



wwPDB EM Validation Summary Report ⓘ

Sep 2, 2025 – 03:02 PM EDT

PDB ID : 9OCH / pdb_00009och
EMDB ID : EMD-70315
Title : Transporter associated with antigen processing (TAP) bound to the viral protein hUS6 in the outward-facing open state
Authors : Lee, J.; Manon, V.; Chen, J.
Deposited on : 2025-04-24
Resolution : 3.30 Å(reported)

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

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A user guide is available at

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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.dev126
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) : 2.45.1

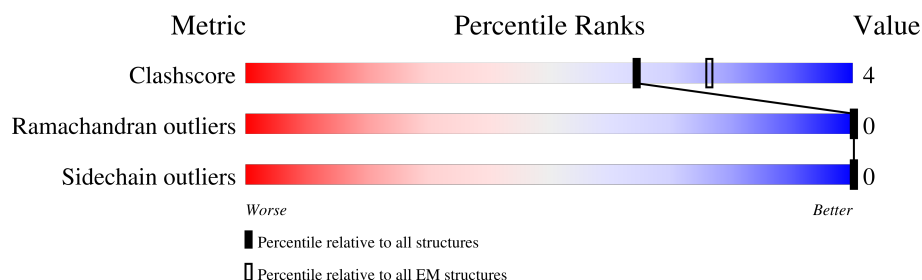
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	B	686	
2	D	239	
3	A	887	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8895 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 Antigen peptide transporter 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	548	Total	C	N	O	S	0	0
			4288	2724	753	788	23		

- Molecule 2 is a protein called TAP transport inhibitor US6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	35	Total	C	N	O	S	0	0
			279	172	56	47	4		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	184	GLY	-	expression tag	UNP P14334
D	185	SER	-	expression tag	UNP P14334
D	186	SER	-	expression tag	UNP P14334
D	187	GLY	-	expression tag	UNP P14334
D	188	GLY	-	expression tag	UNP P14334
D	189	GLY	-	expression tag	UNP P14334
D	190	SER	-	expression tag	UNP P14334
D	191	SER	-	expression tag	UNP P14334
D	192	GLY	-	expression tag	UNP P14334
D	193	SER	-	expression tag	UNP P14334
D	194	GLY	-	expression tag	UNP P14334
D	195	GLY	-	expression tag	UNP P14334
D	196	GLU	-	expression tag	UNP P14334
D	197	ASN	-	expression tag	UNP P14334
D	198	LEU	-	expression tag	UNP P14334
D	199	TYR	-	expression tag	UNP P14334
D	200	PHE	-	expression tag	UNP P14334
D	201	GLN	-	expression tag	UNP P14334
D	202	GLY	-	expression tag	UNP P14334
D	203	SER	-	expression tag	UNP P14334
D	204	GLY	-	expression tag	UNP P14334

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Chain	Residue	Modelled	Actual	Comment	Reference
D	205	GLY	-	expression tag	UNP P14334
D	206	GLY	-	expression tag	UNP P14334
D	207	SER	-	expression tag	UNP P14334
D	208	GLY	-	expression tag	UNP P14334
D	209	GLY	-	expression tag	UNP P14334
D	210	SER	-	expression tag	UNP P14334
D	211	GLY	-	expression tag	UNP P14334
D	212	GLY	-	expression tag	UNP P14334
D	213	GLY	-	expression tag	UNP P14334
D	214	MET	-	expression tag	UNP P14334
D	215	GLY	-	expression tag	UNP P14334
D	216	ARG	-	expression tag	UNP P14334
D	217	GLY	-	expression tag	UNP P14334
D	218	VAL	-	expression tag	UNP P14334
D	219	PRO	-	expression tag	UNP P14334
D	220	HIS	-	expression tag	UNP P14334
D	221	ILE	-	expression tag	UNP P14334
D	222	VAL	-	expression tag	UNP P14334
D	223	VAL	-	expression tag	UNP P14334
D	224	ASP	-	expression tag	UNP P14334
D	225	ALA	-	expression tag	UNP P14334
D	226	TYR	-	expression tag	UNP P14334
D	227	LYS	-	expression tag	UNP P14334
D	228	ARG	-	expression tag	UNP P14334
D	229	TYR	-	expression tag	UNP P14334
D	230	LYS	-	expression tag	UNP P14334
D	231	SER	-	expression tag	UNP P14334
D	232	ALA	-	expression tag	UNP P14334
D	233	GLN	-	expression tag	UNP P14334
D	234	LEU	-	expression tag	UNP P14334
D	235	GLU	-	expression tag	UNP P14334
D	236	VAL	-	expression tag	UNP P14334
D	237	LEU	-	expression tag	UNP P14334
D	238	PHE	-	expression tag	UNP P14334
D	239	GLN	-	expression tag	UNP P14334

- Molecule 3 is a protein called Antigen peptide transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	551	Total	C	N	O	S	0	0
			4268	2726	726	799	17		

There are 139 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	749	SER	-	expression tag	UNP Q03518
A	750	ALA	-	expression tag	UNP Q03518
A	751	GLN	-	expression tag	UNP Q03518
A	752	LEU	-	expression tag	UNP Q03518
A	753	GLU	-	expression tag	UNP Q03518
A	754	GLY	-	expression tag	UNP Q03518
A	755	SER	-	expression tag	UNP Q03518
A	756	GLY	-	expression tag	UNP Q03518
A	757	GLY	-	expression tag	UNP Q03518
A	758	GLY	-	expression tag	UNP Q03518
A	759	ALA	-	expression tag	UNP Q03518
A	760	MET	-	expression tag	UNP Q03518
A	761	VAL	-	expression tag	UNP Q03518
A	762	THR	-	expression tag	UNP Q03518
A	763	THR	-	expression tag	UNP Q03518
A	764	LEU	-	expression tag	UNP Q03518
A	765	SER	-	expression tag	UNP Q03518
A	766	GLY	-	expression tag	UNP Q03518
A	767	LEU	-	expression tag	UNP Q03518
A	768	SER	-	expression tag	UNP Q03518
A	769	GLY	-	expression tag	UNP Q03518
A	770	GLU	-	expression tag	UNP Q03518
A	771	GLN	-	expression tag	UNP Q03518
A	772	GLY	-	expression tag	UNP Q03518
A	773	PRO	-	expression tag	UNP Q03518
A	774	SER	-	expression tag	UNP Q03518
A	775	GLY	-	expression tag	UNP Q03518
A	776	ASP	-	expression tag	UNP Q03518
A	777	MET	-	expression tag	UNP Q03518
A	778	THR	-	expression tag	UNP Q03518
A	779	THR	-	expression tag	UNP Q03518
A	780	GLU	-	expression tag	UNP Q03518
A	781	GLU	-	expression tag	UNP Q03518
A	782	ASP	-	expression tag	UNP Q03518
A	783	SER	-	expression tag	UNP Q03518
A	784	ALA	-	expression tag	UNP Q03518
A	785	THR	-	expression tag	UNP Q03518
A	786	HIS	-	expression tag	UNP Q03518
A	787	ILE	-	expression tag	UNP Q03518
A	788	LYS	-	expression tag	UNP Q03518
A	789	PHE	-	expression tag	UNP Q03518
A	790	SER	-	expression tag	UNP Q03518
A	791	LYS	-	expression tag	UNP Q03518

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Chain	Residue	Modelled	Actual	Comment	Reference
A	792	ARG	-	expression tag	UNP Q03518
A	793	ASP	-	expression tag	UNP Q03518
A	794	GLU	-	expression tag	UNP Q03518
A	795	ASP	-	expression tag	UNP Q03518
A	796	GLY	-	expression tag	UNP Q03518
A	797	ARG	-	expression tag	UNP Q03518
A	798	GLU	-	expression tag	UNP Q03518
A	799	LEU	-	expression tag	UNP Q03518
A	800	ALA	-	expression tag	UNP Q03518
A	801	GLY	-	expression tag	UNP Q03518
A	802	ALA	-	expression tag	UNP Q03518
A	803	THR	-	expression tag	UNP Q03518
A	804	MET	-	expression tag	UNP Q03518
A	805	GLU	-	expression tag	UNP Q03518
A	806	LEU	-	expression tag	UNP Q03518
A	807	ARG	-	expression tag	UNP Q03518
A	808	ASP	-	expression tag	UNP Q03518
A	809	SER	-	expression tag	UNP Q03518
A	810	SER	-	expression tag	UNP Q03518
A	811	GLY	-	expression tag	UNP Q03518
A	812	LYS	-	expression tag	UNP Q03518
A	813	THR	-	expression tag	UNP Q03518
A	814	ILE	-	expression tag	UNP Q03518
A	815	SER	-	expression tag	UNP Q03518
A	816	THR	-	expression tag	UNP Q03518
A	817	TRP	-	expression tag	UNP Q03518
A	818	ILE	-	expression tag	UNP Q03518
A	819	SER	-	expression tag	UNP Q03518
A	820	ASP	-	expression tag	UNP Q03518
A	821	GLY	-	expression tag	UNP Q03518
A	822	HIS	-	expression tag	UNP Q03518
A	823	VAL	-	expression tag	UNP Q03518
A	824	LYS	-	expression tag	UNP Q03518
A	825	ASP	-	expression tag	UNP Q03518
A	826	PHE	-	expression tag	UNP Q03518
A	827	TYR	-	expression tag	UNP Q03518
A	828	LEU	-	expression tag	UNP Q03518
A	829	TYR	-	expression tag	UNP Q03518
A	830	PRO	-	expression tag	UNP Q03518
A	831	GLY	-	expression tag	UNP Q03518
A	832	LYS	-	expression tag	UNP Q03518
A	833	TYR	-	expression tag	UNP Q03518

