



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:33 AM UTC

PDB ID : 8T1F / pdb_00008t1f
EMDB ID : EMD-40962
Title : Cryo-EM structure of full-length human TRPV4 in complex with antagonist HC-067047
Authors : Talyzina, I.A.; Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on : 2023-06-02
Resolution : 3.49 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.dev132
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) : 2.49

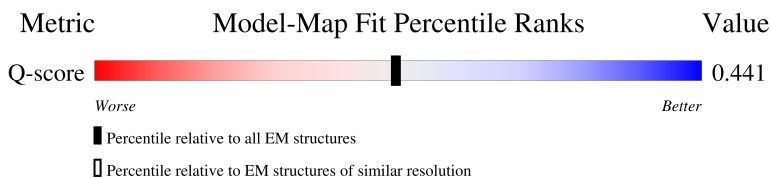
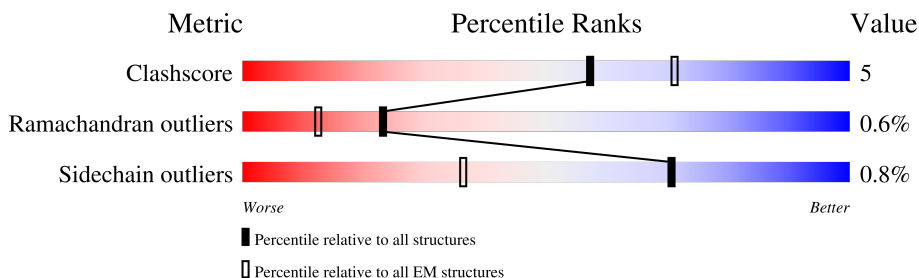
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 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	13600 (2.99 - 3.99)

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	1132	10% 47% 8% 44%
1	B	1132	10% 47% 8% 44%
1	C	1132	11% 48% 8% 44%
1	D	1132	10% 47% 9% 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20790 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 Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	635	Total	C	N	O	S	0	0
			5107	3321	849	911	26		
1	B	636	Total	C	N	O	S	0	0
			5116	3326	850	914	26		
1	C	635	Total	C	N	O	S	0	0
			5107	3321	849	911	26		
1	D	636	Total	C	N	O	S	0	0
			5116	3326	850	914	26		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	872	LEU	-	linker	UNP Q9HBA0
A	873	VAL	-	linker	UNP Q9HBA0
A	874	PRO	-	linker	UNP Q9HBA0
A	875	ARG	-	linker	UNP Q9HBA0
A	876	GLY	-	linker	UNP Q9HBA0
A	877	SER	-	linker	UNP Q9HBA0
A	878	ALA	-	linker	UNP Q9HBA0
A	879	ALA	-	linker	UNP Q9HBA0
A	880	ALA	-	linker	UNP Q9HBA0
A	881	ALA	-	linker	UNP Q9HBA0
A	1087	LYS	ALA	conflict	UNP C5MKY7
A	1120	SER	-	expression tag	UNP C5MKY7
A	1121	GLY	-	expression tag	UNP C5MKY7
A	1122	LEU	-	expression tag	UNP C5MKY7
A	1123	ARG	-	expression tag	UNP C5MKY7
A	1124	SER	-	expression tag	UNP C5MKY7
A	1125	TRP	-	expression tag	UNP C5MKY7
A	1126	SER	-	expression tag	UNP C5MKY7
A	1127	HIS	-	expression tag	UNP C5MKY7
A	1128	PRO	-	expression tag	UNP C5MKY7
A	1129	GLN	-	expression tag	UNP C5MKY7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1130	PHE	-	expression tag	UNP C5MKY7
A	1131	GLU	-	expression tag	UNP C5MKY7
A	1132	LYS	-	expression tag	UNP C5MKY7
B	872	LEU	-	linker	UNP Q9HBA0
B	873	VAL	-	linker	UNP Q9HBA0
B	874	PRO	-	linker	UNP Q9HBA0
B	875	ARG	-	linker	UNP Q9HBA0
B	876	GLY	-	linker	UNP Q9HBA0
B	877	SER	-	linker	UNP Q9HBA0
B	878	ALA	-	linker	UNP Q9HBA0
B	879	ALA	-	linker	UNP Q9HBA0
B	880	ALA	-	linker	UNP Q9HBA0
B	881	ALA	-	linker	UNP Q9HBA0
B	1087	LYS	ALA	conflict	UNP C5MKY7
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B	1126	SER	-	expression tag	UNP C5MKY7
B	1127	HIS	-	expression tag	UNP C5MKY7
B	1128	PRO	-	expression tag	UNP C5MKY7
B	1129	GLN	-	expression tag	UNP C5MKY7
B	1130	PHE	-	expression tag	UNP C5MKY7
B	1131	GLU	-	expression tag	UNP C5MKY7
B	1132	LYS	-	expression tag	UNP C5MKY7
C	872	LEU	-	linker	UNP Q9HBA0
C	873	VAL	-	linker	UNP Q9HBA0
C	874	PRO	-	linker	UNP Q9HBA0
C	875	ARG	-	linker	UNP Q9HBA0
C	876	GLY	-	linker	UNP Q9HBA0
C	877	SER	-	linker	UNP Q9HBA0
C	878	ALA	-	linker	UNP Q9HBA0
C	879	ALA	-	linker	UNP Q9HBA0
C	880	ALA	-	linker	UNP Q9HBA0
C	881	ALA	-	linker	UNP Q9HBA0
C	1087	LYS	ALA	conflict	UNP C5MKY7
C	1120	SER	-	expression tag	UNP C5MKY7
C	1121	GLY	-	expression tag	UNP C5MKY7
C	1122	LEU	-	expression tag	UNP C5MKY7
C	1123	ARG	-	expression tag	UNP C5MKY7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1124	SER	-	expression tag	UNP C5MKY7
C	1125	TRP	-	expression tag	UNP C5MKY7
C	1126	SER	-	expression tag	UNP C5MKY7
C	1127	HIS	-	expression tag	UNP C5MKY7
C	1128	PRO	-	expression tag	UNP C5MKY7
C	1129	GLN	-	expression tag	UNP C5MKY7
C	1130	PHE	-	expression tag	UNP C5MKY7
C	1131	GLU	-	expression tag	UNP C5MKY7
C	1132	LYS	-	expression tag	UNP C5MKY7
D	872	LEU	-	linker	UNP Q9HBA0
D	873	VAL	-	linker	UNP Q9HBA0
D	874	PRO	-	linker	UNP Q9HBA0
D	875	ARG	-	linker	UNP Q9HBA0
D	876	GLY	-	linker	UNP Q9HBA0
D	877	SER	-	linker	UNP Q9HBA0
D	878	ALA	-	linker	UNP Q9HBA0
D	879	ALA	-	linker	UNP Q9HBA0
D	880	ALA	-	linker	UNP Q9HBA0
D	881	ALA	-	linker	UNP Q9HBA0
D	1087	LYS	ALA	conflict	UNP C5MKY7
D	1120	SER	-	expression tag	UNP C5MKY7
D	1121	GLY	-	expression tag	UNP C5MKY7
D	1122	LEU	-	expression tag	UNP C5MKY7
D	1123	ARG	-	expression tag	UNP C5MKY7
D	1124	SER	-	expression tag	UNP C5MKY7
D	1125	TRP	-	expression tag	UNP C5MKY7
D	1126	SER	-	expression tag	UNP C5MKY7
D	1127	HIS	-	expression tag	UNP C5MKY7
D	1128	PRO	-	expression tag	UNP C5MKY7
D	1129	GLN	-	expression tag	UNP C5MKY7
D	1130	PHE	-	expression tag	UNP C5MKY7
D	1131	GLU	-	expression tag	UNP C5MKY7
D	1132	LYS	-	expression tag	UNP C5MKY7

- Molecule 2 is 2-methyl-1-[3-(morpholin-4-yl)propyl]-5-phenyl-N-[3-(trifluoromethyl)phenyl]-1H-pyrrole-3-carboxamide (CCD ID: X7N) (formula: C₂₆H₂₈F₃N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 34	C 26	F 3	N 3	O 2	0
2	B	1	Total 34	C 26	F 3	N 3	O 2	0
2	C	1	Total 34	C 26	F 3	N 3	O 2	0
2	D	1	Total 34	C 26	F 3	N 3	O 2	0

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 52	C 42	N 1	O 8	P 1	0
3	B	1	Total 52	C 42	N 1	O 8	P 1	0
3	C	1	Total 52	C 42	N 1	O 8	P 1	0
3	D	1	Total 52	C 42	N 1	O 8	P 1	0

