U	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
9	V	79/104 (76%)	76 (96%)	3 (4%)	0	100	100
9	W	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
9	X	79/104 (76%)	76 (96%)	3 (4%)	0	100	100
10	h	47/476 (10%)	46 (98%)	1 (2%)	0	100	100
11	c	53/169 (31%)	53 (100%)	0	0	100	100
All	All	5229/6354 (82%)	5014 (96%)	209 (4%)	6 (0%)	54	84

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	289	VAL
2	F	289	VAL
2	D	288	ALA
2	F	288	ALA
7	M	148	ALA

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	A	450/474 (95%)	450 (100%)	0	100	100
1	B	450/474 (95%)	450 (100%)	0	100	100
1	C	452/474 (95%)	452 (100%)	0	100	100
2	D	397/400 (99%)	397 (100%)	0	100	100
2	E	397/400 (99%)	397 (100%)	0	100	100
2	F	397/400 (99%)	397 (100%)	0	100	100
3	G	261/264 (99%)	260 (100%)	1 (0%)	91	96
4	H	131/146 (90%)	131 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	58/66 (88%)	58 (100%)	0	100	100
6	J	132/151 (87%)	132 (100%)	0	100	100
6	K	132/151 (87%)	132 (100%)	0	100	100
6	L	132/151 (87%)	132 (100%)	0	100	100
7	M	202/221 (91%)	202 (100%)	0	100	100
8	N	44/87 (51%)	44 (100%)	0	100	100
9	O	58/76 (76%)	58 (100%)	0	100	100
9	P	58/76 (76%)	58 (100%)	0	100	100
9	Q	58/76 (76%)	58 (100%)	0	100	100
9	R	58/76 (76%)	58 (100%)	0	100	100
9	S	58/76 (76%)	58 (100%)	0	100	100
9	T	58/76 (76%)	58 (100%)	0	100	100
9	U	58/76 (76%)	58 (100%)	0	100	100
9	V	58/76 (76%)	58 (100%)	0	100	100
9	W	58/76 (76%)	58 (100%)	0	100	100
9	X	58/76 (76%)	58 (100%)	0	100	100
10	h	44/414 (11%)	44 (100%)	0	100	100
11	c	52/137 (38%)	52 (100%)	0	100	100
All	All	4311/5170 (83%)	4310 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	19	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
3	G	239	ASN

5.3.3 RNA

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	B	601	13	26,33,33	0.86	0	31,52,52	1.49	4 (12%)
15	TRT	E	600	-	25,25,25	0.61	0	33,33,33	0.71	0
12	ATP	C	601	13	26,33,33	0.88	0	31,52,52	1.62	5 (16%)
12	ATP	F	601	13	26,33,33	1.01	2 (7%)	31,52,52	1.65	7 (22%)
14	ADP	D	601	13	24,29,29	0.97	1 (4%)	29,45,45	1.46	4 (13%)
12	ATP	A	601	13	26,33,33	0.82	0	31,52,52	1.55	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	B	601	13	-	2/18/38/38	0/3/3/3
15	TRT	E	600	-	-	8/23/23/23	0/1/1/1
12	ATP	C	601	13	-	3/18/38/38	0/3/3/3
12	ATP	F	601	13	-	4/18/38/38	0/3/3/3
14	ADP	D	601	13	-	0/12/32/32	0/3/3/3
12	ATP	A	601	13	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	601	ATP	C2'-C1'	-2.55	1.49	1.53
14	D	601	ADP	C5-C4	2.18	1.46	1.40
12	F	601	ATP	C5-C4	2.04	1.46	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	601	ATP	PB-O3B-PG	-4.38	117.81	132.83
12	F	601	ATP	PB-O3B-PG	-4.00	119.09	132.83
12	B	601	ATP	PB-O3B-PG	-3.94	119.31	132.83
12	A	601	ATP	PB-O3B-PG	-3.73	120.02	132.83
12	A	601	ATP	N3-C2-N1	-3.58	123.08	128.68

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	601	ATP	C5'-O5'-PA-O1A
12	F	601	ATP	C5'-O5'-PA-O3A
15	E	600	TRT	O15-C16-C17-O18
12	C	601	ATP	PG-O3B-PB-O1B
15	E	600	TRT	C5-C6-C9-C10

There are no ring outliers.

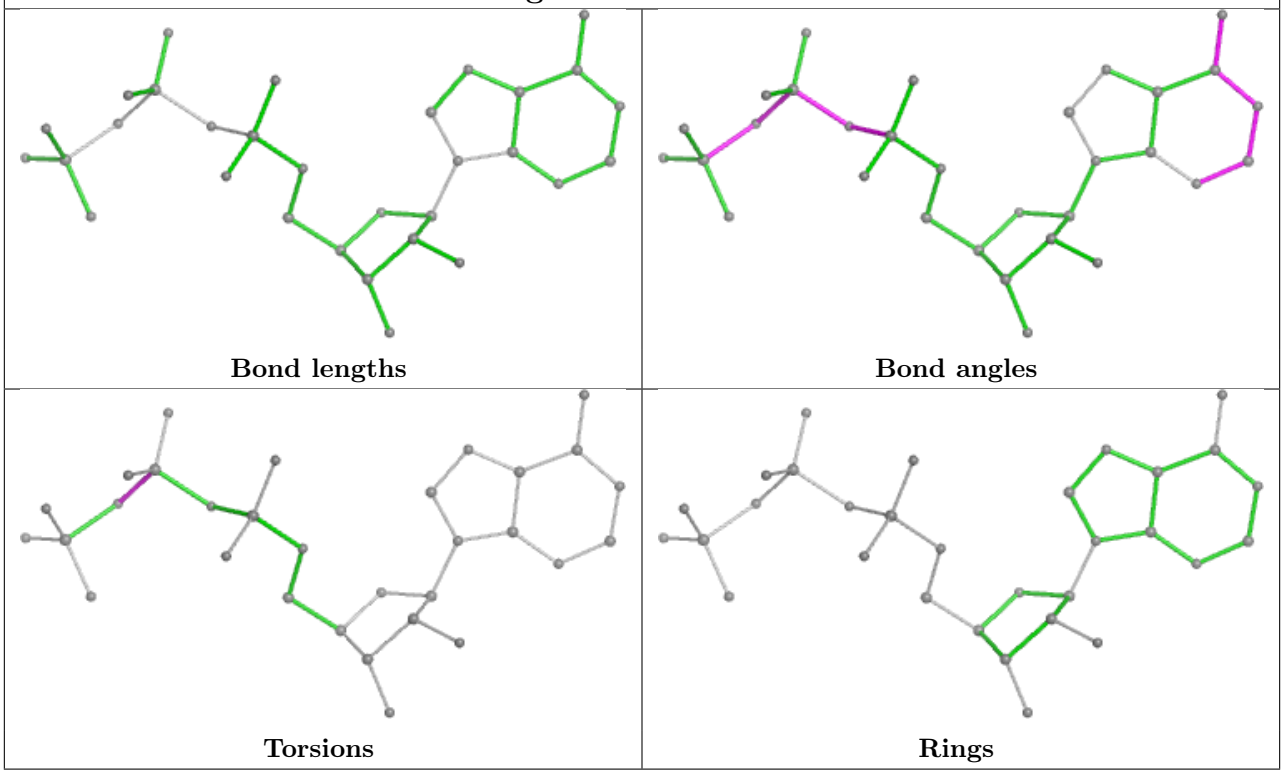
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	600	TRT	2	0
12	F	601	ATP	1	0

