



wwPDB EM Validation Summary Report ⓘ

Aug 13, 2026 – 04:32 PM EDT

PDB ID : 9PEW / pdb_00009pew
EMDB ID : EMD-71580
Title : Porcine ATP synthase with inhibitory protein IF1, DP-state
Authors : Mnatsakanyan, N.; Mello, J.F.R.; Palles, C.
Deposited on : 2025-07-02
Resolution : 2.69 Å(reported)
Based on initial model : .

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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

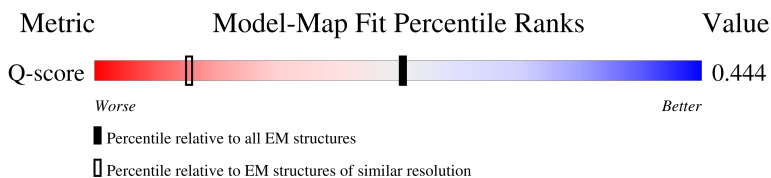
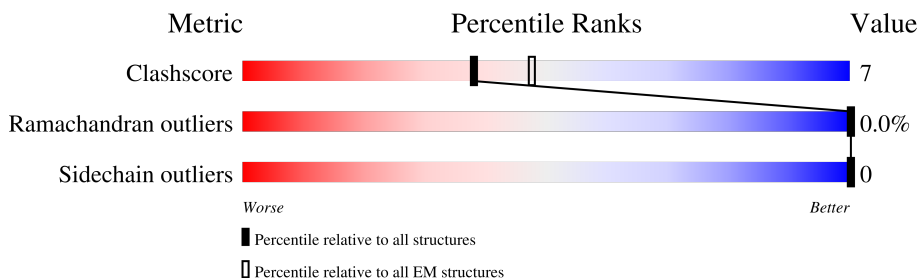
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9309 (2.19 - 3.19)

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	1	73	 71% 29%
1	2	73	 75% 25%
1	3	73	 68% 32%
1	4	73	 79% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	5	73	
1	6	73	
1	7	73	
1	8	73	
2	A	508	
2	B	508	
2	C	508	
3	D	470	
3	E	470	
3	F	470	
4	G	272	
5	H	132	
6	I	47	
7	J	53	
8	K	191	
9	L	68	
10	M	147	
11	N	226	
12	O	187	
13	Q	22	
14	R	84	
15	S	80	
16	T	55	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 38695 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP synthase lipid-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	73	Total	C	N	O	S	0	0
			522	344	81	93	4		
1	2	73	Total	C	N	O	S	0	0
			522	344	81	93	4		
1	3	73	Total	C	N	O	S	0	0
			522	344	81	93	4		
1	4	73	Total	C	N	O	S	0	0
			522	344	81	93	4		
1	5	73	Total	C	N	O	S	0	0
			522	344	81	93	4		
1	6	73	Total	C	N	O	S	0	0
			522	344	81	93	4		
1	7	73	Total	C	N	O	S	0	0
			522	344	81	93	4		
1	8	73	Total	C	N	O	S	0	0
			522	344	81	93	4		

- Molecule 2 is a protein called ATP synthase F(1) complex subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	501	Total	C	N	O	S	0	0
			3820	2406	673	729	12		
2	B	508	Total	C	N	O	S	0	0
			3868	2435	681	740	12		
2	C	488	Total	C	N	O	S	0	0
			3715	2344	656	703	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	470	Total	C	N	O	S	0	0
			3560	2256	604	688	12		
3	E	467	Total	C	N	O	S	0	0
			3532	2240	599	681	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	467	Total	C	N	O	S	0	0
			3532	2240	599	681	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	272	Total	C	N	O	S	0	0
			2112	1332	366	407	7		

- Molecule 5 is a protein called ATP synthase F(1) complex subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	132	Total	C	N	O	S	0	0
			973	610	165	196	2		

- Molecule 6 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	47	Total	C	N	O	S	0	0
			368	235	67	65	1		

- Molecule 7 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	53	Total	C	N	O	S	0	0
			395	237	79	79			

- Molecule 8 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	191	Total	C	N	O	S	0	0
			1553	999	268	281	5		

- Molecule 9 is a protein called ATP synthase peripheral stalk subunit F6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	68	Total	C	N	O	S	0	0
			564	359	95	108	2		

- Molecule 10 is a protein called ATP synthase peripheral stalk subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	147	Total	C	N	O	S	0	0
			1190	769	194	224	3		

- Molecule 11 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	226	Total	C	N	O	S	0	0
			1760	1170	279	298	13		

- Molecule 12 is a protein called ATP synthase peripheral stalk subunit OSCP, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	187	Total	C	N	O	S	0	0
			1435	913	247	266	9		

- Molecule 13 is a protein called ATP synthase F(0) complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	22	Total	C	N	O	S	0	0
			184	127	25	30	2		

- Molecule 14 is a protein called ATP synthase F(0) complex subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	84	Total	C	N	O	S	0	0
			702	458	125	116	3		

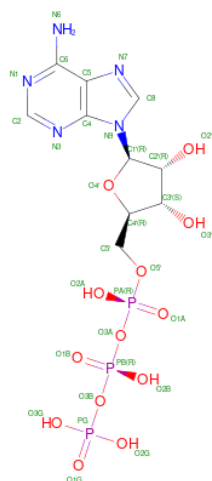
- Molecule 15 is a protein called ATP synthase F(0) complex subunit g, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	80	Total	C	N	O	S	0	0
			626	412	104	109	1		

- Molecule 16 is a protein called ATP synthase F(0) complex subunit e, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	55	Total	C	N	O	S	0	0
			447	288	80	78	1		

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 31	C 10	N 5	O 13	P 3	0
17	B	1	Total 31	C 10	N 5	O 13	P 3	0
17	C	1	Total 31	C 10	N 5	O 13	P 3	0
17	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

3 Residue-property plots

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

- Molecule 1: ATP synthase lipid-binding protein

Chain 1:  71% 29%



- Molecule 1: ATP synthase lipid-binding protein

Chain 2:  75% 25%



- Molecule 1: ATP synthase lipid-binding protein

Chain 3:  68% 32%



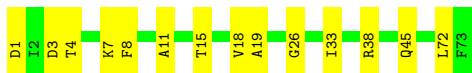
- Molecule 1: ATP synthase lipid-binding protein

Chain 4:  79% 21%



- Molecule 1: ATP synthase lipid-binding protein

Chain 5:  81% 19%



- Molecule 1: ATP synthase lipid-binding protein

Chain 6:  75% 25%



- Molecule 1: ATP synthase lipid-binding protein

Chain 7:  82% 18%



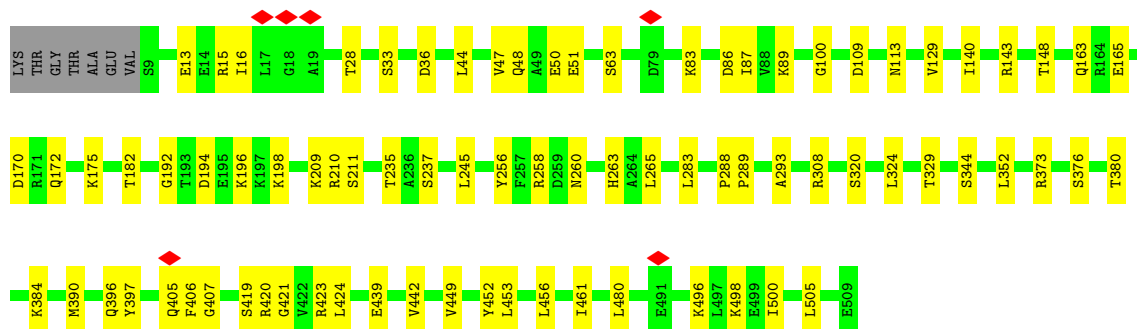
- Molecule 1: ATP synthase lipid-binding protein

Chain 8:  75% 25%



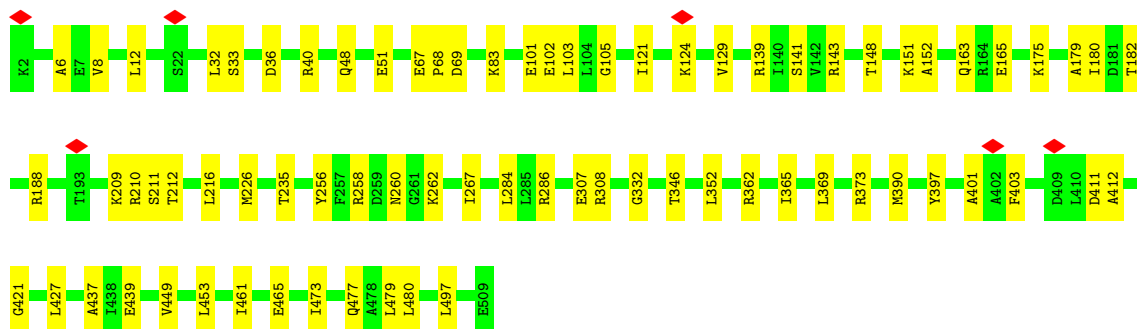
- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial

Chain A:  83% 16%



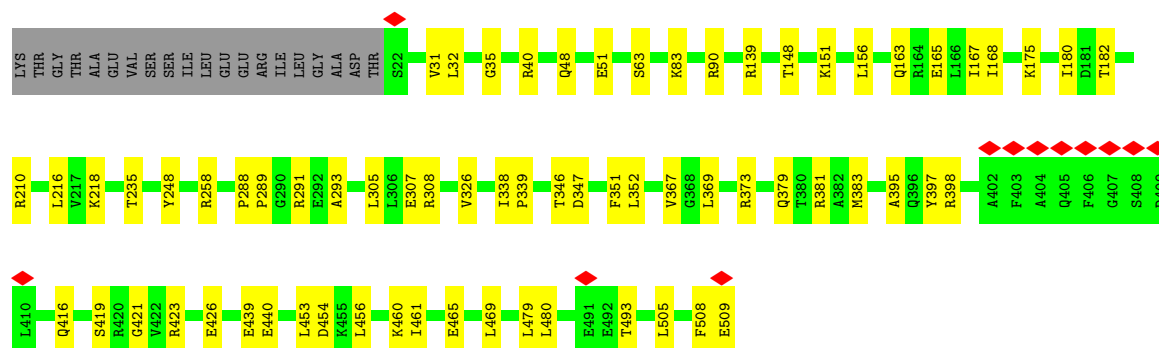
- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial

Chain B:  85% 15%



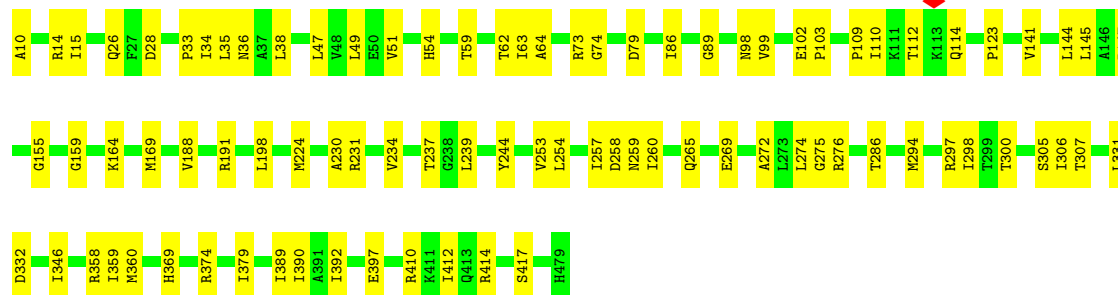
- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial

Chain C:  82% 14%



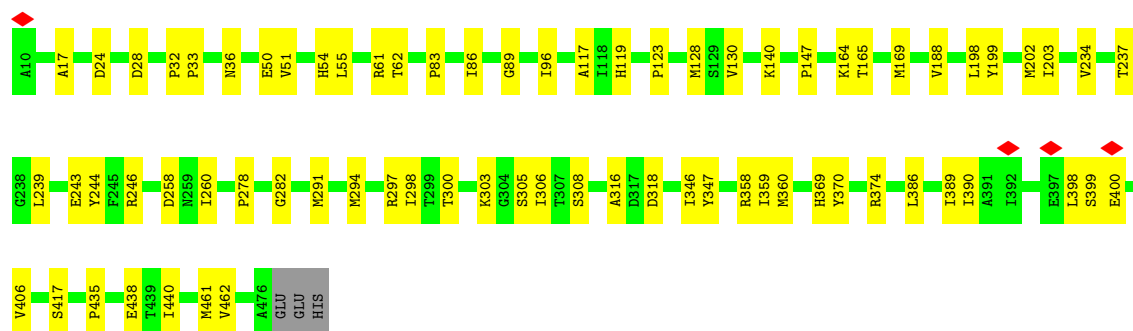
• Molecule 3: ATP synthase subunit beta

Chain D:  81% 19%



• Molecule 3: ATP synthase subunit beta

Chain E:  84% 16%



• Molecule 3: ATP synthase subunit beta

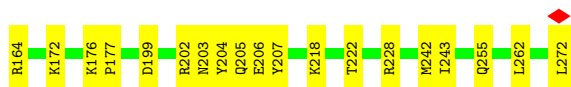
Chain F:  86% 13%





- Molecule 4: ATP synthase subunit gamma

Chain G: 81% 19%



- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial

Chain H: 78% 22%



- Molecule 6: ATP synthase F1 subunit epsilon

Chain I: 79% 21%



- Molecule 7: ATPase inhibitor, mitochondrial

Chain J: 19% 85% 15%



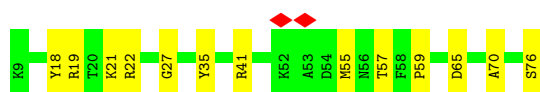
- Molecule 8: ATP synthase subunit b

Chain K: 14% 79% 21%

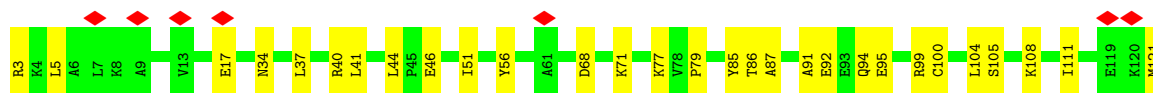
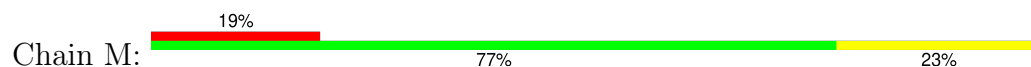


- Molecule 9: ATP synthase peripheral stalk subunit F6, mitochondrial

Chain L: 81% 19%



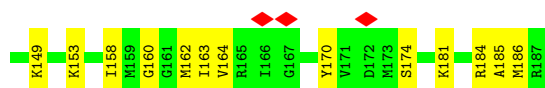
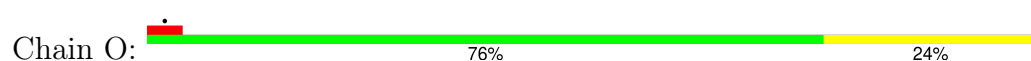
- Molecule 10: ATP synthase peripheral stalk subunit d, mitochondrial



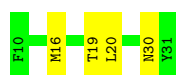
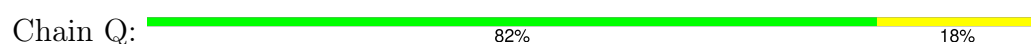
- Molecule 11: ATP synthase subunit a



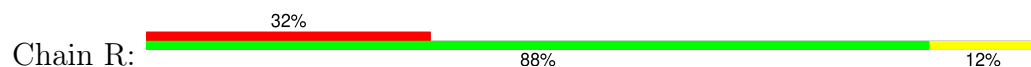
- Molecule 12: ATP synthase peripheral stalk subunit OSCP, mitochondrial

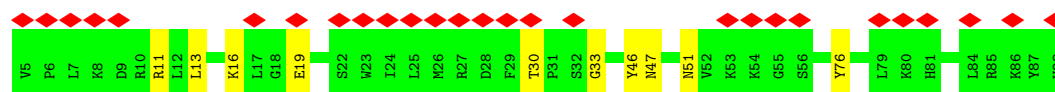


- Molecule 13: ATP synthase F(0) complex subunit 8

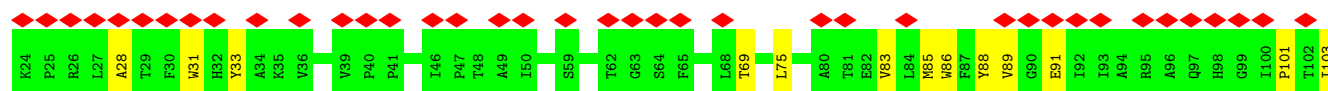
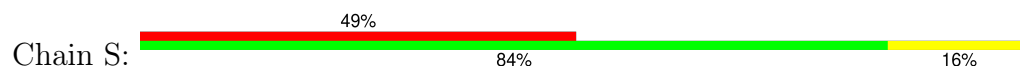


- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial

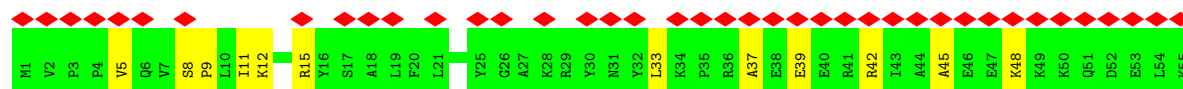
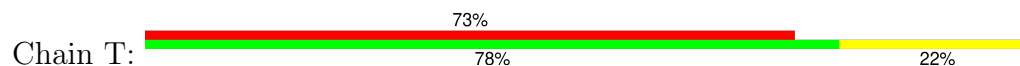




- Molecule 15: ATP synthase F(0) complex subunit g, mitochondrial



- Molecule 16: ATP synthase F(0) complex subunit e, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105447	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	51.984	Depositor
Minimum map value	-24.262	Depositor
Average map value	0.012	Depositor
Map value standard deviation	1.076	Depositor
Recommended contour level	5.1	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ATP

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	1	0.17	0/531	0.32	0/714
1	2	0.17	0/531	0.32	0/714
1	3	0.17	0/531	0.35	0/714
1	4	0.18	0/531	0.34	0/714
1	5	0.18	0/531	0.34	0/714
1	6	0.18	0/531	0.35	0/714
1	7	0.17	0/531	0.31	0/714
1	8	0.18	0/531	0.37	0/714
2	A	0.10	0/3871	0.29	0/5223
2	B	0.11	0/3919	0.29	0/5288
2	C	0.13	0/3766	0.31	0/5082
3	D	0.08	0/3618	0.22	0/4907
3	E	0.12	0/3589	0.24	0/4868
3	F	0.12	0/3589	0.24	0/4868
4	G	0.11	0/2138	0.23	0/2874
5	H	0.12	0/986	0.30	0/1342
6	I	0.11	0/373	0.29	0/500
7	J	0.11	0/399	0.20	0/532
8	K	0.12	0/1577	0.27	0/2121
9	L	0.09	0/577	0.28	0/773
10	M	0.08	0/1214	0.23	0/1639
11	N	0.10	0/1800	0.24	0/2457
12	O	0.11	0/1453	0.29	0/1954
13	Q	0.05	0/187	0.19	0/251
14	R	0.06	0/720	0.18	0/966
15	S	0.10	0/642	0.28	0/875
16	T	0.10	0/455	0.21	0/609
All	All	0.12	0/39121	0.27	0/52841

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	522	0	537	19	0
1	2	522	0	537	17	0
1	3	522	0	537	22	0
1	4	522	0	537	13	0
1	5	522	0	537	14	0
1	6	522	0	537	17	0
1	7	522	0	537	13	0
1	8	522	0	537	16	0
2	A	3820	0	3923	59	0
2	B	3868	0	3973	49	0
2	C	3715	0	3815	50	0
3	D	3560	0	3609	62	0
3	E	3532	0	3590	50	0
3	F	3532	0	3589	43	0
4	G	2112	0	2189	41	0
5	H	973	0	971	24	0
6	I	368	0	387	11	0
7	J	395	0	372	9	0
8	K	1553	0	1614	43	0
9	L	564	0	548	13	0
10	M	1190	0	1216	34	0
11	N	1760	0	1884	48	0
12	O	1435	0	1546	33	0
13	Q	184	0	199	3	0
14	R	702	0	720	7	0
15	S	626	0	656	10	0
16	T	447	0	475	8	0
17	A	31	0	12	1	0
17	B	31	0	12	0	0
17	C	31	0	12	1	0
17	F	31	0	12	3	0
18	A	1	0	0	0	0
18	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	C	1	0	0	0	0
18	D	1	0	0	0	0
18	F	1	0	0	0	0
19	D	27	0	12	1	0
19	E	27	0	12	0	0
All	All	38695	0	39644	576	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 7.