ASN	ARG	ILE	GLU	LEU	GLY	LYS	ILE	ASP	ASP	GLY	ASN	ASN	LEU	GLY	HIS	LYS	LEU	GLU	TYR	TYR	ASN	ASN	ASN	VAL	TYR	ILE	ILE	MET	ALA	ASP	LYS	LYS	GLN	VAL	ASN	ASN	ASP	ASP	GLY	LYS	ARG	ILE	GLU	ILE	ASN	ASN	GLN	VAL	VAL	GLY	ASP	ASP	GLY	ASN	ASN	GLN	VAL	VAL	GLN	LEU	LEU	ALA	ASP
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LEU	ARG	SER	TRP	SER	HIS	PRO	GLN	THR	ASN	GLN	GLY	ASP	GLY	VAL	PRO	LEU	LEU	ASP	ASN	HIS	TRP	LEU	SER	THR	GLN	SER	GLY	LEU	LYS	ASP	PRO	ASN	GLU	LYS	ASP	ARG	ASP	HIS	HIS	VAL	VAL	LEU	LEU	GLY	ILE	ALA	ALA	THR	THR	LEU	GLY	MET	ASP	GLU	LEU	LYS	LYS	SER	GLY
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- Molecule 1: Transient receptor potential cation channel subfamily V member 4/Enhanced green fluorescent protein chimera

[illegible]

Lys	Arg	Trp	Arg	Lys	Lys	Ile	Glu	Lys	Gln	Pro	Gln	Ser	Pro	Pro	Ile	Leu	Lys	V148	L154	F155	D156	R160	G161	S162	T163	A164	D165	L166	D167	G168	L169	L170	L173	L174	T175	H176	K177	K178	R179	E183	E184	F185	R186	S189	T190																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
G191	K192	P196	K197	A198	R206	N207	D208	T209	L210	E218	R219	G221	R224	R232	Y236	R243	E247	L256	Q260	D263	Q267	K268	R269	Q274	E278	Y283	P288	H309	Q317	R320	G321	K322	H326	I331	A332	D333	N334																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			</

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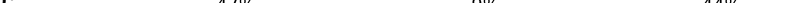
ALA PRO LEU LEU VAL PRO ARG GLY SER ALA ALA ALA VAL SER LYS GLY GLU LEU PHE THR THR THR TYR TYR LYS LEU LEU PHE

CYS	THR	THR	THR	GLY	LEU	PRO	VAL	TRP	PRO	THR	THR	LEU	VAL	THR	THR	LEU	THR	TYR	GLY	VAL	GLN	CYS	PHE	SER	ARG	TYR	PRO	ASP	HIS	HIS	MET	LYS	GLN	ASP	PHE	PHE	LYS	SER	ALA	ALA	MET	PRO	GLU	GLY	GLY	TYR	VAL	GLN	GLU	ARG	THR	ILE	PHE	PHE	LYS	ASP	ASP	GLY	ASN	TYR	TYR
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THR	ARG	ALA	ALA	GLU	VAL	LYS	PHE	GLU	GLY	ASP	THR	LEU	VAL	ASN	ARG	GLU	LEU	LYS	GLY	ILE	ASP	PHE	LYS	GLU	ASP	GLY	ASN	ASN	ILE	LEU	GLY	HIS	HIS	ASN	ASN	VAL	TYR	TYR	ILE	MET	MET	ILE	ALA	ASP	LYS	GLN	LYS	LYS	ASN	ASN	PHE	LYS	ILE	LYS	VAL	ASN	ASN	PHE	LYS	ILE	THR
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ARG	HIS	ASN	ASN	ILE	GLU	ASP	GLY	SER	Gln	LEU	ALA	ASP	HIS	Tyr	Gln	Gln	Asn	Pro	Thr	Pro	Ile	GLY	GLY	GLY	GLY	PRO	VAL	LEU	LEU	LEU	LEU	SER	THR	Gln	SER	SER	Lys	Lys	LEU	LEU	SER	Lys	ASP	PRO	PRO	ASN	GLU	Lys	Arg	ASP	HIS	MET	Val	Val	Leu	Leu	GLU	PHE	Val	Val	Thr	Ala	Ala
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GLY	ILE	THR	LEU	GLY	MET	ASP	GLU	LEU	TYR	LYS	SER	GLY	LEU	ARG	SER	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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- Chain D: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65881	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.891	Depositor
Minimum map value	-0.559	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, X7N

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	0.29	0/5225	0.84	6/7083 (0.1%)
1	B	0.29	0/5234	0.79	8/7095 (0.1%)
1	C	0.29	0/5225	0.84	6/7083 (0.1%)
1	D	0.29	0/5234	0.79	6/7095 (0.1%)
All	All	0.29	0/20918	0.82	26/28356 (0.1%)

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	A	0	2
1	B	0	4
1	C	0	2
1	D	0	4
All	All	0	12

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	721	THR	CA-C-N	6.67	133.98	121.97
1	A	721	THR	C-N-CA	6.67	133.98	121.97
1	C	721	THR	CA-C-N	6.66	133.95	121.97
1	C	721	THR	C-N-CA	6.66	133.95	121.97
1	B	364	ALA	N-CA-C	-6.36	106.74	114.75

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	SER	Peptide
1	A	722	VAL	Peptide
1	B	222	ASN	Peptide
1	B	383	ILE	Peptide
1	B	497	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5107	0	5176	56	0
1	B	5116	0	5182	54	0
1	C	5107	0	5176	49	0
1	D	5116	0	5182	56	0
2	A	34	0	0	0	0
2	B	34	0	0	0	0
2	C	34	0	0	0	0
2	D	34	0	0	0	0
3	A	52	0	82	1	0
3	B	52	0	82	1	0
3	C	52	0	82	1	0
3	D	52	0	82	1	0
All	All	20790	0	21044	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 201 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:249:ARG:NH2	1:B:295:THR:O	2.32	0.63
1:D:249:ARG:NH2	1:D:295:THR:O	2.32	0.63
1:B:552:LEU:HB3	1:B:588:ASN:HD21	1.65	0.62
1:D:552:LEU:HB3	1:D:588:ASN:HD21	1.65	0.61
1:D:544:PHE:O	1:D:736:GLN:NE2	2.34	0.60

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	A	631/1132 (56%)	545 (86%)	80 (13%)	6 (1%)	12	44
1	B	632/1132 (56%)	563 (89%)	67 (11%)	2 (0%)	36	67
1	C	631/1132 (56%)	545 (86%)	80 (13%)	6 (1%)	12	44
1	D	632/1132 (56%)	563 (89%)	67 (11%)	2 (0%)	36	67
All	All	2526/4528 (56%)	2216 (88%)	294 (12%)	16 (1%)	23	54

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	722	VAL
1	A	723	GLY
1	C	722	VAL
1	C	723	GLY
1	A	190	THR

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	A	559/987 (57%)	554 (99%)	5 (1%)	70	76
1	B	560/987 (57%)	555 (99%)	5 (1%)	70	76
1	C	559/987 (57%)	554 (99%)	5 (1%)	70	76
1	D	560/987 (57%)	556 (99%)	4 (1%)	76	78
All	All	2238/3948 (57%)	2219 (99%)	19 (1%)	70	77

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	683	LEU
1	D	696	ILE
1	D	732	ILE
1	D	331	ILE
1	B	696	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	265	HIS
1	C	588	ASN
1	D	784	ASN
1	C	322	ASN
1	C	474	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](#)

8 ligands 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
2	X7N	A	1201	-	37,37,37	0.46	0	50,52,52	0.65	0
3	POV	D	1202	-	51,51,51	0.33	0	57,59,59	0.45	0
2	X7N	C	1201	-	37,37,37	0.52	0	50,52,52	0.67	0
3	POV	A	1202	-	51,51,51	0.33	0	57,59,59	0.41	0
2	X7N	D	1201	-	37,37,37	0.47	0	50,52,52	0.72	2 (4%)
2	X7N	B	1201	-	37,37,37	0.47	0	50,52,52	0.71	1 (2%)
3	POV	B	1202	-	51,51,51	0.33	0	57,59,59	0.43	0
3	POV	C	1202	-	51,51,51	0.32	0	57,59,59	0.43	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
2	X7N	A	1201	-	-	6/24/32/32	0/4/4/4
3	POV	D	1202	-	-	28/55/55/55	-
2	X7N	C	1201	-	-	6/24/32/32	0/4/4/4
3	POV	A	1202	-	-	19/55/55/55	-
2	X7N	D	1201	-	-	6/24/32/32	0/4/4/4
2	X7N	B	1201	-	-	6/24/32/32	0/4/4/4
3	POV	B	1202	-	-	27/55/55/55	-
3	POV	C	1202	-	-	17/55/55/55	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	X7N	C28-N29-C34	2.06	116.72	111.24
2	B	1201	X7N	C28-N29-C34	2.05	116.71	111.24
2	D	1201	X7N	C6-N5-C4	2.03	131.06	127.45

There are no chirality outliers.