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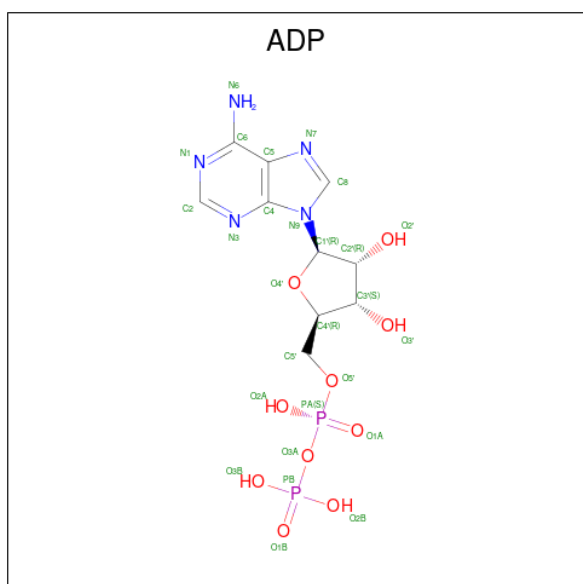
Chain	Residue	Modelled	Actual	Comment	Reference
A	834	THR	-	expression tag	UNP Q03518
A	835	PHE	-	expression tag	UNP Q03518
A	836	VAL	-	expression tag	UNP Q03518
A	837	GLU	-	expression tag	UNP Q03518
A	838	THR	-	expression tag	UNP Q03518
A	839	ALA	-	expression tag	UNP Q03518
A	840	ALA	-	expression tag	UNP Q03518
A	841	PRO	-	expression tag	UNP Q03518
A	842	ASP	-	expression tag	UNP Q03518
A	843	GLY	-	expression tag	UNP Q03518
A	844	TYR	-	expression tag	UNP Q03518
A	845	GLU	-	expression tag	UNP Q03518
A	846	VAL	-	expression tag	UNP Q03518
A	847	ALA	-	expression tag	UNP Q03518
A	848	THR	-	expression tag	UNP Q03518
A	849	PRO	-	expression tag	UNP Q03518
A	850	ILE	-	expression tag	UNP Q03518
A	851	GLU	-	expression tag	UNP Q03518
A	852	PHE	-	expression tag	UNP Q03518
A	853	THR	-	expression tag	UNP Q03518
A	854	VAL	-	expression tag	UNP Q03518
A	855	ASN	-	expression tag	UNP Q03518
A	856	GLU	-	expression tag	UNP Q03518
A	857	ASP	-	expression tag	UNP Q03518
A	858	GLY	-	expression tag	UNP Q03518
A	859	GLN	-	expression tag	UNP Q03518
A	860	VAL	-	expression tag	UNP Q03518
A	861	THR	-	expression tag	UNP Q03518
A	862	VAL	-	expression tag	UNP Q03518
A	863	ASP	-	expression tag	UNP Q03518
A	864	GLY	-	expression tag	UNP Q03518
A	865	GLU	-	expression tag	UNP Q03518
A	866	ALA	-	expression tag	UNP Q03518
A	867	THR	-	expression tag	UNP Q03518
A	868	GLU	-	expression tag	UNP Q03518
A	869	GLY	-	expression tag	UNP Q03518
A	870	ASP	-	expression tag	UNP Q03518
A	871	ALA	-	expression tag	UNP Q03518
A	872	HIS	-	expression tag	UNP Q03518
A	873	THR	-	expression tag	UNP Q03518
A	874	SER	-	expression tag	UNP Q03518
A	875	GLY	-	expression tag	UNP Q03518

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Chain	Residue	Modelled	Actual	Comment	Reference
A	876	GLY	-	expression tag	UNP Q03518
A	877	GLY	-	expression tag	UNP Q03518
A	878	HIS	-	expression tag	UNP Q03518
A	879	HIS	-	expression tag	UNP Q03518
A	880	HIS	-	expression tag	UNP Q03518
A	881	HIS	-	expression tag	UNP Q03518
A	882	HIS	-	expression tag	UNP Q03518
A	883	HIS	-	expression tag	UNP Q03518
A	884	HIS	-	expression tag	UNP Q03518
A	885	HIS	-	expression tag	UNP Q03518
A	886	HIS	-	expression tag	UNP Q03518
A	887	HIS	-	expression tag	UNP Q03518

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

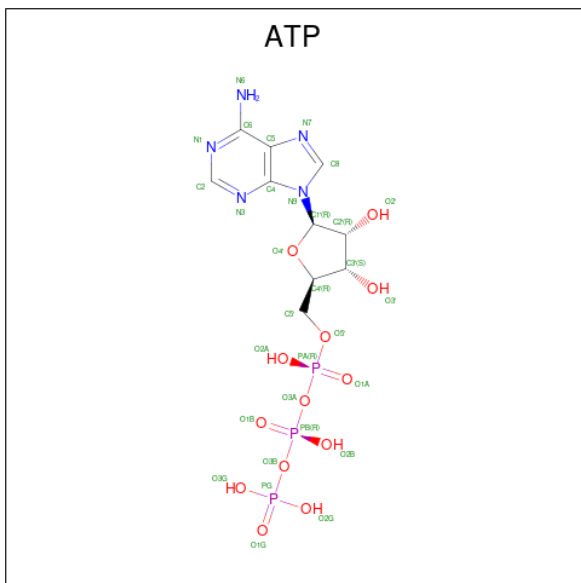
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



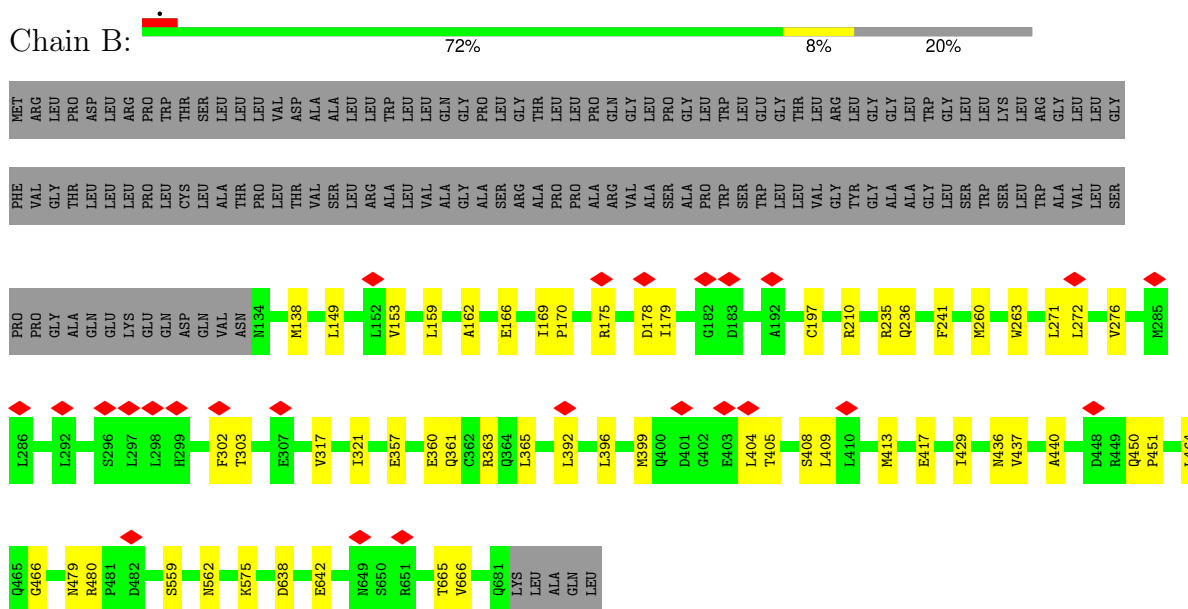
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

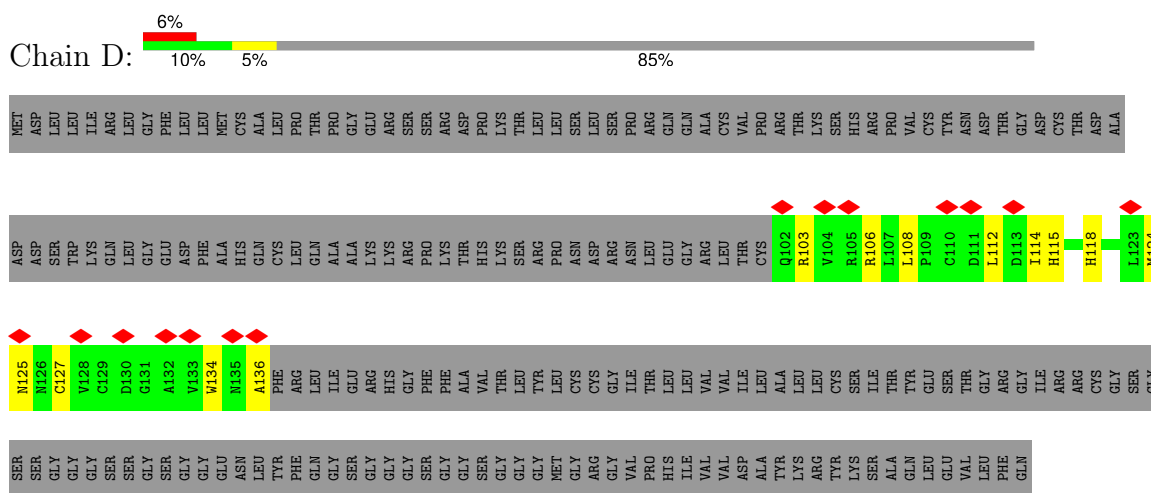
- Molecule 1: Antigen peptide transporter 2