The worst 5 of 576 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)
14:R:30:THR:HG23	14:R:33:GLY:H	1.47	0.78
11:N:174:ILE:HD12	11:N:199:LEU:HD22	1.65	0.78
1:3:33:ILE:HG21	1:4:32:MET:HA	1.65	0.78
2:C:83:LYS:HD2	3:E:33:PRO:HG3	1.66	0.75
3:D:239:LEU:HD13	3:D:298:ILE:HG12	1.69	0.74

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	1	71/73 (97%)	71 (100%)	0	0	100	100
1	2	71/73 (97%)	71 (100%)	0	0	100	100
1	3	71/73 (97%)	71 (100%)	0	0	100	100
1	4	71/73 (97%)	71 (100%)	0	0	100	100
1	5	71/73 (97%)	71 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	71/73 (97%)	71 (100%)	0	0	100	100
1	7	71/73 (97%)	71 (100%)	0	0	100	100
1	8	71/73 (97%)	71 (100%)	0	0	100	100
2	A	499/508 (98%)	490 (98%)	9 (2%)	0	100	100
2	B	506/508 (100%)	497 (98%)	9 (2%)	0	100	100
2	C	486/508 (96%)	473 (97%)	12 (2%)	1 (0%)	43	68
3	D	468/470 (100%)	457 (98%)	11 (2%)	0	100	100
3	E	465/470 (99%)	453 (97%)	12 (3%)	0	100	100
3	F	465/470 (99%)	450 (97%)	15 (3%)	0	100	100
4	G	270/272 (99%)	266 (98%)	4 (2%)	0	100	100
5	H	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
6	I	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
7	J	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
8	K	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
9	L	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
10	M	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
11	N	224/226 (99%)	222 (99%)	2 (1%)	0	100	100
12	O	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
13	Q	20/22 (91%)	20 (100%)	0	0	100	100
14	R	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
15	S	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
16	T	53/55 (96%)	53 (100%)	0	0	100	100
All	All	4995/5082 (98%)	4884 (98%)	110 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	35	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	50/50 (100%)	50 (100%)	0	100	100
1	2	50/50 (100%)	50 (100%)	0	100	100
1	3	50/50 (100%)	50 (100%)	0	100	100
1	4	50/50 (100%)	50 (100%)	0	100	100
1	5	50/50 (100%)	50 (100%)	0	100	100
1	6	50/50 (100%)	50 (100%)	0	100	100
1	7	50/50 (100%)	50 (100%)	0	100	100
1	8	50/50 (100%)	50 (100%)	0	100	100
2	A	405/410 (99%)	405 (100%)	0	100	100
2	B	410/410 (100%)	410 (100%)	0	100	100
2	C	391/410 (95%)	391 (100%)	0	100	100
3	D	378/378 (100%)	378 (100%)	0	100	100
3	E	375/378 (99%)	375 (100%)	0	100	100
3	F	375/378 (99%)	375 (100%)	0	100	100
4	G	230/230 (100%)	230 (100%)	0	100	100
5	H	105/105 (100%)	105 (100%)	0	100	100
6	I	37/37 (100%)	37 (100%)	0	100	100
7	J	35/38 (92%)	35 (100%)	0	100	100
8	K	167/167 (100%)	167 (100%)	0	100	100
9	L	61/61 (100%)	61 (100%)	0	100	100
10	M	127/127 (100%)	127 (100%)	0	100	100
11	N	199/199 (100%)	199 (100%)	0	100	100
12	O	163/163 (100%)	163 (100%)	0	100	100
13	Q	22/22 (100%)	22 (100%)	0	100	100
14	R	73/73 (100%)	73 (100%)	0	100	100
15	S	67/67 (100%)	67 (100%)	0	100	100
16	T	46/46 (100%)	46 (100%)	0	100	100
All	All	4066/4099 (99%)	4066 (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. 5 of 28

such sidechains are listed below:

Mol	Chain	Res	Type
3	E	310	GLN
14	R	88	HIS
4	G	225	GLN
9	L	75	GLN
4	G	150	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
19	ADP	E	601	-	28,29,29	1.41	4 (14%)	43,45,45	1.79	8 (18%)
17	ATP	C	601	18	32,33,33	0.38	0	48,52,52	0.29	0
19	ADP	D	601	18	28,29,29	1.43	5 (17%)	43,45,45	1.77	8 (18%)
17	ATP	B	601	18	32,33,33	0.31	0	48,52,52	0.29	0
17	ATP	F	502	18	32,33,33	0.39	0	48,52,52	0.28	0
17	ATP	A	601	18	32,33,33	0.31	0	48,52,52	0.29	0

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
19	ADP	E	601	-	-	4/16/32/32	0/3/3/3
17	ATP	C	601	18	-	1/22/38/38	0/3/3/3
19	ADP	D	601	18	-	2/16/32/32	0/3/3/3
17	ATP	B	601	18	-	0/22/38/38	0/3/3/3
17	ATP	F	502	18	-	2/22/38/38	0/3/3/3
17	ATP	A	601	18	-	1/22/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	601	ADP	C5-C4	4.72	1.47	1.39
19	E	601	ADP	C5-C4	4.67	1.47	1.39
19	D	601	ADP	C5-C6	2.76	1.48	1.41
19	E	601	ADP	C5-C6	2.68	1.48	1.41
19	D	601	ADP	C8-N7	2.36	1.36	1.31

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	601	ADP	C5-C4-N3	-5.85	118.66	126.72
19	E	601	ADP	C5-C4-N3	-5.83	118.69	126.72
19	E	601	ADP	N3-C4-N9	4.64	135.07	127.17
19	D	601	ADP	N3-C4-N9	4.60	134.99	127.17
19	E	601	ADP	C2-N3-C4	3.71	120.90	111.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

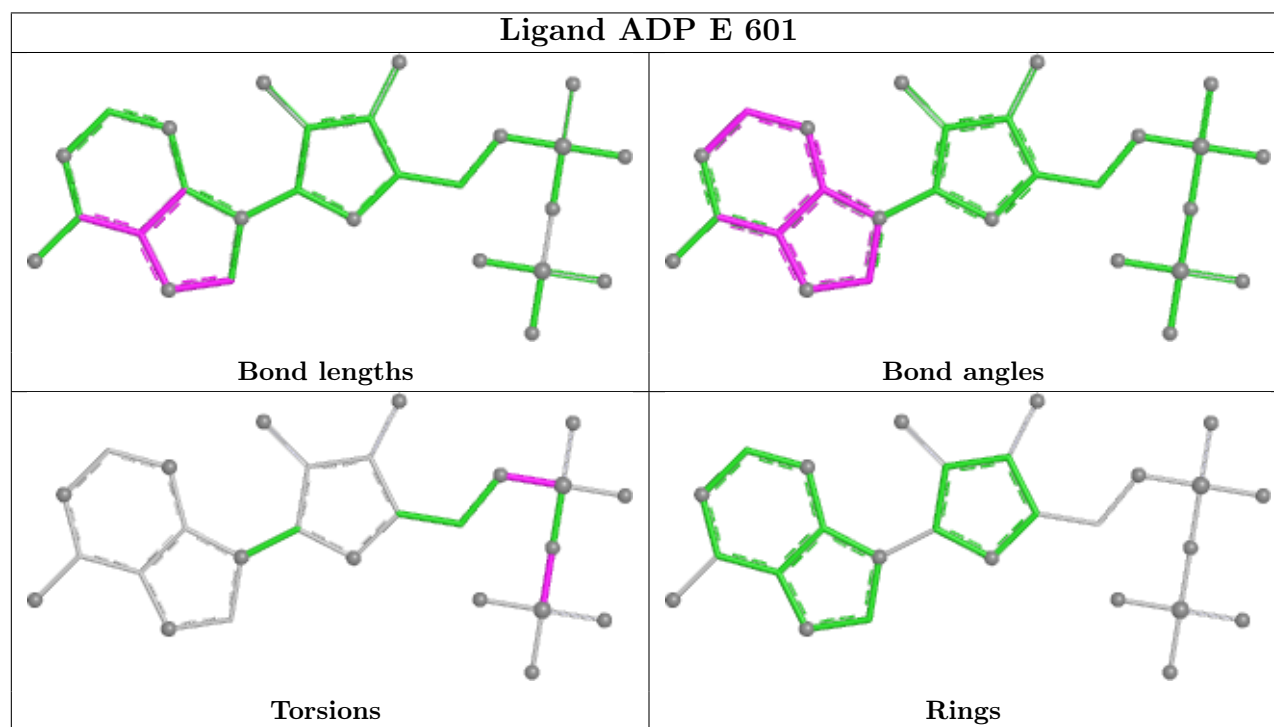
Mol	Chain	Res	Type	Atoms
19	E	601	ADP	C5'-O5'-PA-O1A
19	E	601	ADP	C5'-O5'-PA-O2A
19	E	601	ADP	C5'-O5'-PA-O3A
17	F	502	ATP	PA-O3A-PB-O1B
19	D	601	ADP	PA-O3A-PB-O3B

There are no ring outliers.

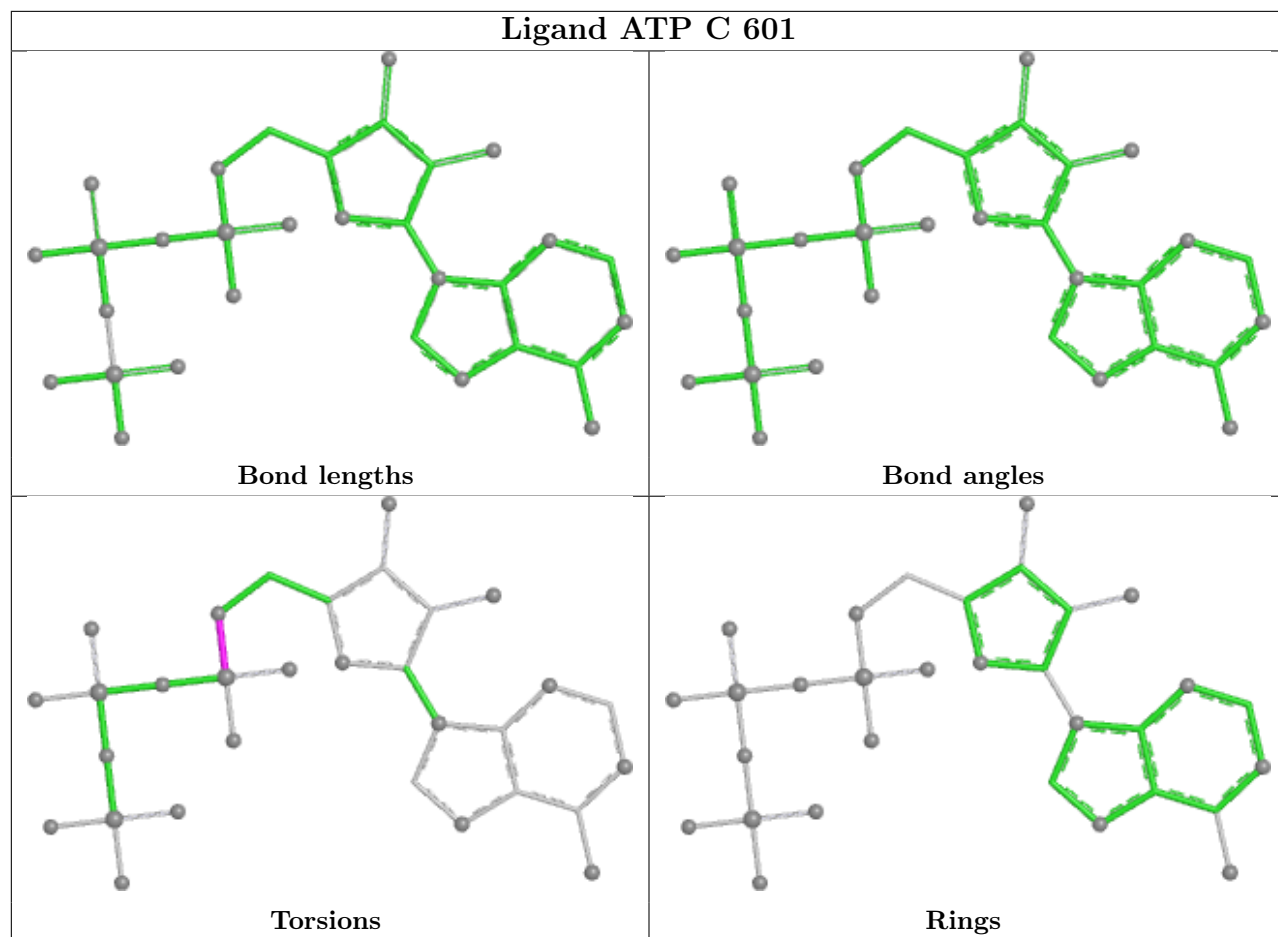
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	601	ATP	1	0
19	D	601	ADP	1	0
17	F	502	ATP	3	0
17	A	601	ATP	1	0