5 of 115 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	POV	C1-O11-P-O12
3	A	1202	POV	C1-O11-P-O13
3	A	1202	POV	C1-O11-P-O14

Continued on next page...

Continued from previous page...

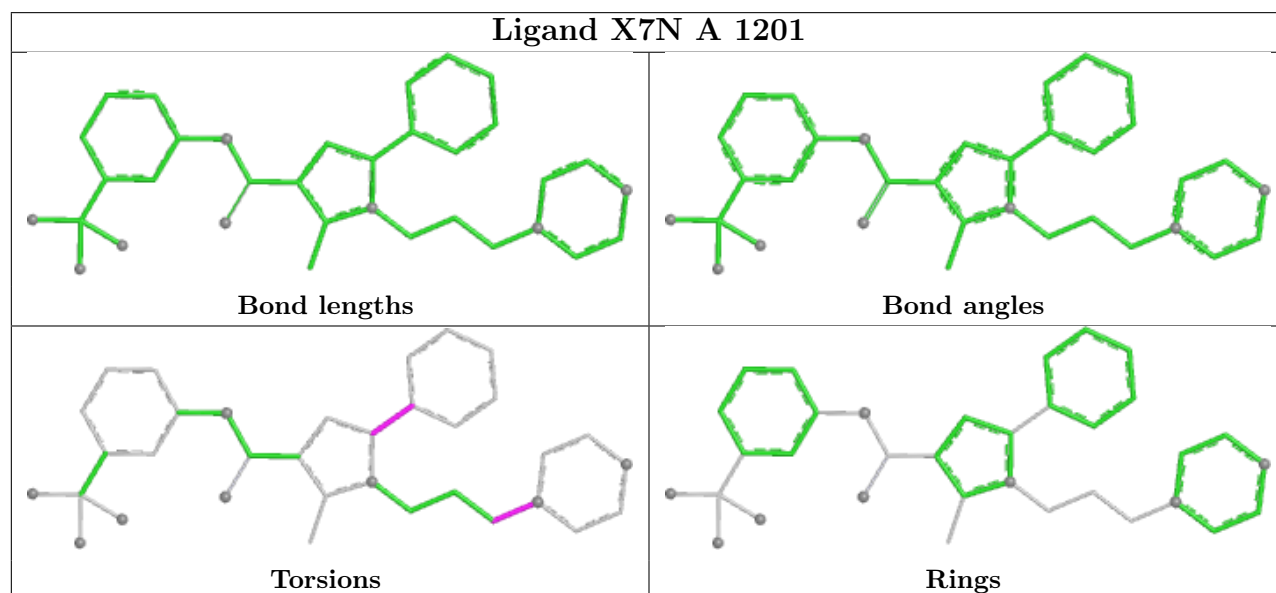
Mol	Chain	Res	Type	Atoms
3	A	1202	POV	C11-O12-P-O14
3	A	1202	POV	C22-C21-O21-C2

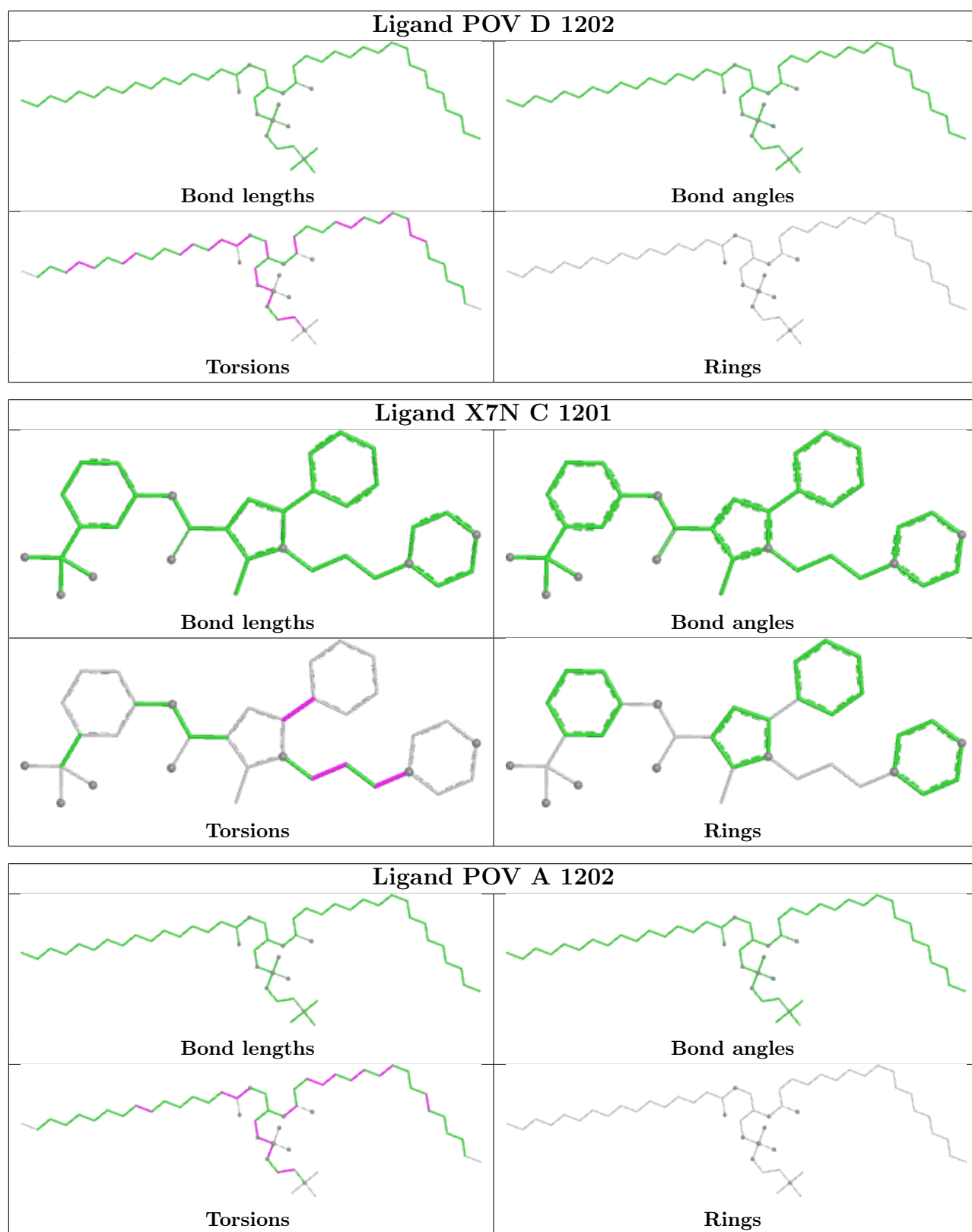
There are no ring outliers.