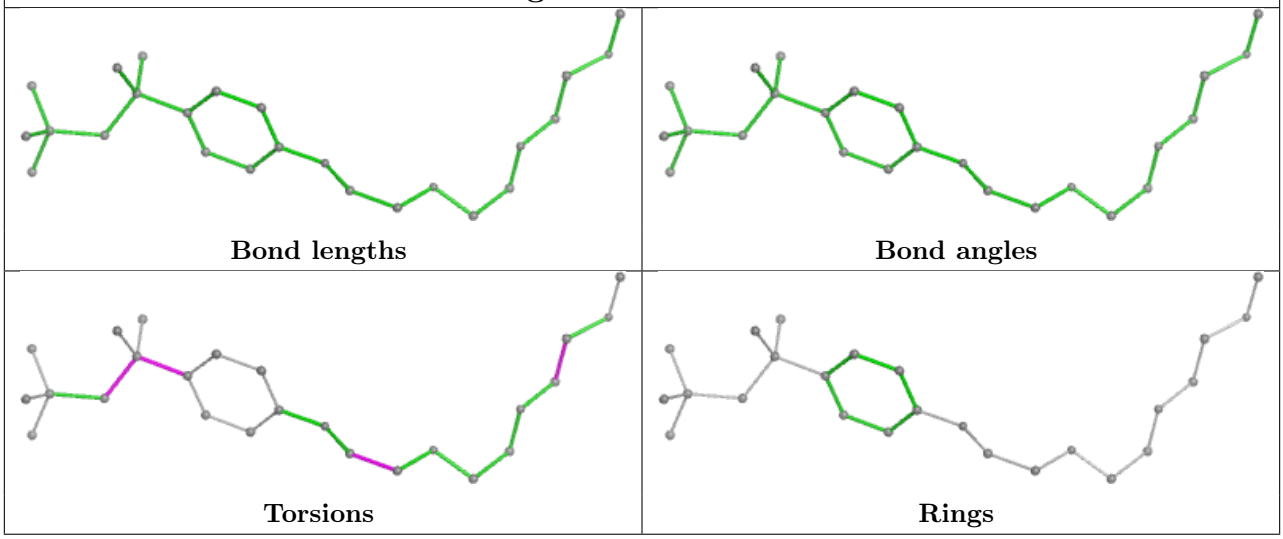
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