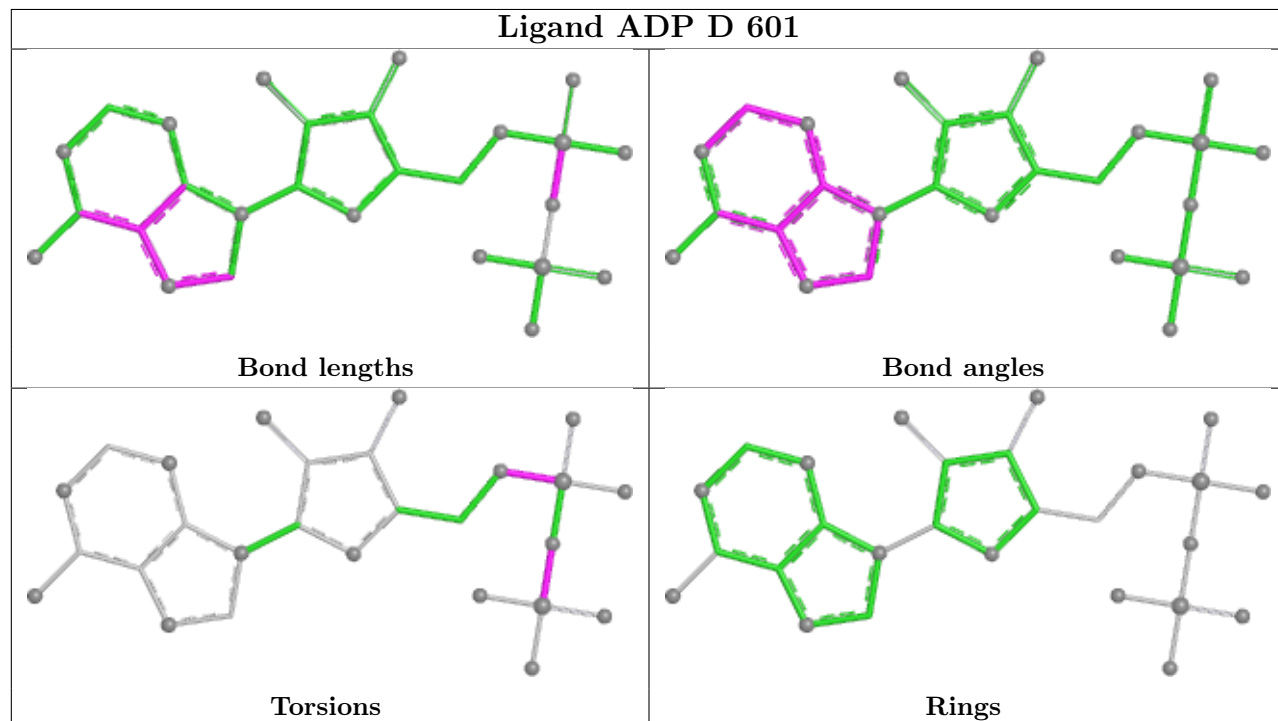
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