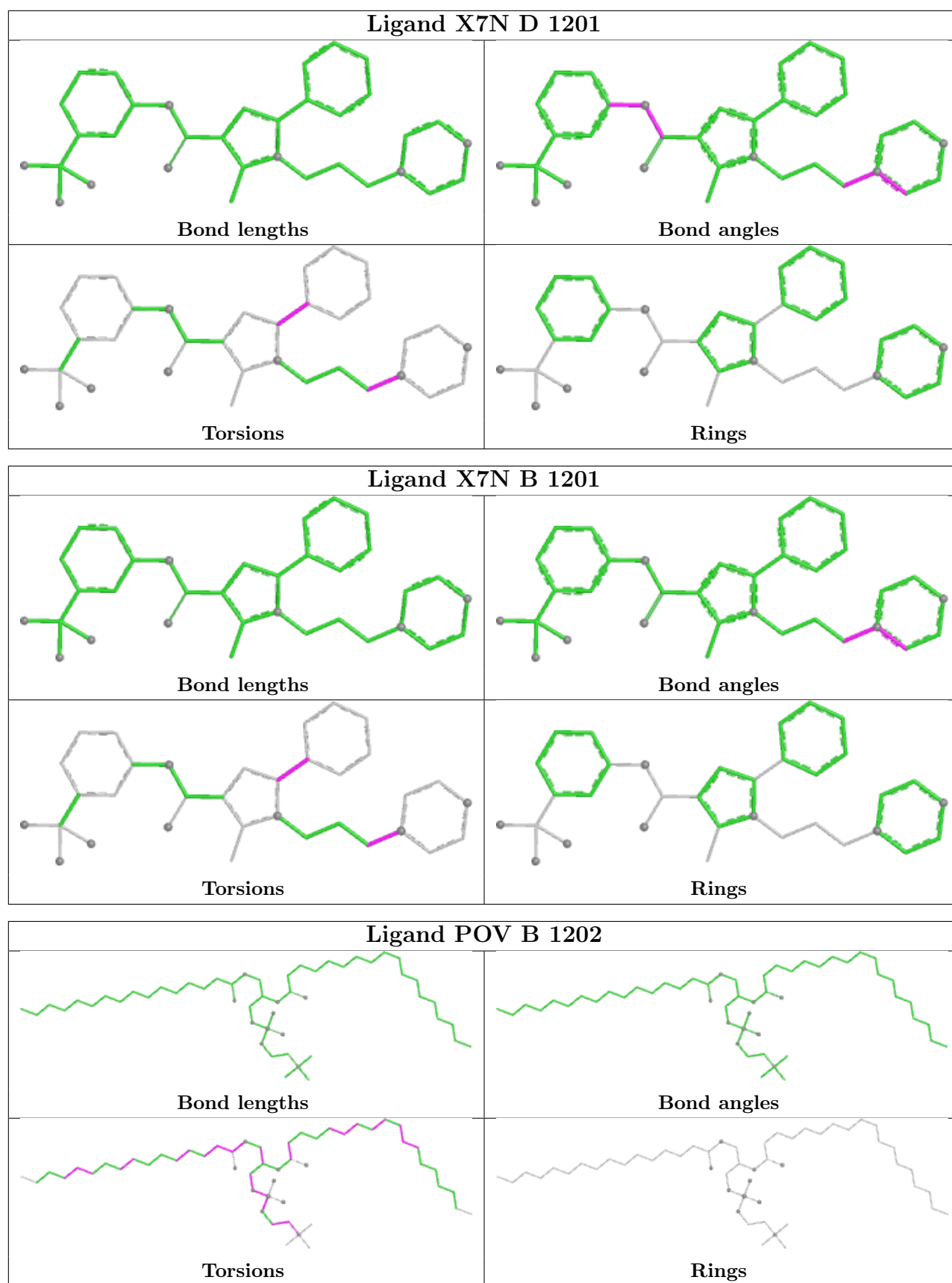
4 monomers are involved in 4 short contacts:

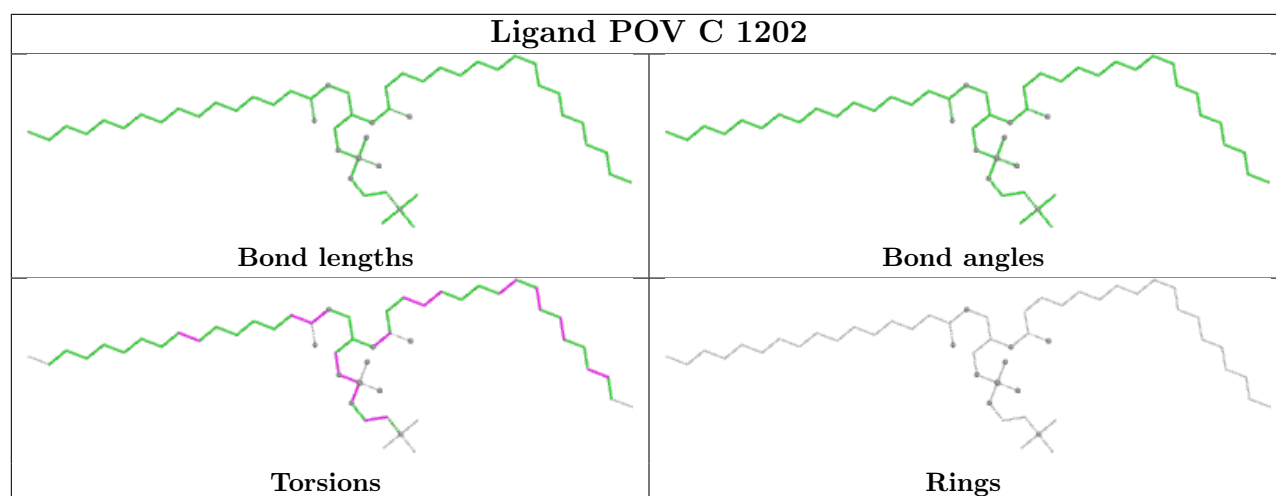
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1202	POV	1	0
3	A	1202	POV	1	0
3	B	1202	POV	1	0
3	C	1202	POV	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

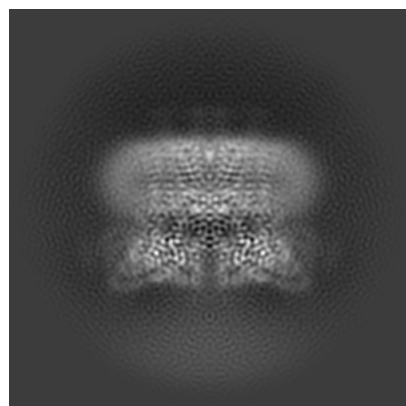
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40962. These allow visual inspection of the internal detail of the map and identification of artifacts.

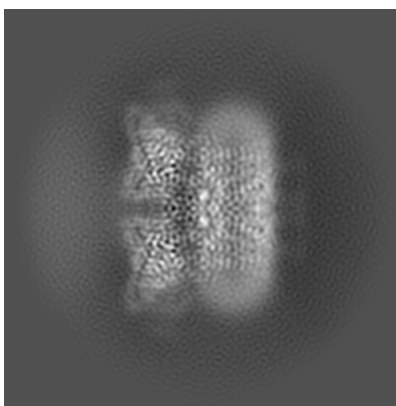
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

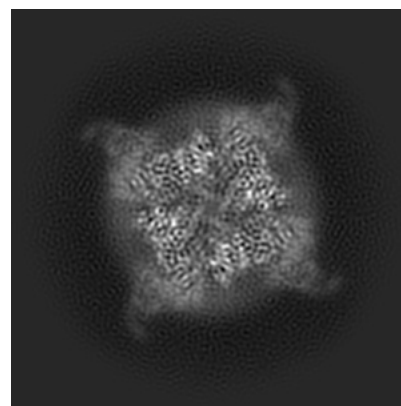
6.1.1 Primary map



X

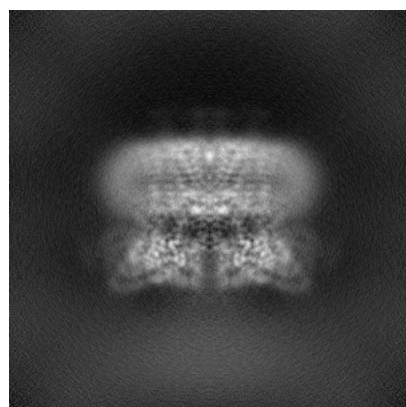


Y

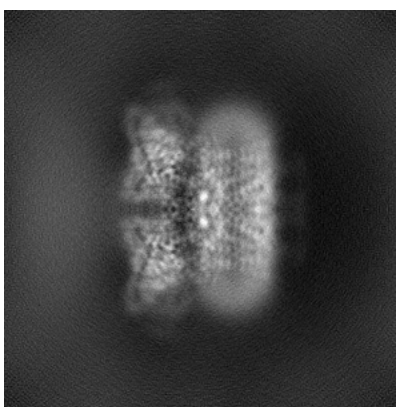


Z

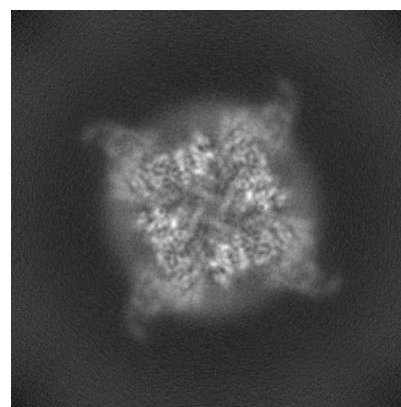
6.1.2 Raw map



X



Y

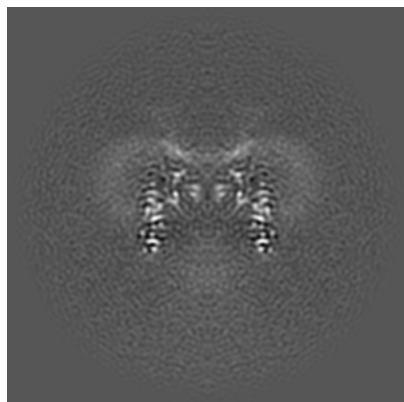


Z

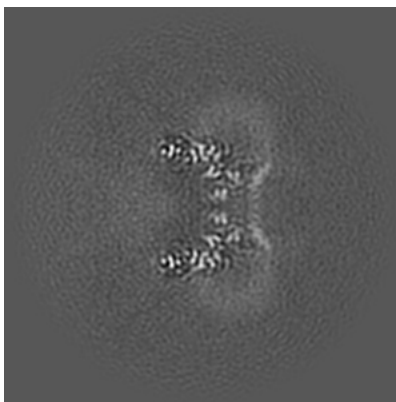
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