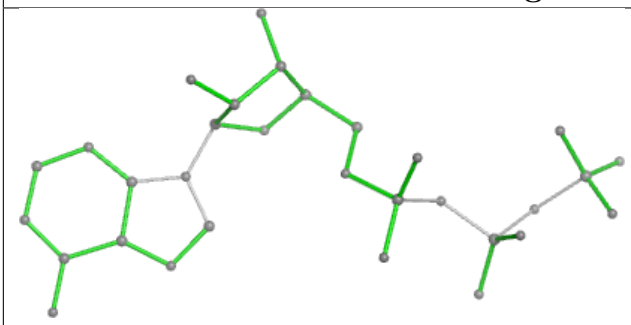
Ligand ATP B 601



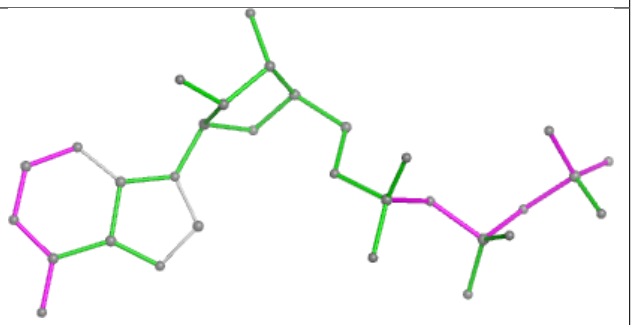
Ligand TRT E 600



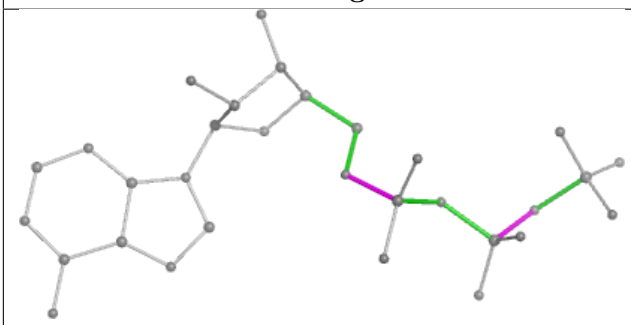
Ligand ATP C 601



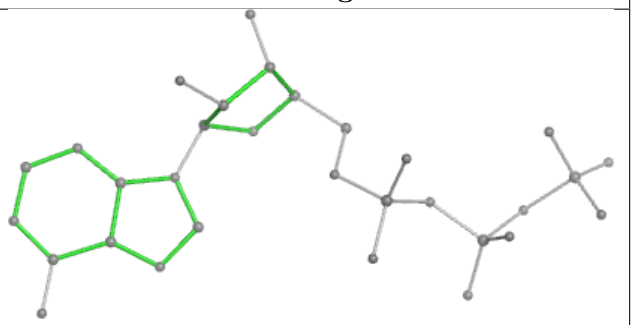
Bond lengths



Bond angles

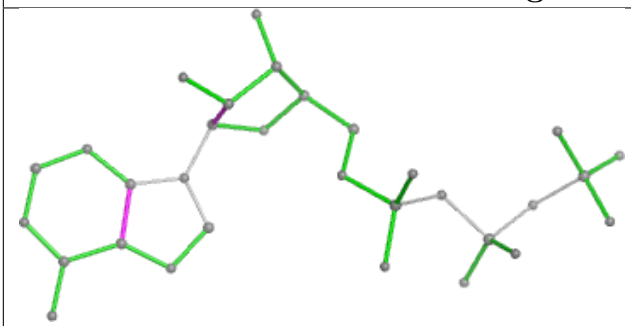


Torsions

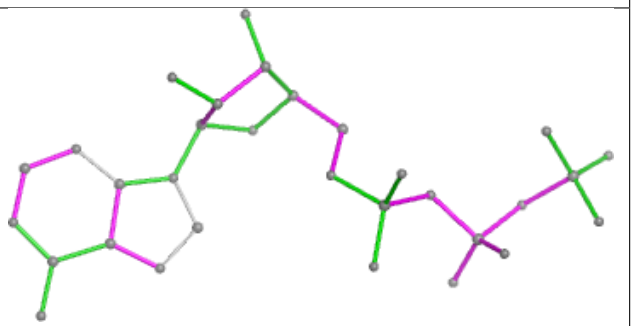


Rings

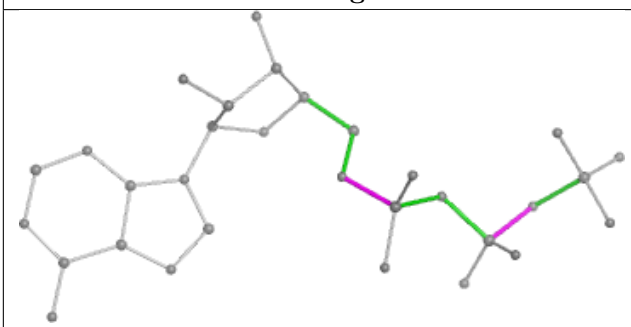
Ligand ATP F 601



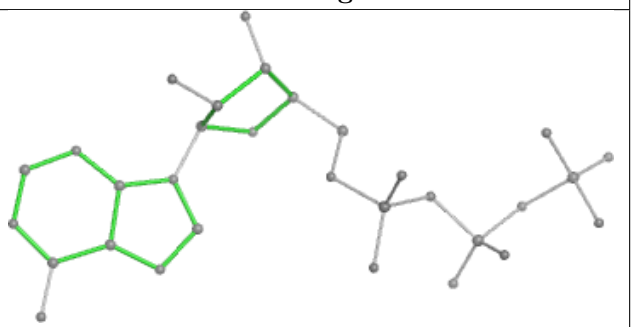
Bond lengths



Bond angles

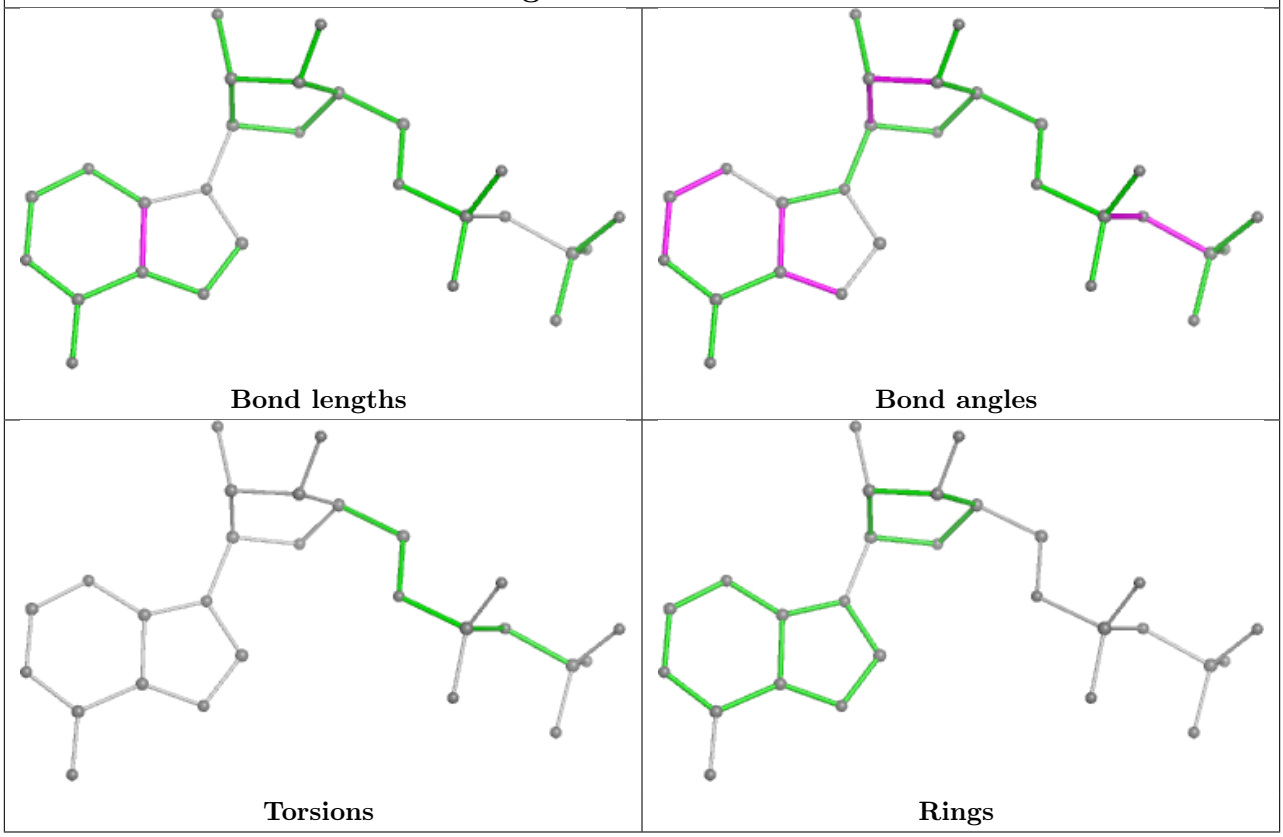


Torsions

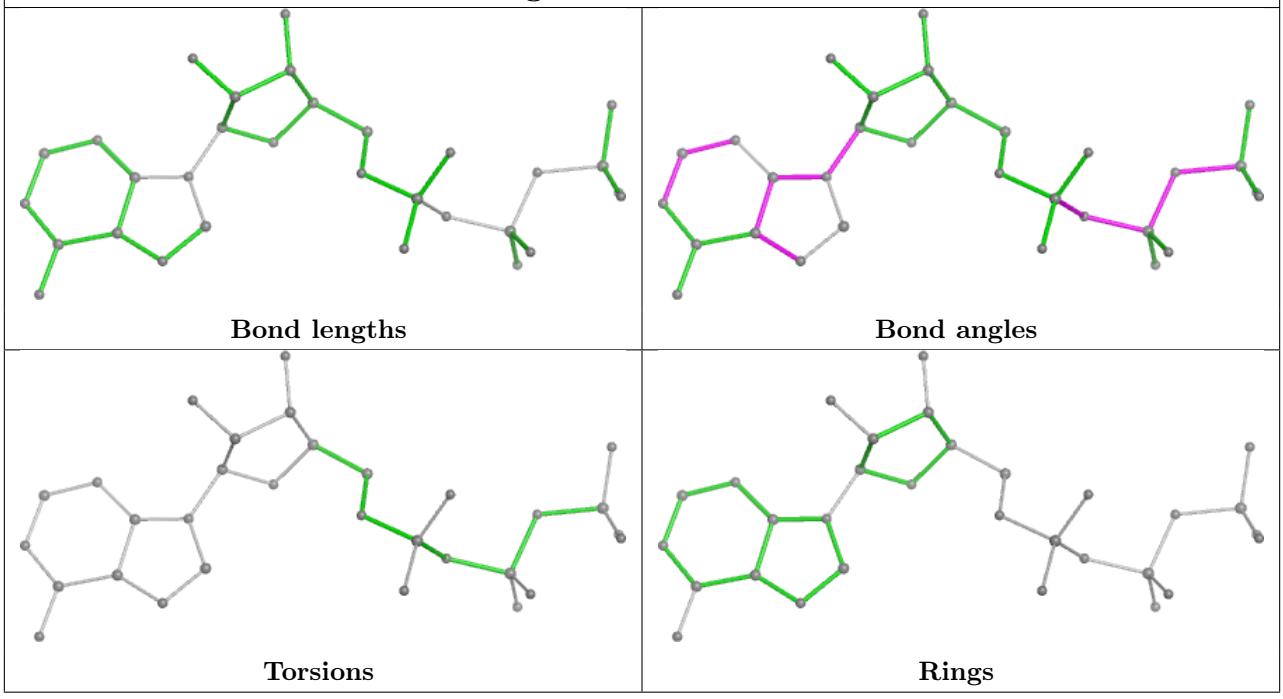


Rings

Ligand ADP D 601



Ligand ATP A 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

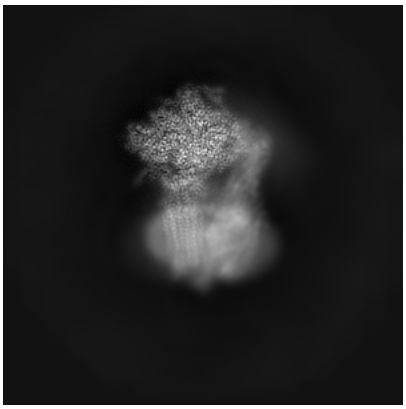
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10471. These allow visual inspection of the internal detail of the map and identification of artifacts.

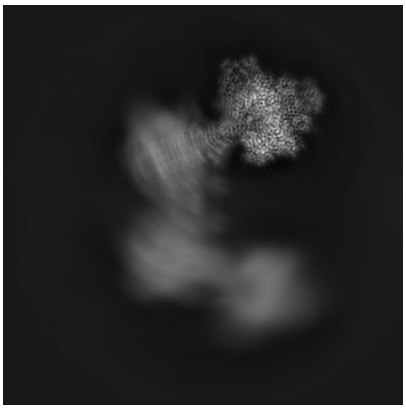
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