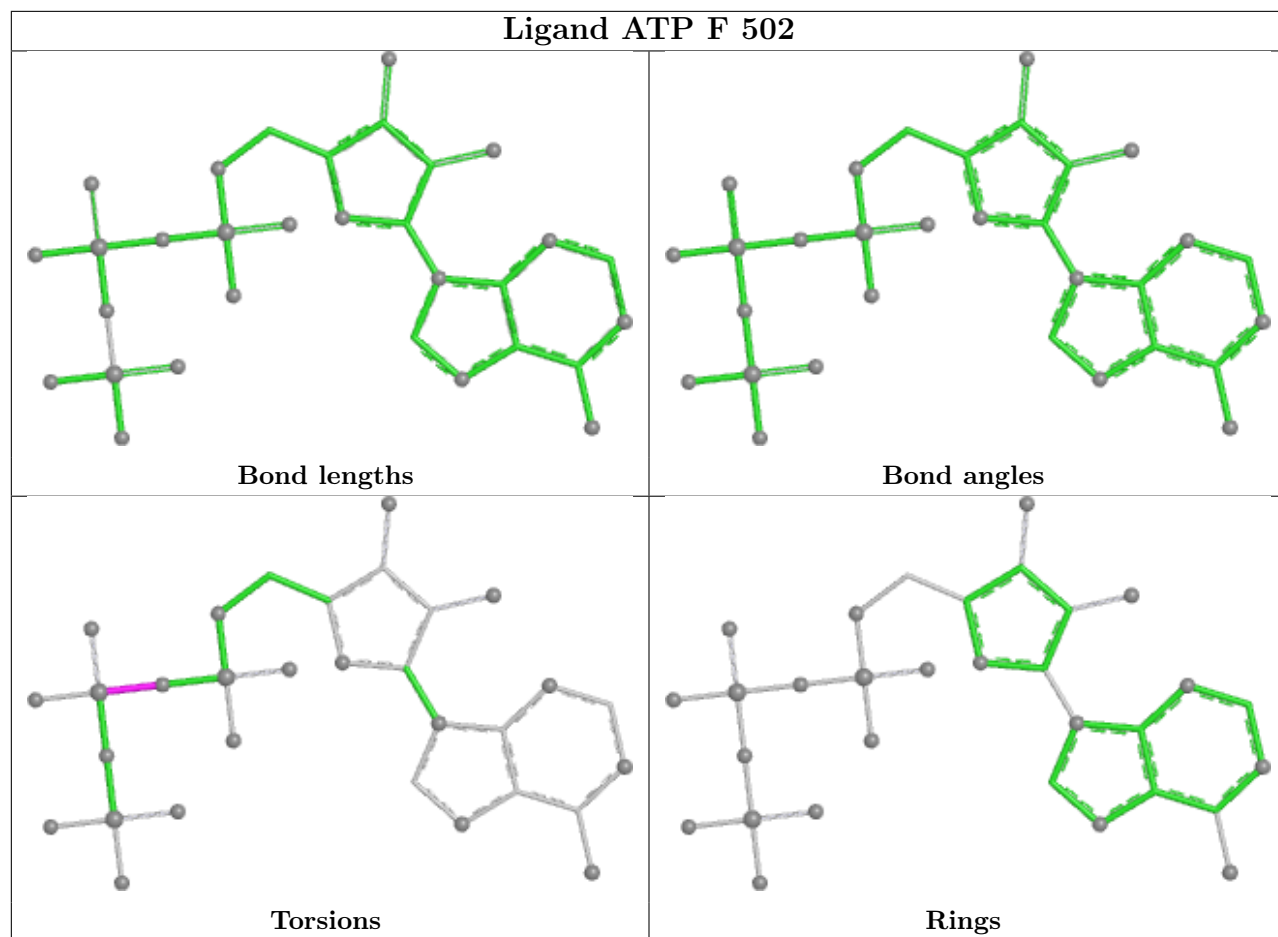


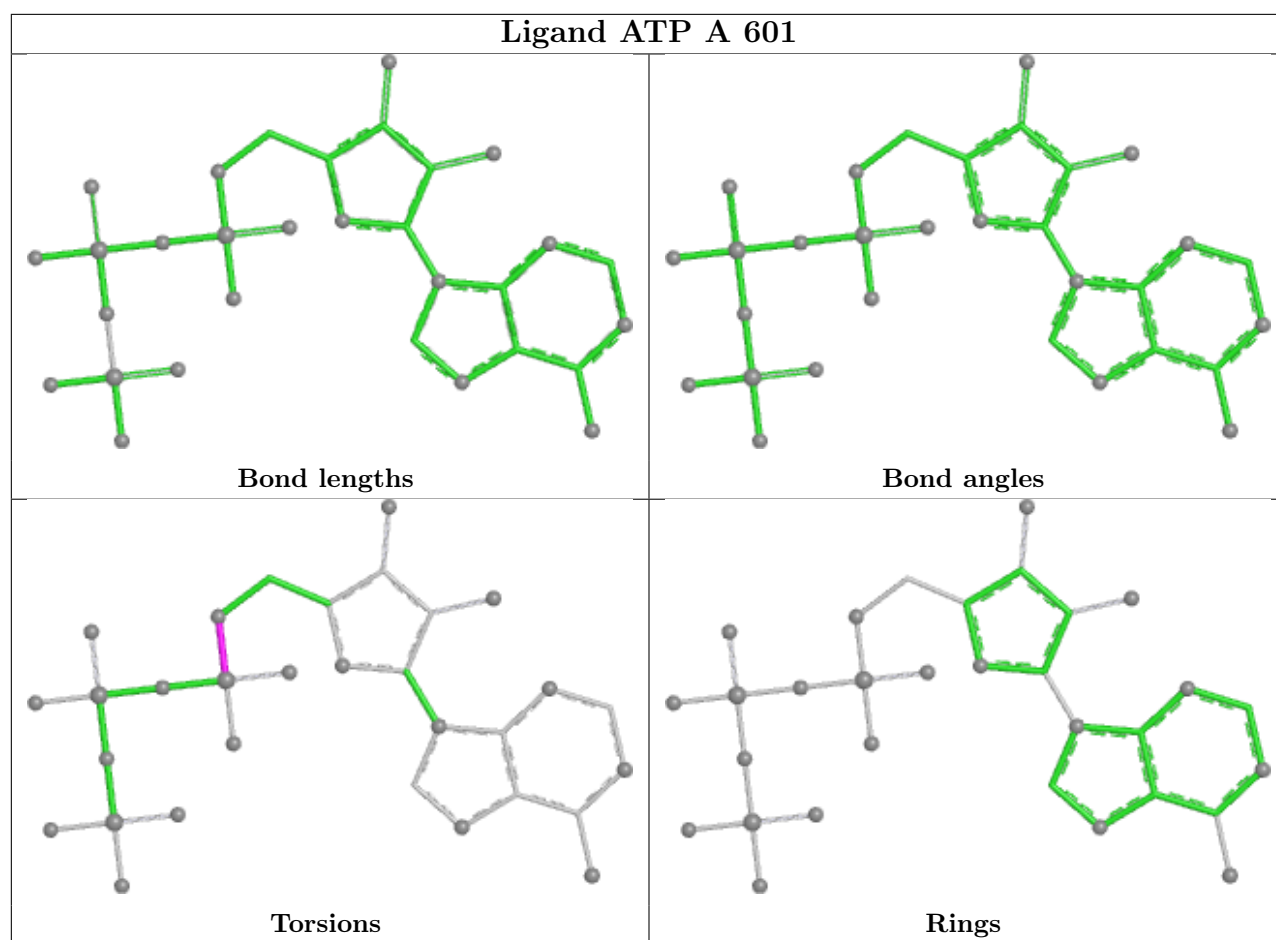
Ligand ATP C 601



Ligand ADP D 601







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.

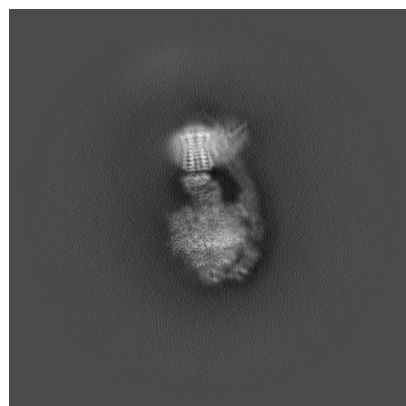
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71580. These allow visual inspection of the internal detail of the map and identification of artifacts.

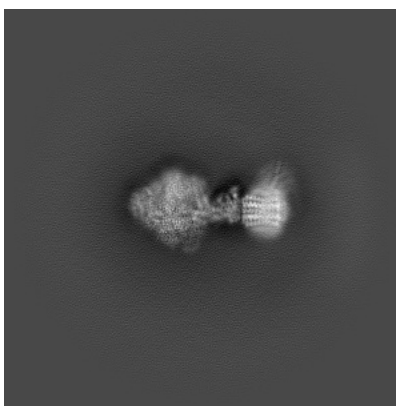
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

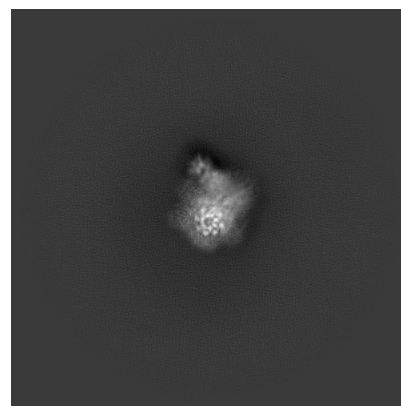
6.1.1 Primary map



X

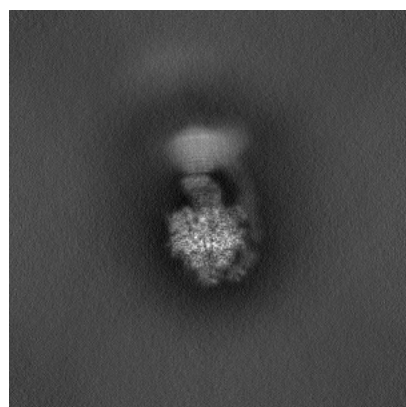


Y

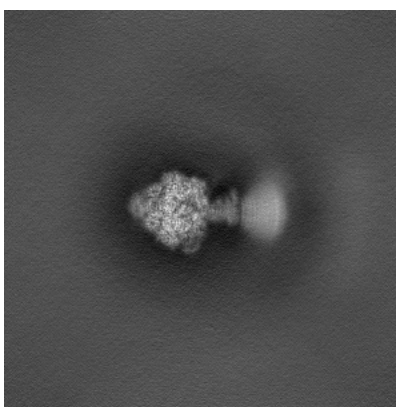


Z

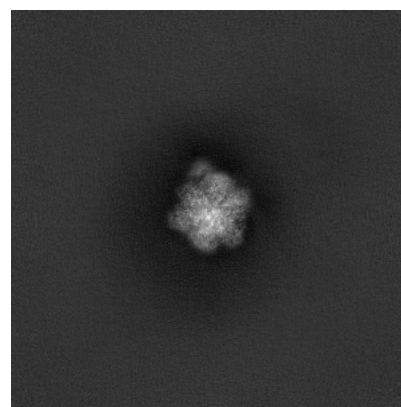
6.1.2 Raw map



X



Y

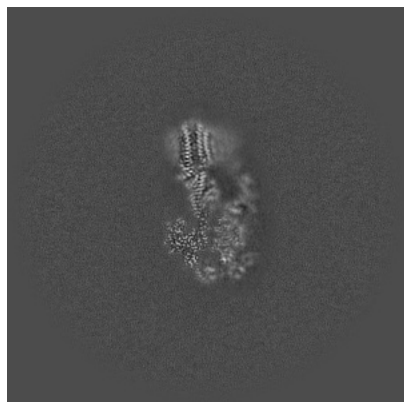


Z

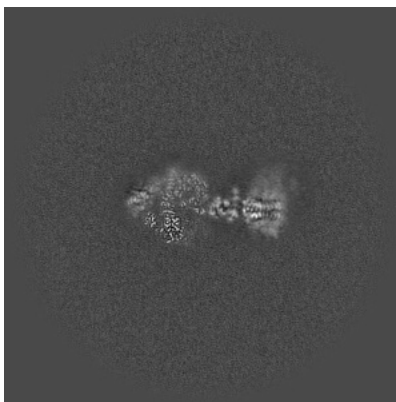
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

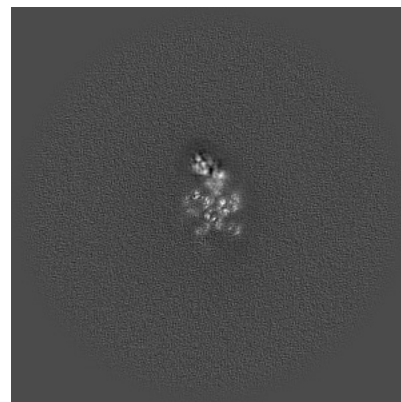
6.2.1 Primary map



X Index: 256



Y Index: 256

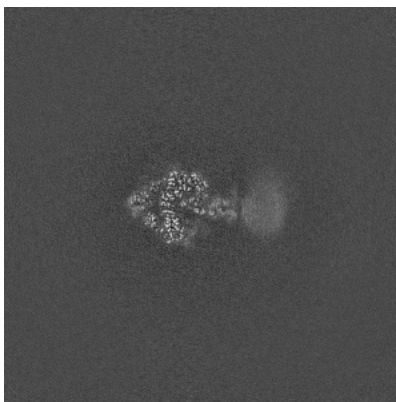


Z Index: 256

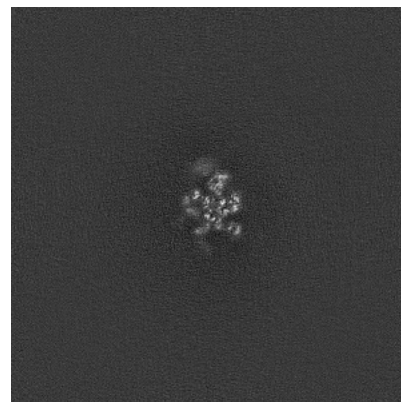
6.2.2 Raw map



X Index: 256



Y Index: 256

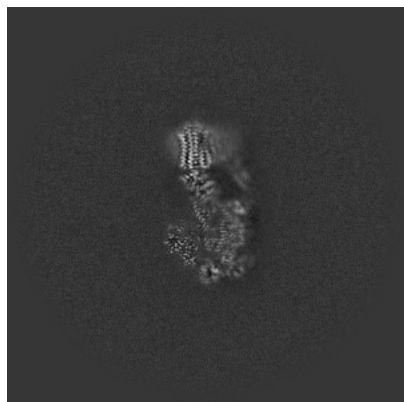


Z Index: 256

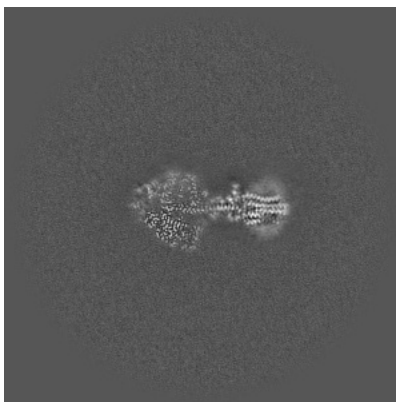
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

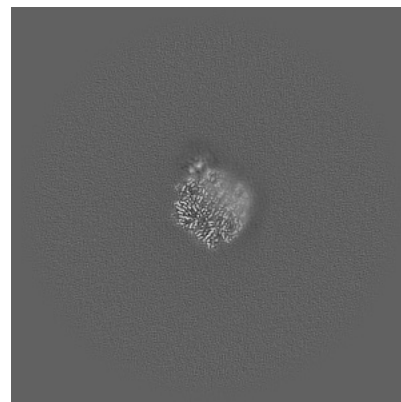
6.3.1 Primary map



X Index: 260



Y Index: 247

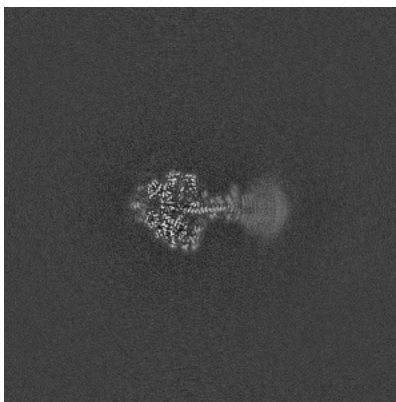


Z Index: 212

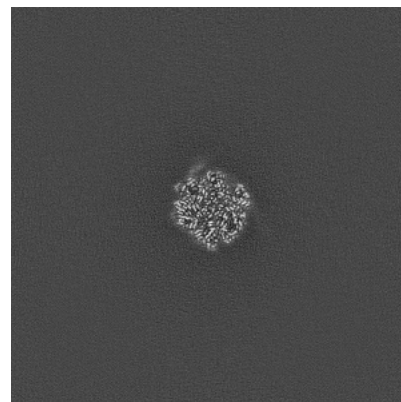
6.3.2 Raw map



X Index: 257



Y Index: 246



Z Index: 212

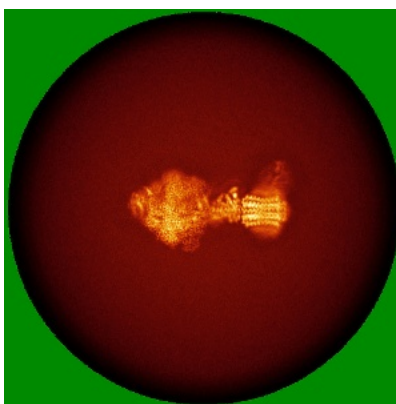
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