Chain B:

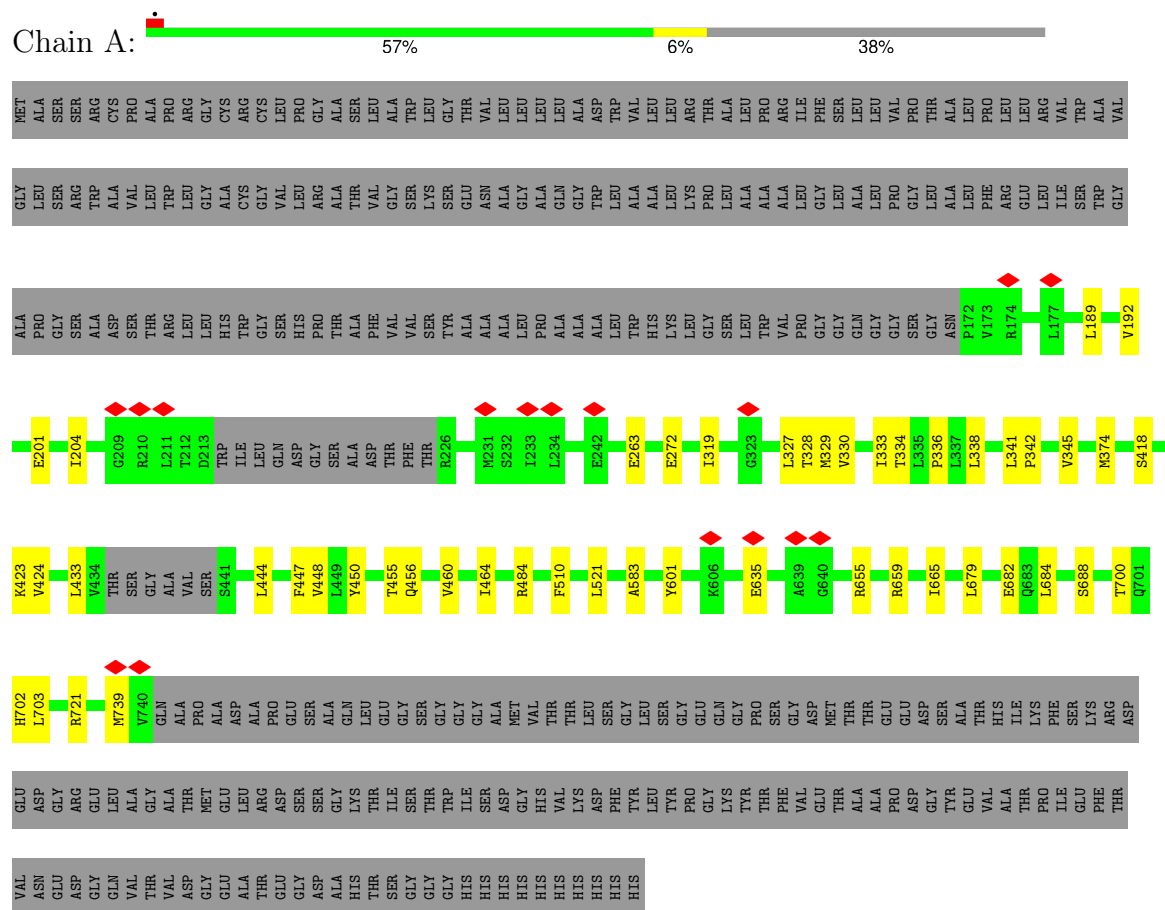


- Molecule 2: TAP transport inhibitor US6

Chain D:



- Molecule 3: Antigen peptide transporter 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14445	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.468	Depositor
Minimum map value	-0.803	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	296.96, 296.96, 296.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.16, 1.16, 1.16	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, ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.16	0/4368	0.44	4/5917 (0.1%)
2	D	0.23	0/284	0.66	1/386 (0.3%)
3	A	0.13	0/4344	0.33	0/5891
All	All	0.15	0/8996	0.40	5/12194 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	THR	N-CA-C	10.49	122.71	111.28
2	D	125	ASN	CB-CA-C	-5.47	109.79	117.23
1	B	436	ASN	N-CA-C	-5.12	105.59	111.07
1	B	302	PHE	N-CA-C	5.03	116.45	110.97
1	B	303	THR	N-CA-CB	-5.00	102.77	110.12

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	B	4288	0	4331	34	0
2	D	279	0	280	9	0
3	A	4268	0	4347	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	31	0	12	0	0
All	All	8895	0	8982	70	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 70 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:MET:HB3	2:D:124:MET:HE1	1.17	1.16
1:B:413:MET:CB	2:D:124:MET:HE1	1.99	0.91
3:A:601:TYR:O	3:A:659:ARG:NH2	2.22	0.72
3:A:510:PHE:HB3	3:A:521:LEU:HD13	1.74	0.69
3:A:655:ARG:O	3:A:659:ARG:NH1	2.32	0.63

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	546/686 (80%)	539 (99%)	7 (1%)	0	100	100
2	D	33/239 (14%)	27 (82%)	6 (18%)	0	100	100
3	A	545/887 (61%)	536 (98%)	9 (2%)	0	100	100
All	All	1124/1812 (62%)	1102 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	466/573 (81%)	466 (100%)	0	100	100
2	D	32/198 (16%)	32 (100%)	0	100	100
3	A	469/719 (65%)	469 (100%)	0	100	100
All	All	967/1490 (65%)	967 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	563	ASN
3	A	411	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	B	701	5	24,29,29	0.88	0	29,45,45	1.24	2 (6%)
6	ATP	A	901	5	28,33,33	0.64	0	34,52,52	0.61	1 (2%)

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	B	701	5	-	2/12/32/32	0/3/3/3
6	ATP	A	901	5	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	ADP	N3-C2-N1	-3.60	123.78	128.67
4	B	701	ADP	C4-C5-N7	-2.56	106.64	109.34
6	A	901	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

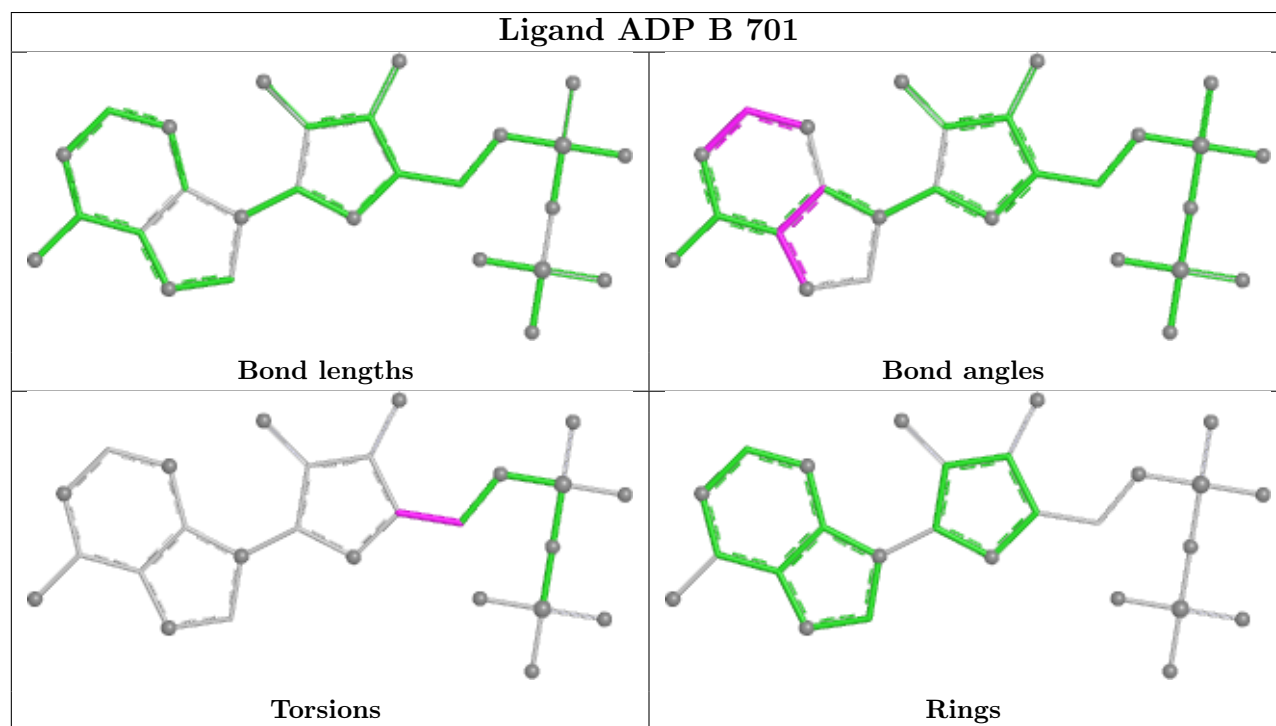
Mol	Chain	Res	Type	Atoms
4	B	701	ADP	O4'-C4'-C5'-O5'
6	A	901	ATP	PA-O3A-PB-O2B
6	A	901	ATP	PA-O3A-PB-O1B
4	B	701	ADP	C3'-C4'-C5'-O5'