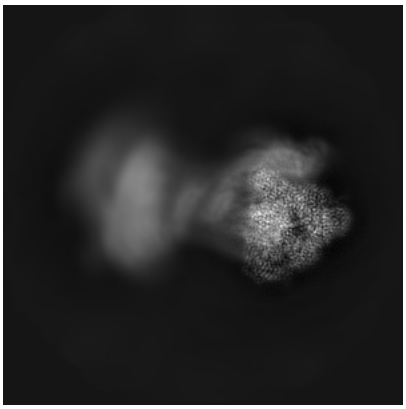
6.1.1 Primary map



X

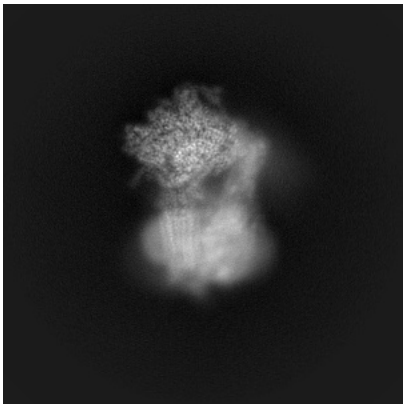


Y

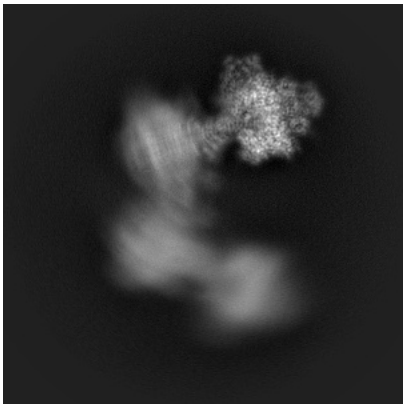


Z

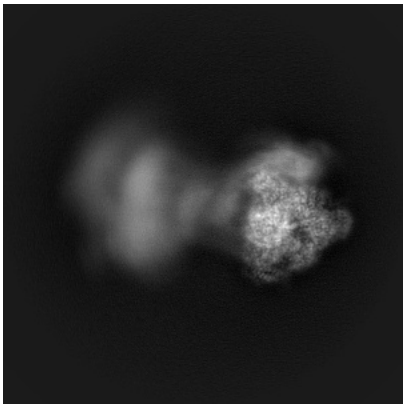
6.1.2 Raw map



X



Y

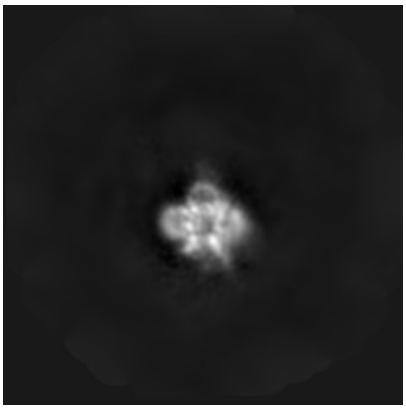


Z

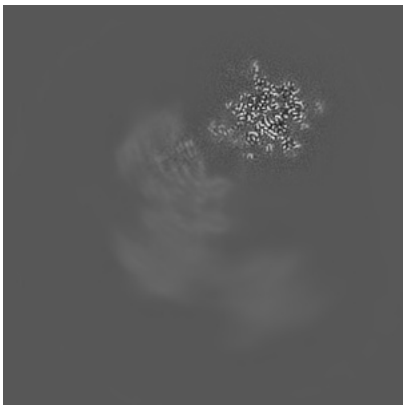
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

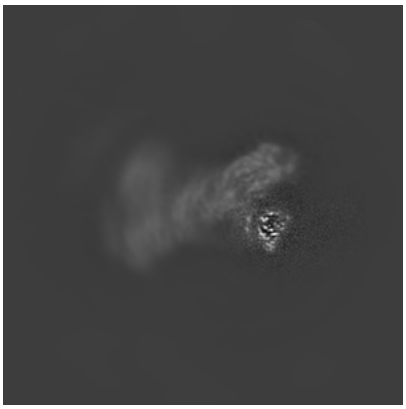
6.2.1 Primary map



X Index: 220

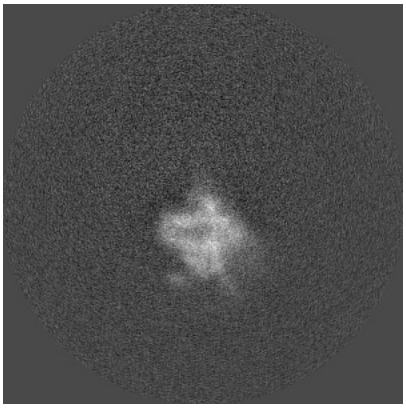


Y Index: 220

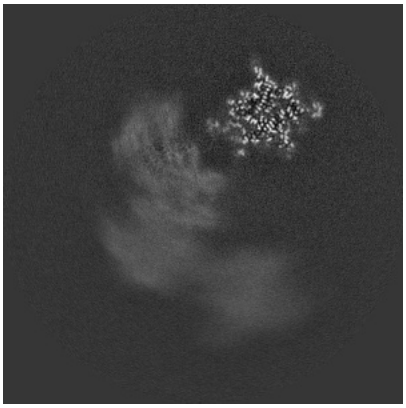


Z Index: 220

6.2.2 Raw map



X Index: 220



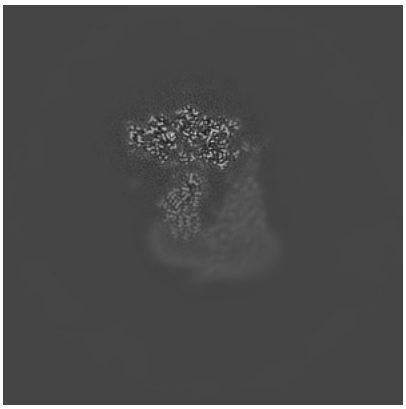
Y Index: 220

Z Index: 220

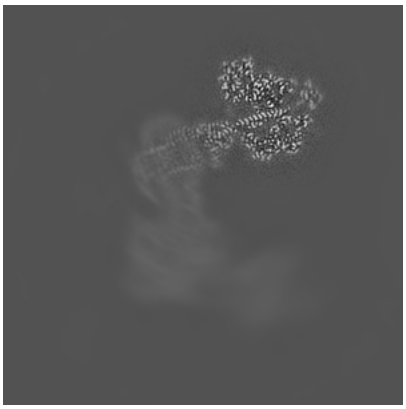
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

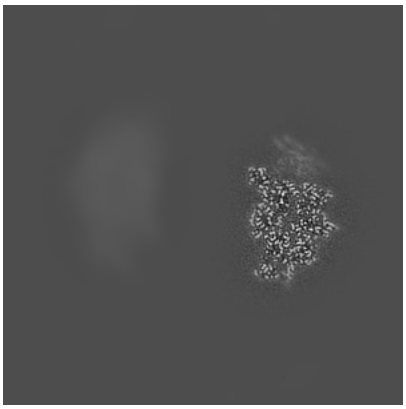
6.3.1 Primary map



X Index: 295

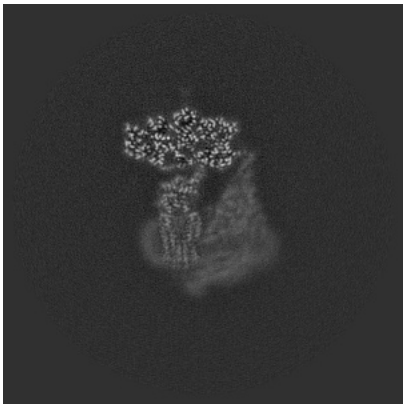


Y Index: 198

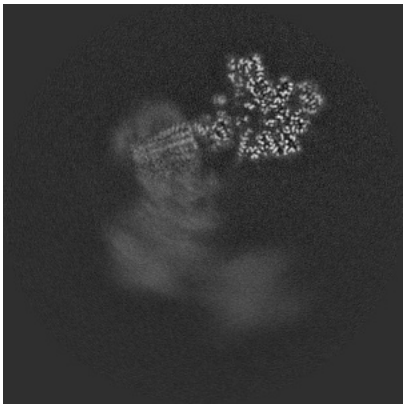


Z Index: 294

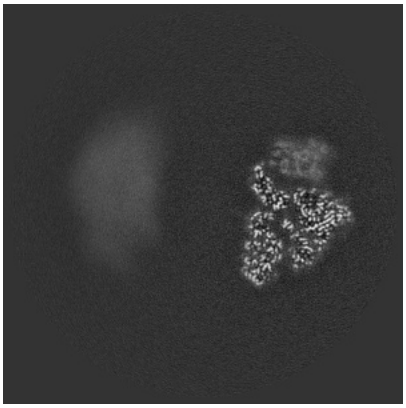
6.3.2 Raw map



X Index: 291



Y Index: 207

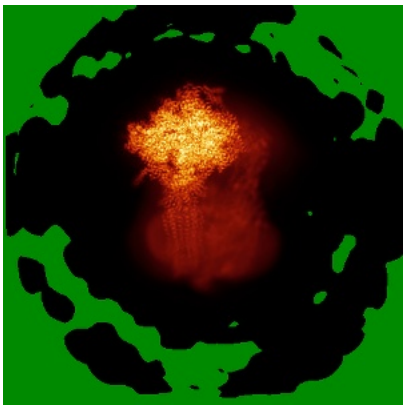


Z Index: 281

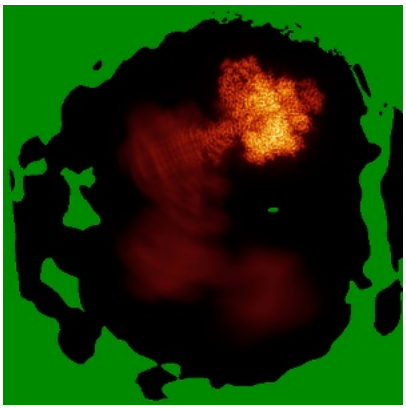
The images above show the largest variance slices of the map in three orthogonal directions.