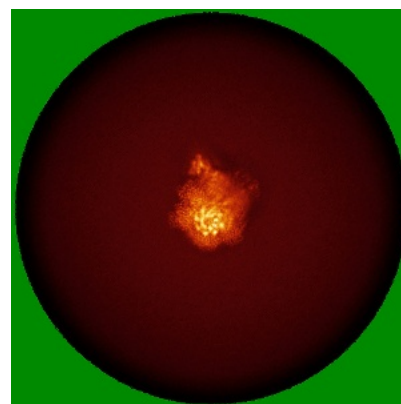
6.4.1 Primary map



X



Y

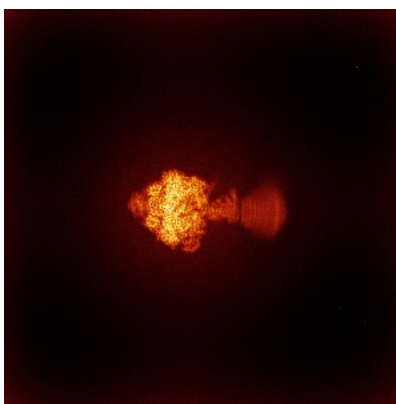


Z

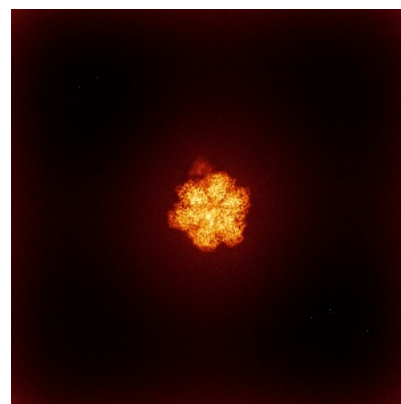
6.4.2 Raw map



X



Y

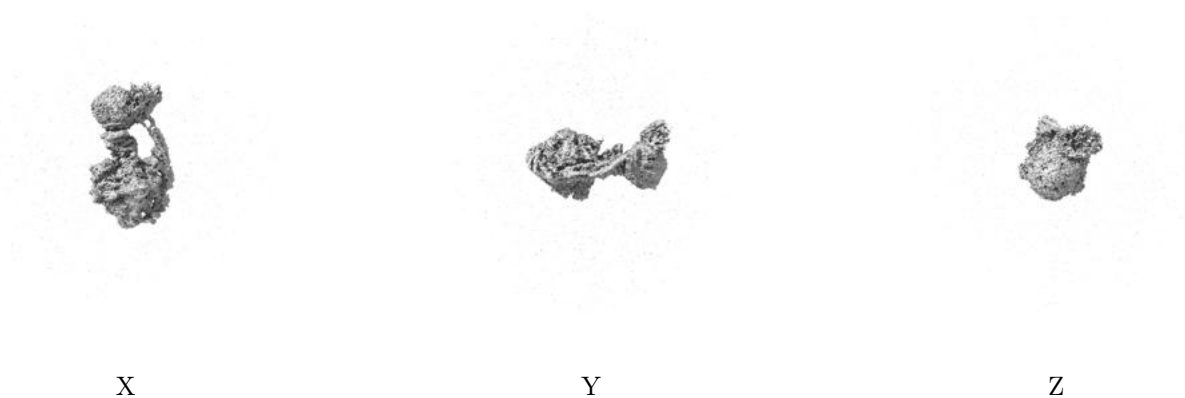


Z

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.

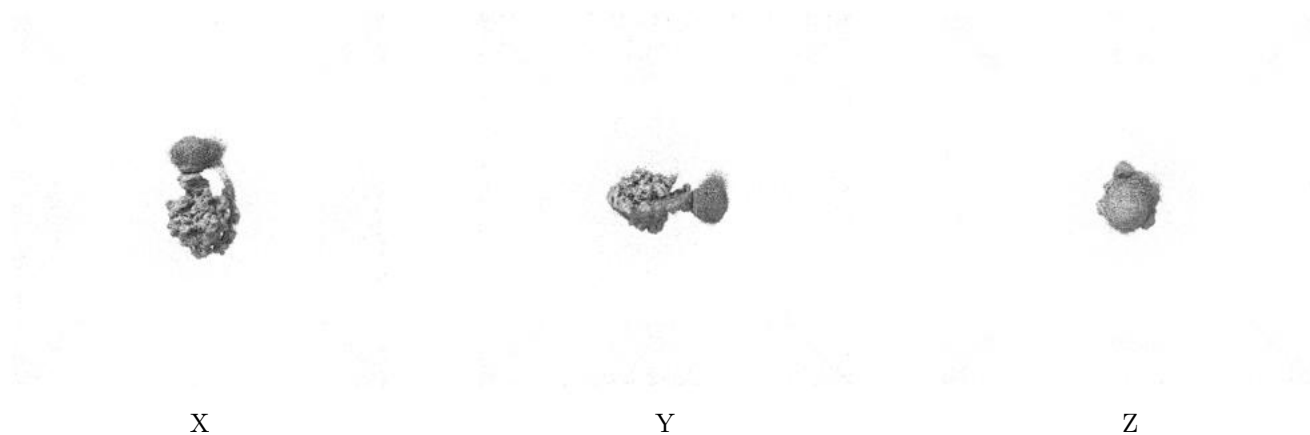
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.1. 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



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.

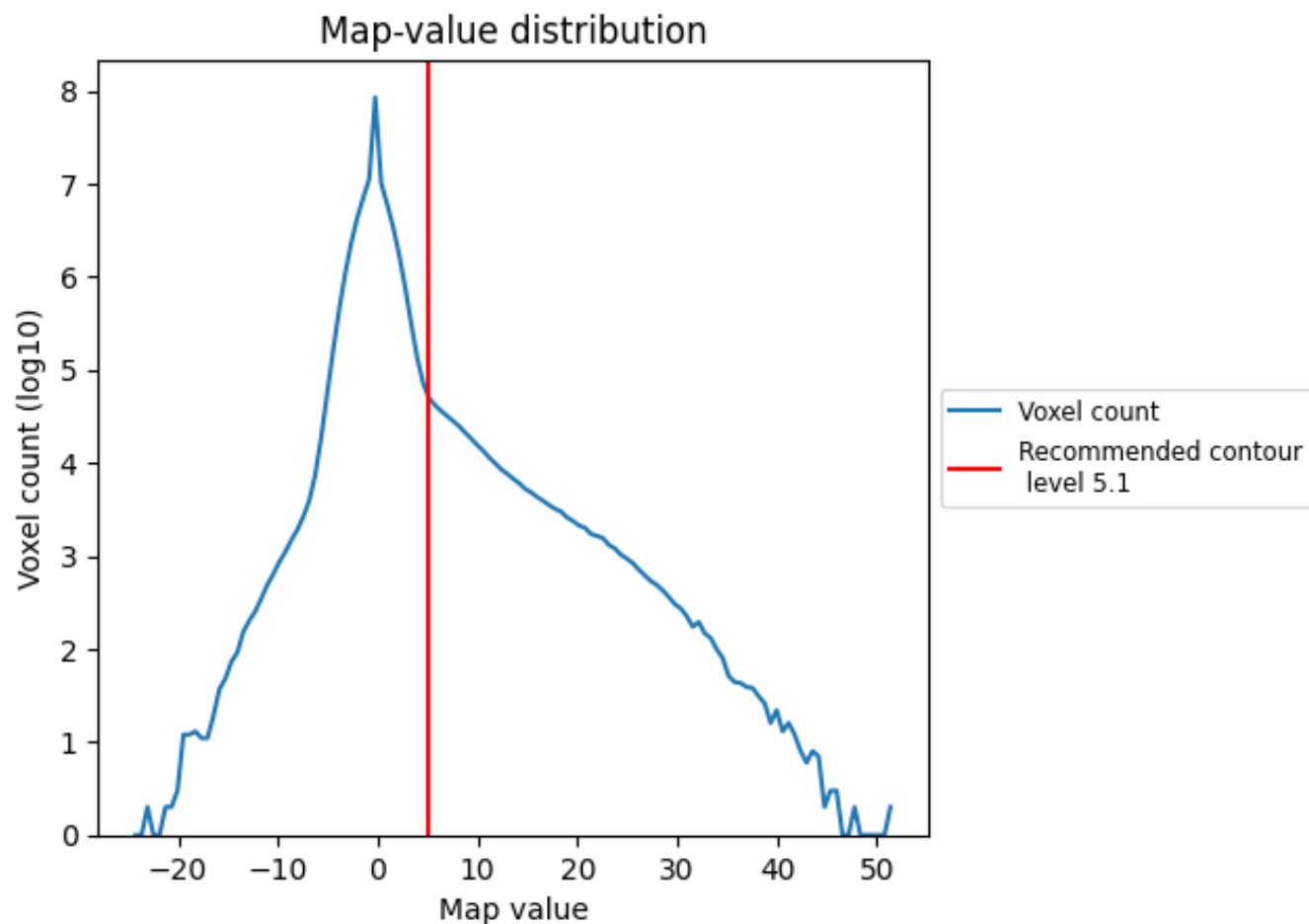
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

