



wwPDB EM Validation Summary Report ⓘ

May 13, 2025 – 08:51 AM EDT

PDB ID : 9AZP / pdb_00009azp
EMDB ID : EMD-44018
Title : INF2 at the Barbed End of F-Actin with Incoming Profilin-Actin
Authors : Palmer, N.J.; Barrie, K.R.; Dominguez, R.
Deposited on : 2024-03-11
Resolution : 3.79 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

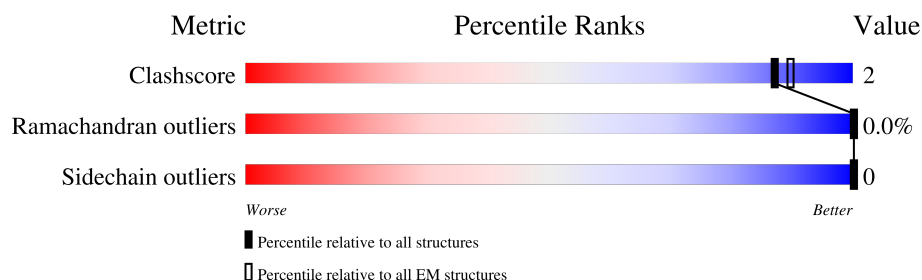
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.79 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.



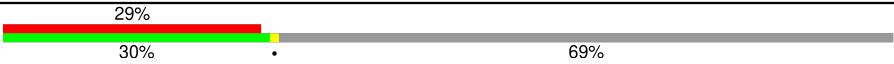

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	371	
1	B	371	
1	C	371	
1	D	371	
1	E	371	
1	F	371	
1	I	371	
2	G	1249	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	1249	
3	J	139	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27674 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	B	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	C	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	D	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	E	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	F	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		
1	I	371	Total	C	N	O	S	0	0
			2900	1837	489	553	21		

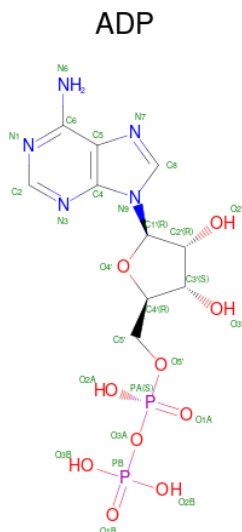
- Molecule 2 is a protein called Inverted formin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	382	Total	C	N	O	S	0	0
			3057	1928	536	580	13		
2	H	384	Total	C	N	O	S	0	0
			3071	1937	539	582	13		

- Molecule 3 is a protein called Profilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	139	Total	C	N	O	S	0	0
			1046	657	180	202	7		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0
4	E	1	Total 27	C 10	N 5	O 10	P 2	0
4	F	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

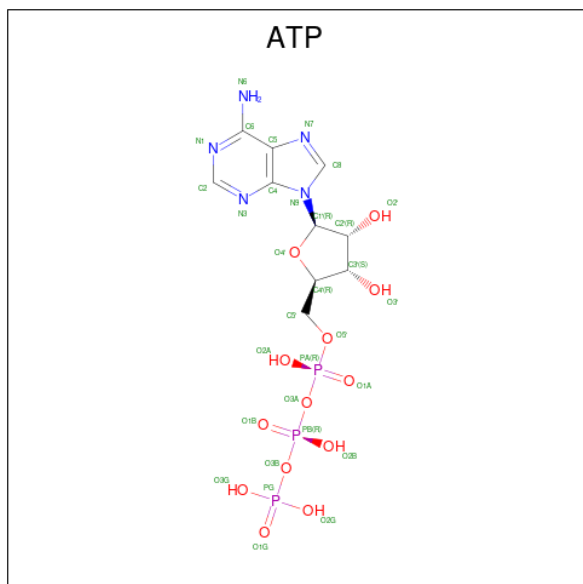
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Mg 1 1	0
5	B	1	Total Mg 1 1	0
5	C	1	Total Mg 1 1	0
5	D	1	Total Mg 1 1	0
5	E	1	Total Mg 1 1	0
5	F	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	I	1	1	1	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

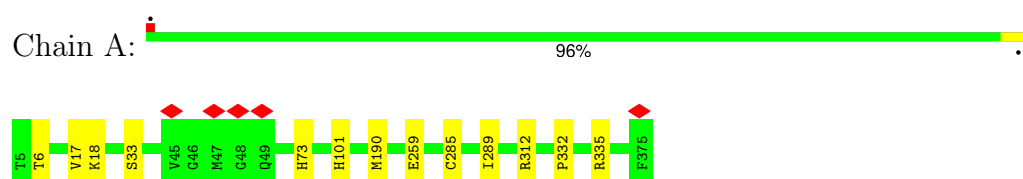


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	I	1	31	10	5	13	3	0

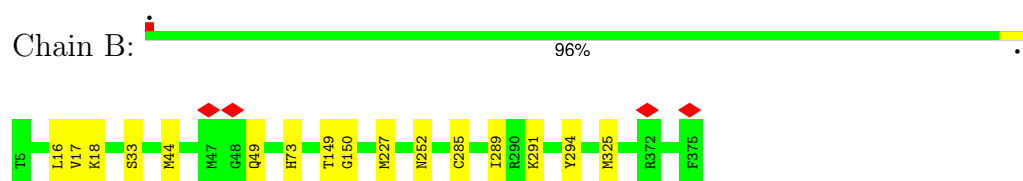
3 Residue-property plots

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

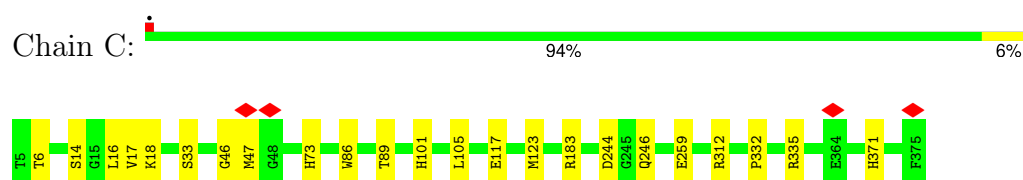
- Molecule 1: Actin, alpha skeletal muscle



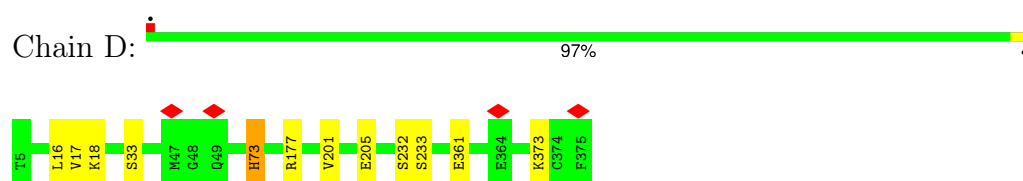
- Molecule 1: Actin, alpha skeletal muscle



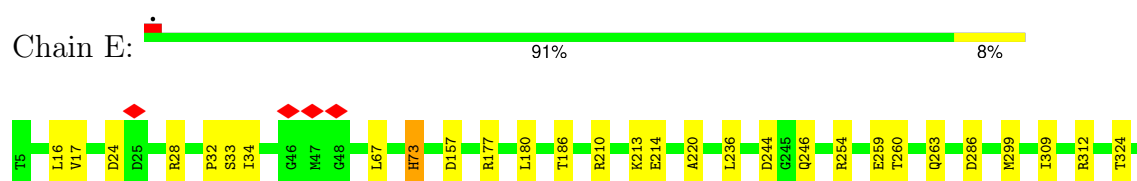
- Molecule 1: Actin, alpha skeletal muscle

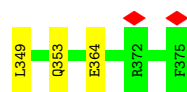


- Molecule 1: Actin, alpha skeletal muscle

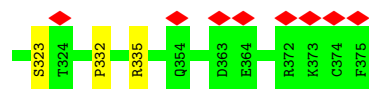


- Molecule 1: Actin, alpha skeletal muscle

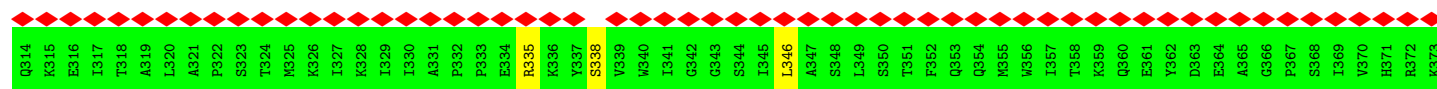
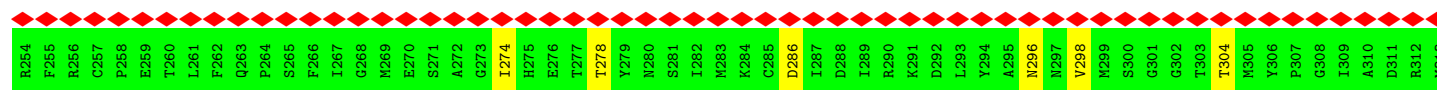
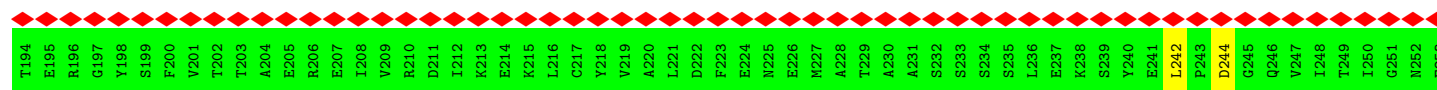
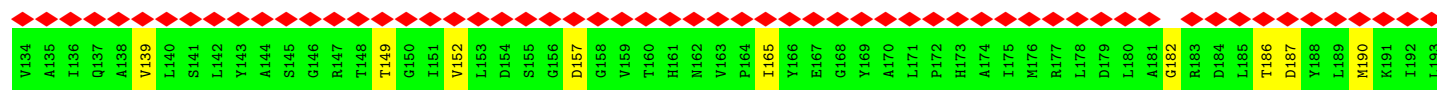
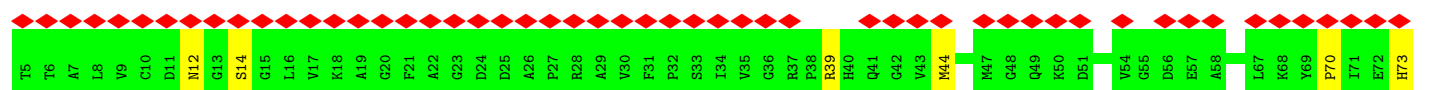
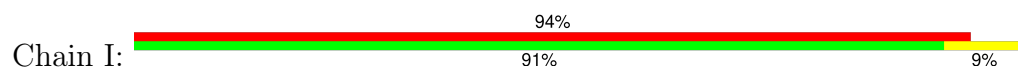




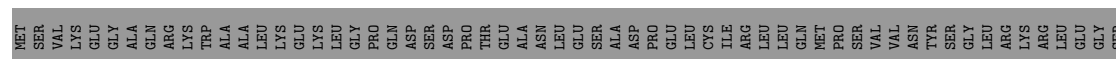
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Inverted formin-2