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

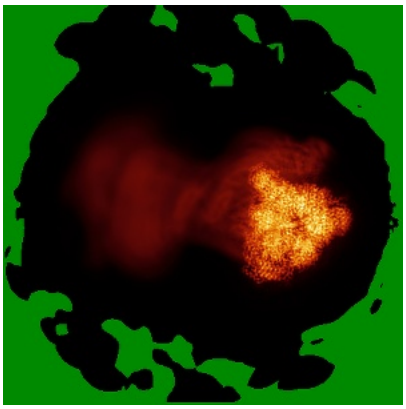
6.4.1 Primary map



X

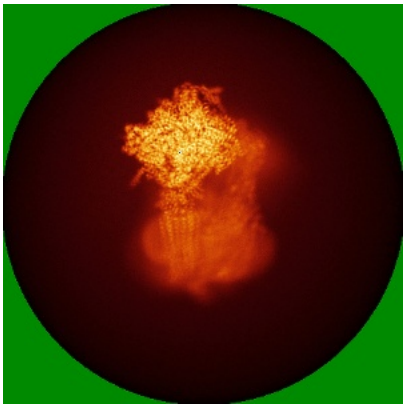


Y

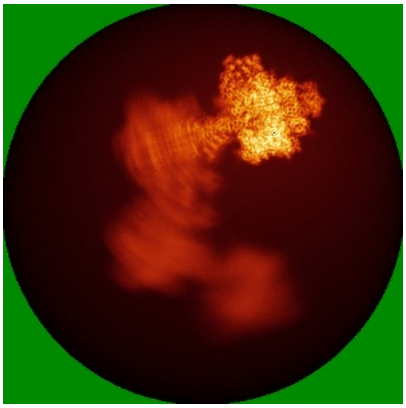


Z

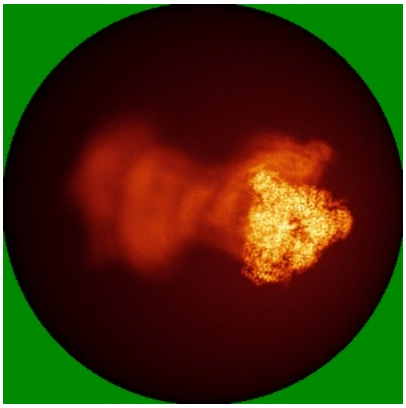
6.4.2 Raw map



X



Y

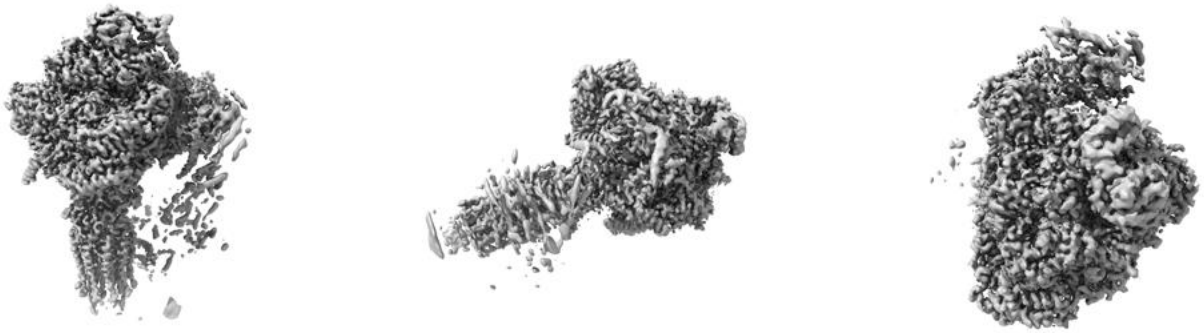


Z

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)

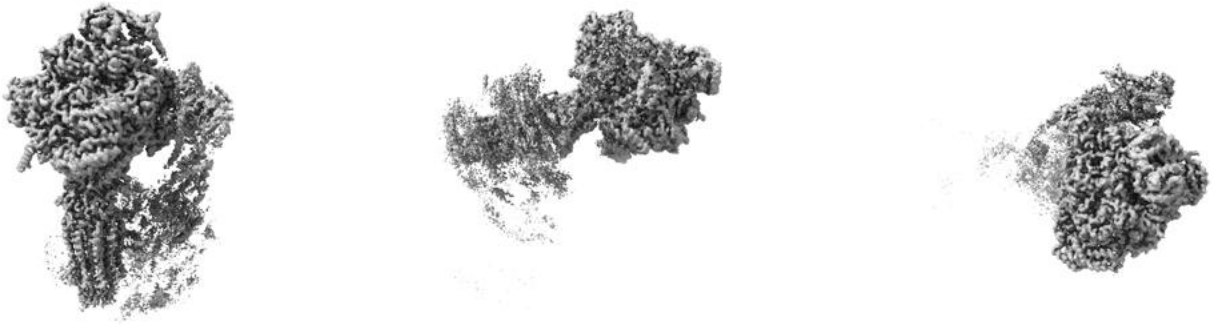
6.5.1 Primary map



X Y Z

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

6.5.2 Raw map



X Y Z

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.

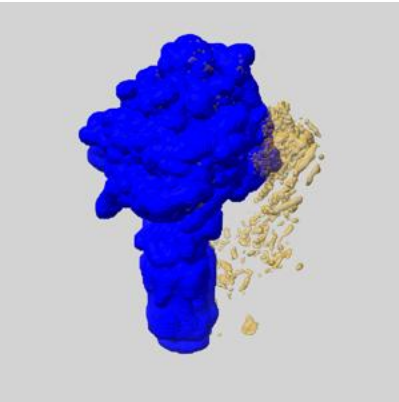
6.6 Mask visualisation (i)

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

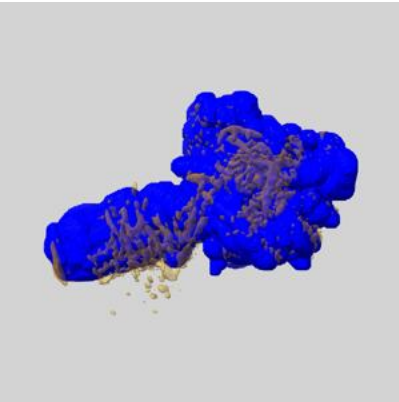
A mask typically either:

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

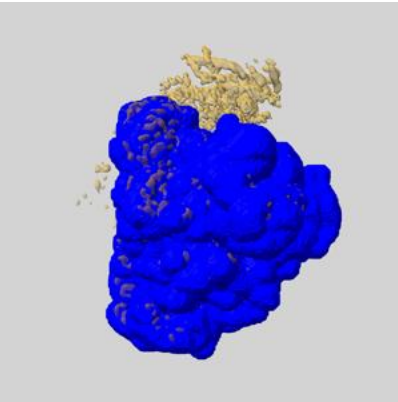
6.6.1 emd_10471_msk_1.map (i)