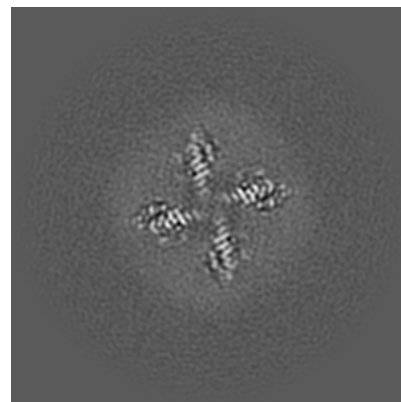
6.2.1 Primary map



X Index: 160

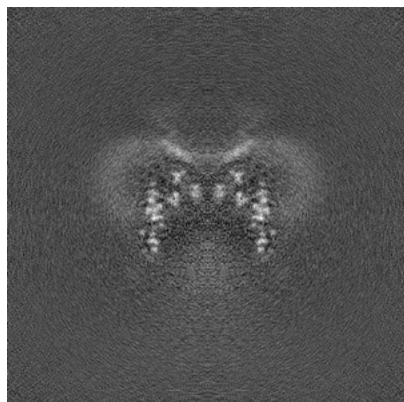


Y Index: 160

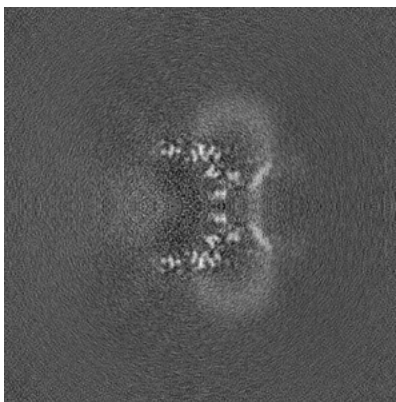


Z Index: 160

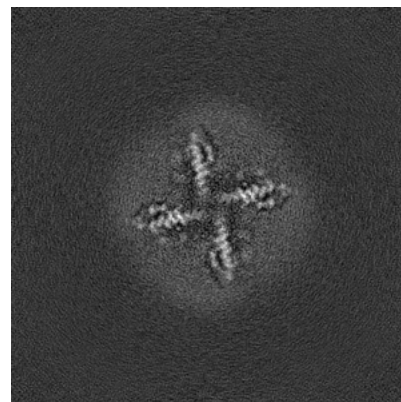
6.2.2 Raw map



X Index: 160



Y Index: 160

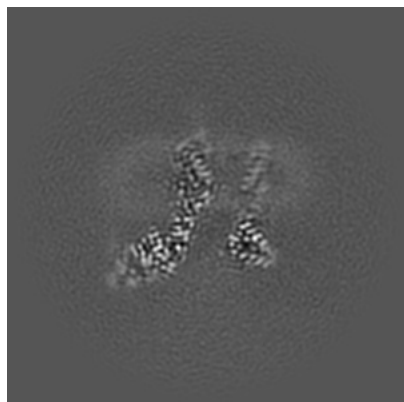


Z Index: 160

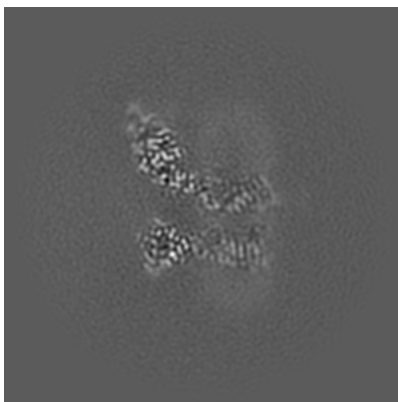
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

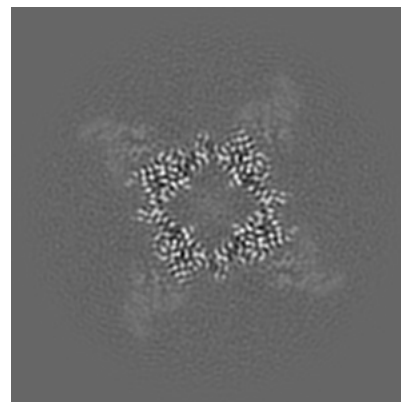
6.3.1 Primary map



X Index: 134

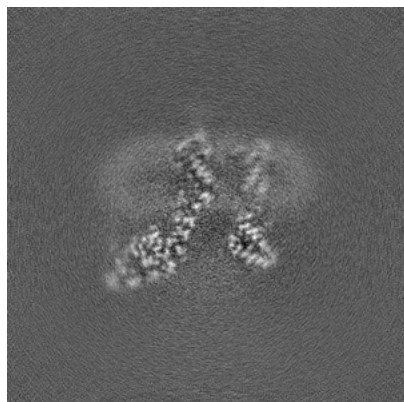


Y Index: 134

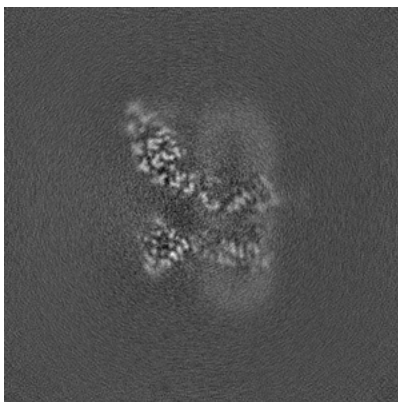


Z Index: 129

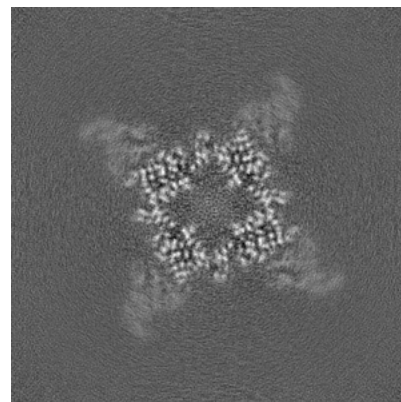
6.3.2 Raw map



X Index: 135



Y Index: 134

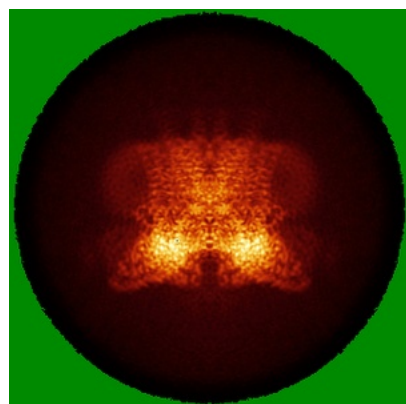


Z Index: 129

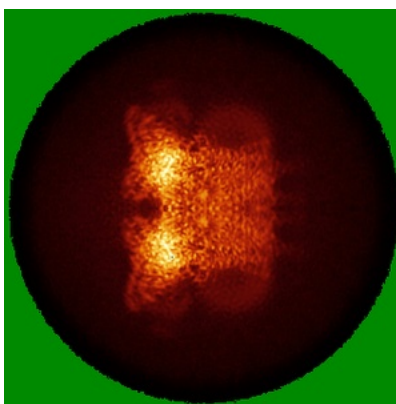
The images above show the largest variance slices of the map in three orthogonal directions.

