wwPDB EM Validation Summary Report

Aug 8, 2026 – 04:08 PM EDT

PDB ID	:	9YVK / pdb_00009yvk
EMDB ID	:	EMD-73526
Title	:	Cryo-EM structure of the human TRPM4 channel bound to NC1 in the presence of EGTA.
Authors	:	Teixeira-Duarte, C.M.; Jiang, Y.
Deposited on	:	2025-10-23
Resolution	:	2.69 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:

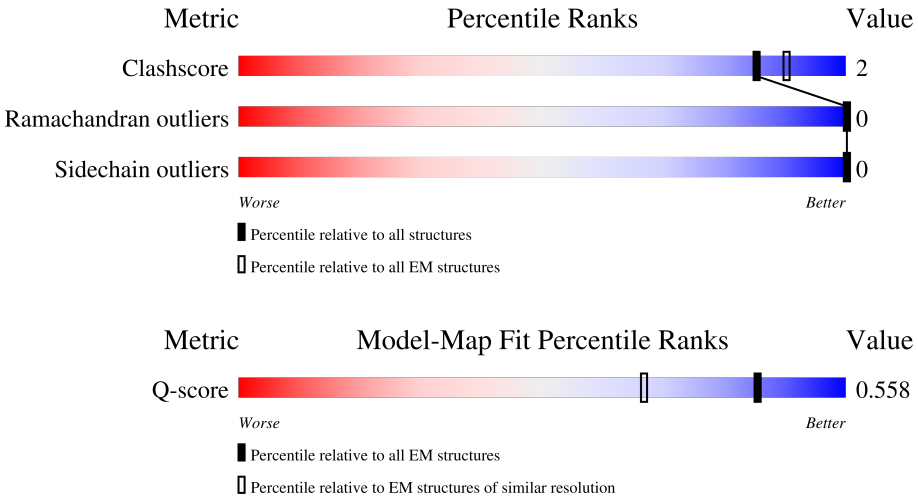
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9309 (2.19 - 3.19)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1231	16% 73% 5% 22%
1	B	1231	16% 74% 5% 22%
1	C	1231	16% 74% 5% 22%
1	D	1231	16% 74% 5% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 30856 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 M member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	965	Total	C	N	O	S	0	0
			7687	4961	1344	1342	40		
1	A	965	Total	C	N	O	S	0	0
			7687	4961	1344	1342	40		
1	B	965	Total	C	N	O	S	0	0
			7687	4961	1344	1342	40		
1	D	965	Total	C	N	O	S	0	0
			7687	4961	1344	1342	40		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP Q8TD43
C	-15	ASP	-	expression tag	UNP Q8TD43
C	-14	TYR	-	expression tag	UNP Q8TD43
C	-13	LYS	-	expression tag	UNP Q8TD43
C	-12	ASP	-	expression tag	UNP Q8TD43
C	-11	ASP	-	expression tag	UNP Q8TD43
C	-10	ASP	-	expression tag	UNP Q8TD43
C	-9	ASP	-	expression tag	UNP Q8TD43
C	-8	LYS	-	expression tag	UNP Q8TD43
C	-7	GLY	-	expression tag	UNP Q8TD43
C	-6	SER	-	expression tag	UNP Q8TD43
C	-5	GLY	-	expression tag	UNP Q8TD43
C	-4	LEU	-	expression tag	UNP Q8TD43
C	-3	VAL	-	expression tag	UNP Q8TD43
C	-2	PRO	-	expression tag	UNP Q8TD43
C	-1	ARG	-	expression tag	UNP Q8TD43
C	0	GLY	-	expression tag	UNP Q8TD43
C	1	SER	-	expression tag	UNP Q8TD43
A	-16	MET	-	initiating methionine	UNP Q8TD43
A	-15	ASP	-	expression tag	UNP Q8TD43
A	-14	TYR	-	expression tag	UNP Q8TD43

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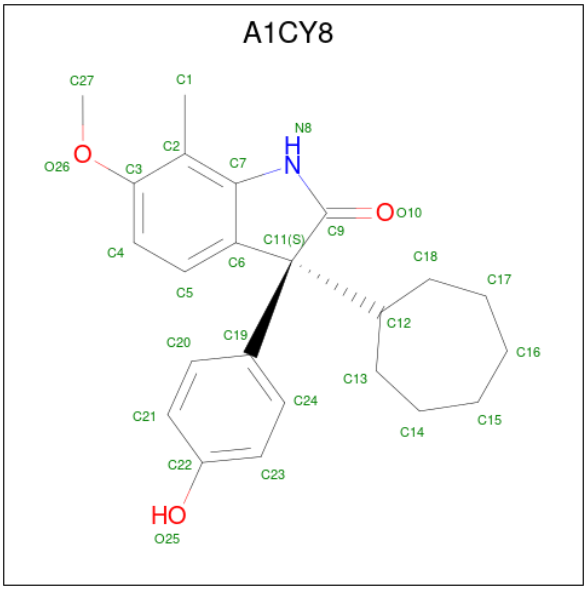
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	LYS	-	expression tag	UNP Q8TD43
A	-12	ASP	-	expression tag	UNP Q8TD43
A	-11	ASP	-	expression tag	UNP Q8TD43
A	-10	ASP	-	expression tag	UNP Q8TD43
A	-9	ASP	-	expression tag	UNP Q8TD43
A	-8	LYS	-	expression tag	UNP Q8TD43
A	-7	GLY	-	expression tag	UNP Q8TD43
A	-6	SER	-	expression tag	UNP Q8TD43
A	-5	GLY	-	expression tag	UNP Q8TD43
A	-4	LEU	-	expression tag	UNP Q8TD43
A	-3	VAL	-	expression tag	UNP Q8TD43
A	-2	PRO	-	expression tag	UNP Q8TD43
A	-1	ARG	-	expression tag	UNP Q8TD43
A	0	GLY	-	expression tag	UNP Q8TD43
A	1	SER	-	expression tag	UNP Q8TD43
B	-16	MET	-	initiating methionine	UNP Q8TD43
B	-15	ASP	-	expression tag	UNP Q8TD43
B	-14	TYR	-	expression tag	UNP Q8TD43
B	-13	LYS	-	expression tag	UNP Q8TD43
B	-12	ASP	-	expression tag	UNP Q8TD43
B	-11	ASP	-	expression tag	UNP Q8TD43
B	-10	ASP	-	expression tag	UNP Q8TD43
B	-9	ASP	-	expression tag	UNP Q8TD43
B	-8	LYS	-	expression tag	UNP Q8TD43
B	-7	GLY	-	expression tag	UNP Q8TD43
B	-6	SER	-	expression tag	UNP Q8TD43
B	-5	GLY	-	expression tag	UNP Q8TD43
B	-4	LEU	-	expression tag	UNP Q8TD43
B	-3	VAL	-	expression tag	UNP Q8TD43
B	-2	PRO	-	expression tag	UNP Q8TD43
B	-1	ARG	-	expression tag	UNP Q8TD43
B	0	GLY	-	expression tag	UNP Q8TD43
B	1	SER	-	expression tag	UNP Q8TD43
D	-16	MET	-	initiating methionine	UNP Q8TD43
D	-15	ASP	-	expression tag	UNP Q8TD43
D	-14	TYR	-	expression tag	UNP Q8TD43
D	-13	LYS	-	expression tag	UNP Q8TD43
D	-12	ASP	-	expression tag	UNP Q8TD43
D	-11	ASP	-	expression tag	UNP Q8TD43
D	-10	ASP	-	expression tag	UNP Q8TD43
D	-9	ASP	-	expression tag	UNP Q8TD43
D	-8	LYS	-	expression tag	UNP Q8TD43

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	GLY	-	expression tag	UNP Q8TD43
D	-6	SER	-	expression tag	UNP Q8TD43
D	-5	GLY	-	expression tag	UNP Q8TD43
D	-4	LEU	-	expression tag	UNP Q8TD43
D	-3	VAL	-	expression tag	UNP Q8TD43
D	-2	PRO	-	expression tag	UNP Q8TD43
D	-1	ARG	-	expression tag	UNP Q8TD43
D	0	GLY	-	expression tag	UNP Q8TD43
D	1	SER	-	expression tag	UNP Q8TD43

- Molecule 2 is Necrocide 1 (CCD ID: A1CY8) (formula: $C_{23}H_{27}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total C N O 27 23 1 3	0
2	A	1	Total C N O 27 23 1 3	0
2	B	1	Total C N O 27 23 1 3	0
2	D	1	Total C N O 27 23 1 3	0