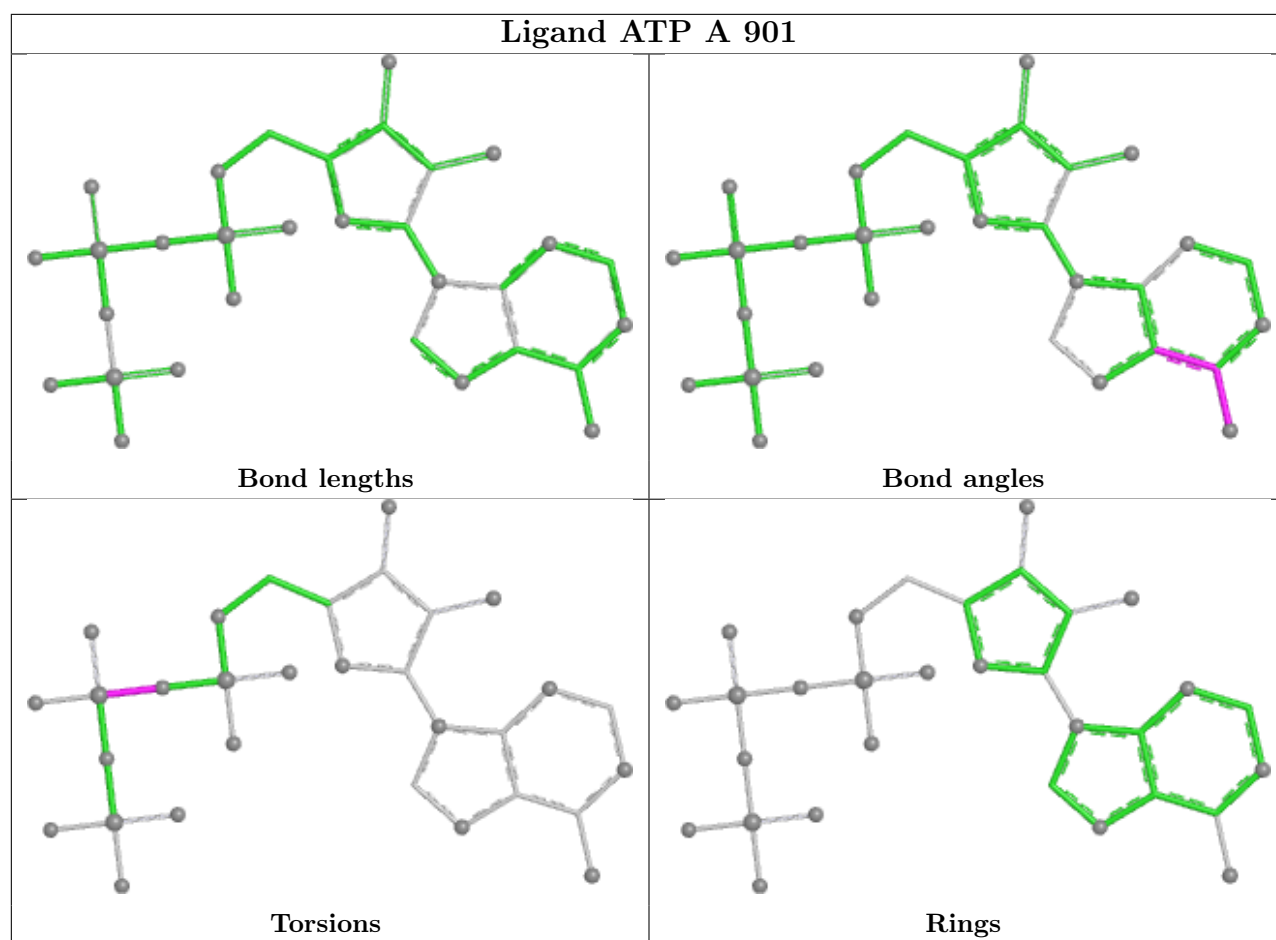
There are no ring outliers.

No monomer is involved in short contacts.

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

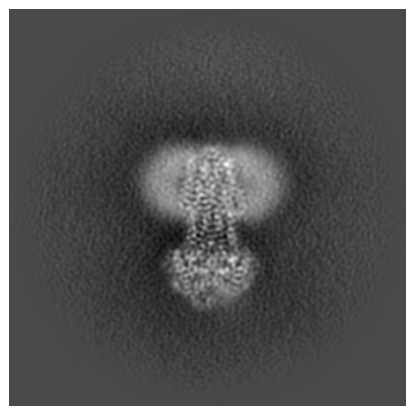
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70315. These allow visual inspection of the internal detail of the map and identification of artifacts.

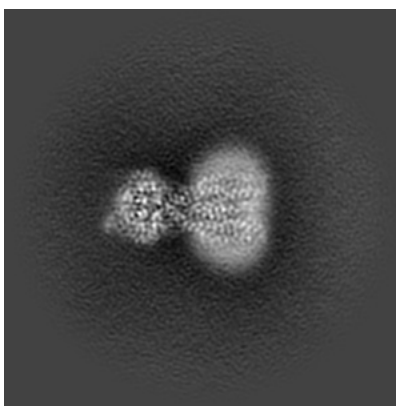
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

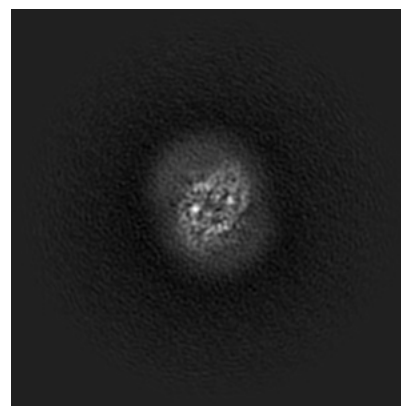
6.1.1 Primary map



X

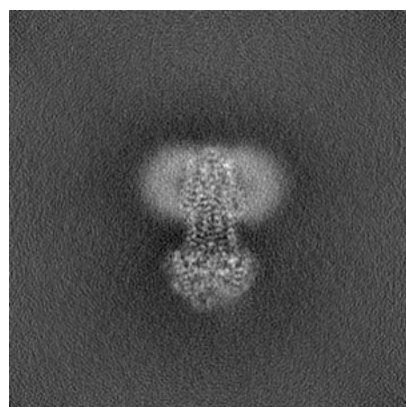


Y

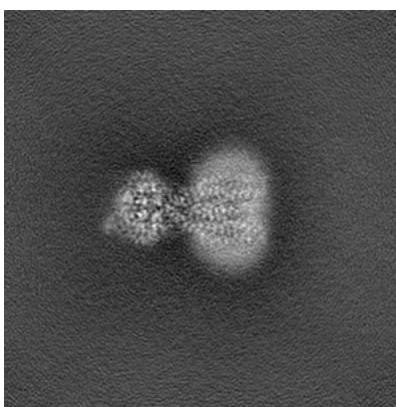


Z

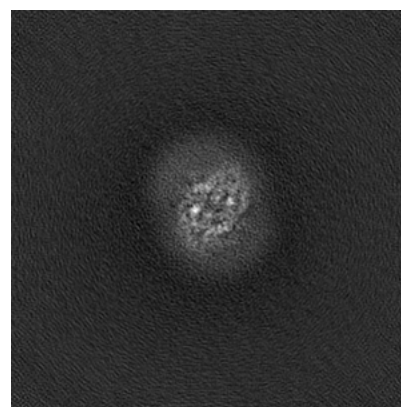
6.1.2 Raw map



X



Y

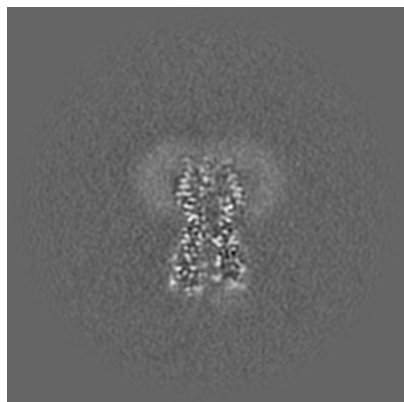


Z

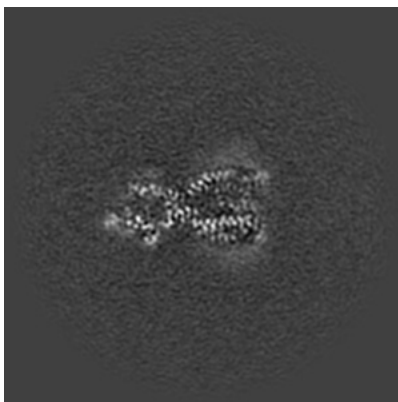
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