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

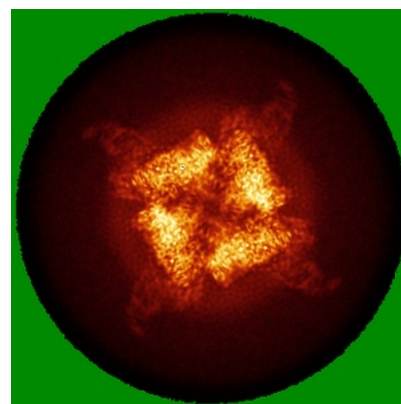
6.4.1 Primary map



X

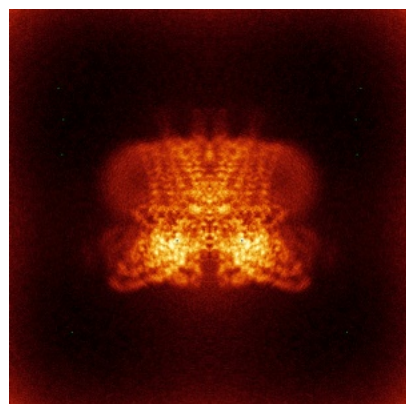


Y

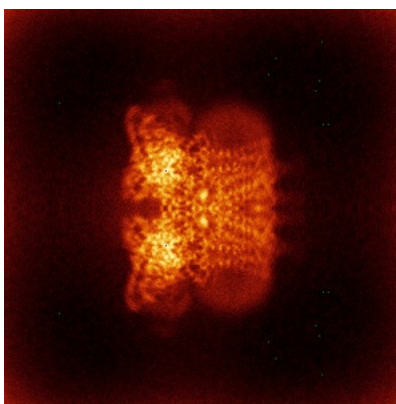


Z

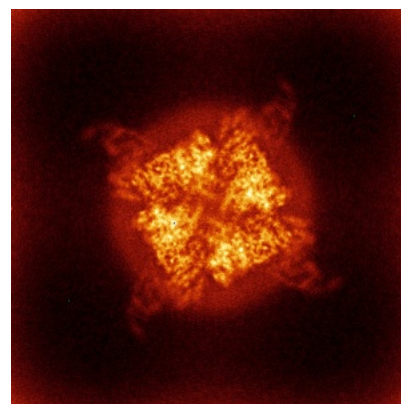
6.4.2 Raw map



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](#)

This section was not generated.

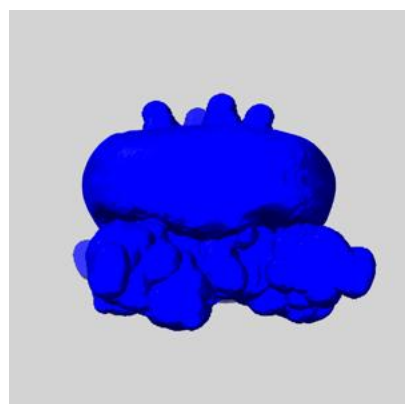
6.6 Mask visualisation [i](#)

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

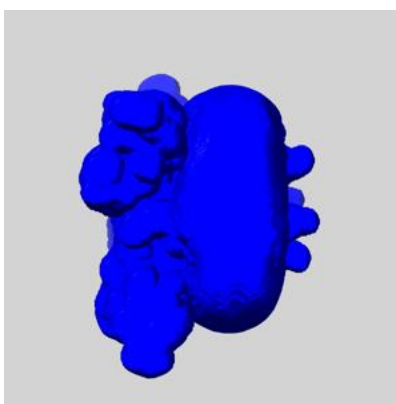
A mask typically either:

- 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_40962_msk_1.map [i](#)



X



Y

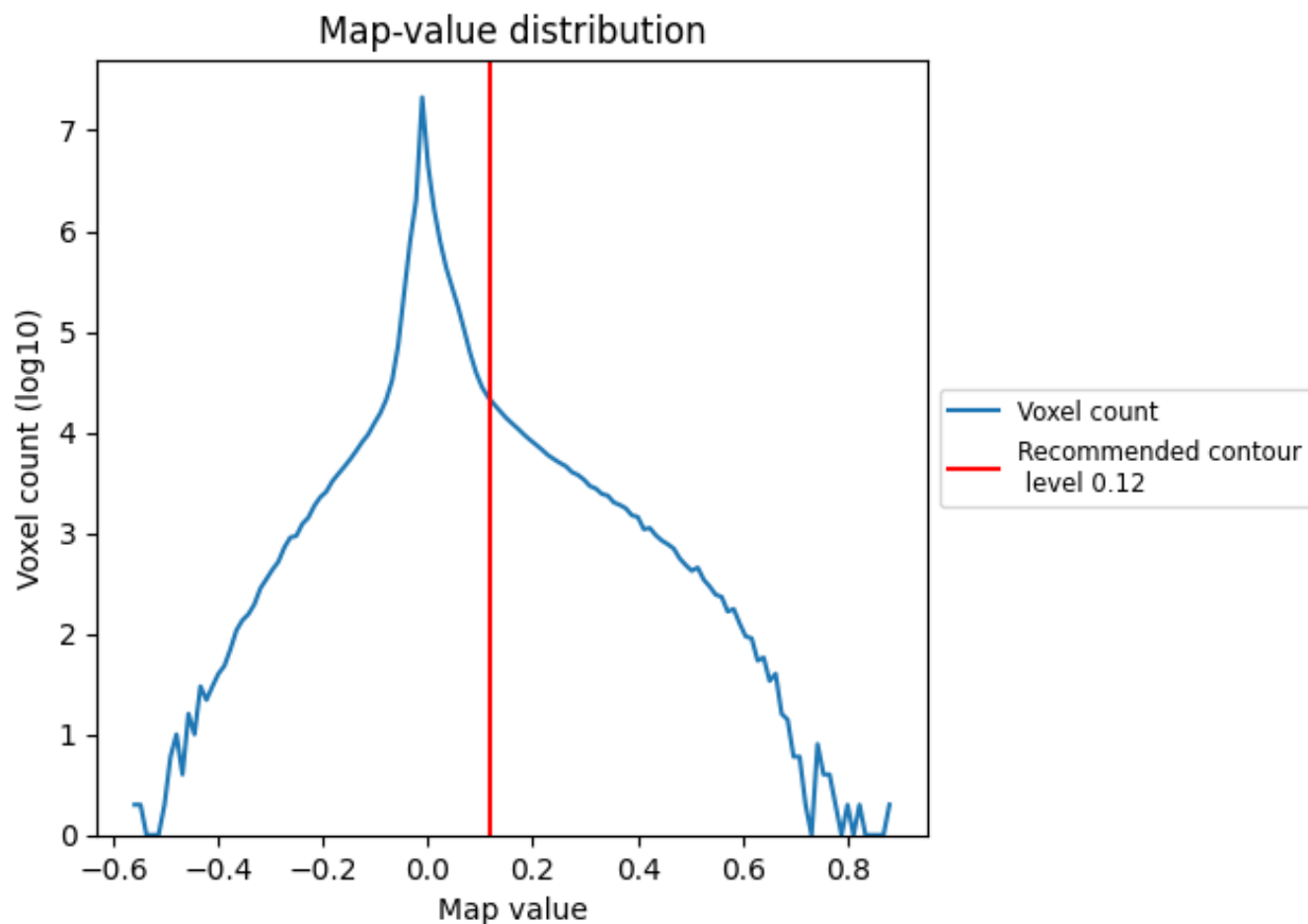


Z

7 Map analysis [i](#)

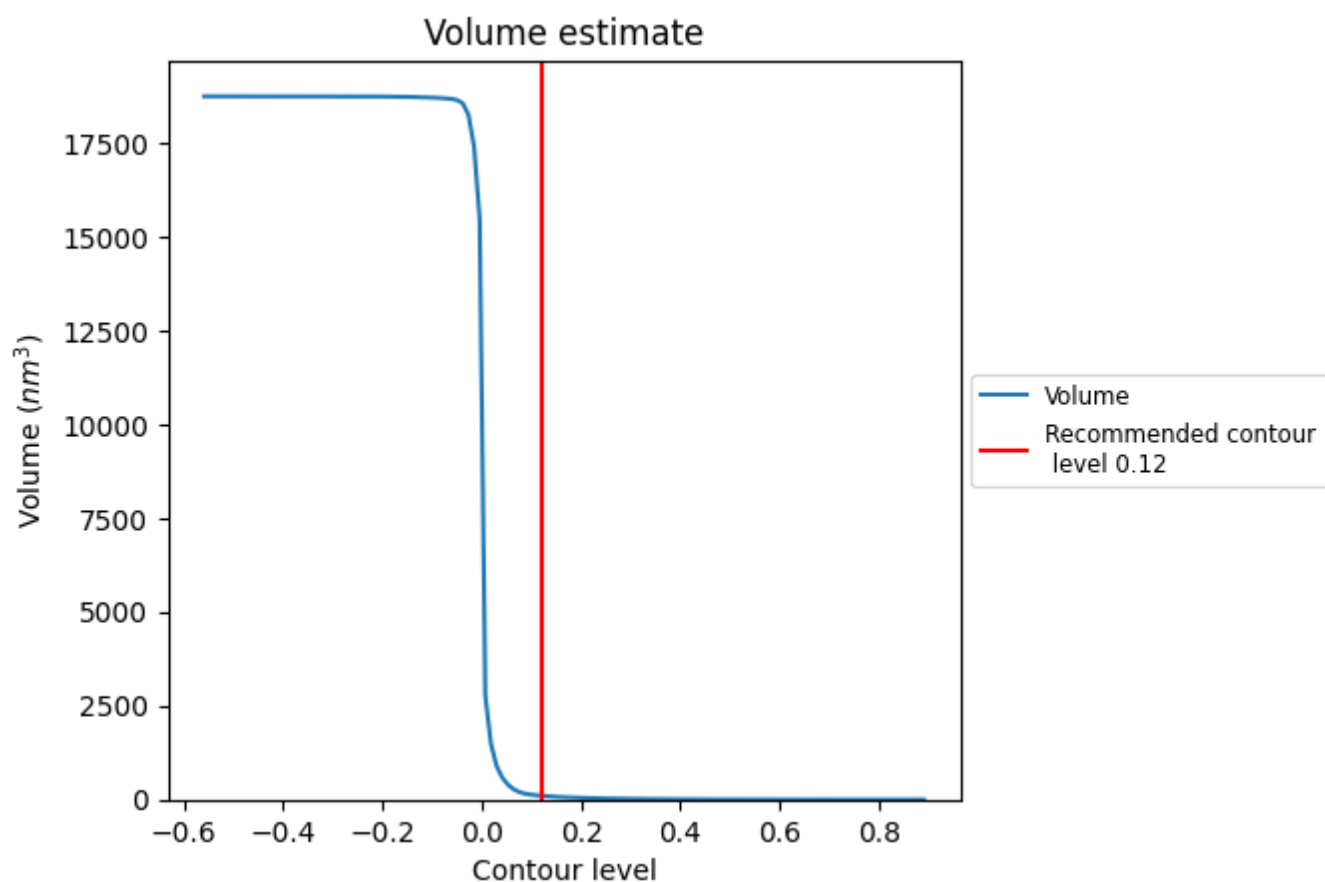
This section contains the results of statistical analysis of the map.