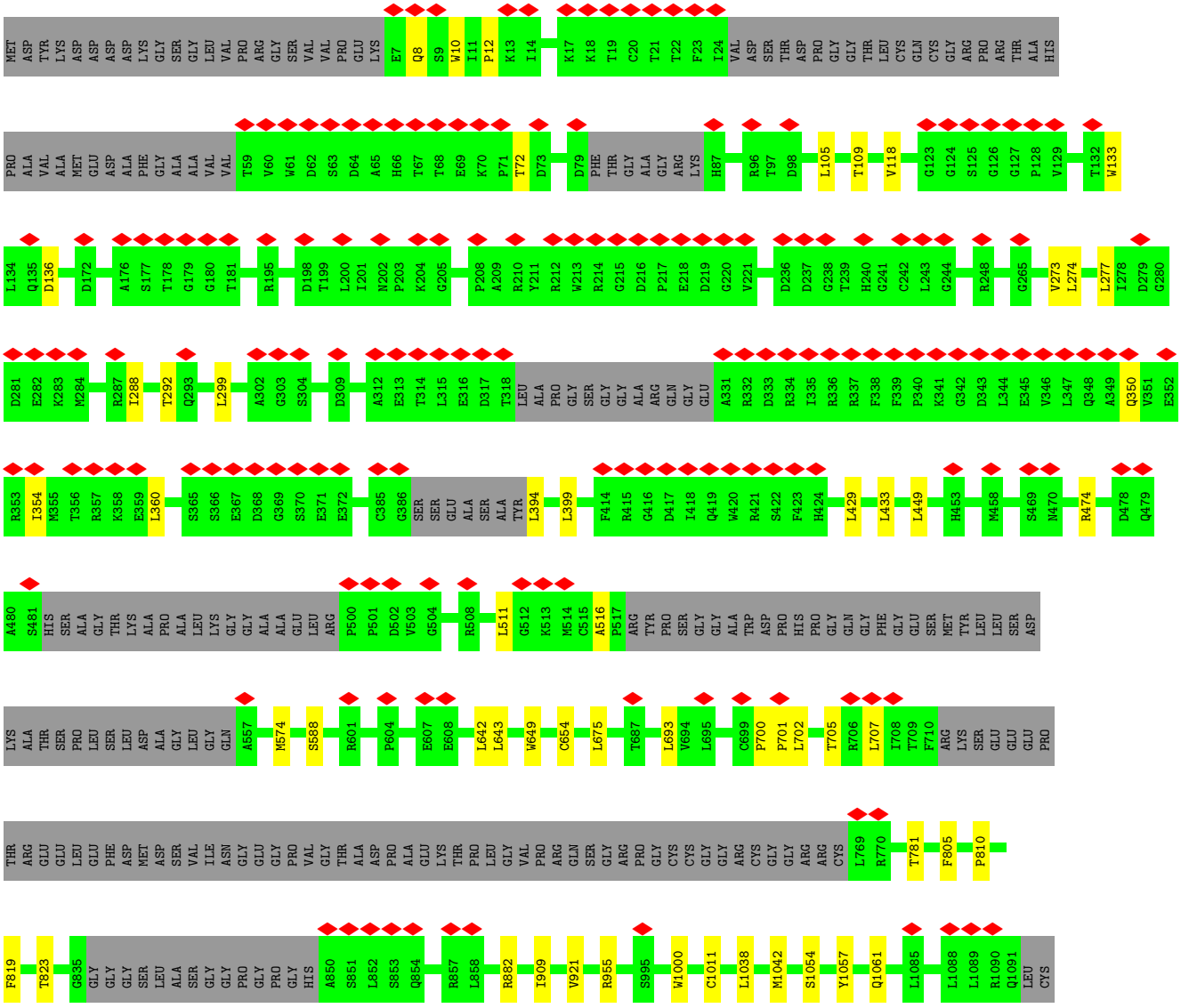
3 Residue-property plots (i)

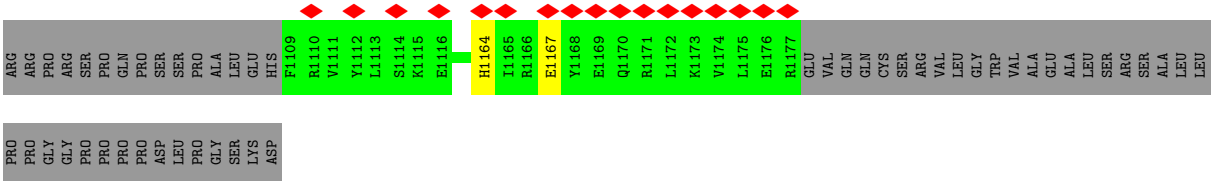
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain C:



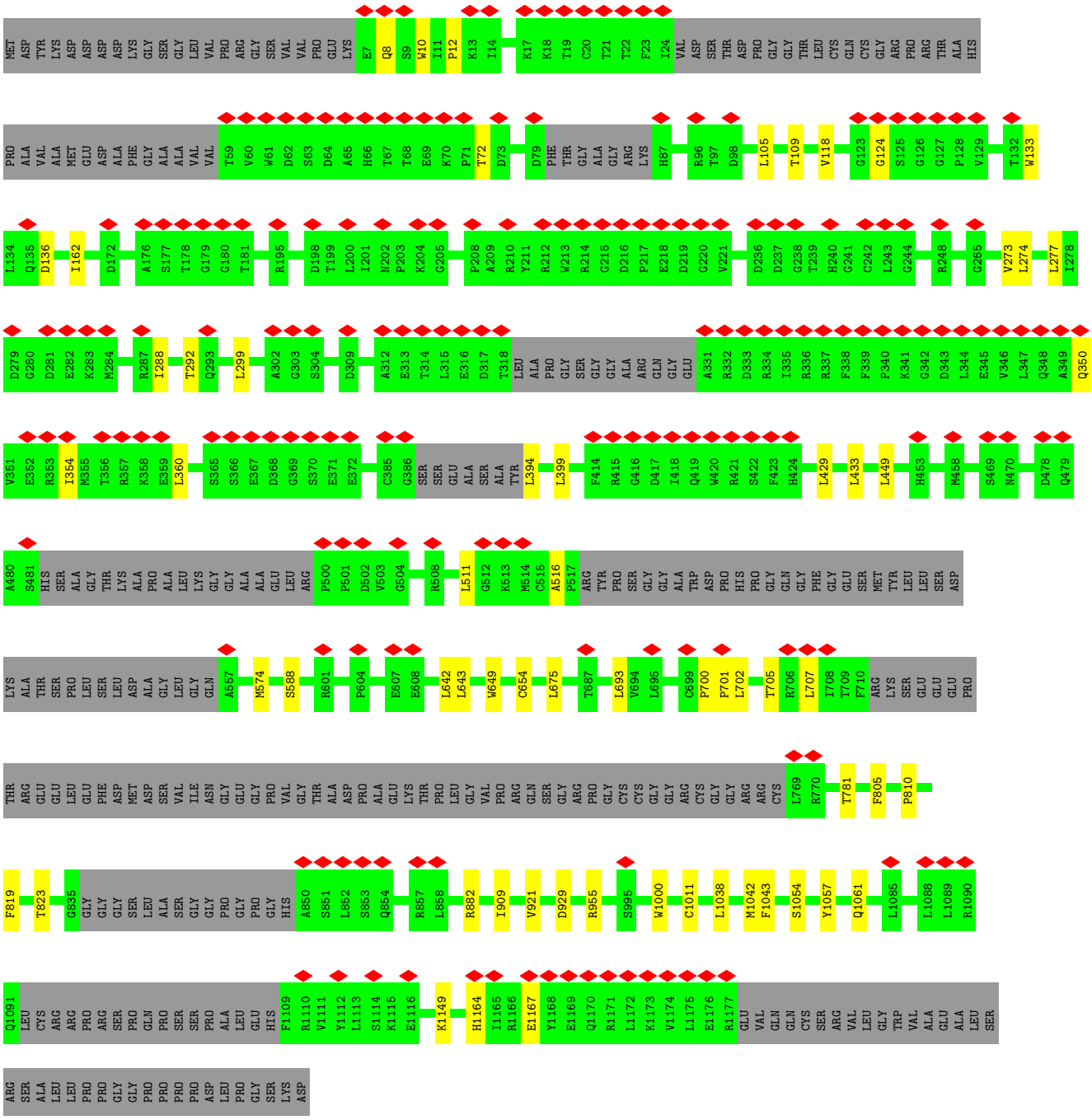




• Molecule 1: Transient receptor potential cation channel subfamily M member 4

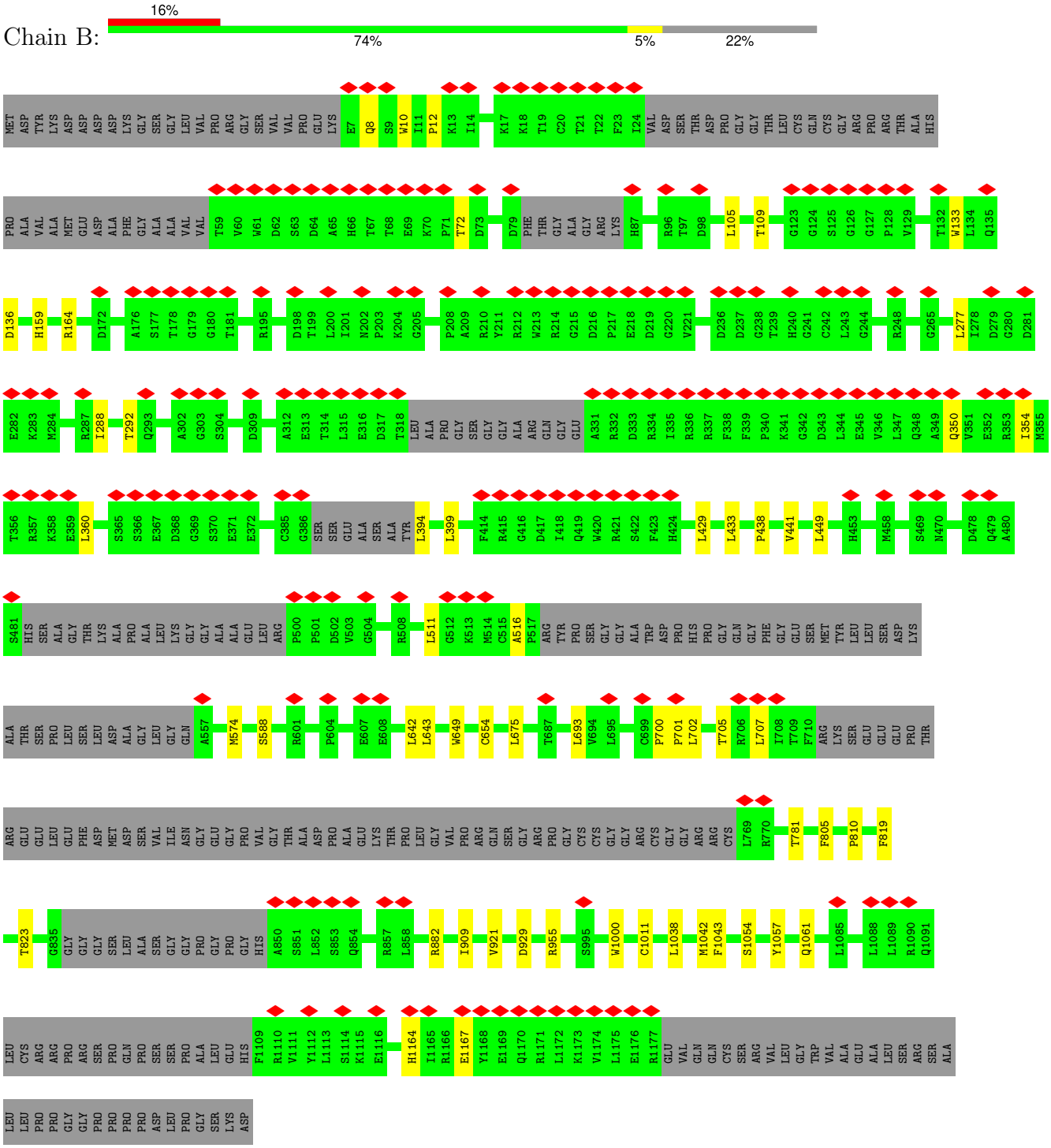
Chain A:





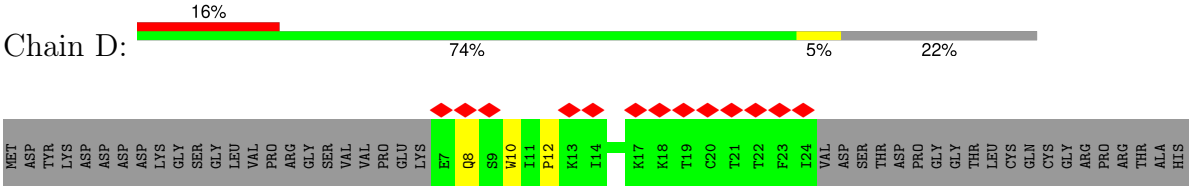
• Molecule 1: Transient receptor potential cation channel subfamily M member 4

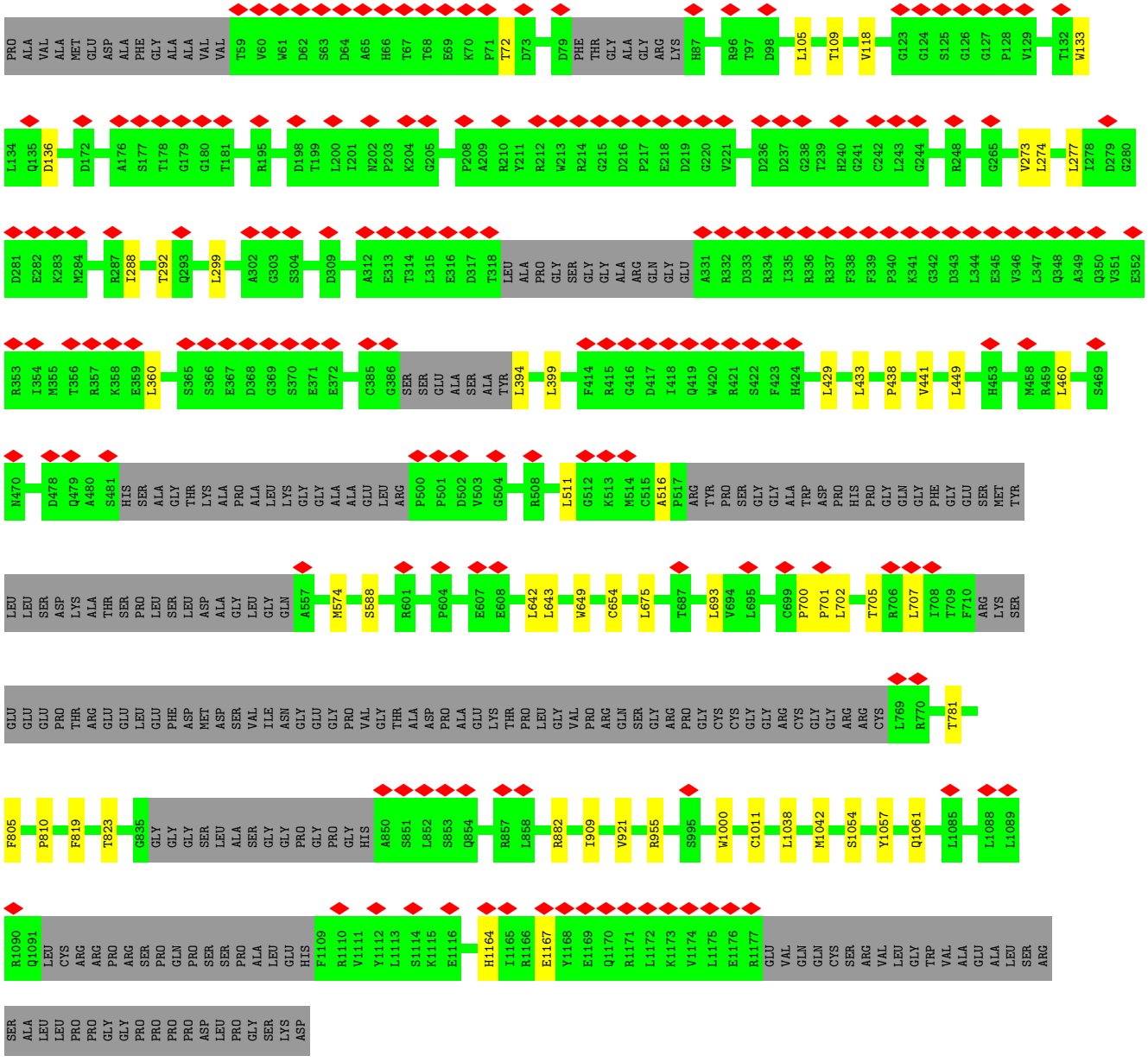
Chain B:



• Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain D:




PRO ALA VAL ALA MET GLU ASP ALA PHE GLY ALA ALA VAL T59 V60 W61 D62 S63 D64 A65 H66 T67 T68 E69 K70 P71 T72 D73 D79 PHE THR GLY ALA GLY ARG LYS H87 R96 T97 D98 L105 T109 V118 G123 G124 S125 G126 G127 P128 V129 T132 W133
L134 Q135 D136 D172 A176 S177 T178 G179 G180 T181 R195 D198 T199 L200 I201 N202 P203 K204 G205 P208 A209 R210 Y211 R212 W213 R214 G215 D216 P217 E218 D219 G220 V221 D236 D237 G238 T239 H240 G241 C242 L243 G244 R248 G265 V273 L274 L277 I278 D279 G280
D281 E282 K283 M284 R287 I288 T292 Q293 L299 A302 G303 S304 D309 A312 E313 T314 L315 E316 D317 T318 LEU ALA PRO GLY SER GLY GLY ALA ARG GLN GLY GLU A331 R332 D333 R334 I335 R336 R337 F338 F339 P340 K341 G342 D343 L344 E345 V346 L347 Q348 A349 Q350 V351 E352
R353 I354 M355 T356 R357 K358 E359 L360 S365 S366 E367 D368 G369 S370 E371 E372 C385 G386 SER SER GLU ALA SER ALA TYR L394 L399 F414 R415 G416 D417 I418 Q419 W420 R421 S422 F423 H424 L429 L433 P438 V441 L449 H453 M458 R459 L460 S469
N470 D478 Q479 A480 S481 HIS SER ALA GLY THR LYS ALA PRO ALA LEU LYS GLY GLY ALA ALA GLU LEU ARG P500 P501 D502 V503 G504 R508 L511 G512 K513 M514 C515 A516 P517 ARG TYR PRO SER GLY GLY ALA TRP ASP PRO HIS PRO GLY GLN GLY PHE GLY GLU SER MET TYR
LEU LEU SER ASP LYS ALA THR SER PRO LEU SER LEU ASP ALA GLY LEU GLY GLN A557 M574 S588 R601 P604 E607 E608 L642 L643 W649 C654 L675 T687 L693 V694 L695 C699 P700 P701 L702 T705 R706 L707 I708 T709 F710 ARG LYS SER
GLU GLU GLU PRO THR ARG GLU GLU LEU GLU PHE ASP MET ASP SER VAL ILE ASN GLY GLU GLY PRO VAL GLY THR ALA ASP PRO ALA GLU LYS THR PRO LEU GLY VAL PRO ARG GLN SER GLY ARG PRO GLY CYS CYS GLY GLY ARG CYS GLY GLY ARG ARG CYS L769 R770 T781
F805 P810 F819 T823 G835 GLY GLY GLY SER LEU ALA SER GLY GLY PRO GLY PRO GLY HIS A850 S851 L852 S853 Q854 R857 L858 R882 I909 V921 R955 S995 W1000 C1011 L1038 M1042 S1054 Y1057 Q1061 L1085 L1088 L1099
R1090 Q1091 LEU CYS ARG ARG PRO ARG SER PRO GLN PRO SER SER PRO ALA LEU GLU HIS F1109 R1110 V1111 Y1112 L1113 S1114 K1115 E1116 H1164 I1165 R1166 E1167 Y1168 E1169 Q1170 R1171 L1172 K1173 V1174 L1175 E1176 R1177 GLU VAL GLN GLN CYS SER ARG VAL LEU GLY TRP VAL ALA GLU ALA LEU SER ARG
SER ALA LEU LEU PRO PRO GLY GLY PRO PRO PRO PRO ASP ASP LEU PRO GLY SER LYS ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	112765	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.244	Depositor
Minimum map value	-0.933	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	307.008, 307.008, 307.008	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.738, 0.738, 0.738	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1CY8

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	0.17	0/7864	0.31	0/10656
1	B	0.17	0/7864	0.32	0/10656
1	C	0.18	0/7864	0.32	0/10656
1	D	0.17	0/7864	0.31	0/10656
All	All	0.18	0/31456	0.31	0/42624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7687	0	7766	34	0
1	B	7687	0	7766	32	0
1	C	7687	0	7766	32	0
1	D	7687	0	7766	32	0
2	A	27	0	0	2	0
2	B	27	0	0	2	0
2	C	27	0	0	2	0
2	D	27	0	0	2	0
All	All	30856	0	31064	134	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 134 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:D:292:THR:HG23	1:D:360:LEU:HD12	1.77	0.66
1:A:292:THR:HG23	1:A:360:LEU:HD12	1.78	0.66
1:B:643:LEU:HD21	1:B:675:LEU:HD11	1.79	0.65
1:C:292:THR:HG23	1:C:360:LEU:HD12	1.78	0.65
1:C:643:LEU:HD21	1:C:675:LEU:HD11	1.79	0.65

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	945/1231 (77%)	930 (98%)	15 (2%)	0	100	100
1	B	945/1231 (77%)	930 (98%)	15 (2%)	0	100	100
1	C	945/1231 (77%)	929 (98%)	16 (2%)	0	100	100
1	D	945/1231 (77%)	930 (98%)	15 (2%)	0	100	100
All	All	3780/4924 (77%)	3719 (98%)	61 (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	A	818/1014 (81%)	818 (100%)	0	100	100
1	B	818/1014 (81%)	818 (100%)	0	100	100
1	C	818/1014 (81%)	818 (100%)	0	100	100
1	D	818/1014 (81%)	818 (100%)	0	100	100
All	All	3272/4056 (81%)	3272 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	908	HIS
1	A	908	HIS
1	B	908	HIS
1	D	908	HIS

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)

4 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	A1CY8	C	2001	-	29,30,30	0.37	0	36,44,44	0.61	0
2	A1CY8	A	2001	-	29,30,30	0.37	0	36,44,44	0.61	0
2	A1CY8	B	2001	-	29,30,30	0.36	0	36,44,44	0.62	0
2	A1CY8	D	2001	-	29,30,30	0.36	0	36,44,44	0.63	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	A1CY8	C	2001	-	-	2/8/39/39	0/4/4/4
2	A1CY8	A	2001	-	-	2/8/39/39	0/4/4/4
2	A1CY8	B	2001	-	-	2/8/39/39	0/4/4/4
2	A1CY8	D	2001	-	-	2/8/39/39	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	A1CY8	C12-C11-C19-C24
2	A	2001	A1CY8	C12-C11-C19-C24
2	D	2001	A1CY8	C12-C11-C19-C24
2	B	2001	A1CY8	C12-C11-C19-C24
2	C	2001	A1CY8	C6-C11-C19-C20

There are no ring outliers.

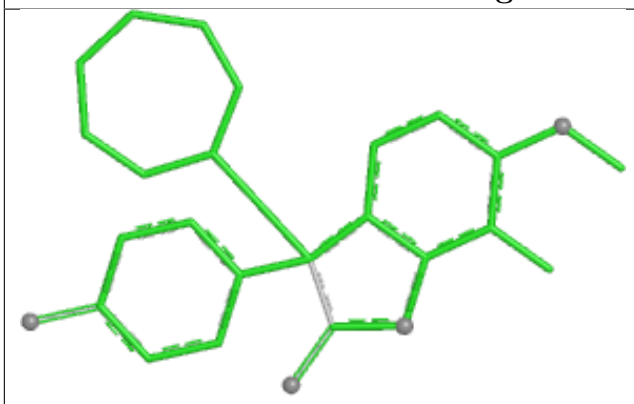
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	A1CY8	2	0
2	A	2001	A1CY8	2	0
2	B	2001	A1CY8	2	0
2	D	2001	A1CY8	2	0

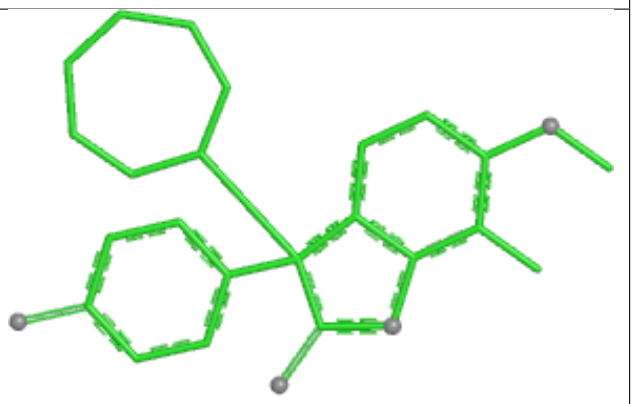
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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