X



Y

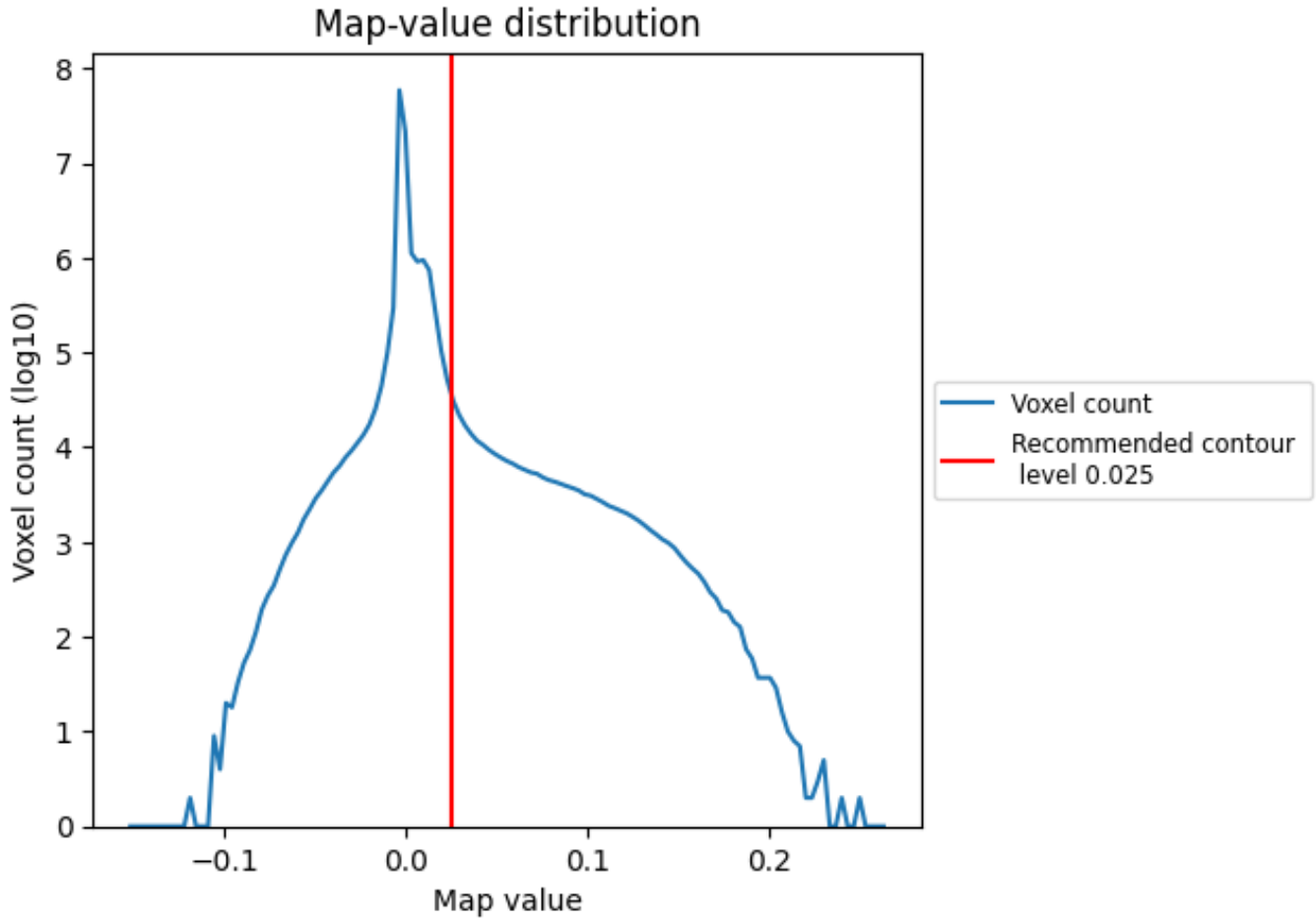


Z

7 Map analysis

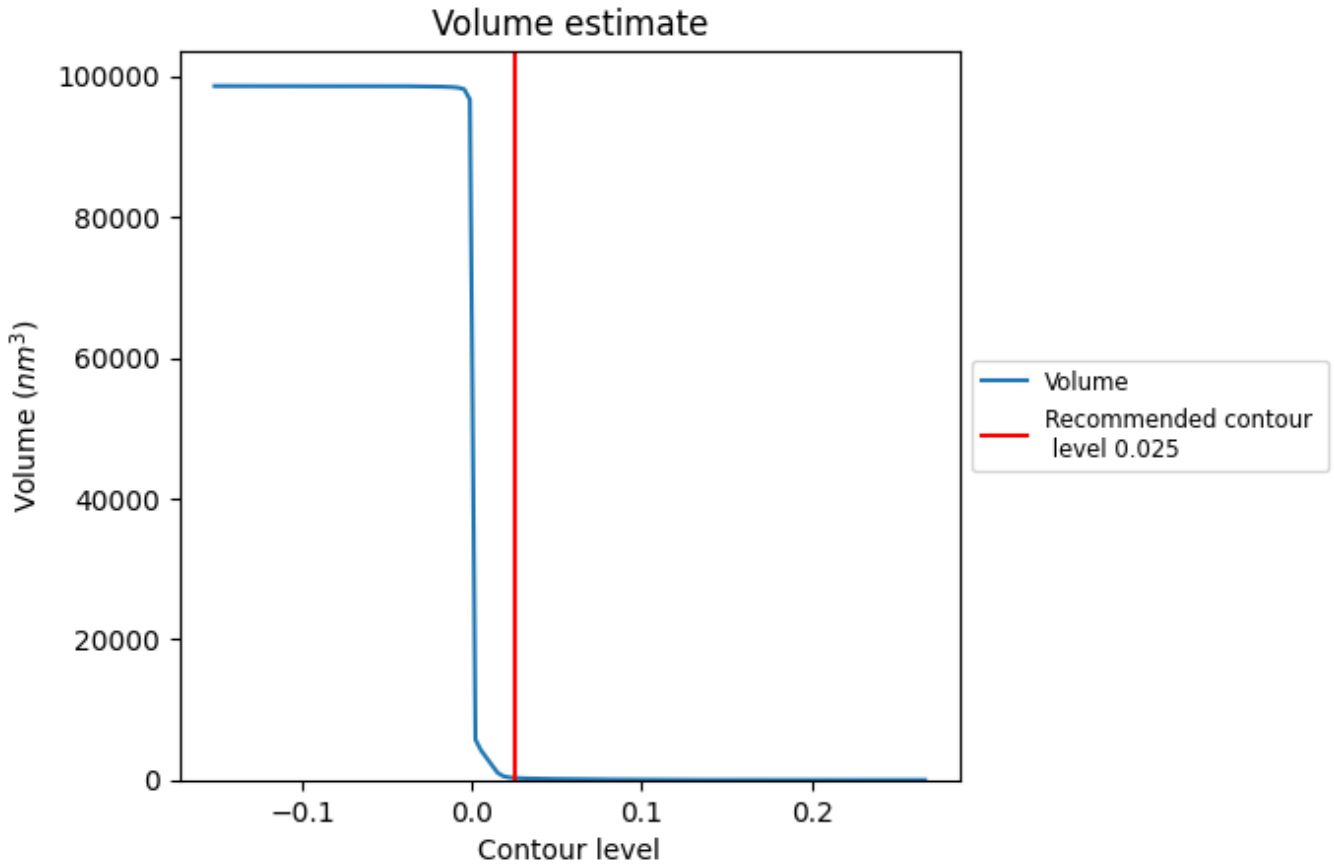
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