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.

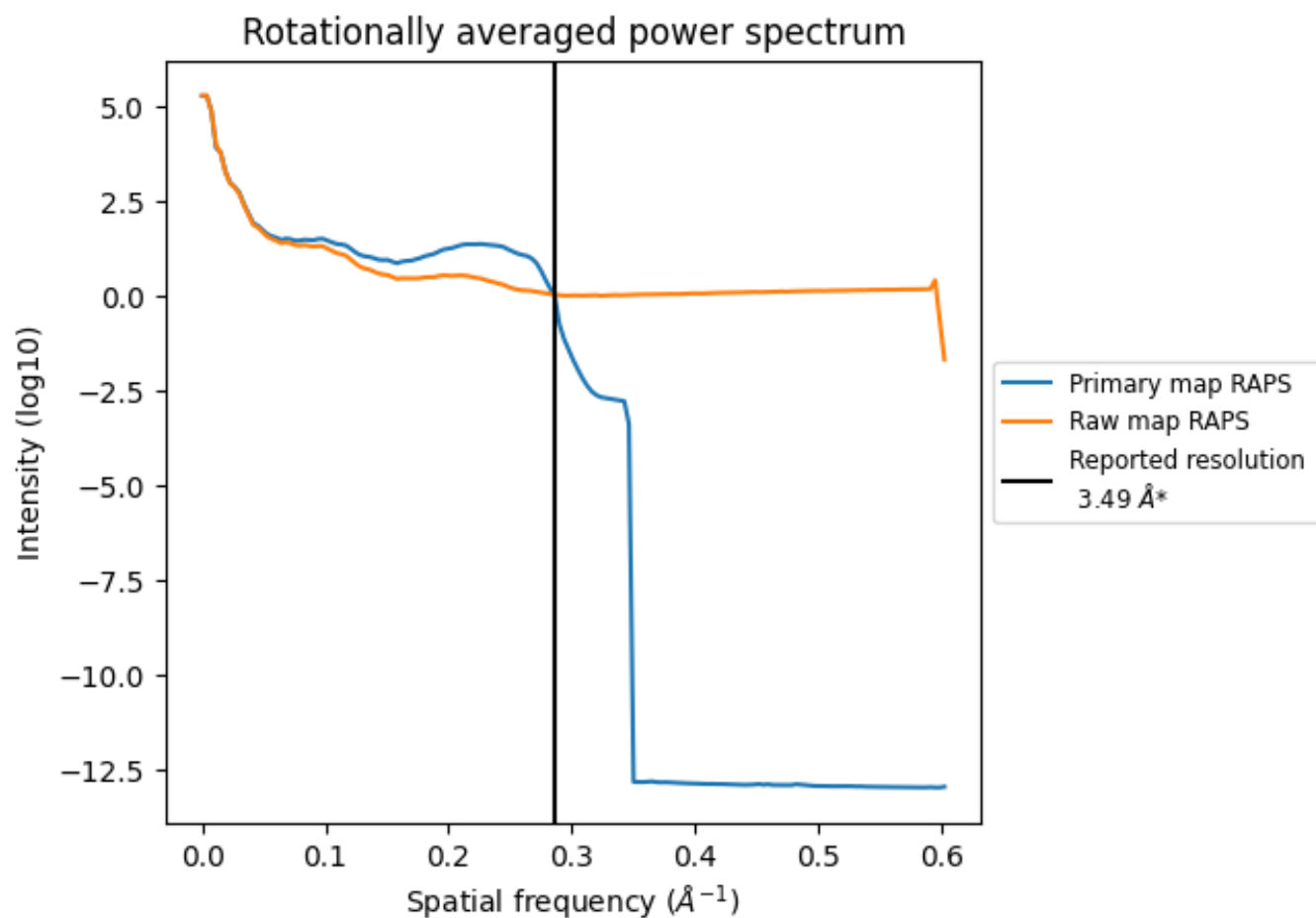
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm³; this corresponds to an approximate mass of 91 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 ⓘ

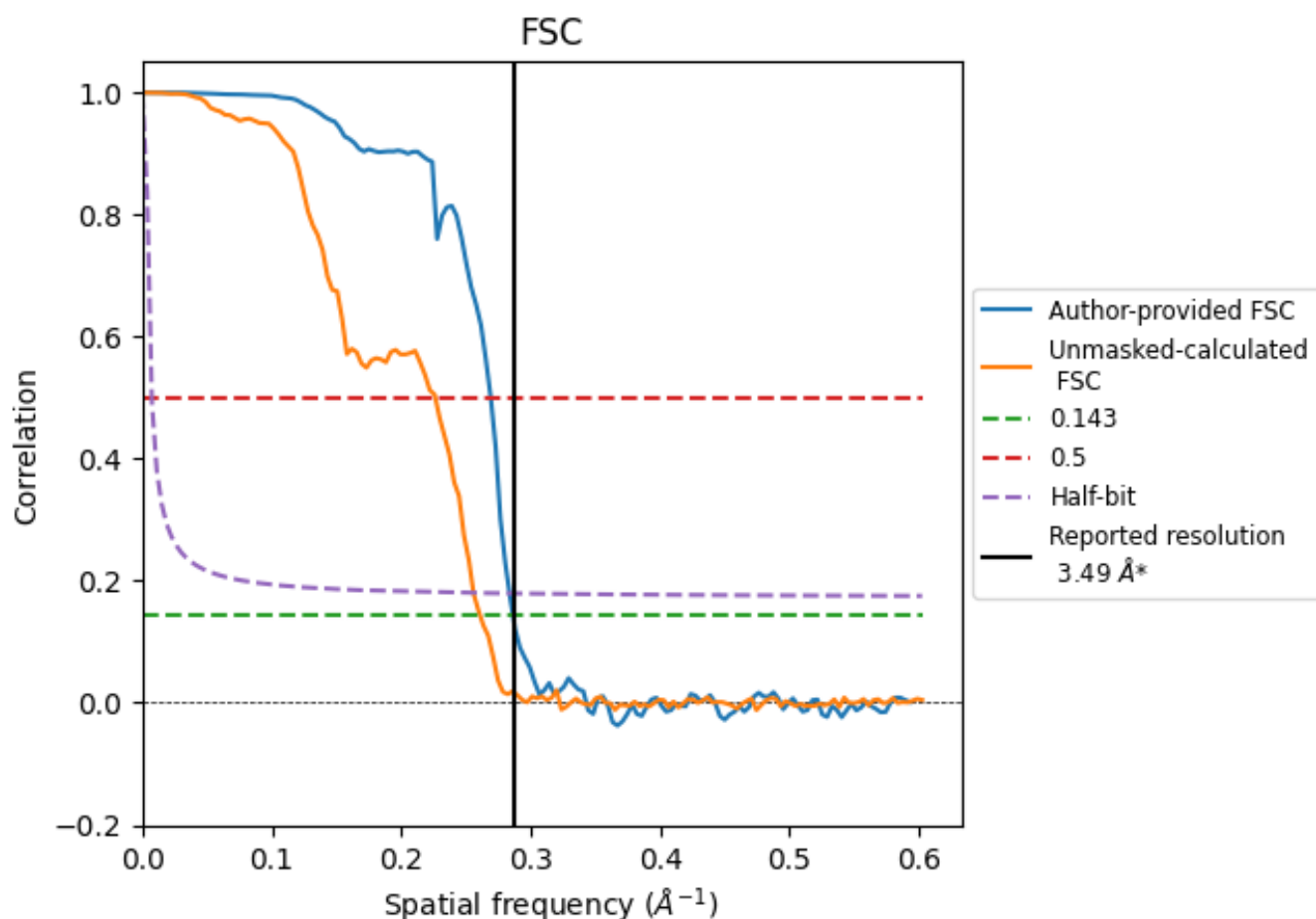


*Reported resolution corresponds to spatial frequency of 0.287 $\text{\AA}^{-1}$

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 0.287 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	3.71	3.52
Unmasked-calculated*	3.83	4.42	3.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