SER	SER	GLY	SER	GLY	THR	LEU	PRO	ARG	ALA	ARG	GLY	ARG	ALA	SER	LYS	GLY	THR	GLY	LYS	ARG	LYS	LYS	ARG	PRO	SER	ARG	GLN	GLU	GLU	VAL	PRO	PRO	ASP	SER	ASP	ASN	LYS	THR	LYS	LYS	LEU	CYS	VAL	LE	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----

- Molecule 2: Inverted formin-2



ASP	GLY	GLY	TRP	MET	VAL	GLN	PHE	LEU	GLU	GLN	SER	GLY	LEU	ASP	ARG	ALA	GLU	ALA	ARG	GLY	VAL	VAL	ALA	ALA	LEU	GLN	THR	CYS	VAL	SER	CYS	VAL	ASP	GLY	SER	GLY	LEU	GLU	GLN	THR	TYR	GLU	ILE	LEU	LEU	FEA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN	GLN	GLY	TYR	VAL	ARG	GLN	LEU	SER	SER	ASN	ASN	VAL	MET	VAL	LYS	LYS	GLN	VAL	PHE	GLU	LEU	ALA	ALA	CYS	ILE	TYR	SER	PRO	GLU	GLY	HIS	VAL	LEU	THR	LEU	ASP	ASP	HIS	CYS	VAL	THR	LYS	TYR	GLN	GLN	ARG	PHE	SER	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	MEI	ASN	GLU	LEU	SER	GLY	SER	ASP	ASN	VAL	PRO	TYR	VAL	VAL	ILE	ASN	ALA	ILE	GLY	GLU	PRO	ASP	LEU	ARG	ALA	THR	GLN	LEU	ARG	GLN	GLU	PHE	ILE	GLY	LEU	GLN	LEU	LEU	ASP	VAL	ALA	LEU	ARG	LEU	LEU	ASP	ASP	ALA	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LEU	LEU	LEU	GLN	LEU	GLU	ALA	PHE	GLU	GLU	ALA	LYS	ALA	ASP	GLU	GLU	GLU	LEU	LEU	ARG	SER	SER	GLY	GLY	VAL	ASP	MET	SER	SER	HIS	GLN	GLU	VAL	PHE	ALA	SER	SER	CYS	SER	PRO	VAL	SER	SER	VAL	LEU	LEU	GLN	GLY	LEU	LEU	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LEU	GLU	PRO	THR	LEU	ARG	SER	SER	GLN	LEU	LEU	TRP	GLU	ALA	LEU	GLU	SER	LEU	VAL	ASN	ARG	ALA	VAL	LEU	ALA	SER	ASP	GLN	GLU	CYS	THR	LEU	GLU	GLY	VAL	VAL	GLU	ARG	LEU	LEU	SER	VAL	GLY	LYS	ARG	PRO	ARG	PRO	SER	PRO	LEU	VAL	LYS	ALA	HIS	LYS	SER	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLN	ALA	ASN	LEU	ASP	GLN	SER	GLN	ARG	GLY	SER	SER	PRO	GLN	ASN	THR	THR	PRO	LYS	PRO	SER	VAL	GLU	GLY	GLN	GLN	PRO	ALA	ALA	ALA	ALA	CYS	GLU	PRO	VAL	ASP	HIS	ALA	GLN	SER	GLU	SER	ILE	LEU	LYS	VAL	SER	PRO	ARG	ALA	ALA	LEU	GLU	GLN	ALA	SER	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible][illegible]

CLN	VAL	ASP	HIS	GLY	LEU	GLY	SER	ALA	TRP
V551	P552	S553	H554	R555	R556	V557	N558	P559	T560
L562	R563	K564	K565	K566	L567	N568	M569	Q570	K571
L572	P573	S574	N575	V576	A577	R578	E579	H580	N581
S582	M583	A584	A585	S586	L587	S588	S589	P590	D591
A592	E593	A594	V595	E596	E597	D598	F599	G600	

S601	I602	E603	B604	L605	F606	S607	F608	P609	A610	A611	L612	P613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	F632	L633	L634	D635	A636	K637	S638	L639	L640	L641	M642	L643	F644	L645	K646	Q647	F648	K649	C650	S651	M652	E653	E654	V655	A656	A657	M658	L659	R660	A661
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

G662	D663	T664	T665	G666	F667	D668	V669	E670	V671	L675	L676	K677	L678	L679	P680	E681	K682	H683	E684	E685	E686	N687	L688	R689	A690	F691	T692	E693	E694	R695	A696	K697	L698	A699	S700	A701	D702	H703	F704	L705	L706	L707	L708	L709	A710	L711	F712	G713	L714	Q715	L716	L717	L718	E719	G720	C721	L722
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

E725	G726	A727	A728	A729	D732	M733	V734	R735	P736	K737	A738	V741	L742	A743	A744	E745	C746	S747	L748	L749	T750	S751	R752	Q753	L754	P755	T756	F757	C758	Q759	L760	T761	L762	R763	T764	G765	M766	F767	L768	M769	Y770	G771	S772	H773	T774	G775	D776	A777	D778	G779	F780	K781	T782	T784	L785	L786
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

K787	L788	T789	E790	T791	K792	S793	Q794	Q795	M796	T797	T798	L800	L801	H802	H803	V804	L805	E806	E807	A808	E809	K810	S811	H812	H813	D814	L815	L816	Q817	L818	P819	R820	D821	L822	E823	Q824	P825	S826	Q827	A828	A829	G830	T831	M832	L833	P834	T835	T836	H837	R838	E839	A840	S841	S842	M843	L844	K845	K846
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.614	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.164	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/2950	0.52	1/3994 (0.0%)
1	B	0.25	0/2950	0.55	0/3994
1	C	0.23	0/2950	0.53	3/3994 (0.1%)
1	D	0.24	0/2950	0.55	0/3994
1	E	0.26	0/2950	0.61	1/3994 (0.0%)
1	F	0.24	0/2950	0.57	1/3994 (0.0%)
1	I	0.31	0/2950	0.69	0/3994
2	G	0.32	0/3104	0.61	1/4182 (0.0%)
2	H	0.29	0/3118	0.62	3/4200 (0.1%)
3	J	0.31	0/1064	0.65	0/1437
All	All	0.27	0/27936	0.59	10/37777 (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	E	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	736	PRO	CA-N-CD	-9.22	99.09	112.00
1	F	44	MET	CB-CG-SD	6.64	132.61	112.70
2	H	658	MET	CA-CB-CG	6.33	126.77	114.10
1	C	47	MET	CA-CB-CG	5.68	125.45	114.10
1	E	364	GLU	N-CA-CB	5.48	118.02	110.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	324	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2900	0	2871	6	0
1	B	2900	0	2871	9	0
1	C	2900	0	2872	10	0
1	D	2900	0	2871	8	0
1	E	2900	0	2872	16	0
1	F	2900	0	2871	12	0
1	I	2900	0	2872	18	0
2	G	3057	0	3109	15	0
2	H	3071	0	3127	5	0
3	J	1046	0	1048	10	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	0	0
4	D	27	0	12	2	0
4	E	27	0	12	1	0
4	F	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
6	I	31	0	12	0	0
All	All	27674	0	27468	104	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 2.

The worst 5 of 104 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)
3:J:77:LEU:HD13	3:J:85:MET:HB2	1.82	0.61
2:G:660:ARG:NH1	2:G:660:ARG:O	2.36	0.58
1:I:88:HIS:HD2	1:I:92:ASN:HB2	1.71	0.56
3:J:18:ASP:HB3	3:J:113:MET:HB3	1.89	0.55
1:F:323:SER:O	2:H:737:LYS:NZ	2.38	0.55

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	368/371 (99%)	353 (96%)	15 (4%)	0	100	100
1	B	368/371 (99%)	353 (96%)	15 (4%)	0	100	100
1	C	368/371 (99%)	354 (96%)	14 (4%)	0	100	100
1	D	368/371 (99%)	355 (96%)	13 (4%)	0	100	100
1	E	368/371 (99%)	354 (96%)	14 (4%)	0	100	100
1	F	368/371 (99%)	355 (96%)	13 (4%)	0	100	100
1	I	368/371 (99%)	362 (98%)	5 (1%)	1 (0%)	37	69
2	G	378/1249 (30%)	371 (98%)	7 (2%)	0	100	100
2	H	380/1249 (30%)	367 (97%)	13 (3%)	0	100	100
3	J	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
All	All	3471/5234 (66%)	3357 (97%)	113 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	44	MET

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	313/313 (100%)	313 (100%)	0	100	100
1	B	313/313 (100%)	313 (100%)	0	100	100
1	C	313/313 (100%)	313 (100%)	0	100	100
1	D	313/313 (100%)	313 (100%)	0	100	100
1	E	313/313 (100%)	313 (100%)	0	100	100
1	F	313/313 (100%)	313 (100%)	0	100	100
1	I	313/313 (100%)	313 (100%)	0	100	100
2	G	336/1057 (32%)	336 (100%)	0	100	100
2	H	337/1057 (32%)	337 (100%)	0	100	100
3	J	113/113 (100%)	113 (100%)	0	100	100
All	All	2977/4418 (67%)	2977 (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 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	812	HIS
2	H	827	GLN
2	H	817	GLN
1	I	49	GLN
1	D	263	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	HIC	C	73	1	8,11,12	1.64	2 (25%)	5,14,16	0.93	0
1	HIC	E	73	1	8,11,12	1.63	2 (25%)	5,14,16	0.98	0
1	HIC	F	73	1	8,11,12	1.63	2 (25%)	5,14,16	0.95	0
1	HIC	B	73	1	8,11,12	1.61	2 (25%)	5,14,16	1.05	0
1	HIC	I	73	1	8,11,12	1.63	2 (25%)	5,14,16	0.96	0
1	HIC	D	73	1	8,11,12	1.65	2 (25%)	5,14,16	0.92	0
1	HIC	A	73	1	8,11,12	1.60	2 (25%)	5,14,16	0.97	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
1	HIC	C	73	1	-	2/5/6/8	0/1/1/1
1	HIC	E	73	1	-	2/5/6/8	0/1/1/1
1	HIC	F	73	1	-	0/5/6/8	0/1/1/1
1	HIC	B	73	1	-	2/5/6/8	0/1/1/1
1	HIC	I	73	1	-	0/5/6/8	0/1/1/1
1	HIC	D	73	1	-	2/5/6/8	0/1/1/1
1	HIC	A	73	1	-	3/5/6/8	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	HIC	CD2-CG	3.58	1.41	1.36
1	E	73	HIC	CD2-CG	3.57	1.41	1.36
1	C	73	HIC	CD2-CG	3.54	1.41	1.36
1	F	73	HIC	CD2-CG	3.54	1.41	1.36
1	I	73	HIC	CD2-CG	3.53	1.41	1.36