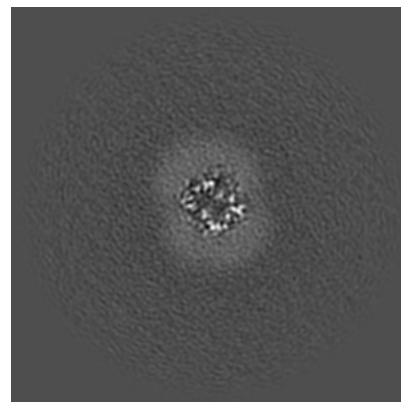
6.2.1 Primary map



X Index: 128

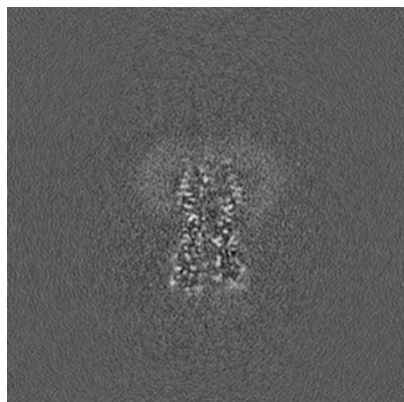


Y Index: 128

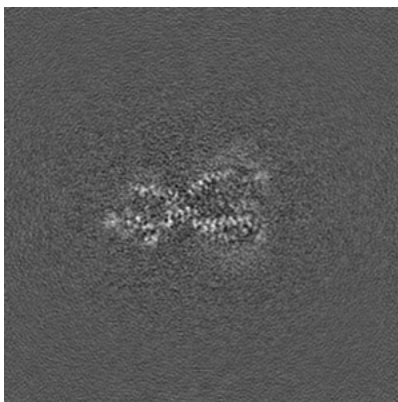


Z Index: 128

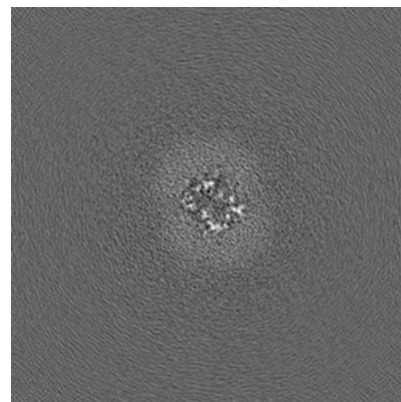
6.2.2 Raw map



X Index: 128



Y Index: 128

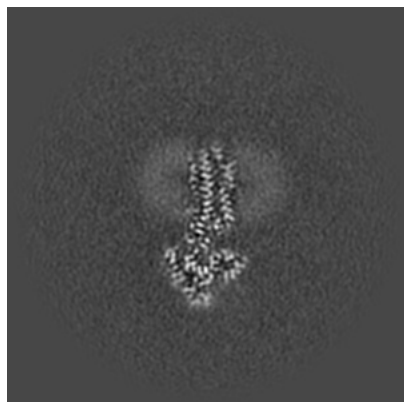


Z Index: 128

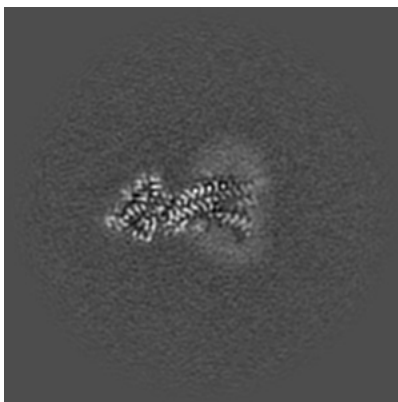
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

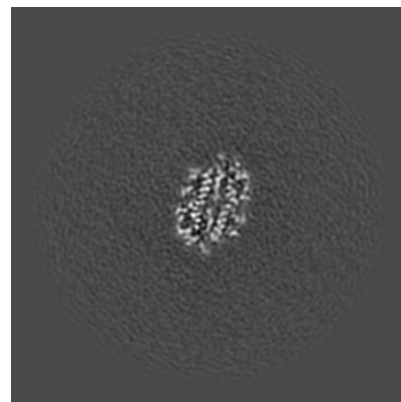
6.3.1 Primary map



X Index: 118

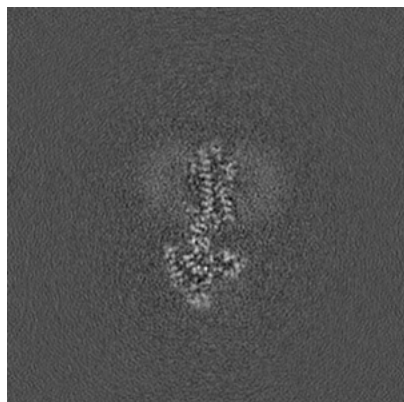


Y Index: 118

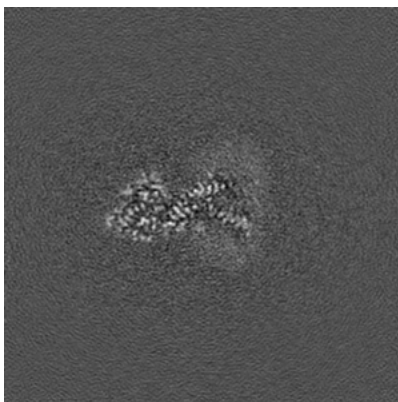


Z Index: 89

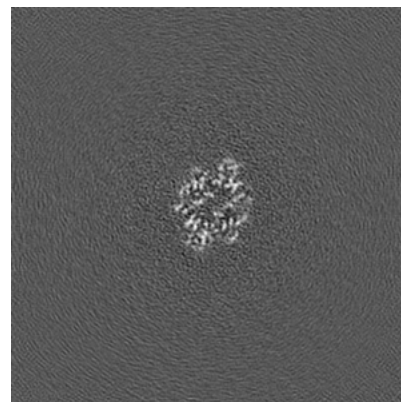
6.3.2 Raw map



X Index: 117



Y Index: 119

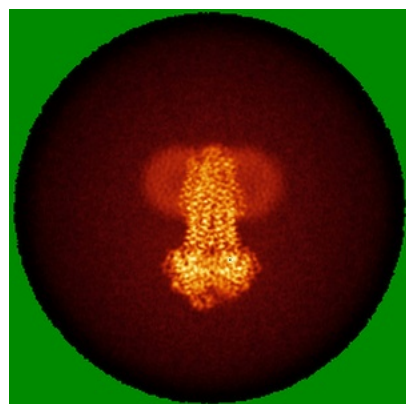


Z Index: 95

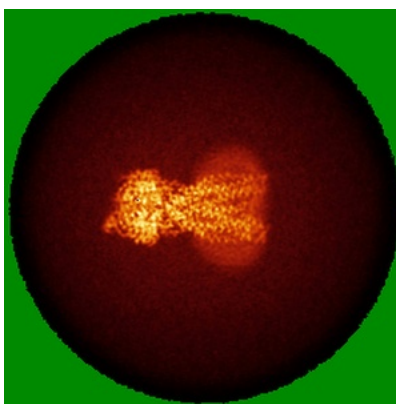
The images above show the largest variance slices of the map in three orthogonal directions.