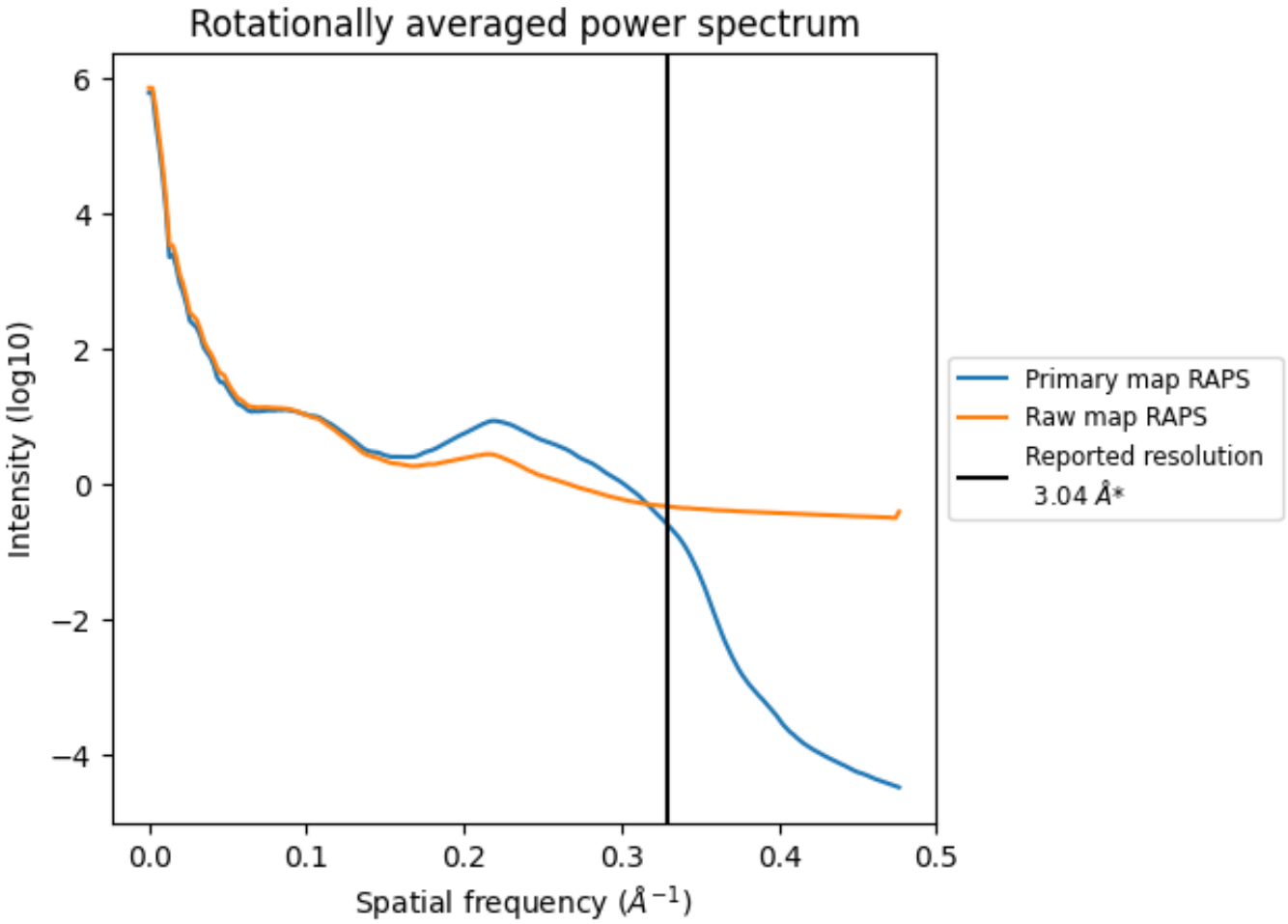
7.2 Volume estimate (i)



The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 263 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)

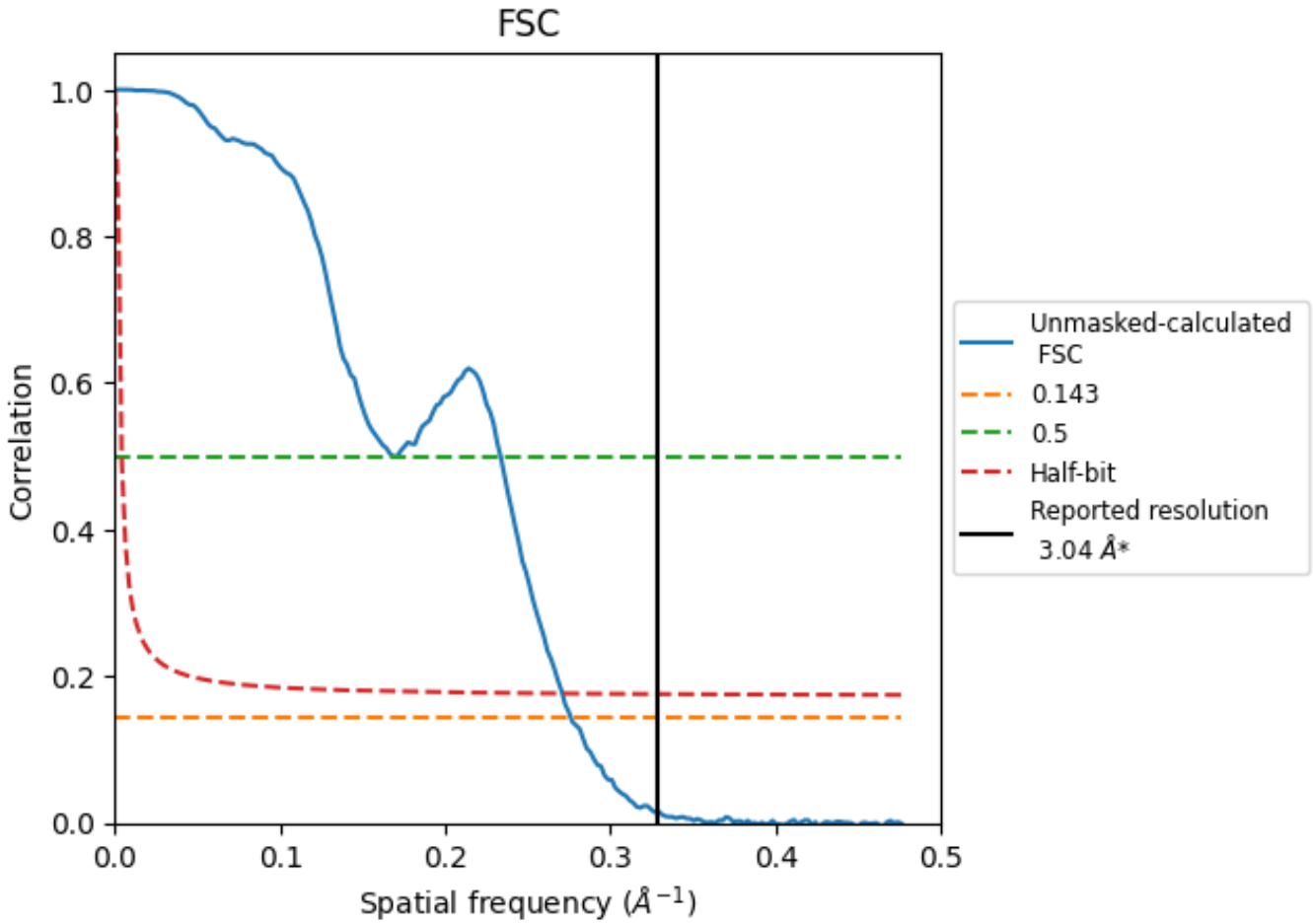


*Reported resolution corresponds to spatial frequency of 0.329 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.329 Å^{-1}

8.2 Resolution estimates (i)

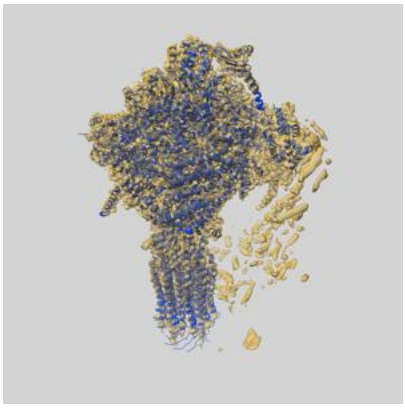
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.62	5.93	3.69

*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 3.62 differs from the reported value 3.04 by more than 10 %

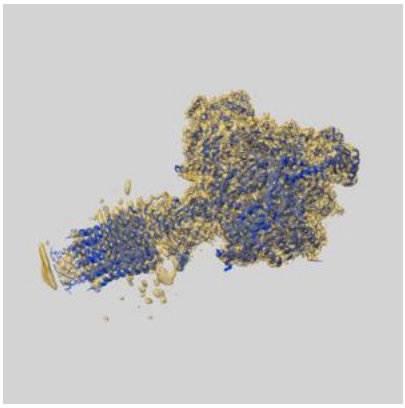
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10471 and PDB model 6TDY. Per-residue inclusion information can be found in section 3 on page 9.