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	CA-CB-CG-ND1
1	A	73	HIC	CA-CB-CG-CD2
1	B	73	HIC	CA-CB-CG-ND1
1	B	73	HIC	CA-CB-CG-CD2
1	C	73	HIC	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	73	HIC	1	0
1	D	73	HIC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\# Z > 2$
4	ADP	D	401	5	24,29,29	0.80	0	29,45,45	1.31	2 (6%)
4	ADP	C	401	5	24,29,29	0.84	0	29,45,45	1.19	2 (6%)
4	ADP	F	401	5	24,29,29	0.89	0	29,45,45	1.24	3 (10%)
6	ATP	I	1001	5	28,33,33	0.69	0	34,52,52	0.61	1 (2%)
4	ADP	A	401	5	24,29,29	0.80	0	29,45,45	1.29	2 (6%)
4	ADP	E	401	5	24,29,29	0.86	0	29,45,45	1.20	2 (6%)
4	ADP	B	401	5	24,29,29	0.82	0	29,45,45	1.26	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	401	5	-	2/12/32/32	0/3/3/3
4	ADP	C	401	5	-	4/12/32/32	0/3/3/3
4	ADP	F	401	5	-	5/12/32/32	0/3/3/3
6	ATP	I	1001	5	-	6/18/38/38	0/3/3/3
4	ADP	A	401	5	-	2/12/32/32	0/3/3/3
4	ADP	E	401	5	-	3/12/32/32	0/3/3/3
4	ADP	B	401	5	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	ADP	N3-C2-N1	-4.00	123.24	128.67
4	F	401	ADP	N3-C2-N1	-3.90	123.37	128.67
4	A	401	ADP	N3-C2-N1	-3.87	123.42	128.67
4	C	401	ADP	N3-C2-N1	-3.84	123.46	128.67
4	B	401	ADP	N3-C2-N1	-3.83	123.47	128.67

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

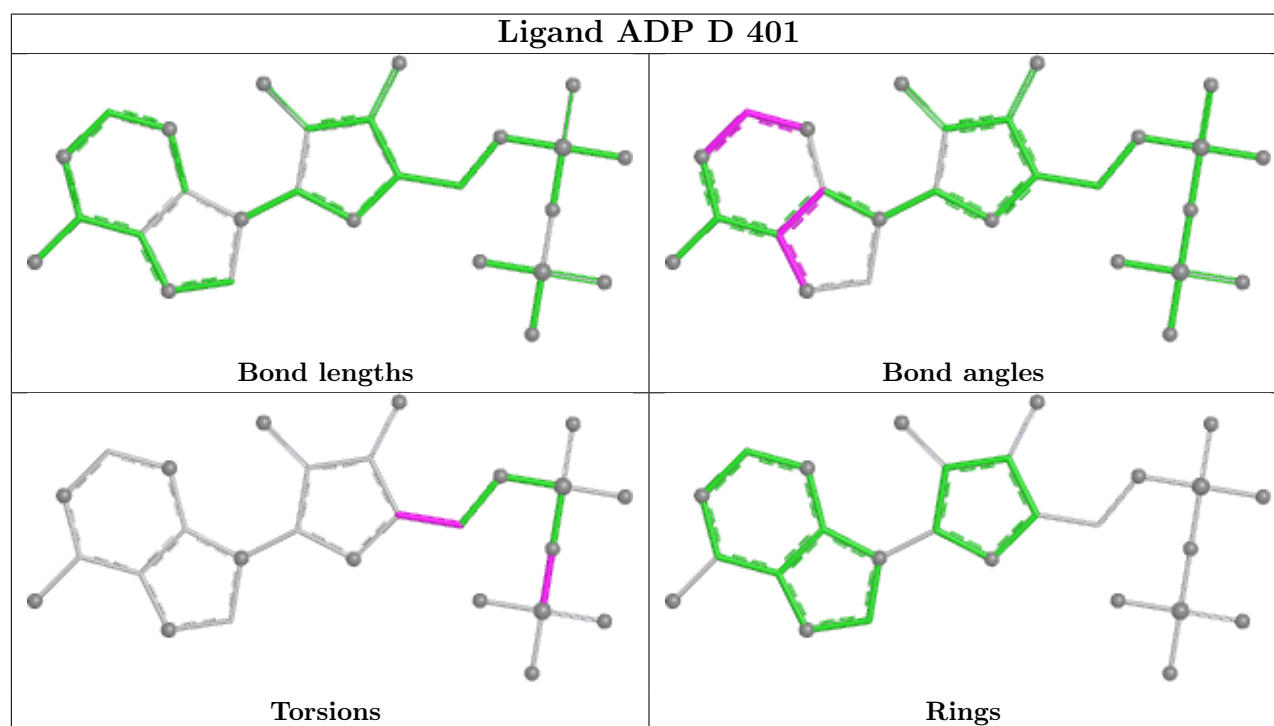
Mol	Chain	Res	Type	Atoms
4	C	401	ADP	C5'-O5'-PA-O1A
4	C	401	ADP	C5'-O5'-PA-O3A
4	D	401	ADP	PA-O3A-PB-O3B
4	E	401	ADP	C5'-O5'-PA-O3A
4	F	401	ADP	PA-O3A-PB-O3B

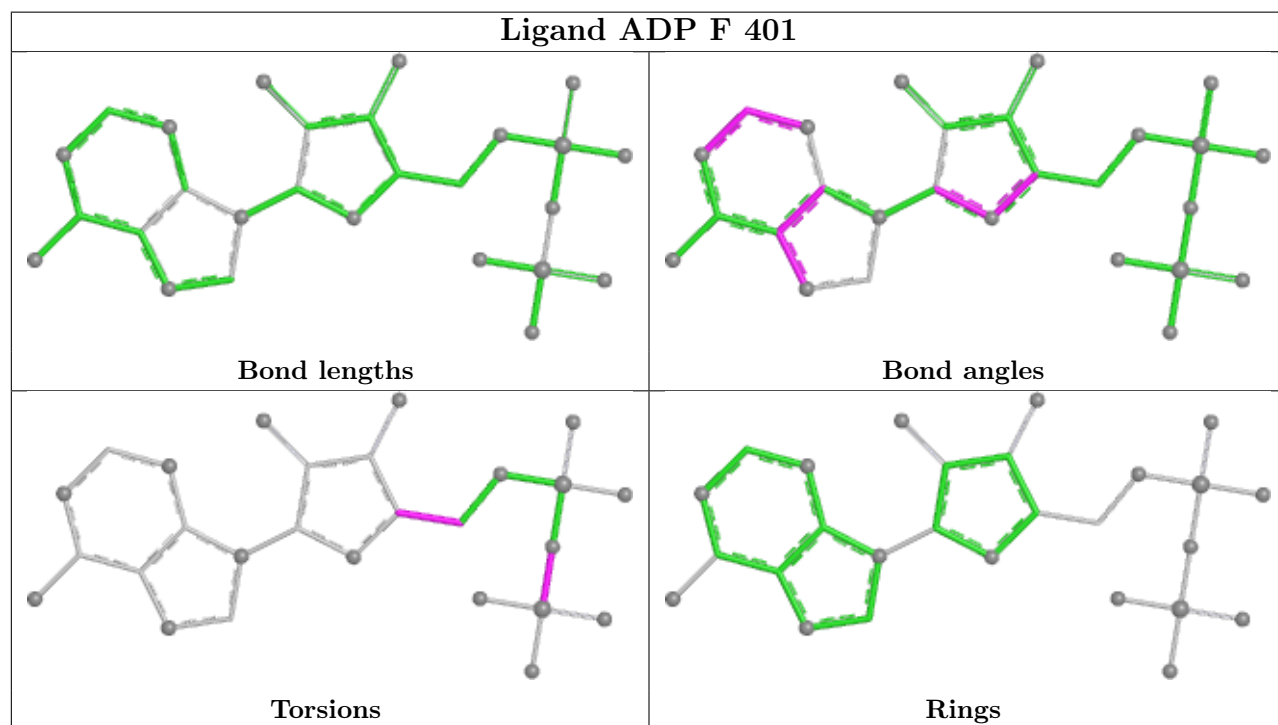
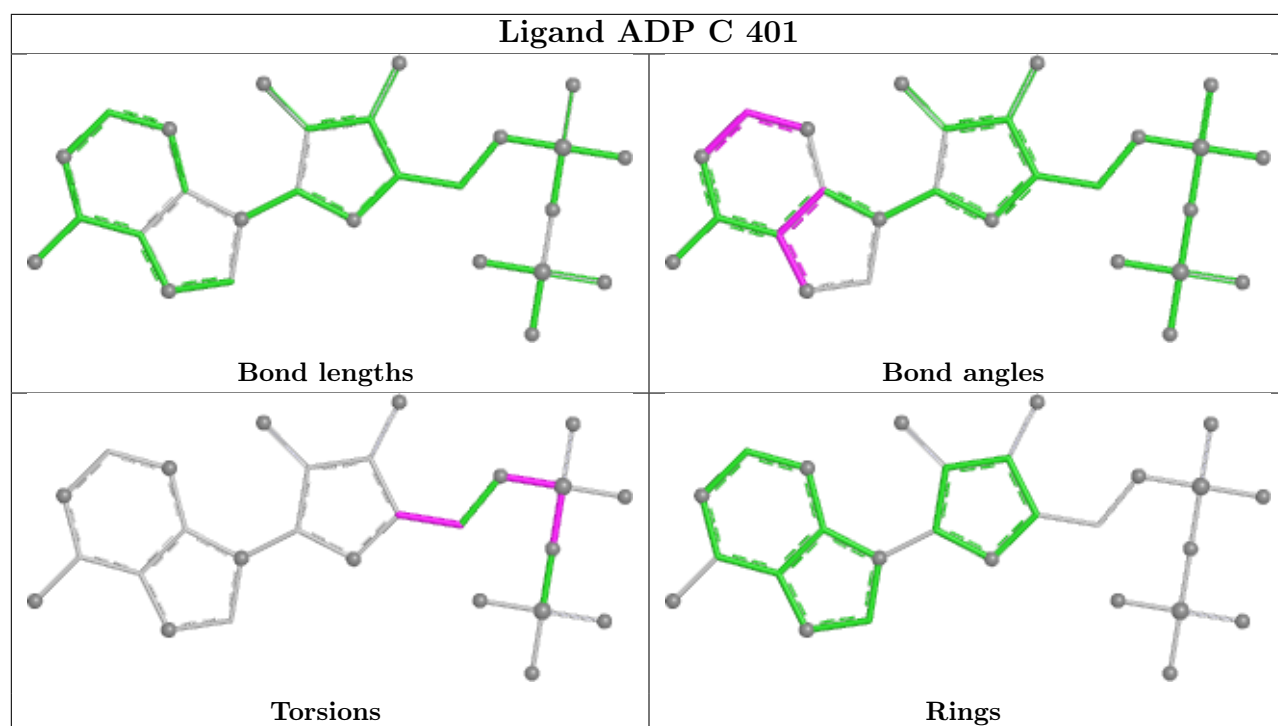
There are no ring outliers.