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

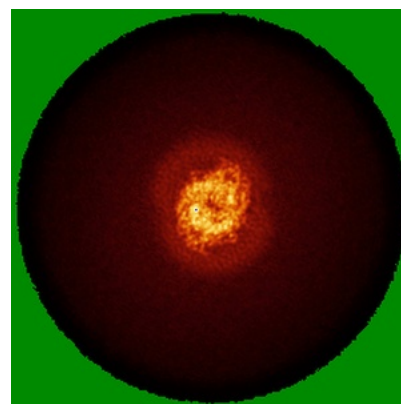
6.4.1 Primary map



X

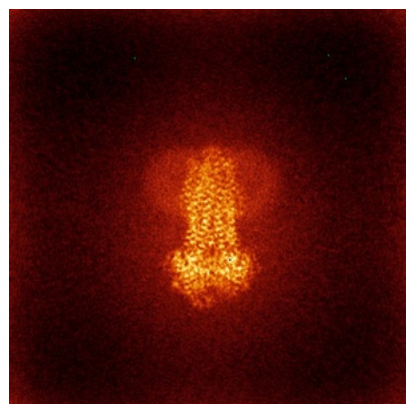


Y

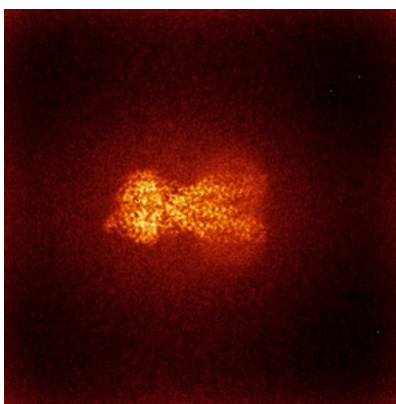


Z

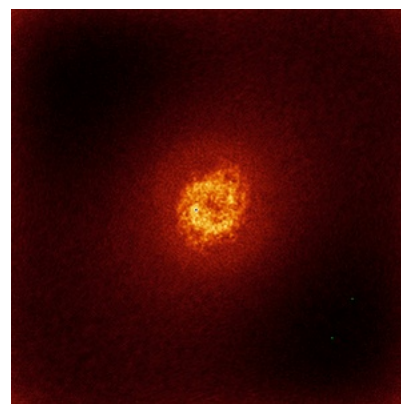
6.4.2 Raw map



X



Y

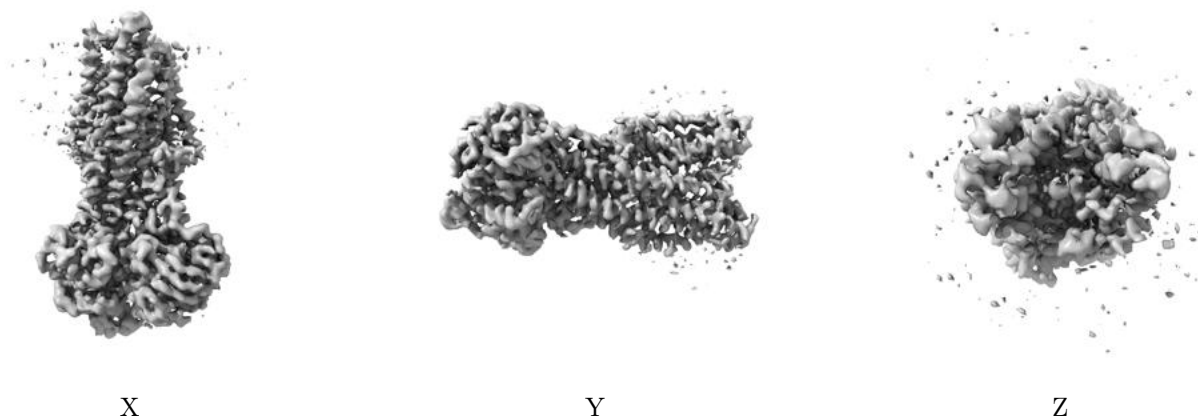


Z

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.

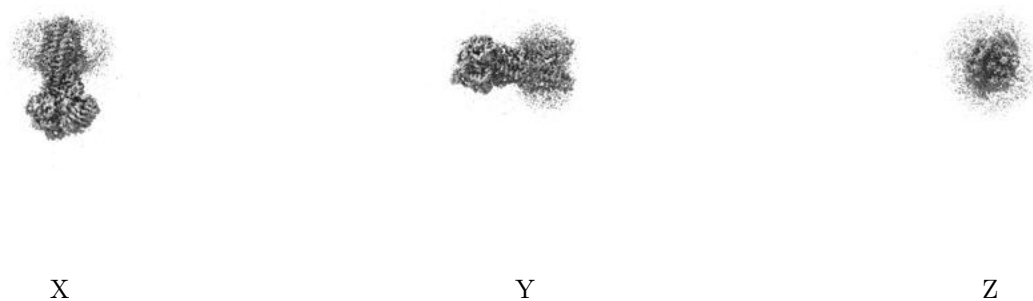
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

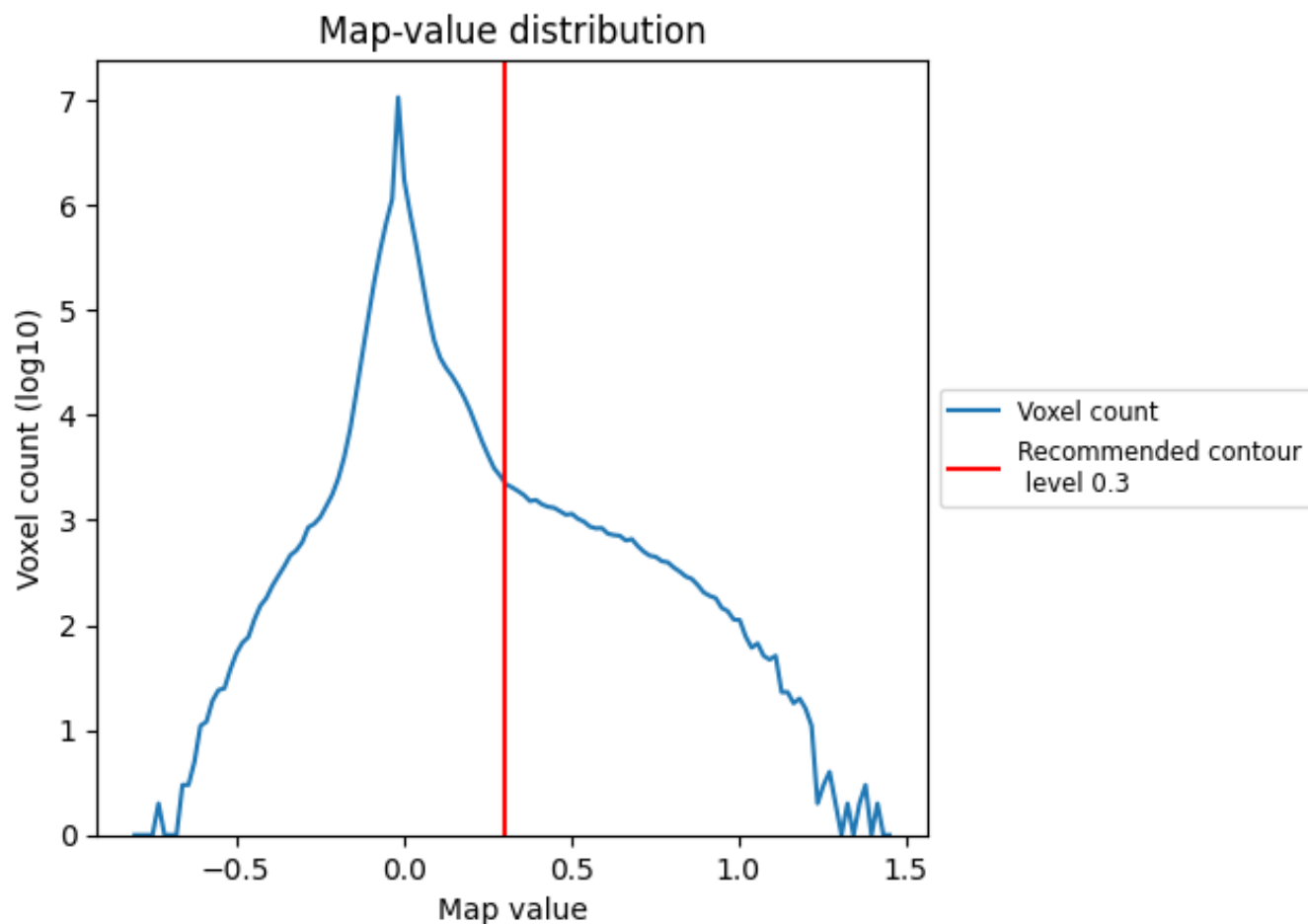
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

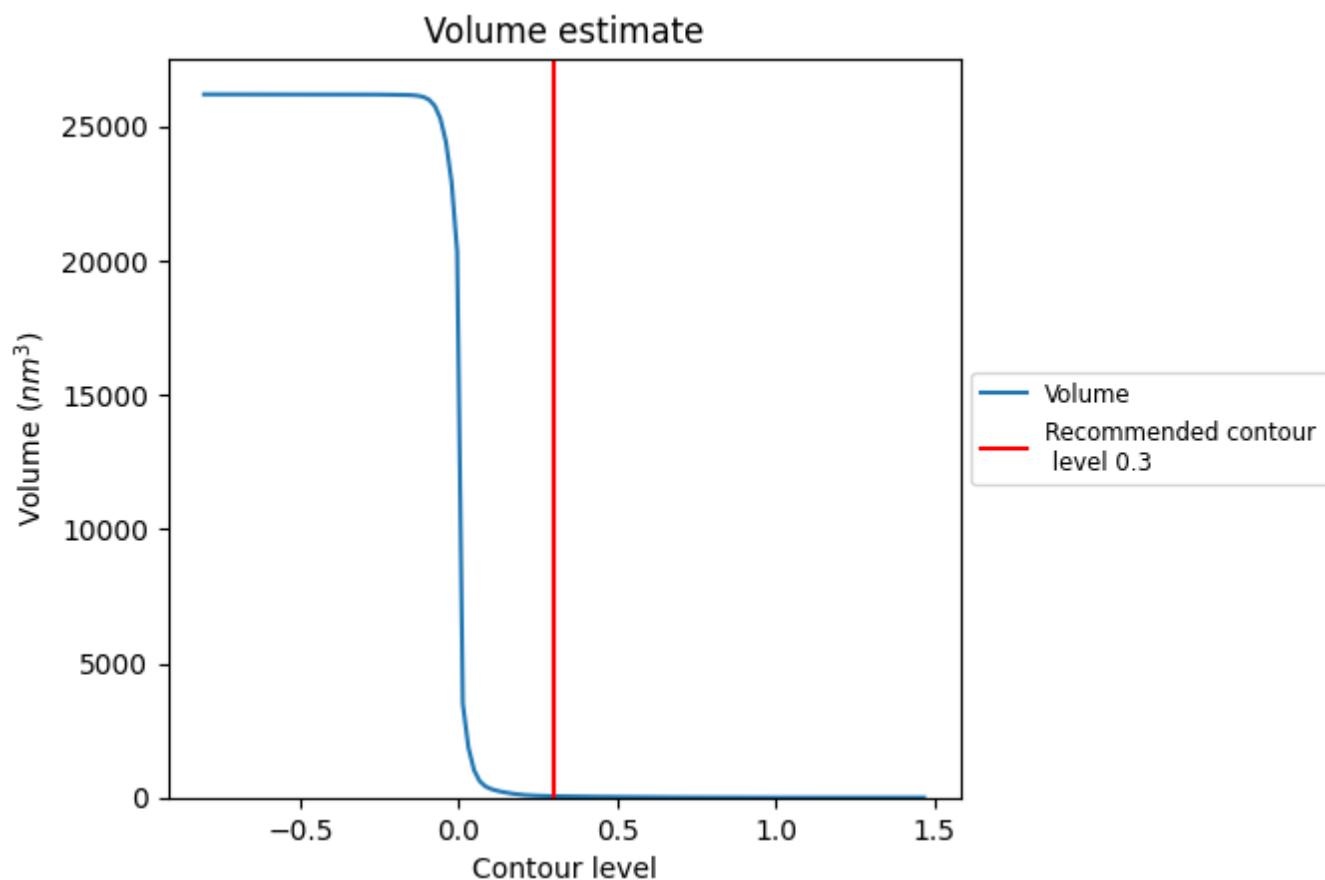
This section contains the results of statistical analysis of the map.