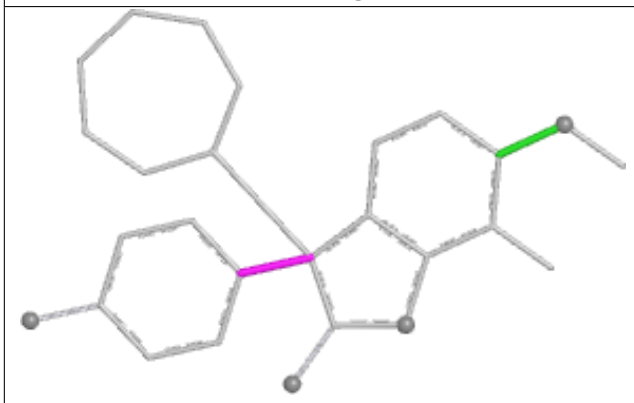
Ligand A1CY8 C 2001



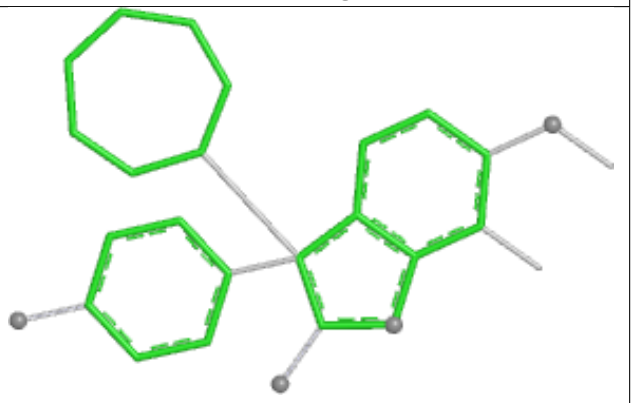
Bond lengths



Bond angles

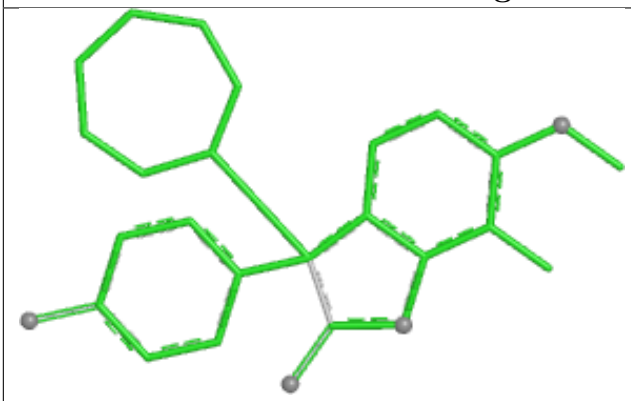


Torsions

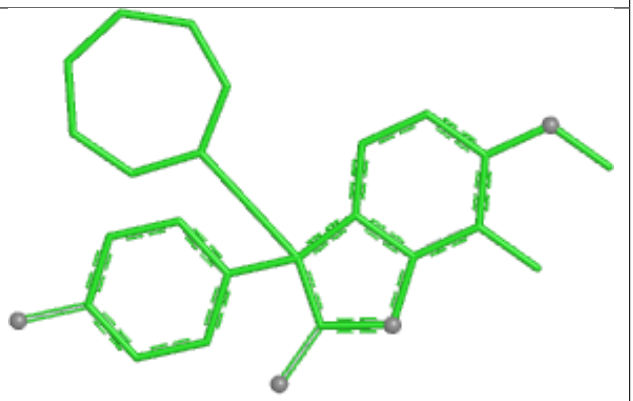


Rings

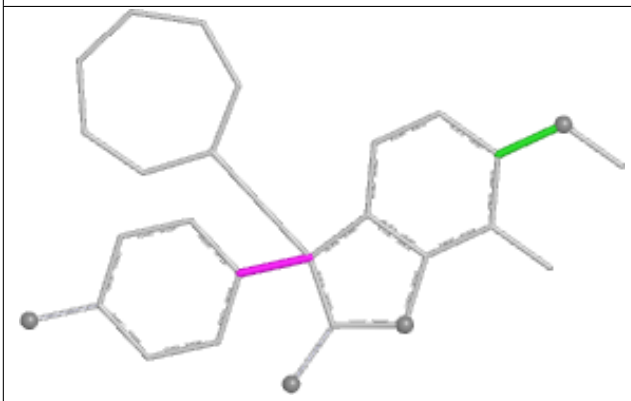
Ligand A1CY8 A 2001



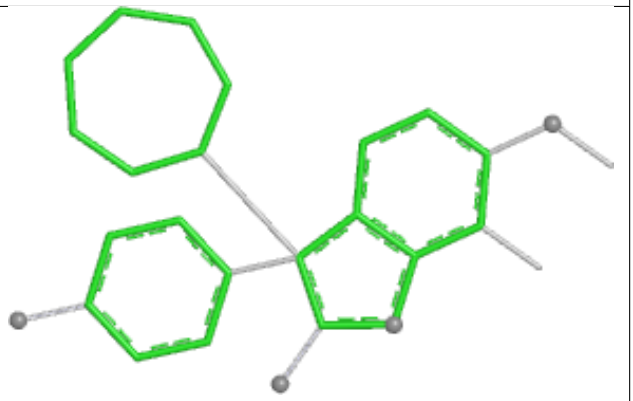
Bond lengths



Bond angles

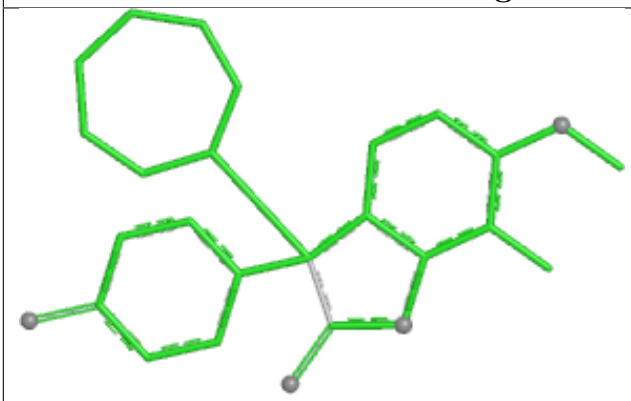


Torsions

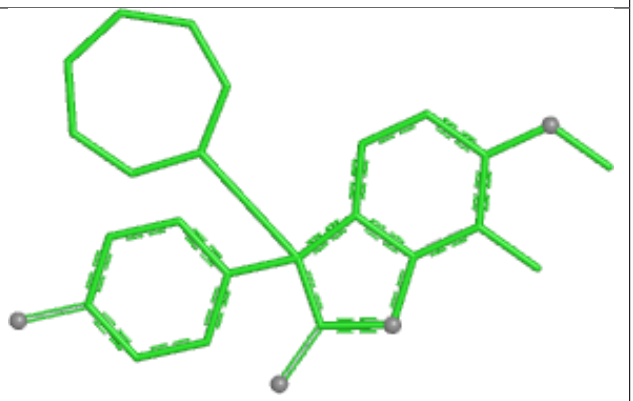


Rings

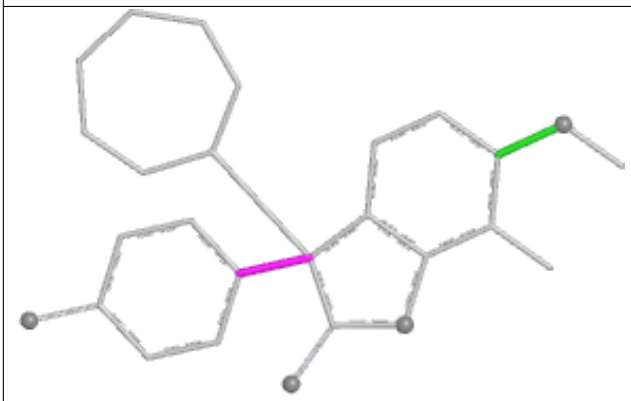
Ligand A1CY8 B 2001



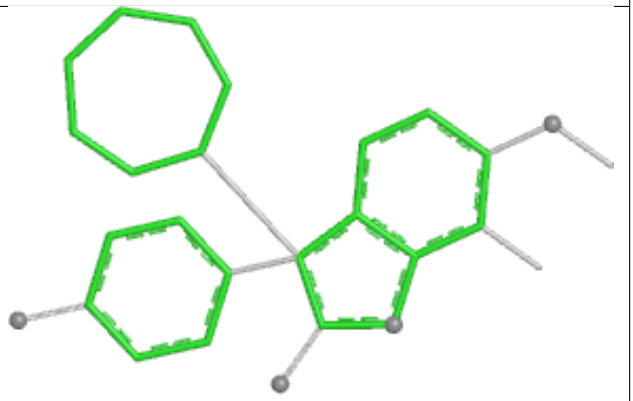
Bond lengths



Bond angles

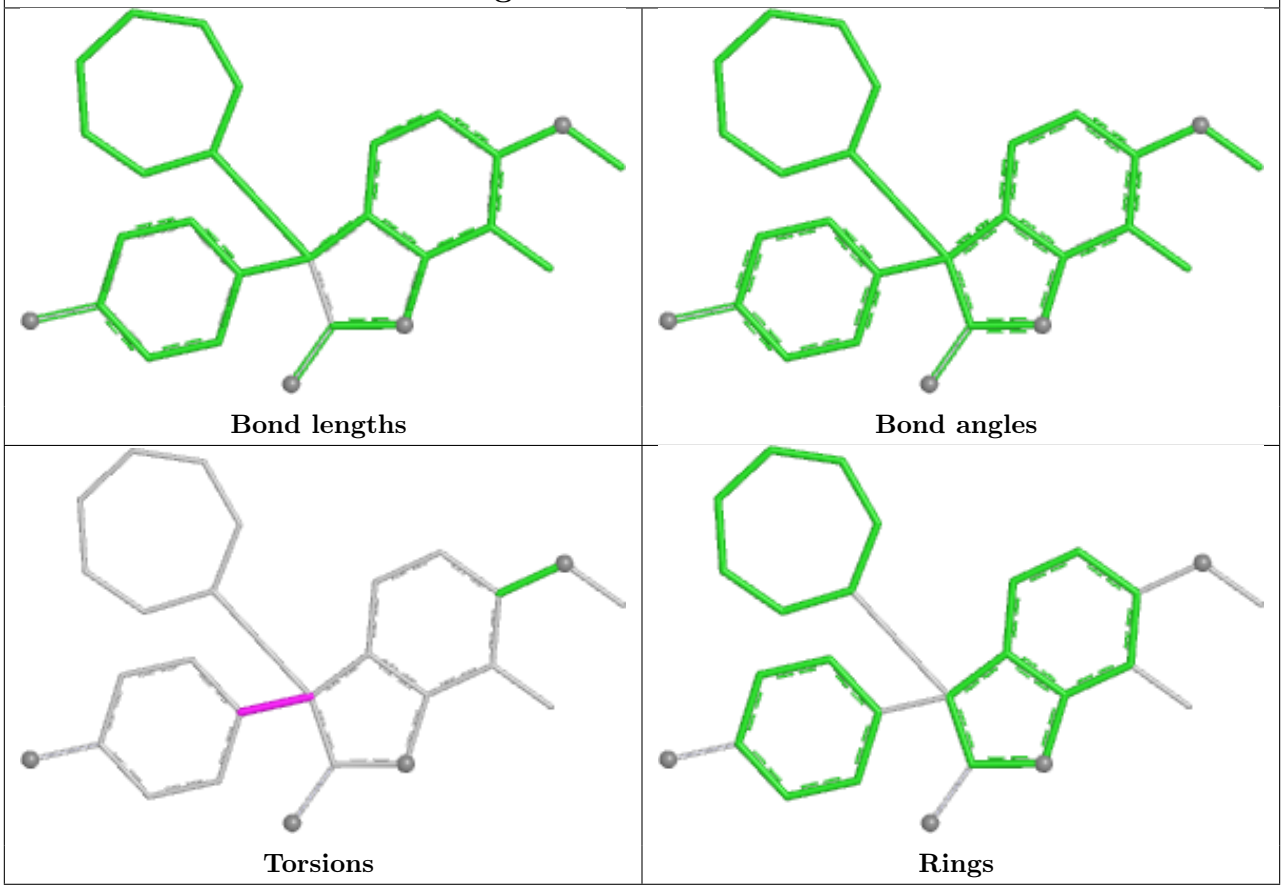


Torsions



Rings

Ligand A1CY8 D 2001