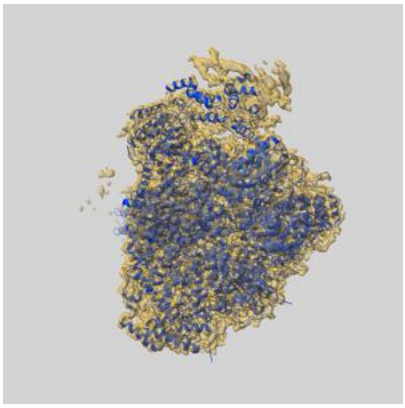
9.1 Map-model overlay



X



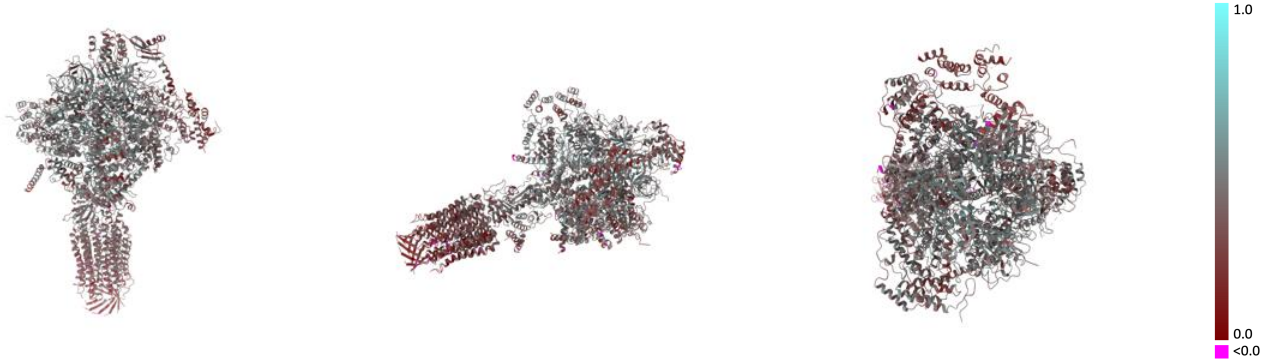
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

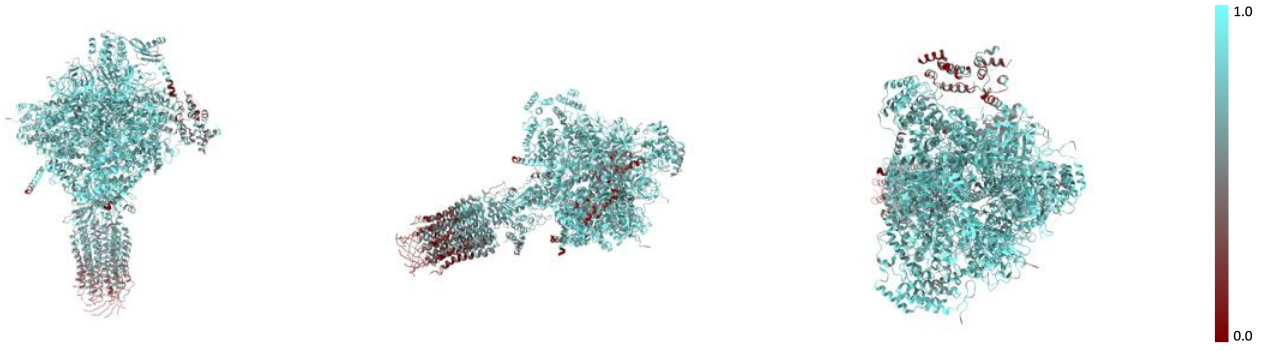
9.2 Q-score mapped to coordinate model



X Y Z

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.

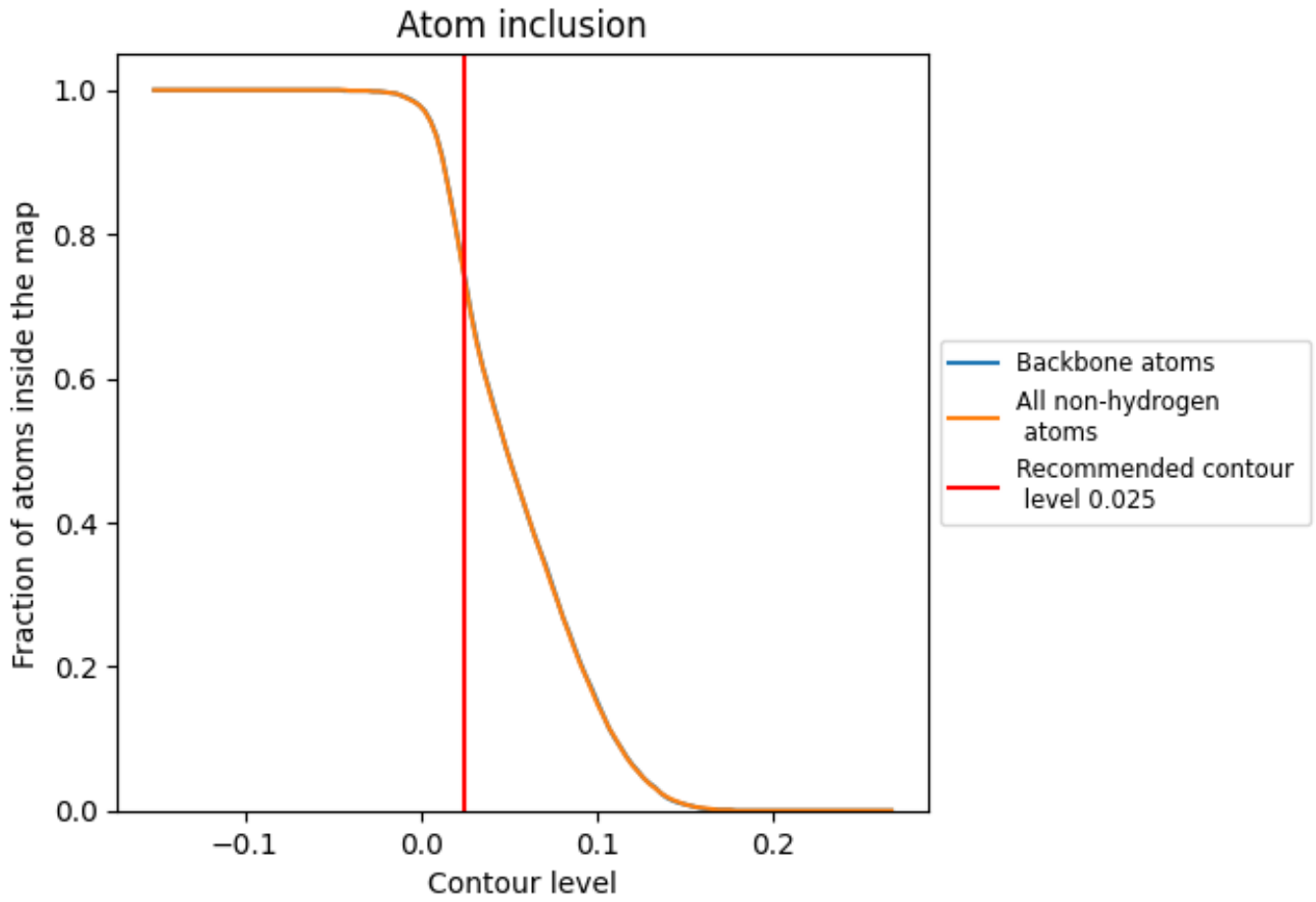
9.3 Atom inclusion mapped to coordinate model



X Y Z

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, 74% of all backbone atoms, 73% 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	0.7330	0.4000
A	0.8310	0.4500
B	0.8400	0.4650
C	0.8190	0.4360
D	0.8050	0.4380
E	0.8260	0.4640
F	0.8240	0.4560
G	0.7820	0.4250
H	0.6710	0.3690
I	0.7200	0.3760
J	0.7880	0.3810
K	0.7840	0.3840
L	0.7380	0.3300
M	0.6470	0.3380
N	0.6770	0.3870
O	0.3510	0.2240
P	0.4050	0.2470
Q	0.4450	0.2730
R	0.4630	0.2910
S	0.4540	0.2760
T	0.4630	0.2790
U	0.4970	0.2690
V	0.4500	0.2230
W	0.4160	0.2310
X	0.3500	0.2100
c	0.4700	0.2570
h	0.3430	0.2660