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.

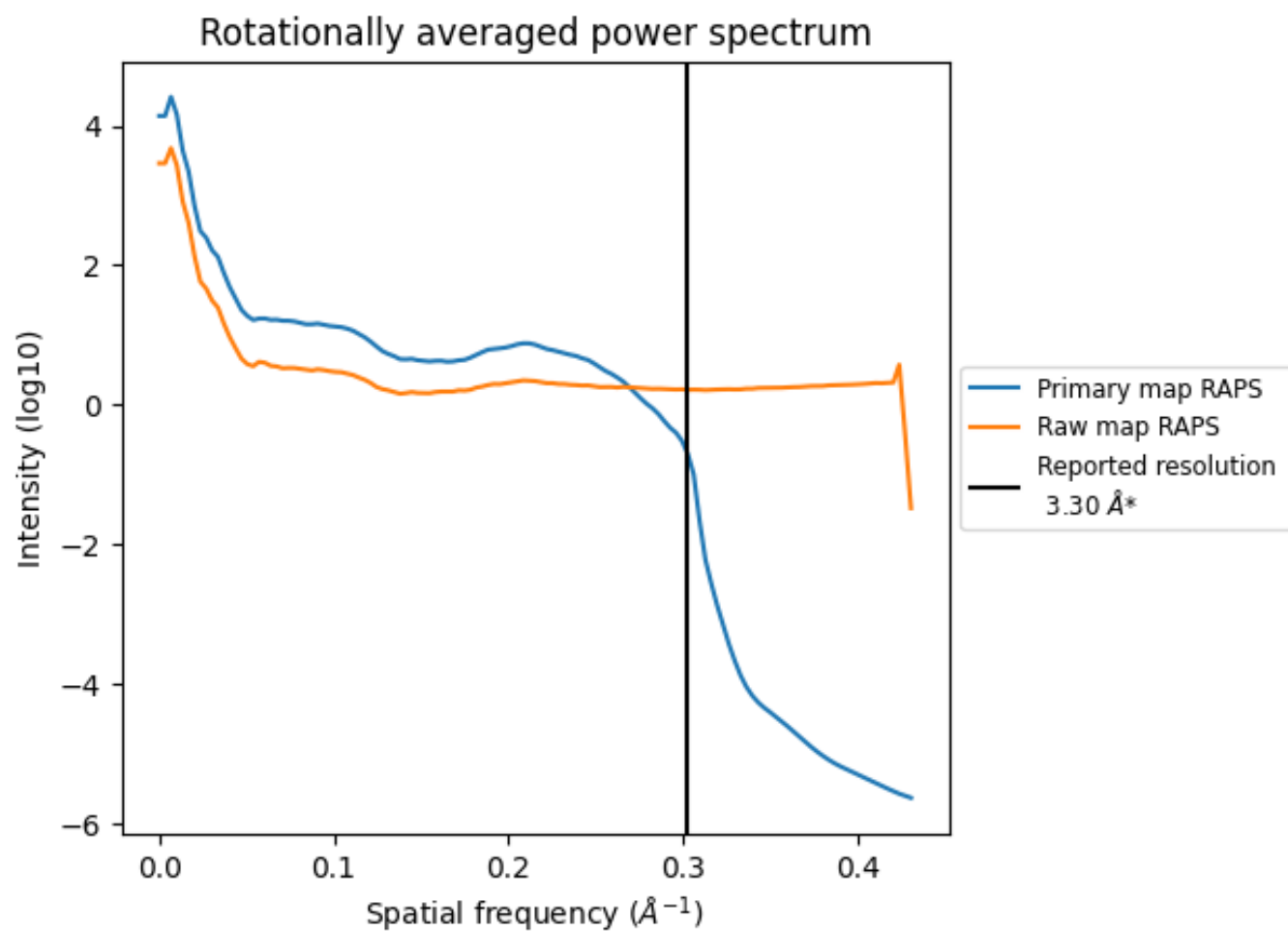
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm³; this corresponds to an approximate mass of 47 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 ⓘ

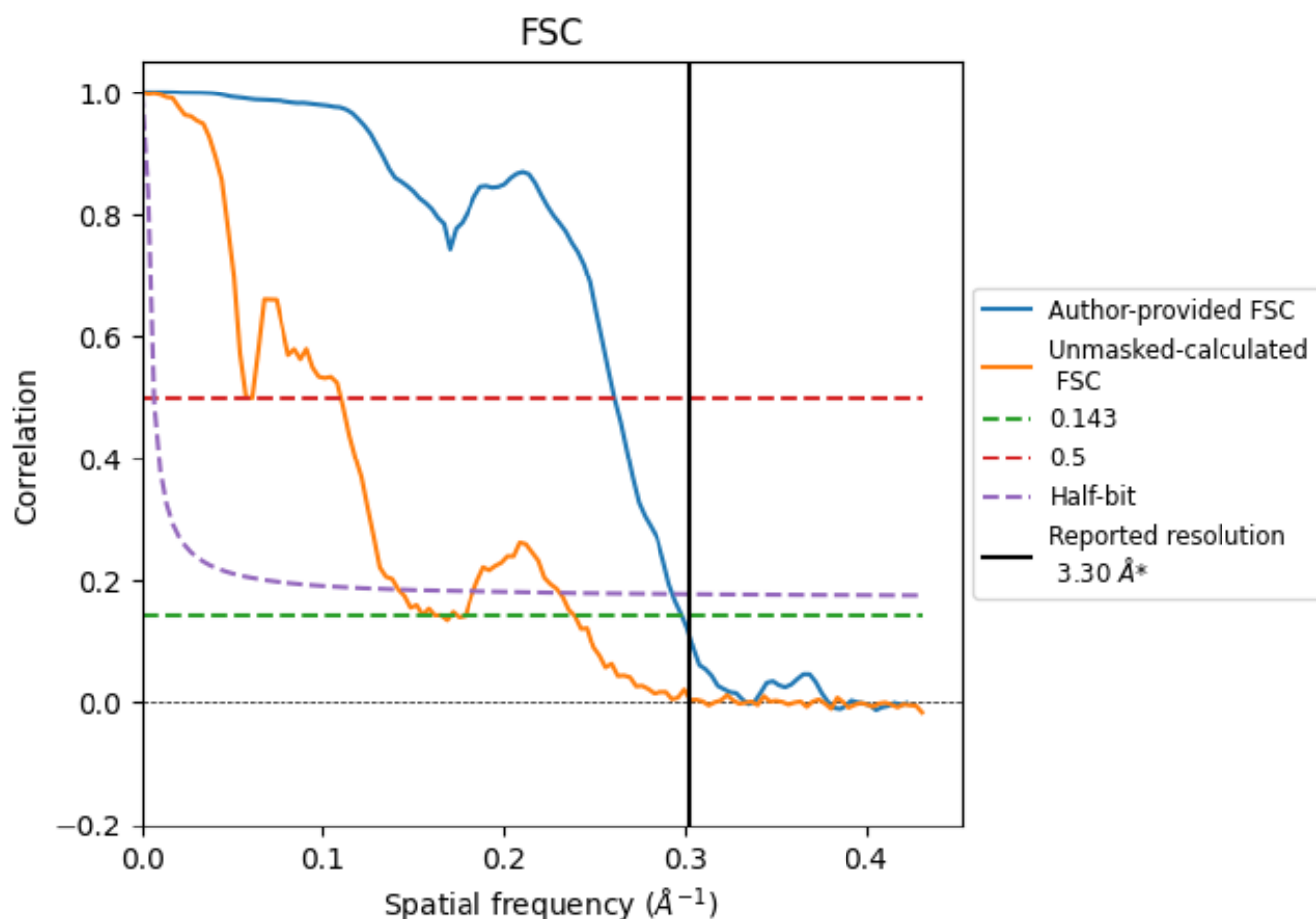


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

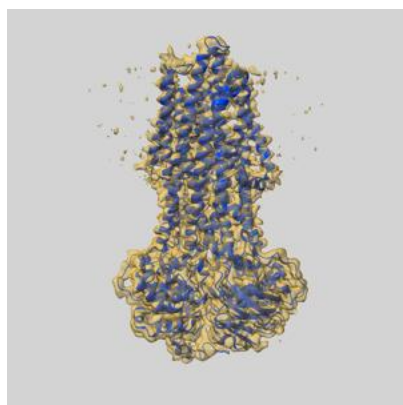
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.35	3.83	3.41
Unmasked-calculated*	6.05	17.27	7.06