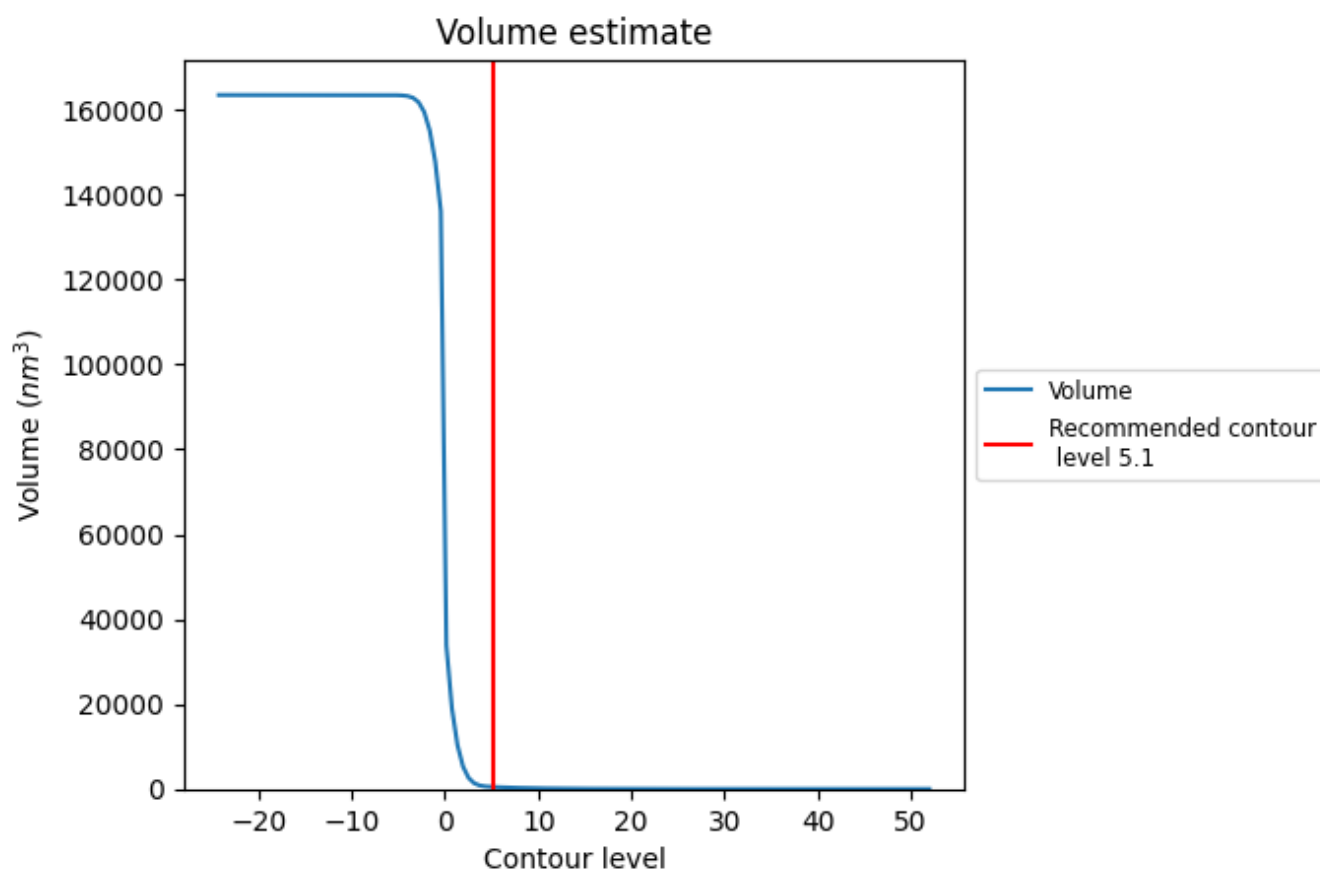
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

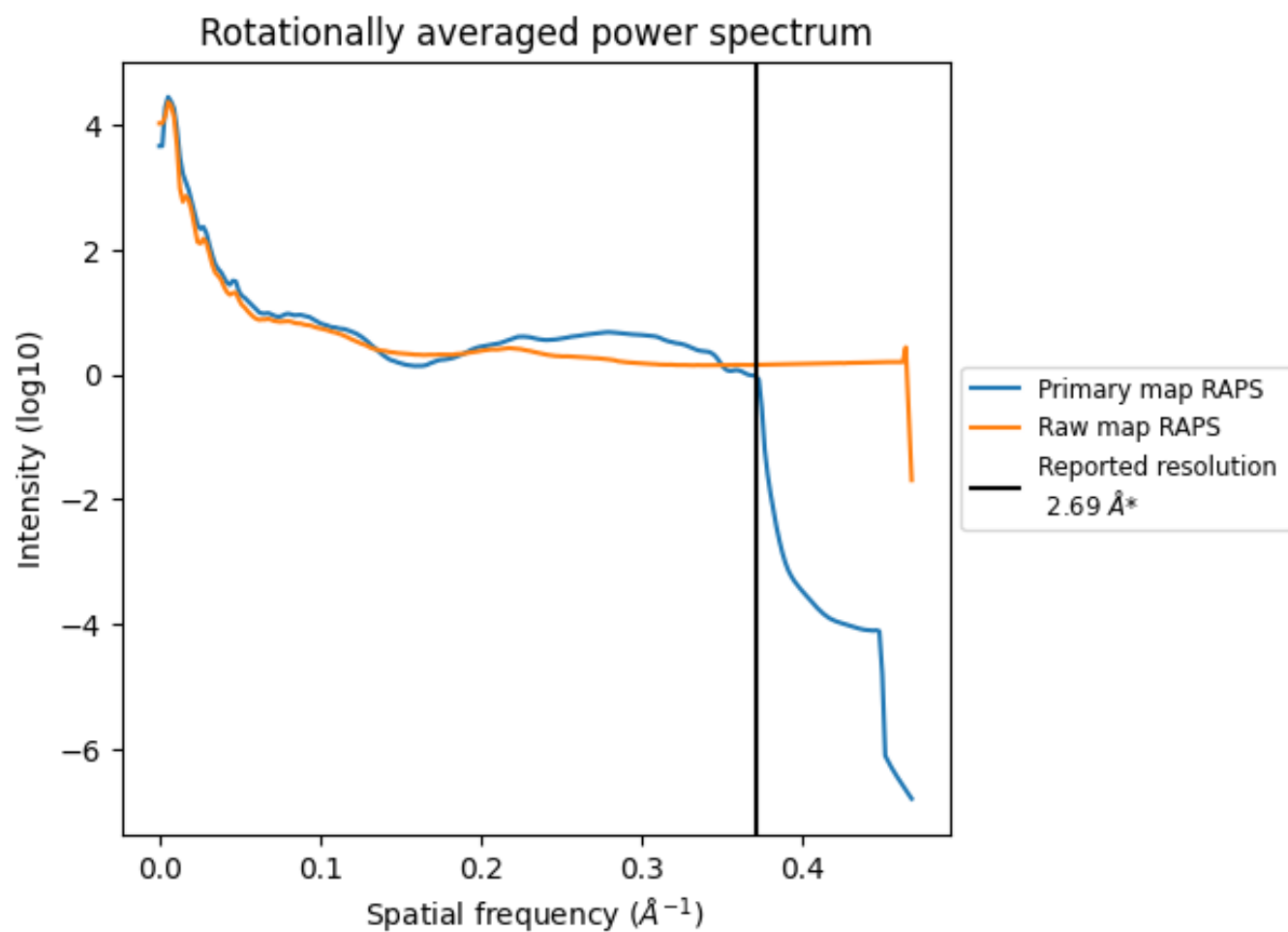
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 476 nm^3 ; this corresponds to an approximate mass of 430 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

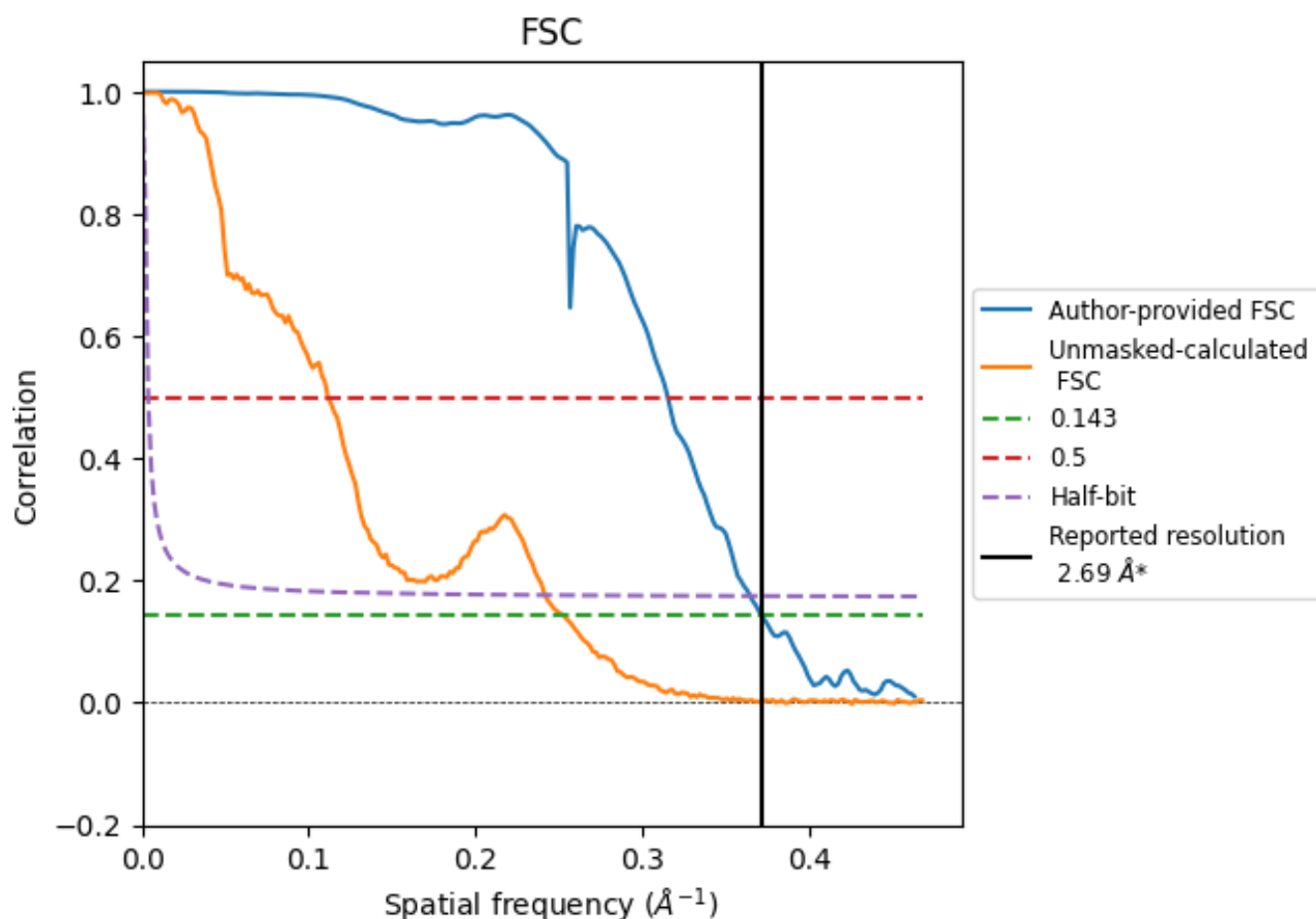


*Reported resolution corresponds to spatial frequency of 0.372 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.372 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