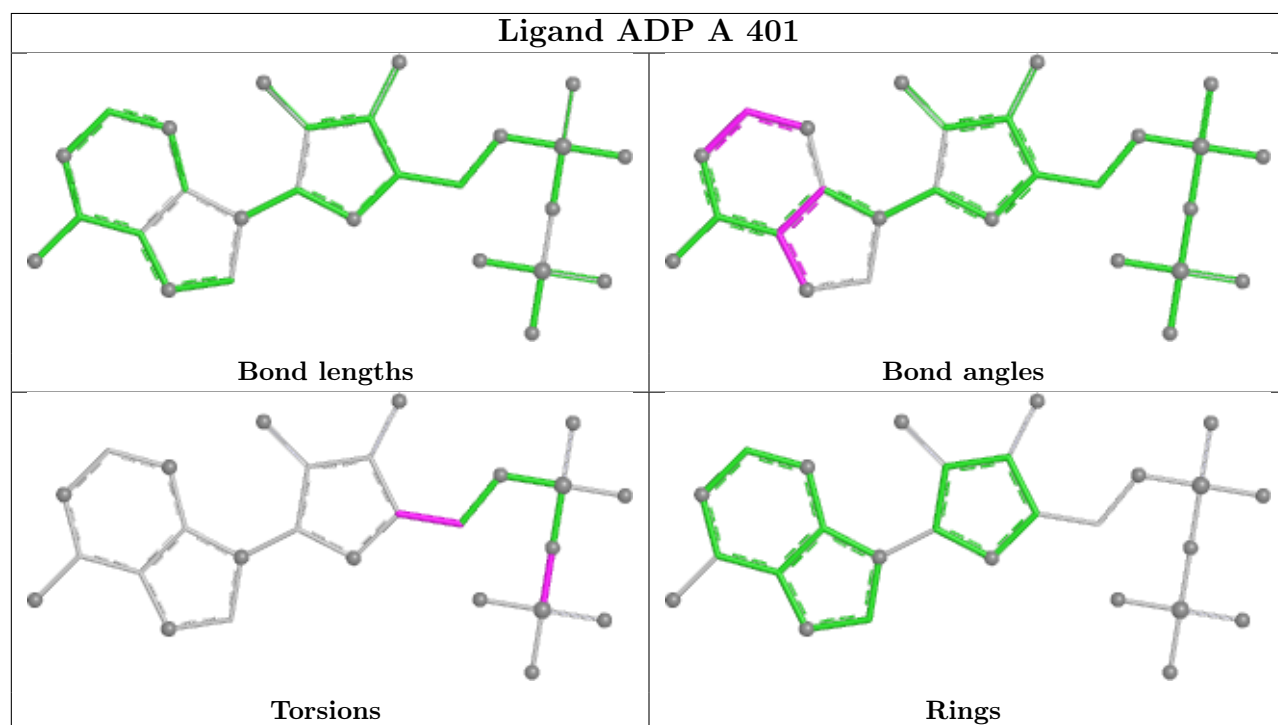
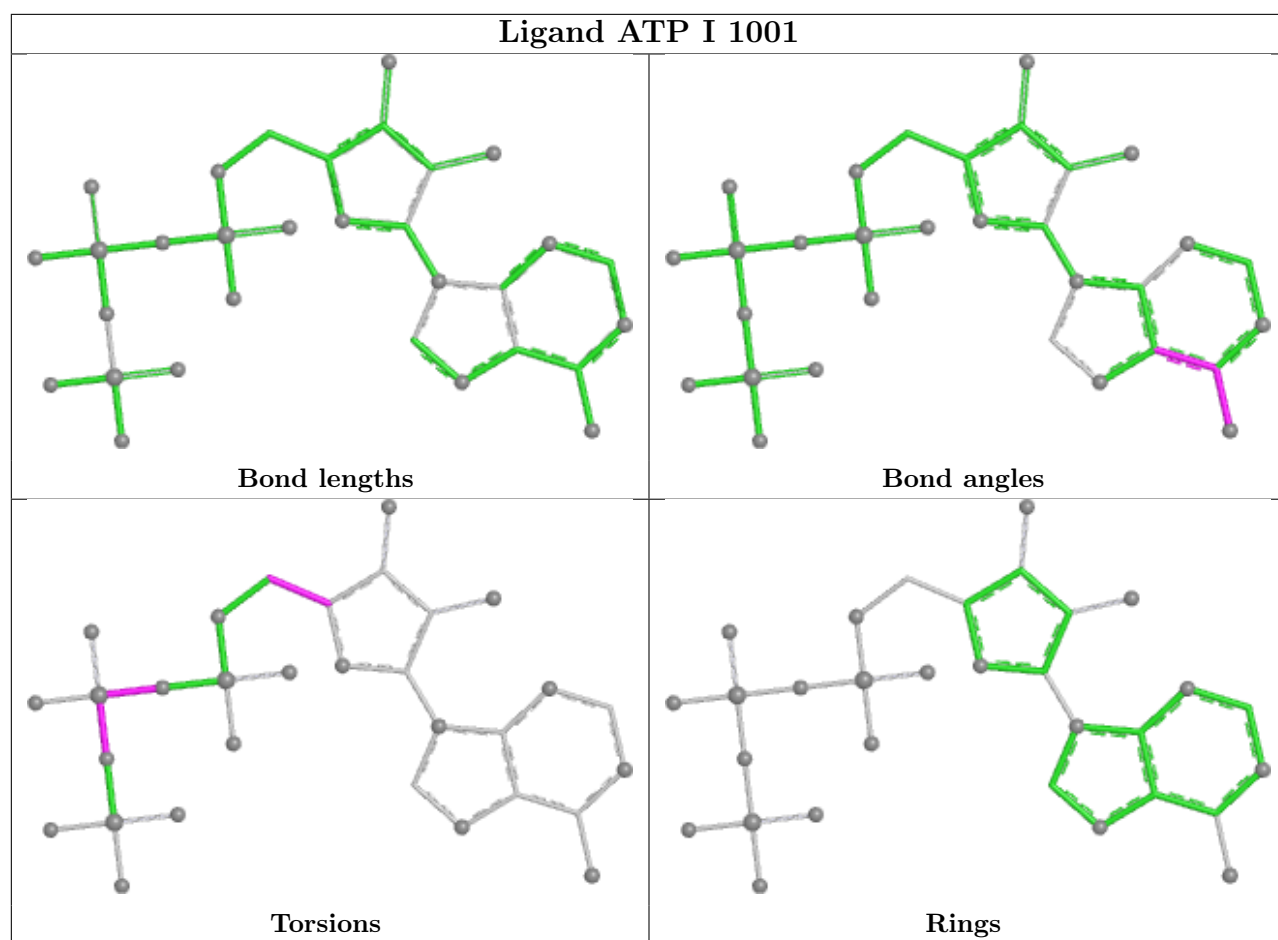
4 monomers are involved in 5 short contacts:

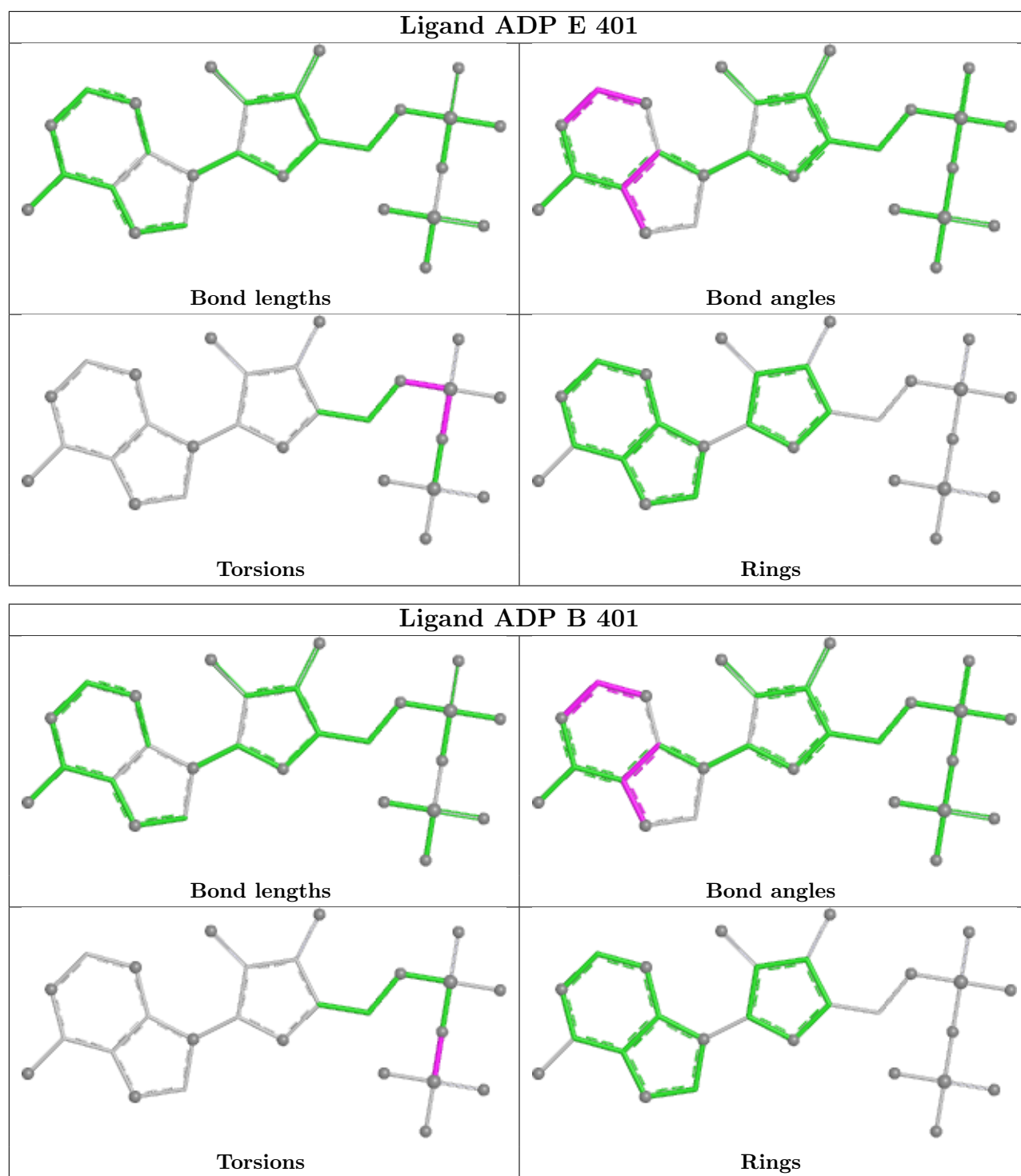
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	ADP	2	0
4	A	401	ADP	1	0
4	E	401	ADP	1	0
4	B	401	ADP	1	0

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.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

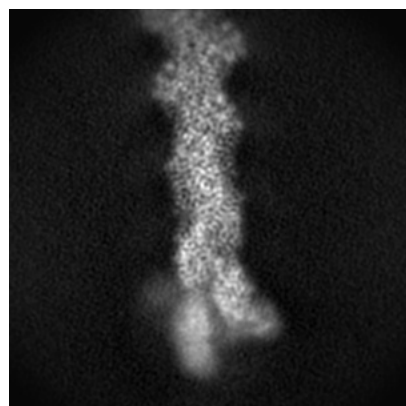
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44018. These allow visual inspection of the internal detail of the map and identification of artifacts.