*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 6.05 differs from the reported value 3.3 by more than 10 %

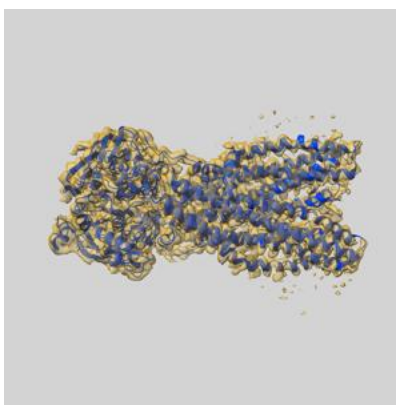
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70315 and PDB model 9OCH. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

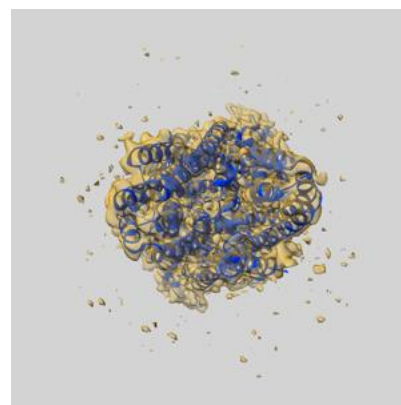
9.1 Map-model overlay [i](#)



X



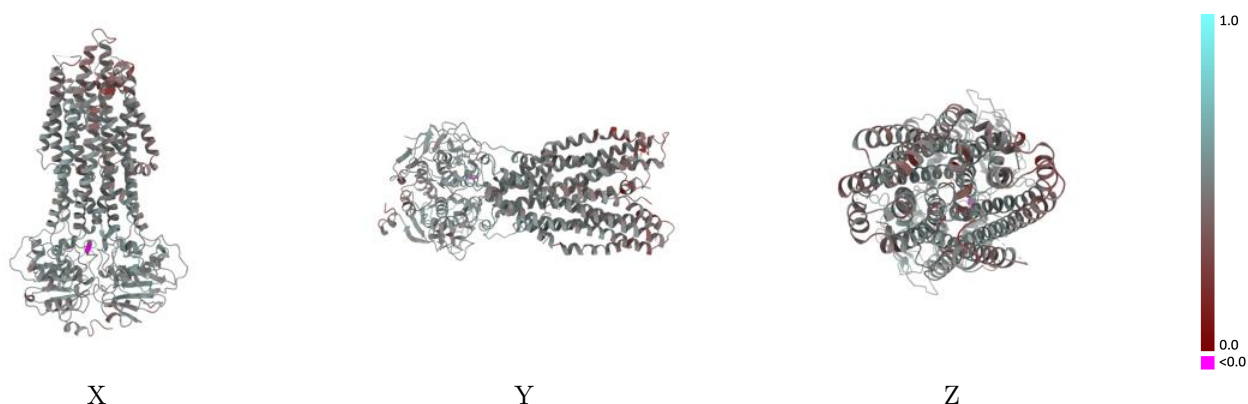
Y



Z

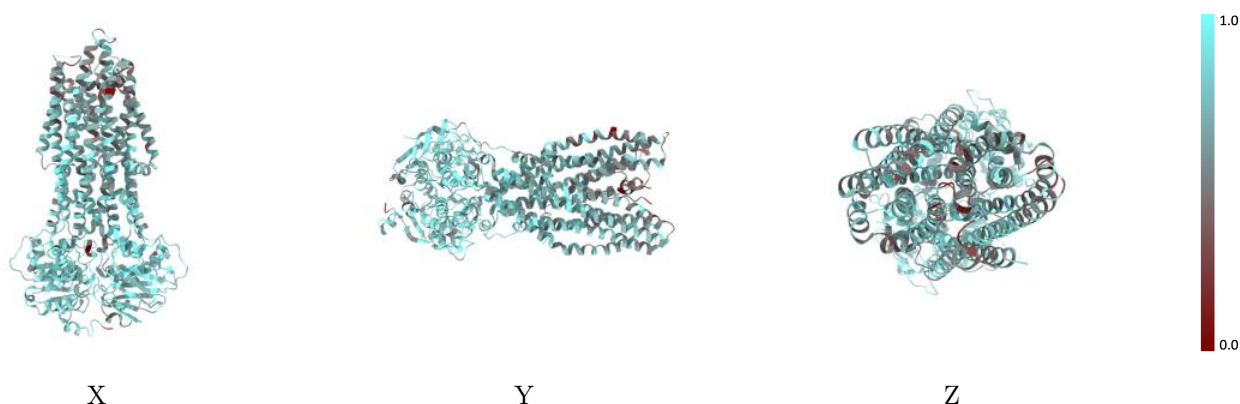
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



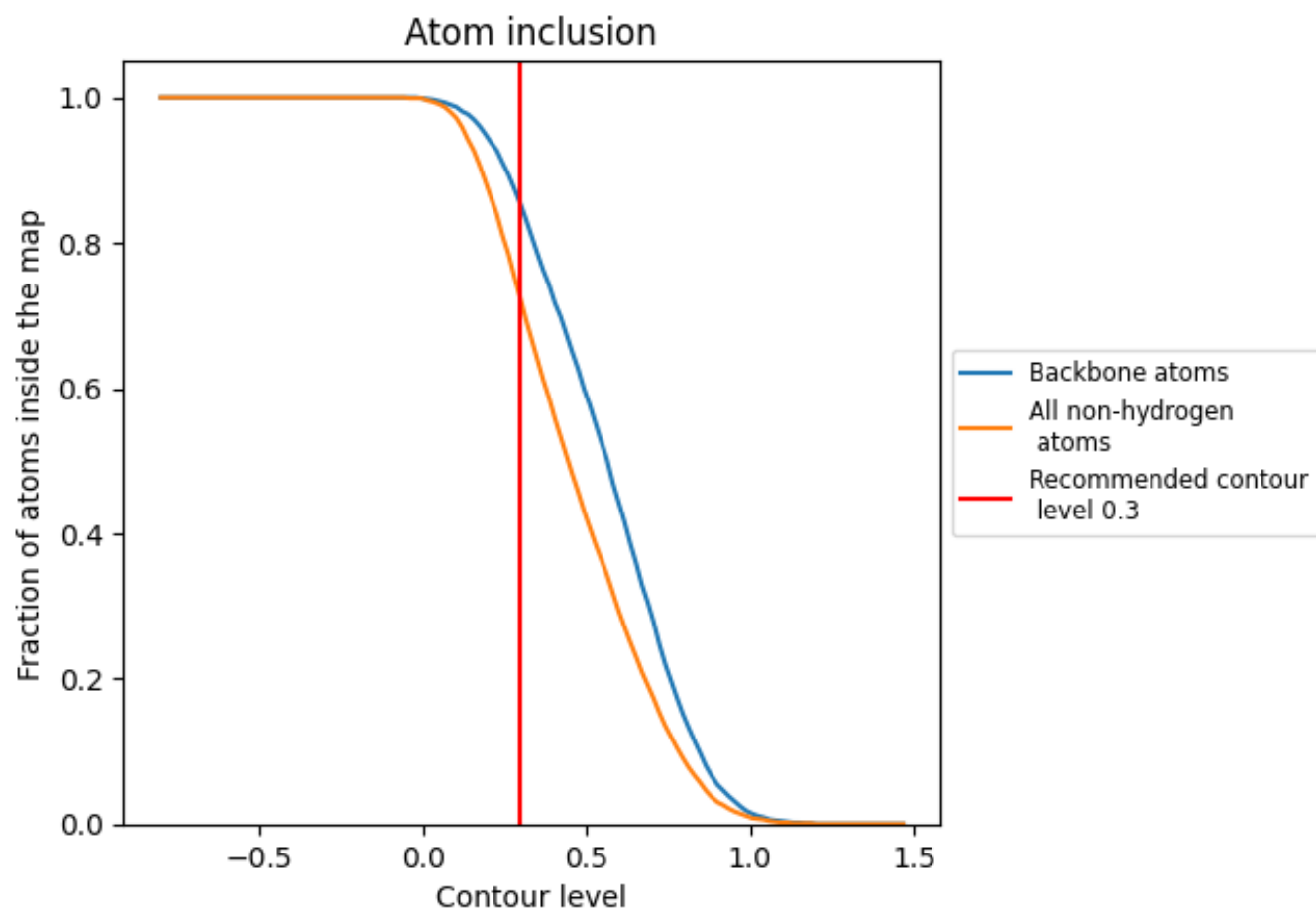
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7210	<div><div></div></div> 0.4840
A	<div><div></div></div> 0.7440	<div><div></div></div> 0.4910
B	<div><div></div></div> 0.7140	<div><div></div></div> 0.4800
D	<div><div></div></div> 0.4740	<div><div></div></div> 0.4350