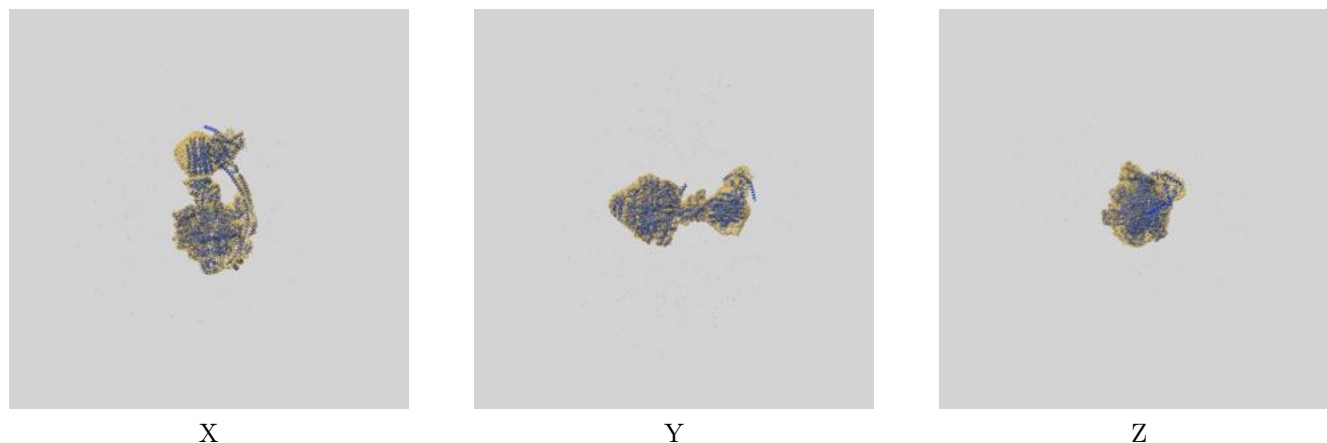
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	3.17	2.74
Unmasked-calculated*	3.96	8.97	4.13

*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 3.96 differs from the reported value 2.69 by more than 10 %

9 Map-model fit [i](#)

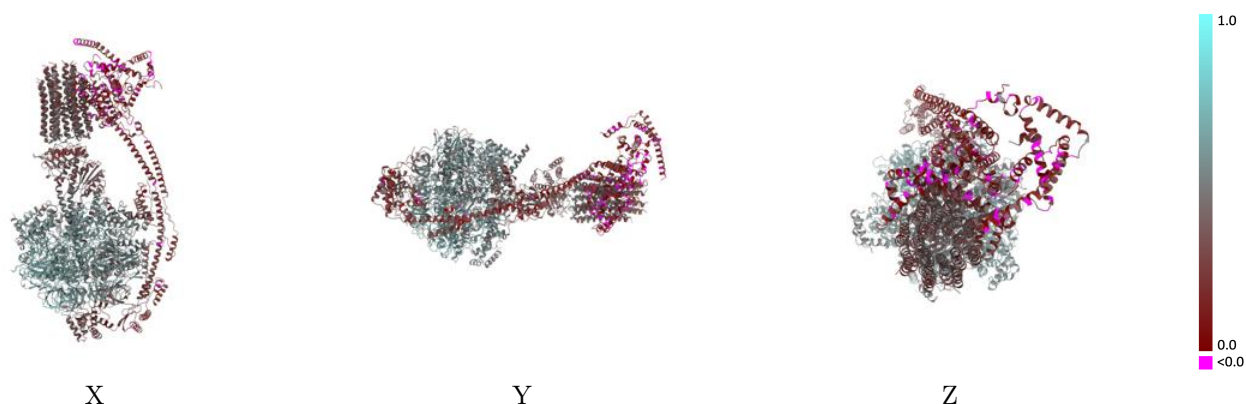
This section contains information regarding the fit between EMDB map EMD-71580 and PDB model 9PEW. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



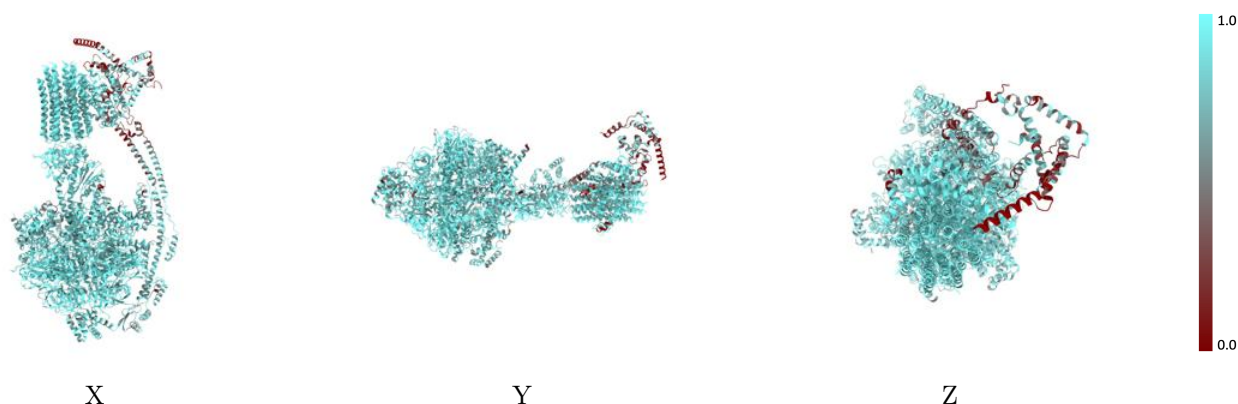
The images above show the 3D surface view of the map at the recommended contour level 5.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



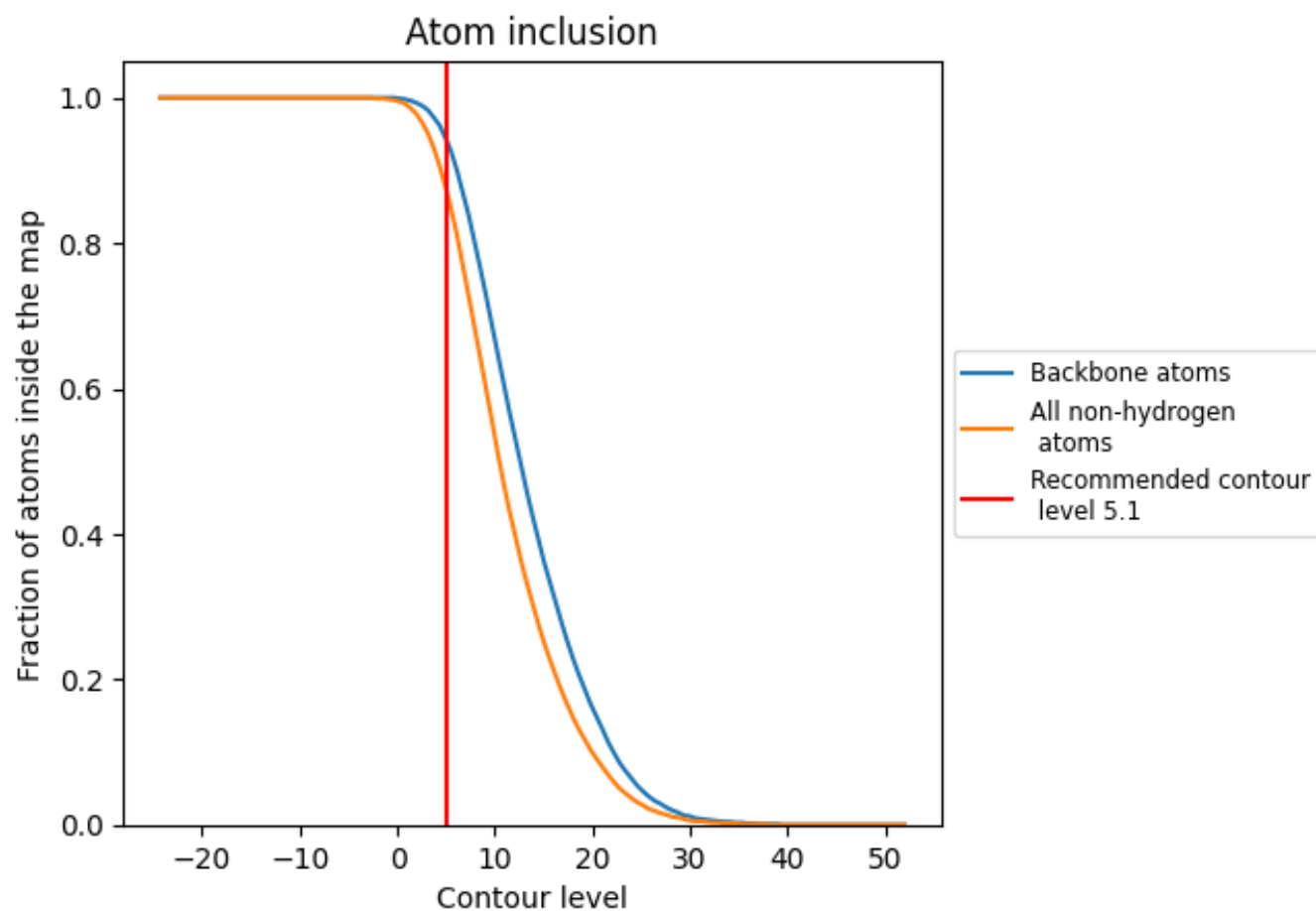
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (5.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.4440
1	 0.9540	 0.3470
2	 0.9480	 0.3530
3	 0.9320	 0.3510
4	 0.9580	 0.3640
5	 0.9600	 0.3820
6	 0.9340	 0.3880
7	 0.9360	 0.3620
8	 0.9440	 0.3420
A	 0.9020	 0.4770
B	 0.9070	 0.5660
C	 0.8840	 0.5770
D	 0.9470	 0.5330
E	 0.9030	 0.5880
F	 0.9490	 0.6080
G	 0.9040	 0.4290
H	 0.9210	 0.3540
I	 0.9360	 0.3660
J	 0.7020	 0.5070
K	 0.7080	 0.1850
L	 0.8680	 0.2710
M	 0.6740	 0.2180
N	 0.8440	 0.1400
O	 0.8120	 0.3240
Q	 0.8690	 0.1670
R	 0.5490	 0.1260
S	 0.4320	 0.1540
T	 0.2030	 0.1410