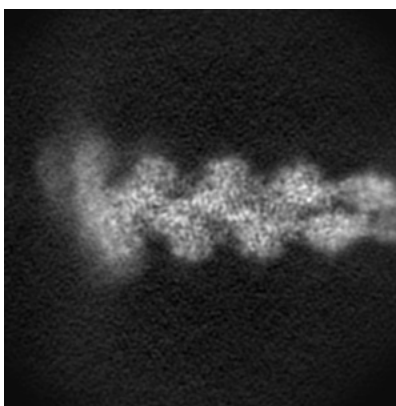
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

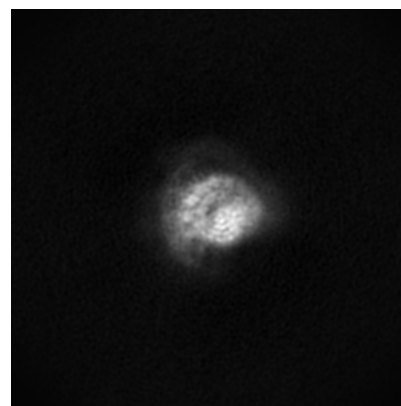
6.1.1 Primary map



X

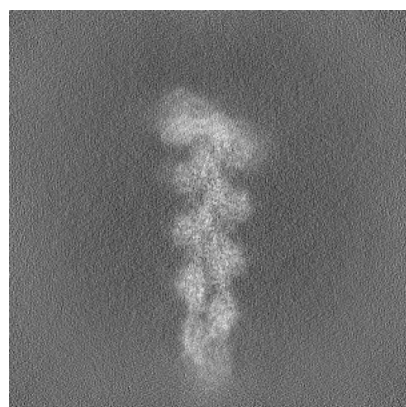


Y

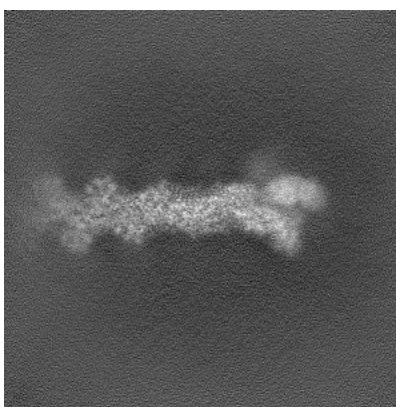


Z

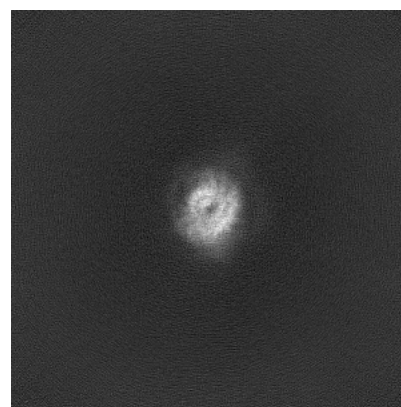
6.1.2 Raw map



X



Y

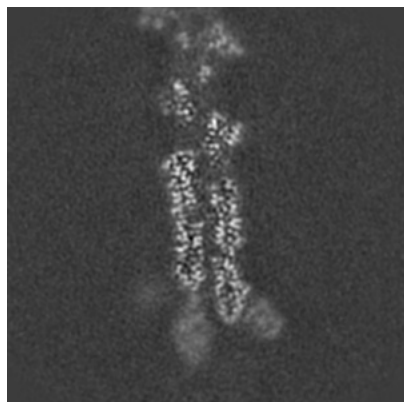


Z

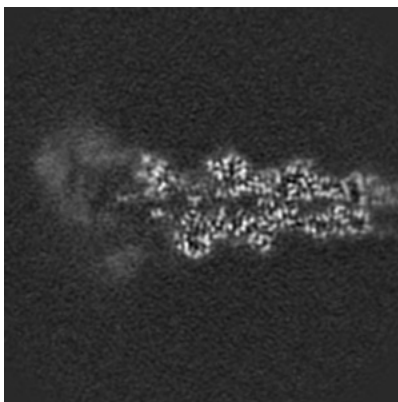
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

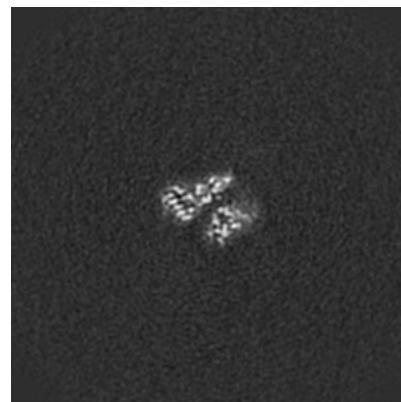
6.2.1 Primary map



X Index: 144

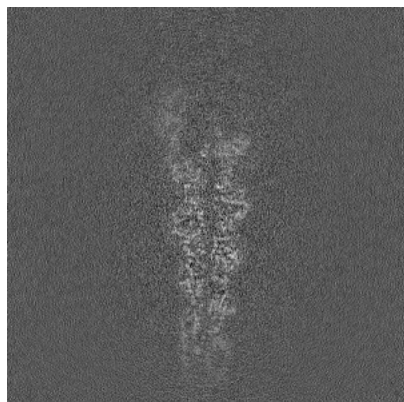


Y Index: 144

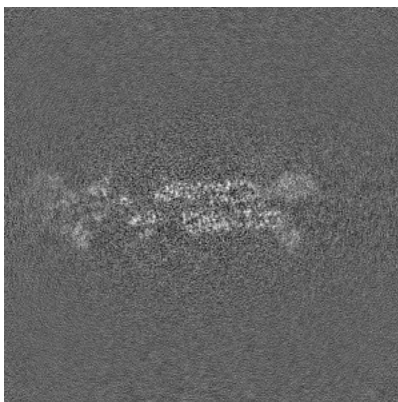


Z Index: 144

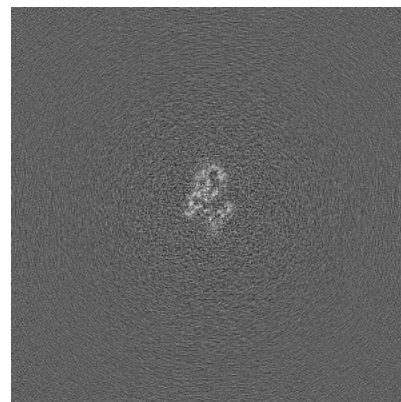
6.2.2 Raw map



X Index: 192



Y Index: 192

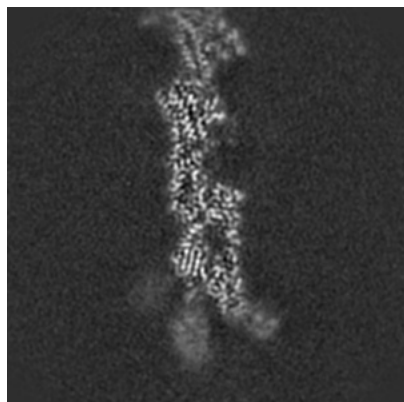


Z Index: 192

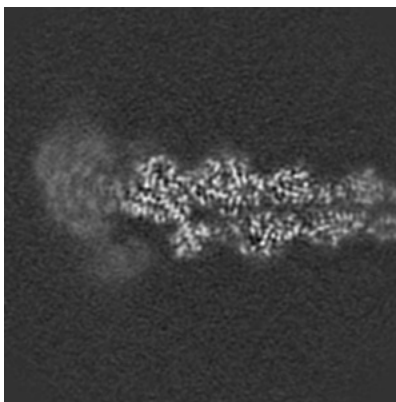
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

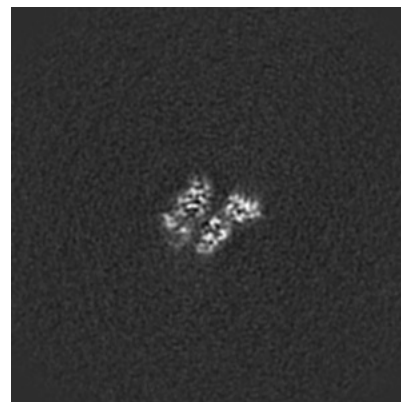
6.3.1 Primary map



X Index: 150

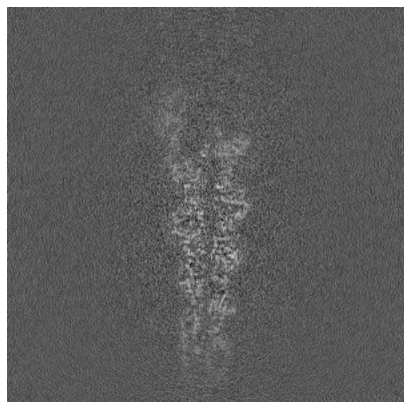


Y Index: 136

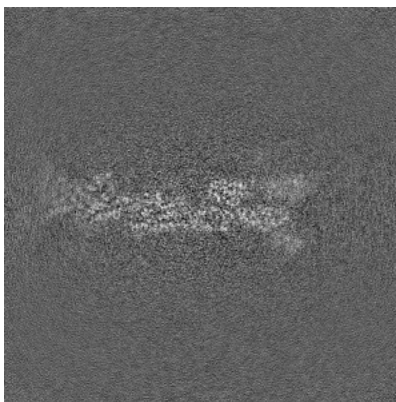


Z Index: 172

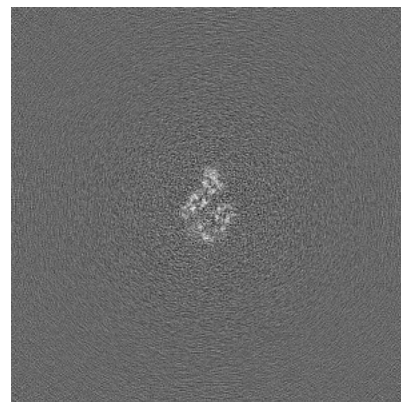
6.3.2 Raw map



X Index: 192



Y Index: 199

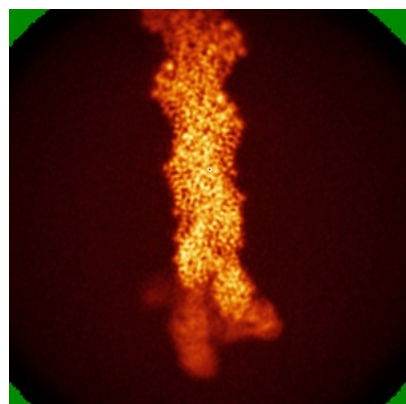


Z Index: 183

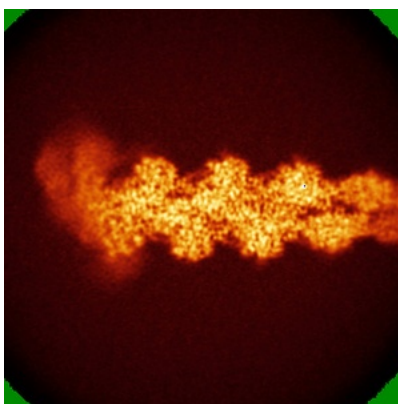
The images above show the largest variance slices of the map in three orthogonal directions.