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.

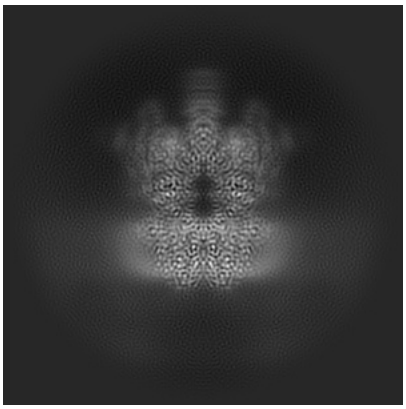
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73526. These allow visual inspection of the internal detail of the map and identification of artifacts.

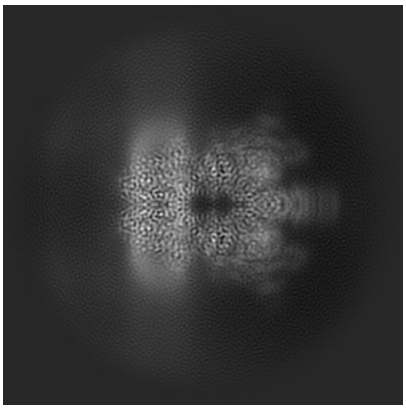
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

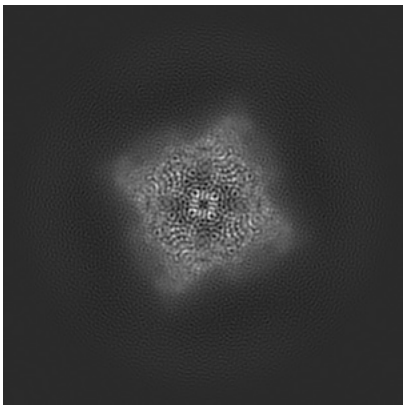
6.1.1 Primary map



X

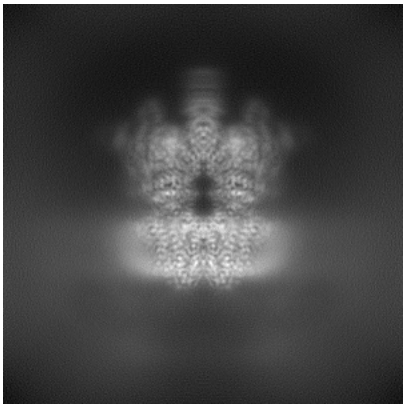


Y

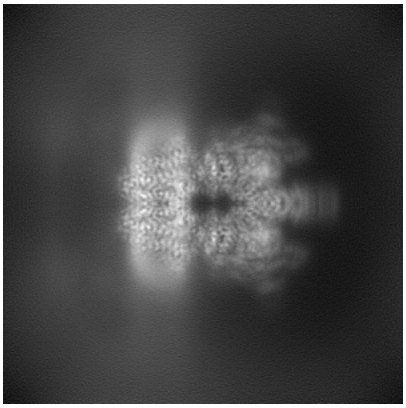


Z

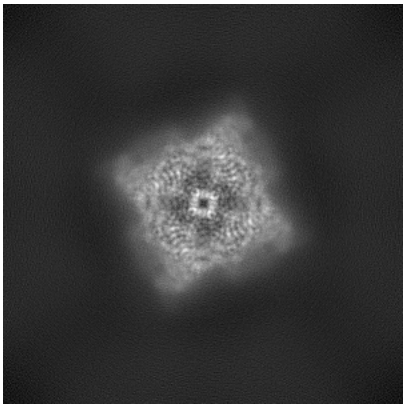
6.1.2 Raw map



X



Y

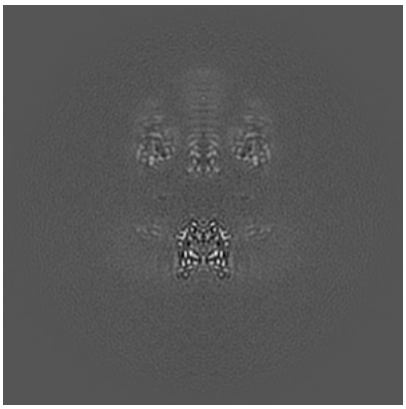


Z

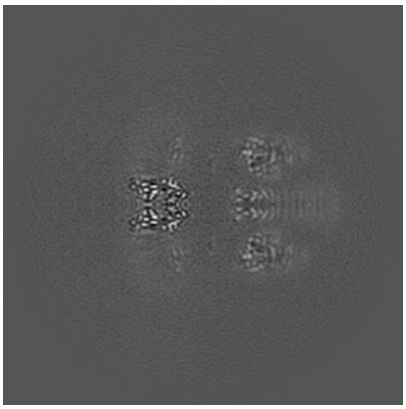
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