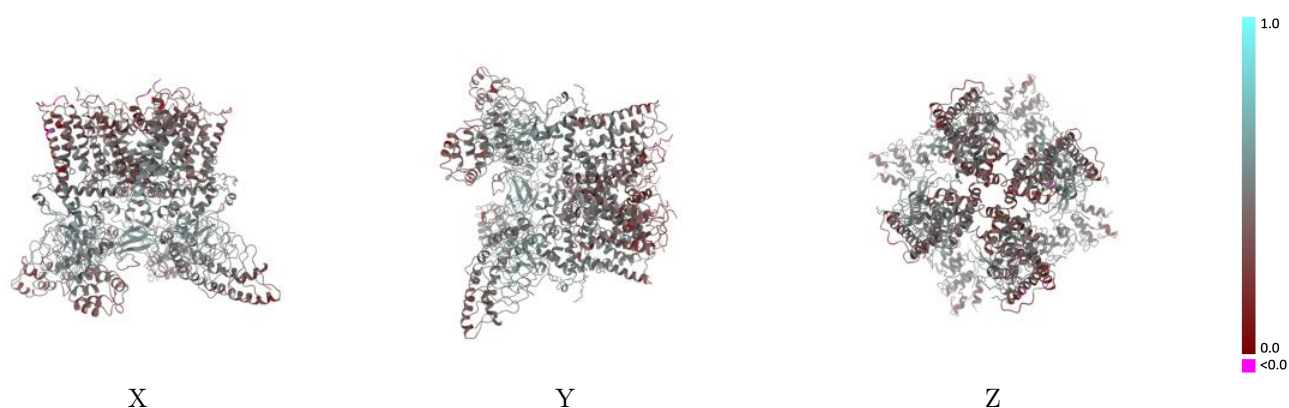
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-40962 and PDB model 8T1F. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

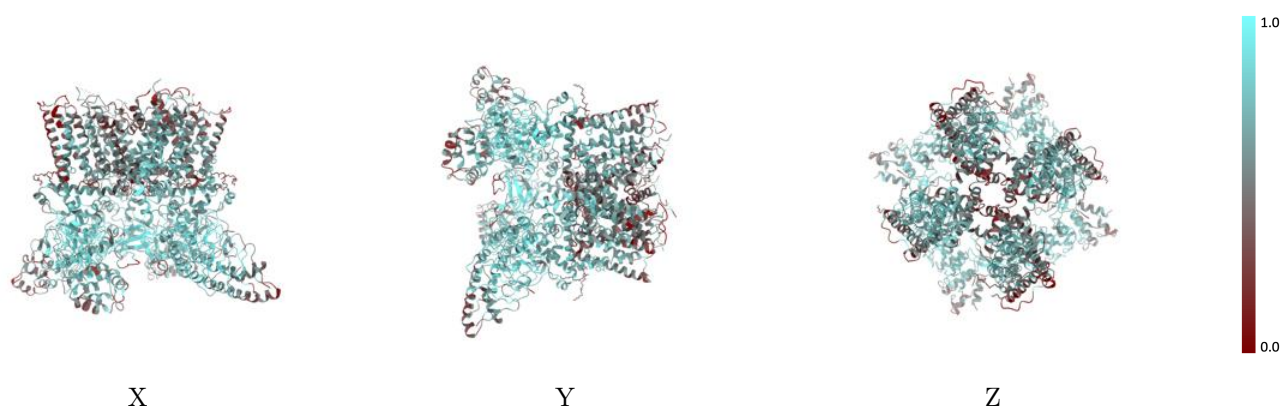
This section was not generated.

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



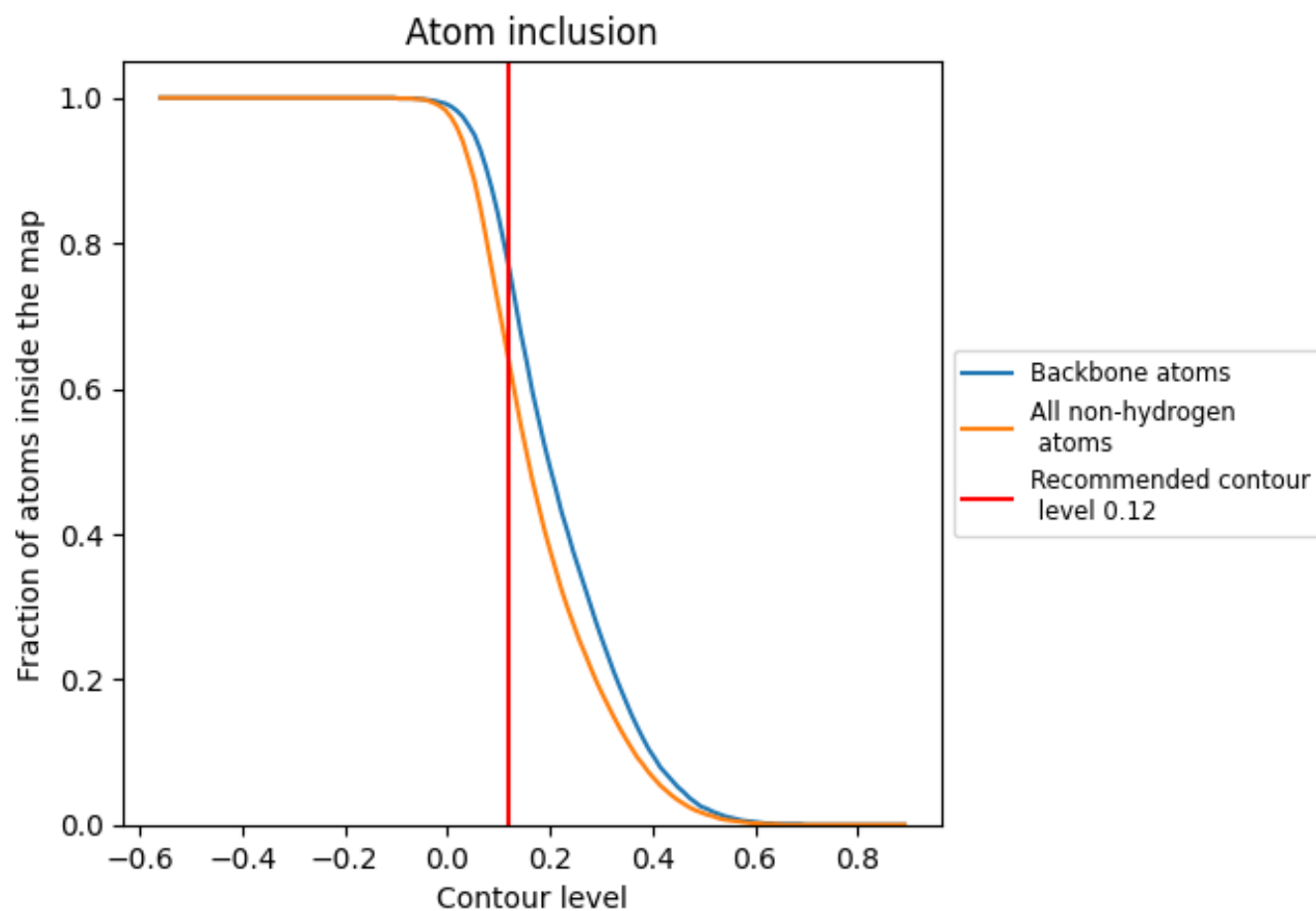
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6370	0.4410
A	0.6330	0.4430
B	0.6410	0.4420
C	0.6230	0.4280
D	0.6490	0.4520