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

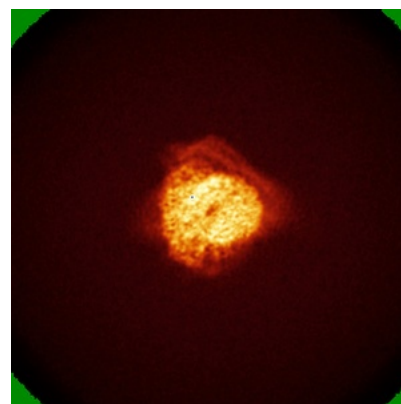
6.4.1 Primary map



X

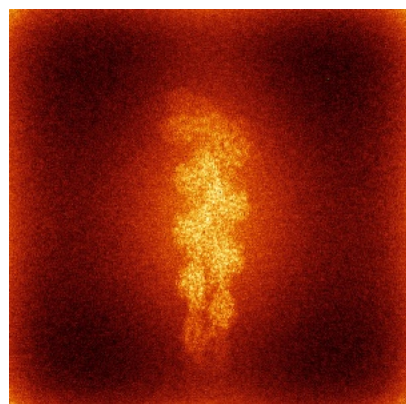


Y

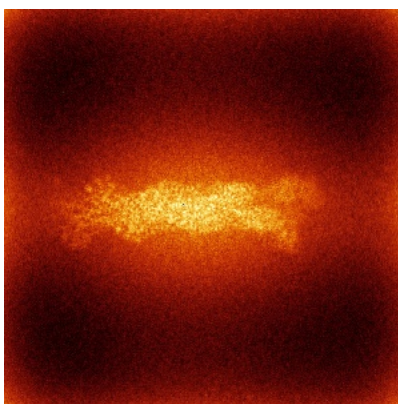


Z

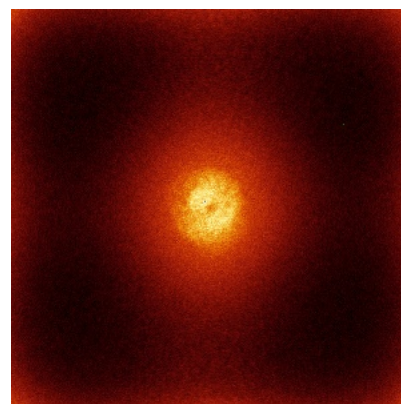
6.4.2 Raw map



X



Y

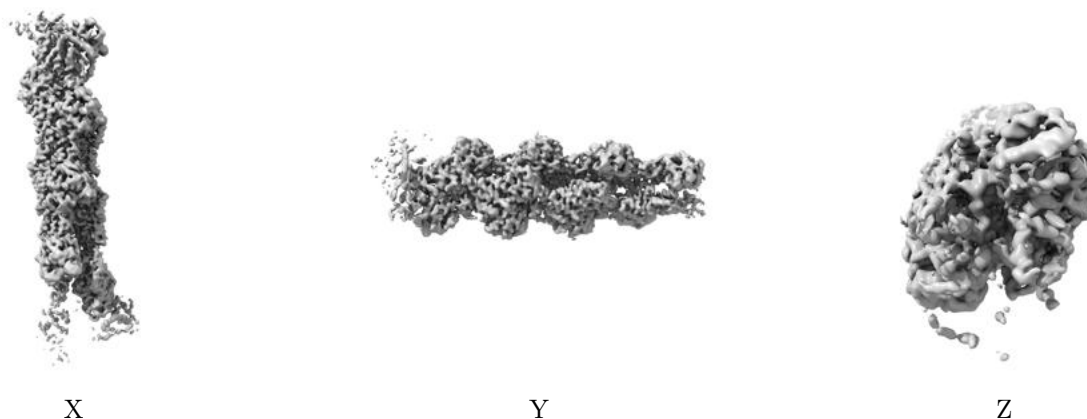


Z

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.

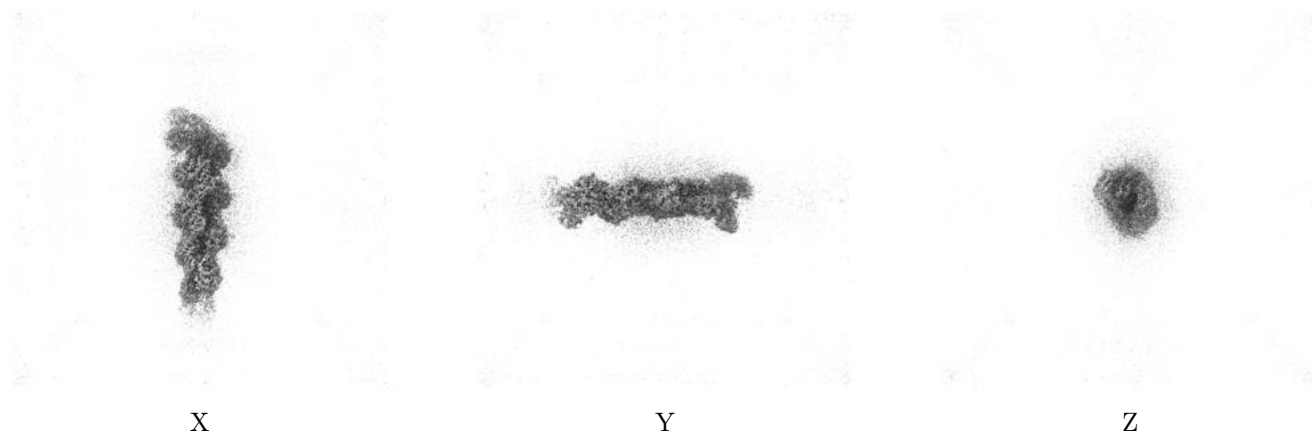
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.164. 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.

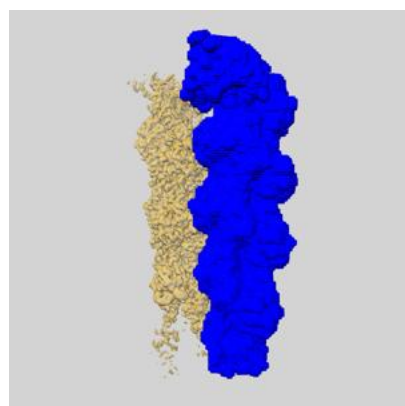
6.6 Mask visualisation [i](#)

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

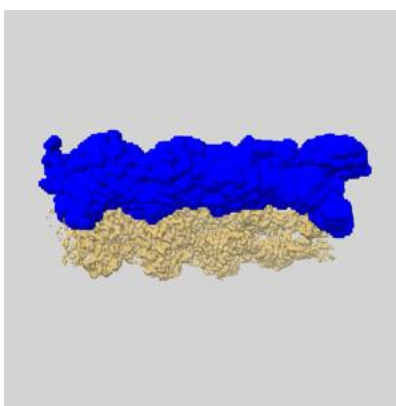
A mask typically either:

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

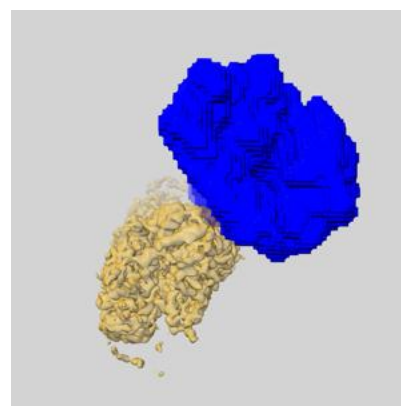
6.6.1 emd_44018_msk_1.map [i](#)