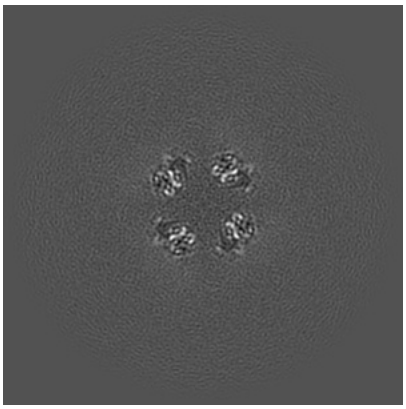
6.2.1 Primary map



X Index: 208

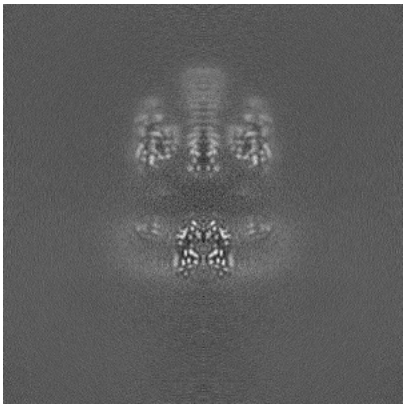


Y Index: 208

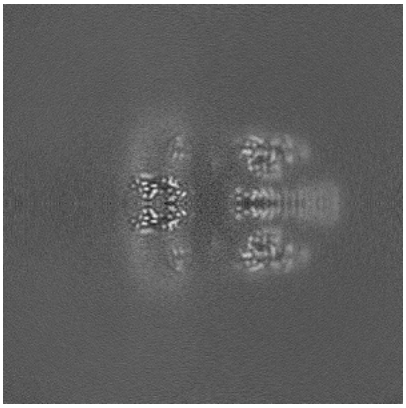


Z Index: 208

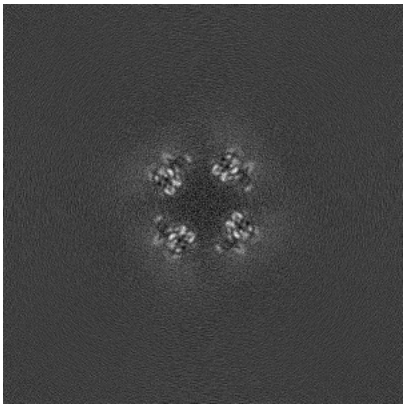
6.2.2 Raw map



X Index: 208



Y Index: 208

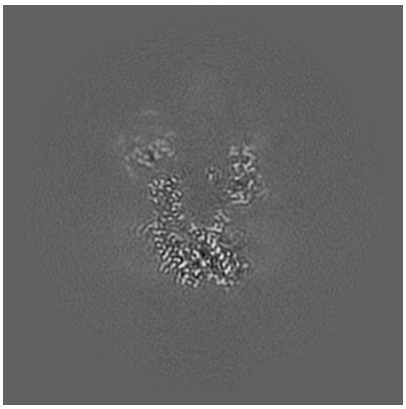


Z Index: 208

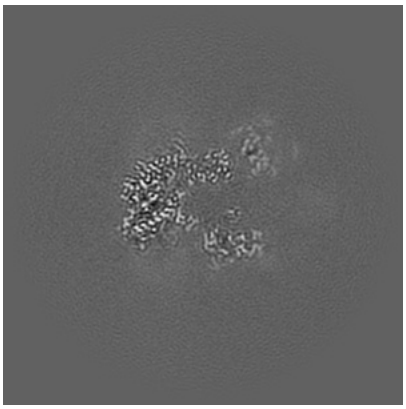
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

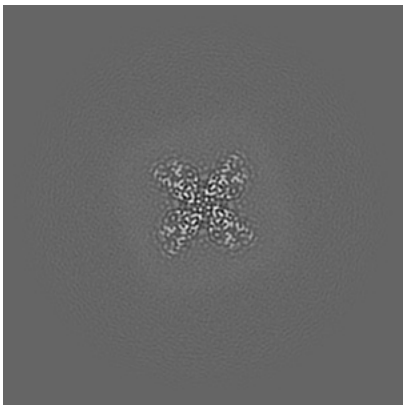
6.3.1 Primary map



X Index: 187

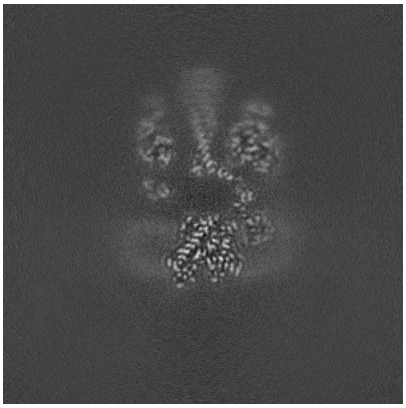


Y Index: 187

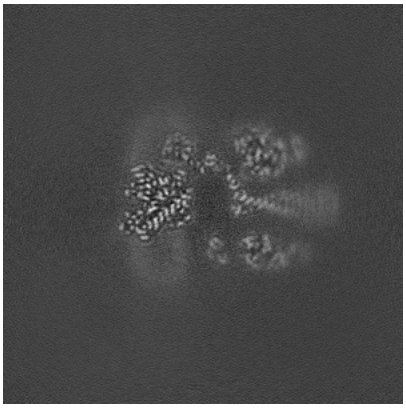


Z Index: 151

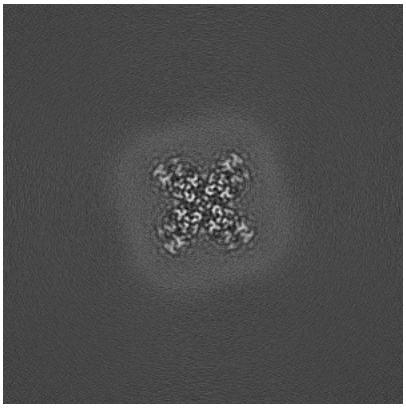
6.3.2 Raw map



X Index: 218



Y Index: 198

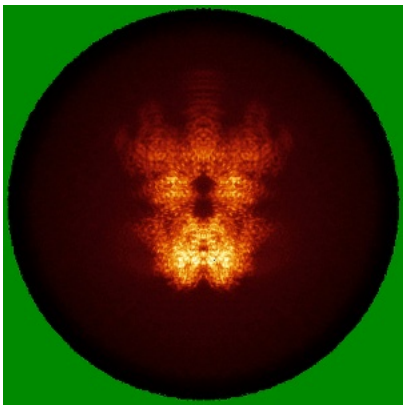


Z Index: 152

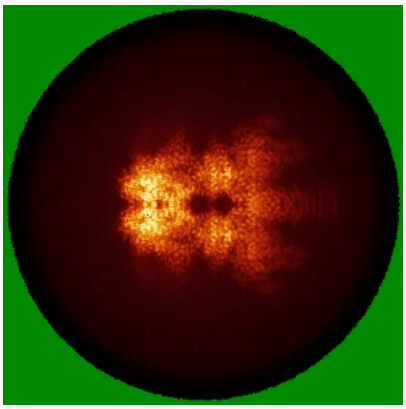
The images above show the largest variance slices of the map in three orthogonal directions.