X



Y

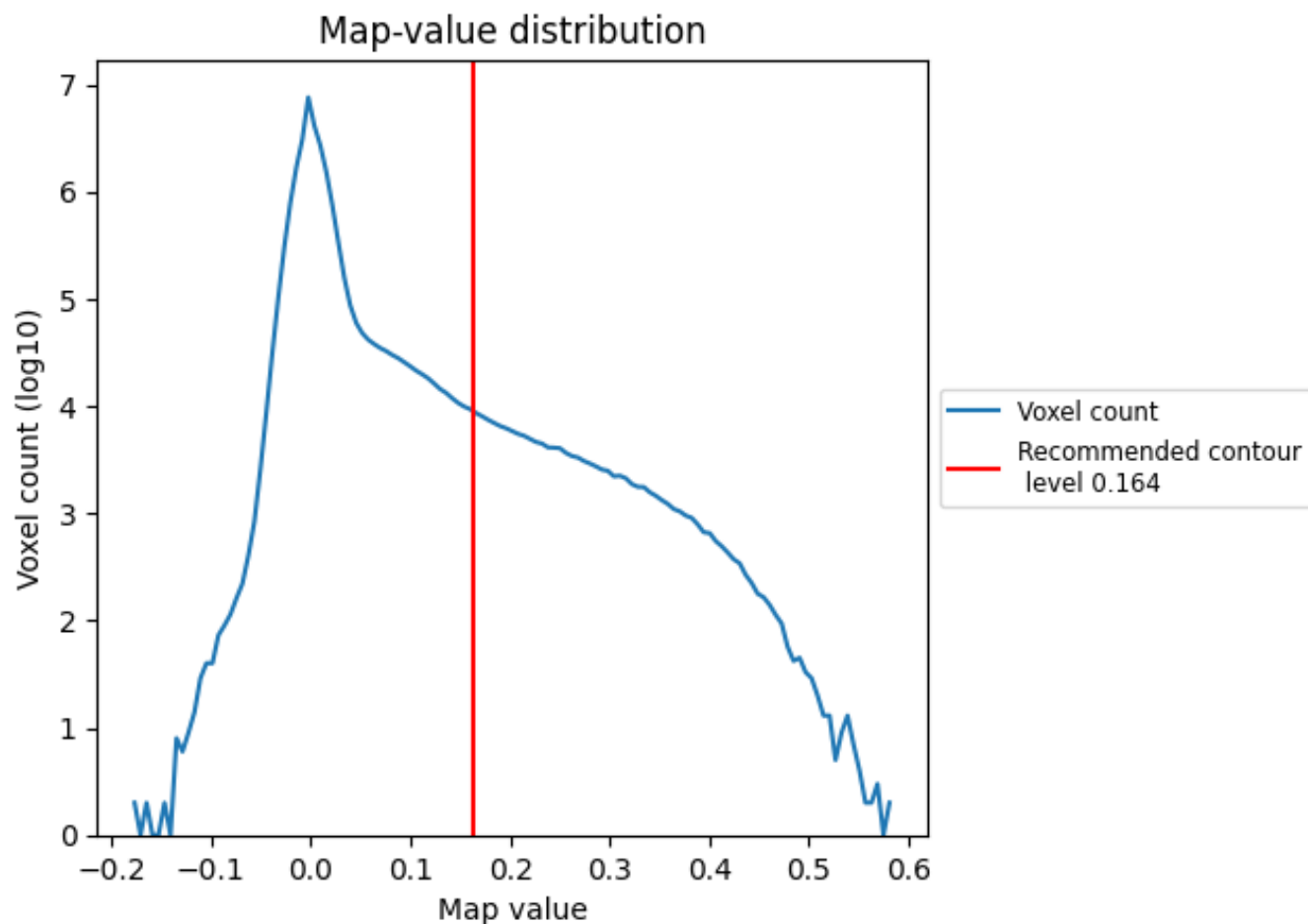


Z

7 Map analysis [i](#)

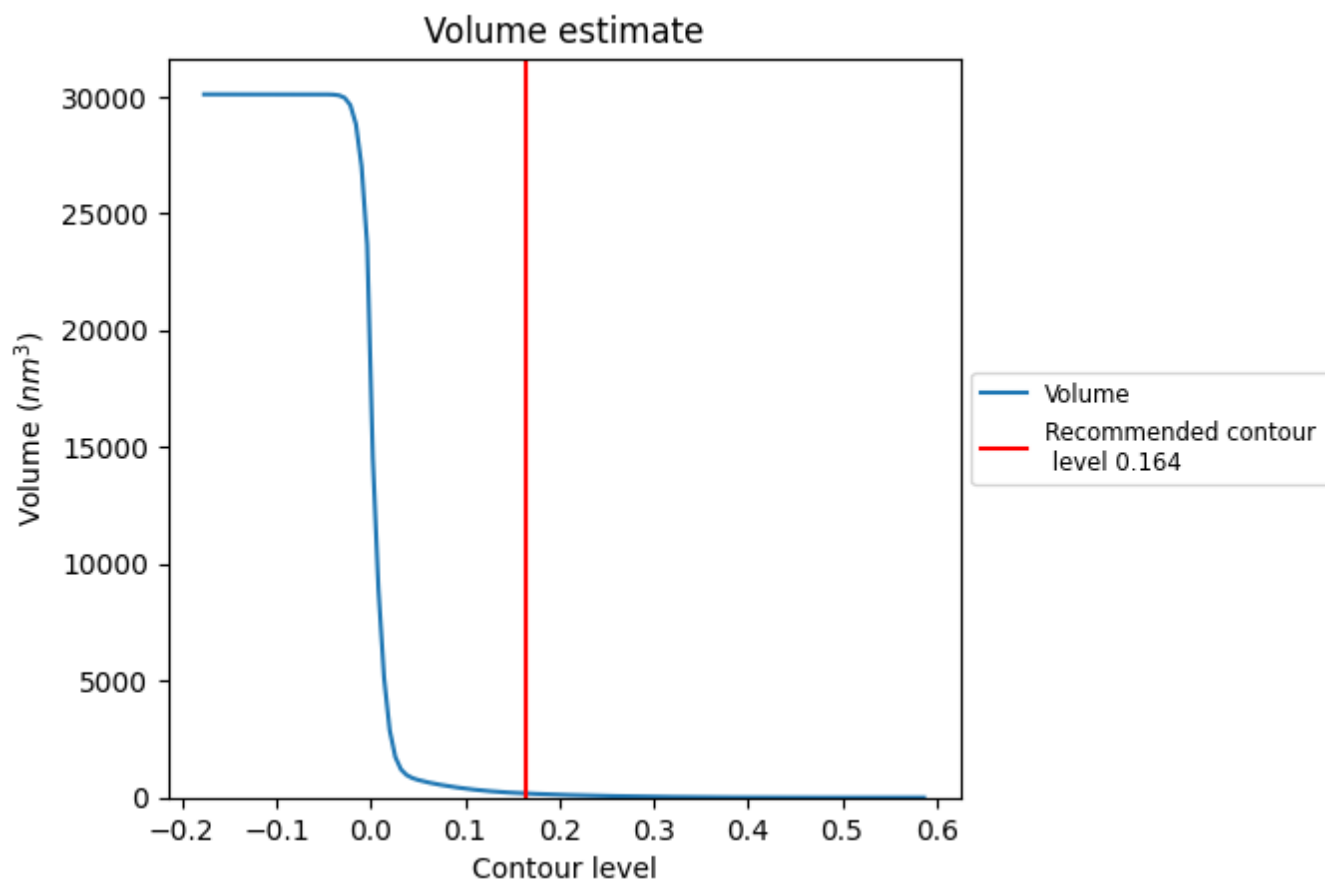
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

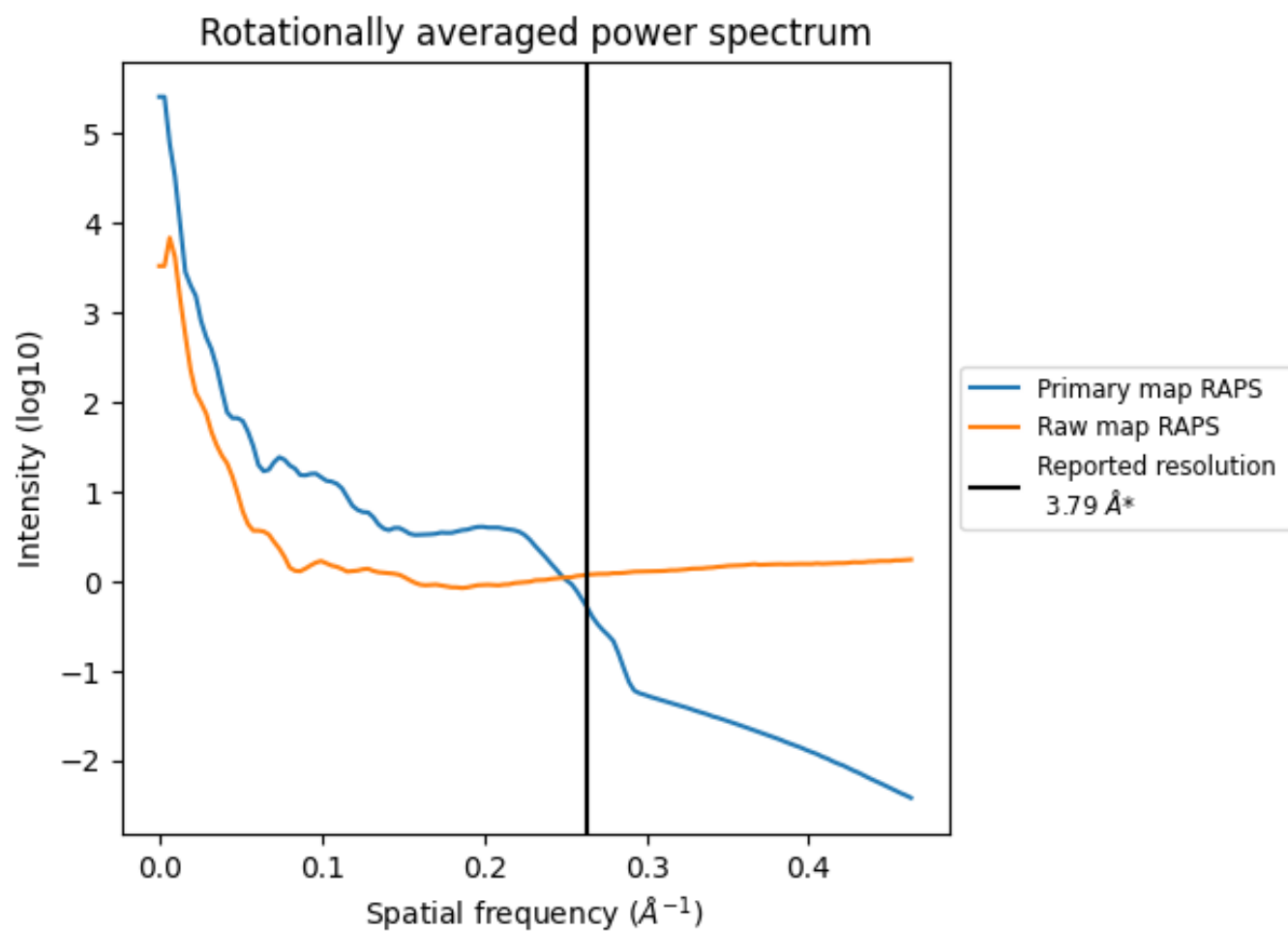
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm³; this corresponds to an approximate mass of 161 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](#)

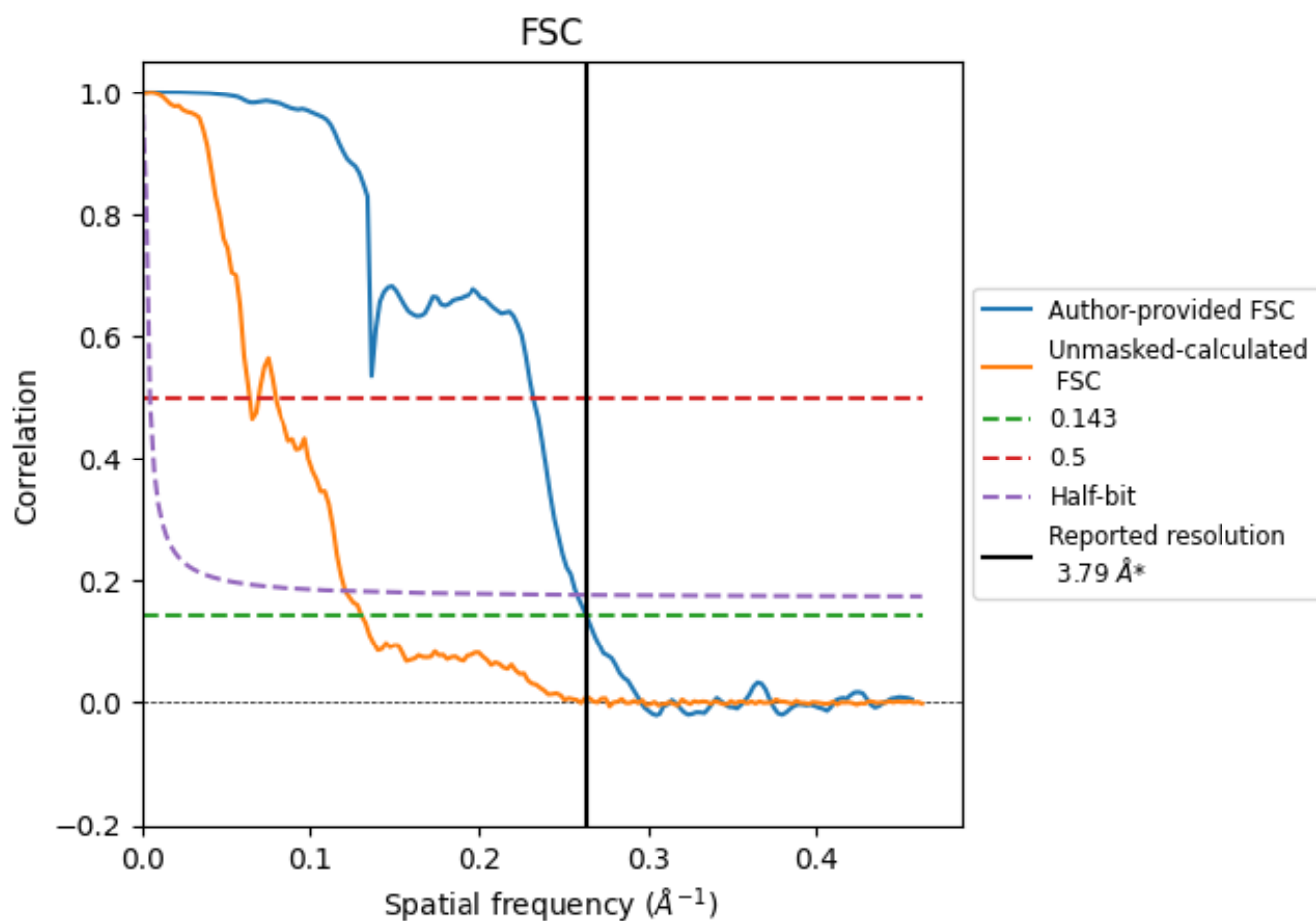


*Reported resolution corresponds to spatial frequency of 0.264 \AA^{-1}

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 0.264 \AA^{-1}

8.2 Resolution estimates [i](#)

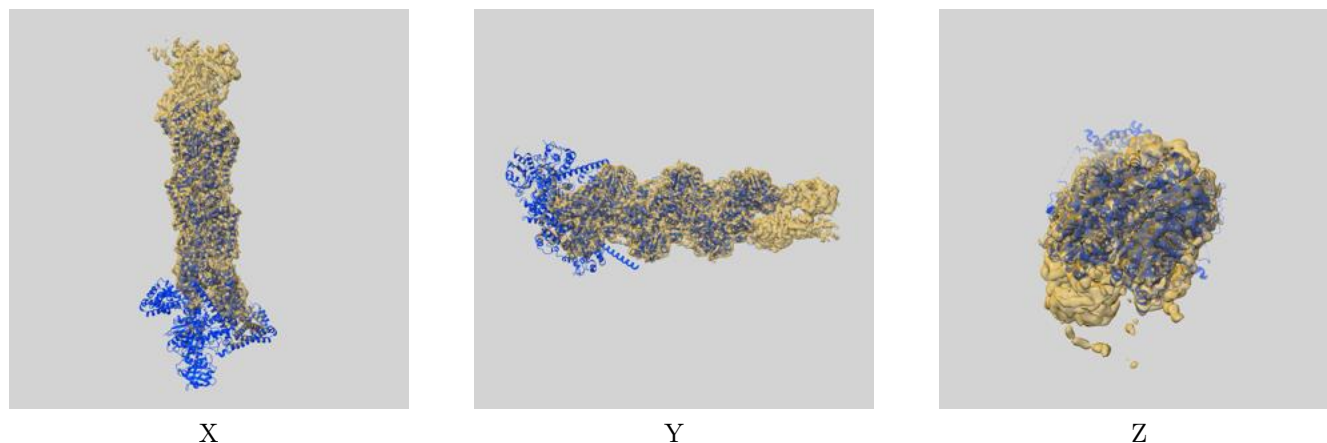
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.79	-	-
Author-provided FSC curve	3.79	4.31	3.87
Unmasked-calculated*	7.67	15.72	8.29

*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 7.67 differs from the reported value 3.79 by more than 10 %

9 Map-model fit [i](#)

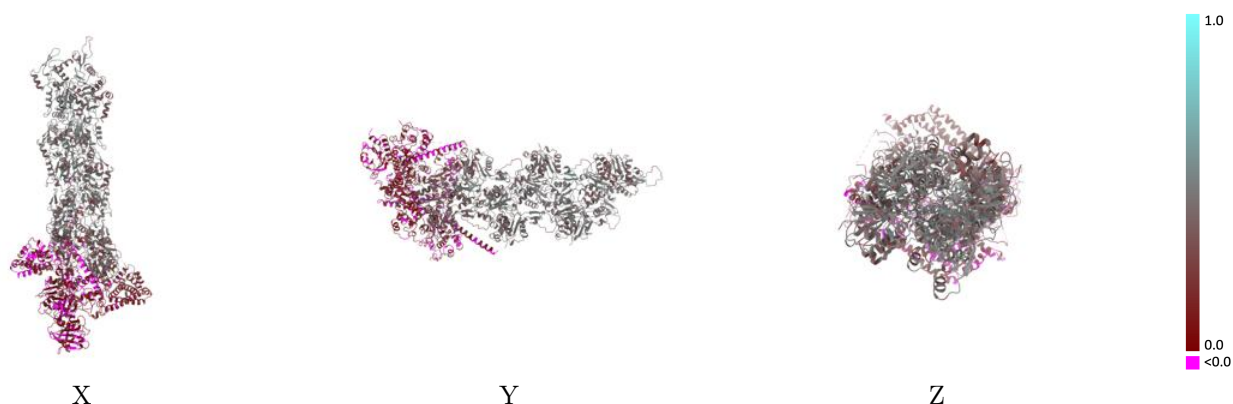
This section contains information regarding the fit between EMDB map EMD-44018 and PDB model 9AZP. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



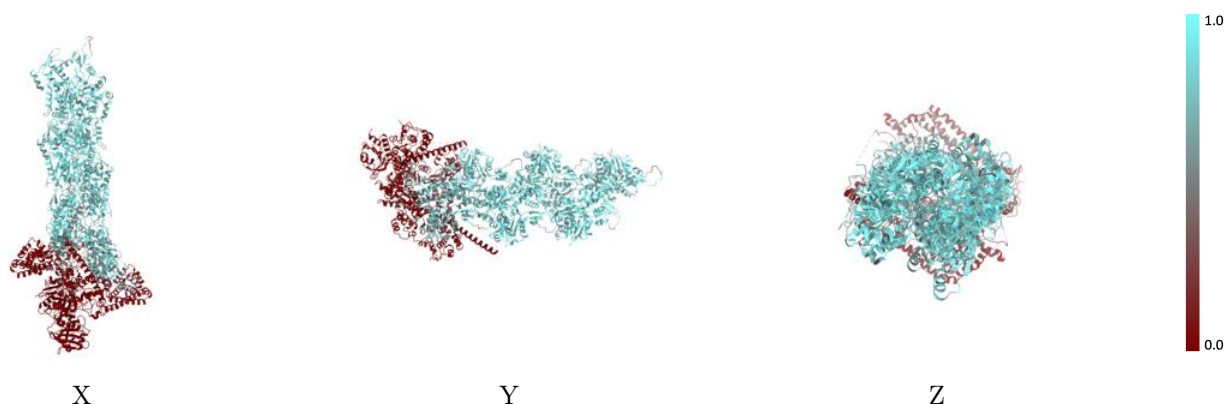
The images above show the 3D surface view of the map at the recommended contour level 0.164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



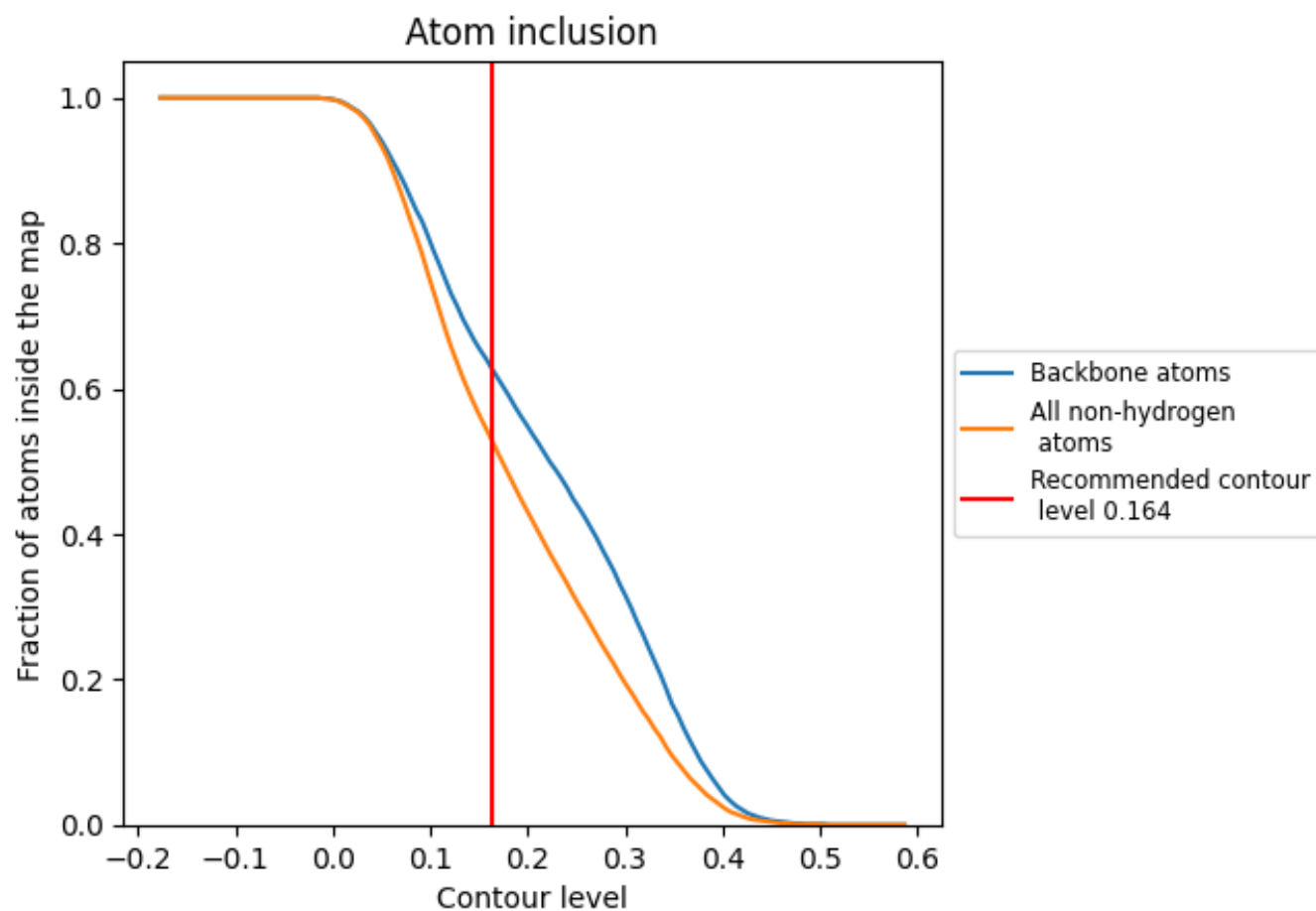
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.164).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 53% 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 (0.164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5270	<div></div> 0.3070
A	<div></div> 0.8010	<div></div> 0.4350
B	<div></div> 0.8310	<div></div> 0.4450
C	<div></div> 0.8360	<div></div> 0.4500
D	<div></div> 0.8330	<div></div> 0.4400
E	<div></div> 0.8170	<div></div> 0.4250
F	<div></div> 0.7350	<div></div> 0.3820
G	<div></div> 0.0000	<div></div> 0.0690
H	<div></div> 0.0680	<div></div> 0.1130
I	<div></div> 0.0550	<div></div> 0.1090
J	<div></div> 0.0000	<div></div> 0.0680

1.0

0.0

<0.0