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

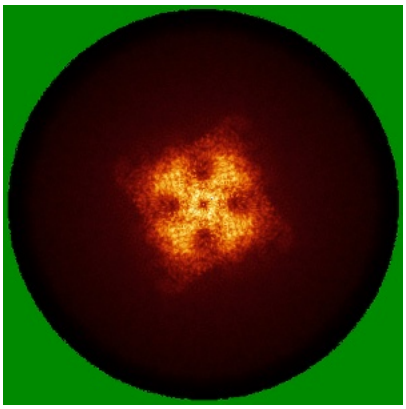
6.4.1 Primary map



X

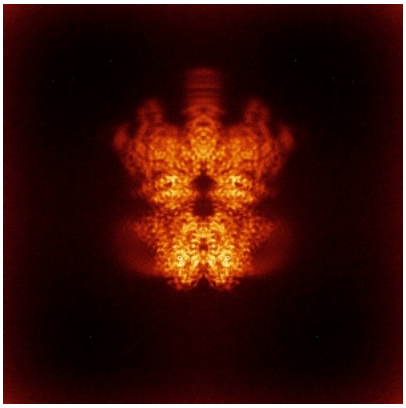


Y

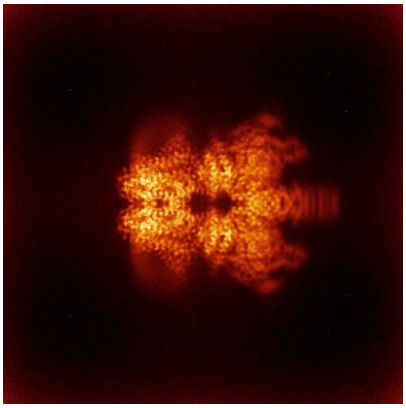


Z

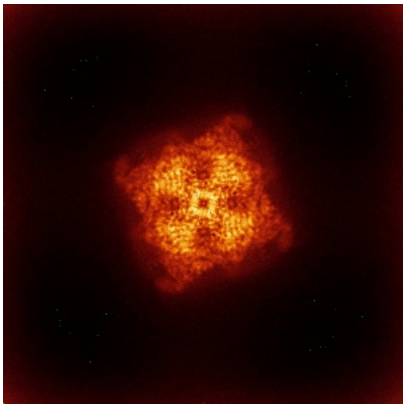
6.4.2 Raw map



X



Y

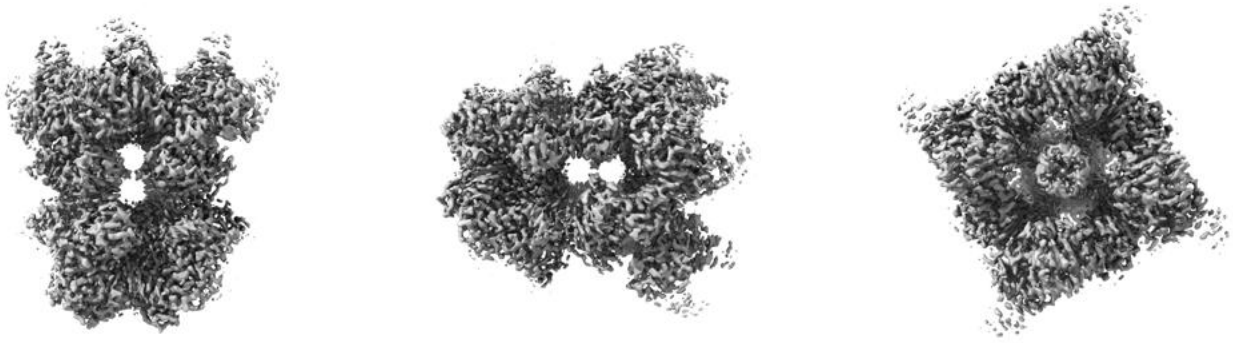


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

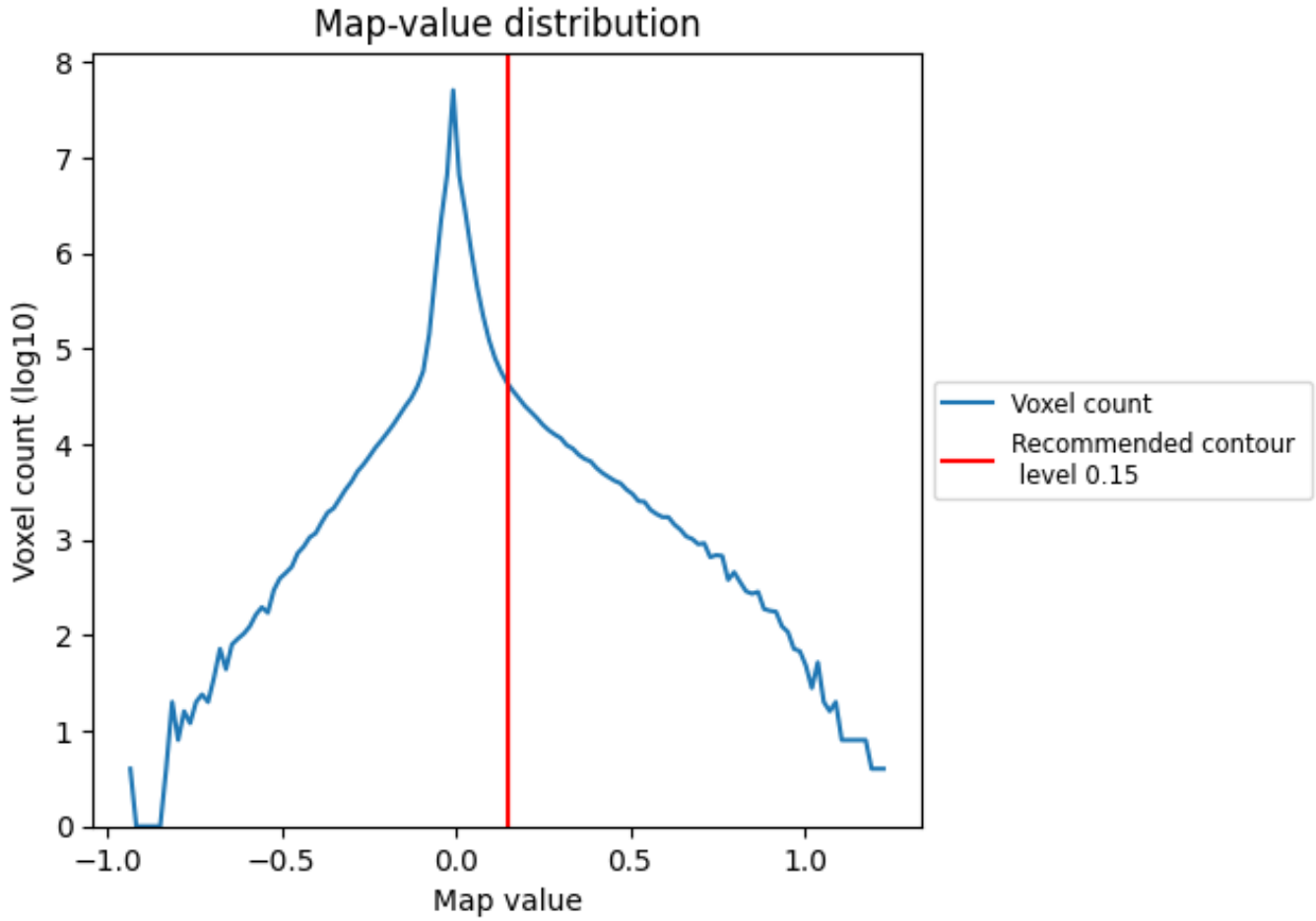
6.6 Mask visualisation (i)

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

7 Map analysis

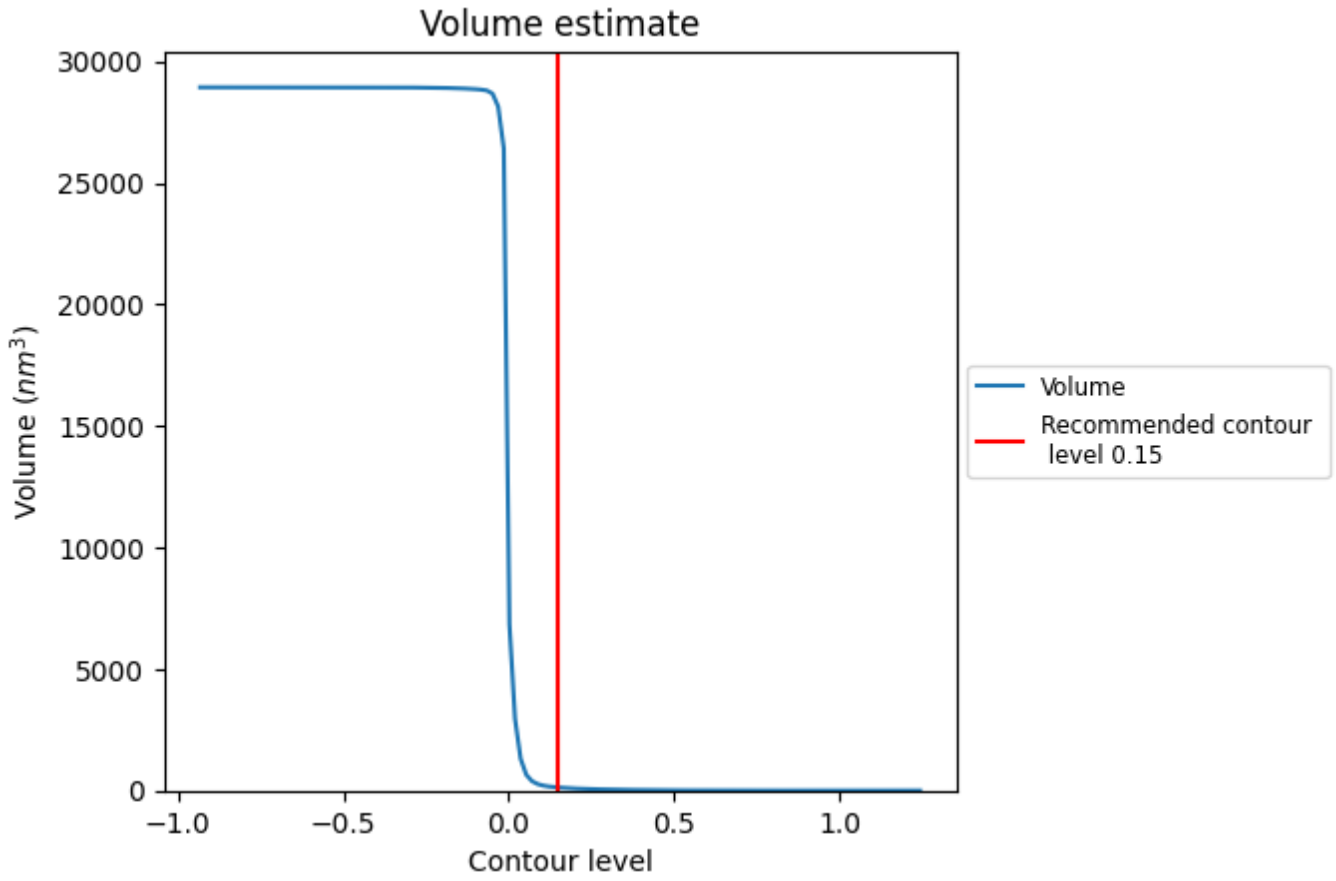
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

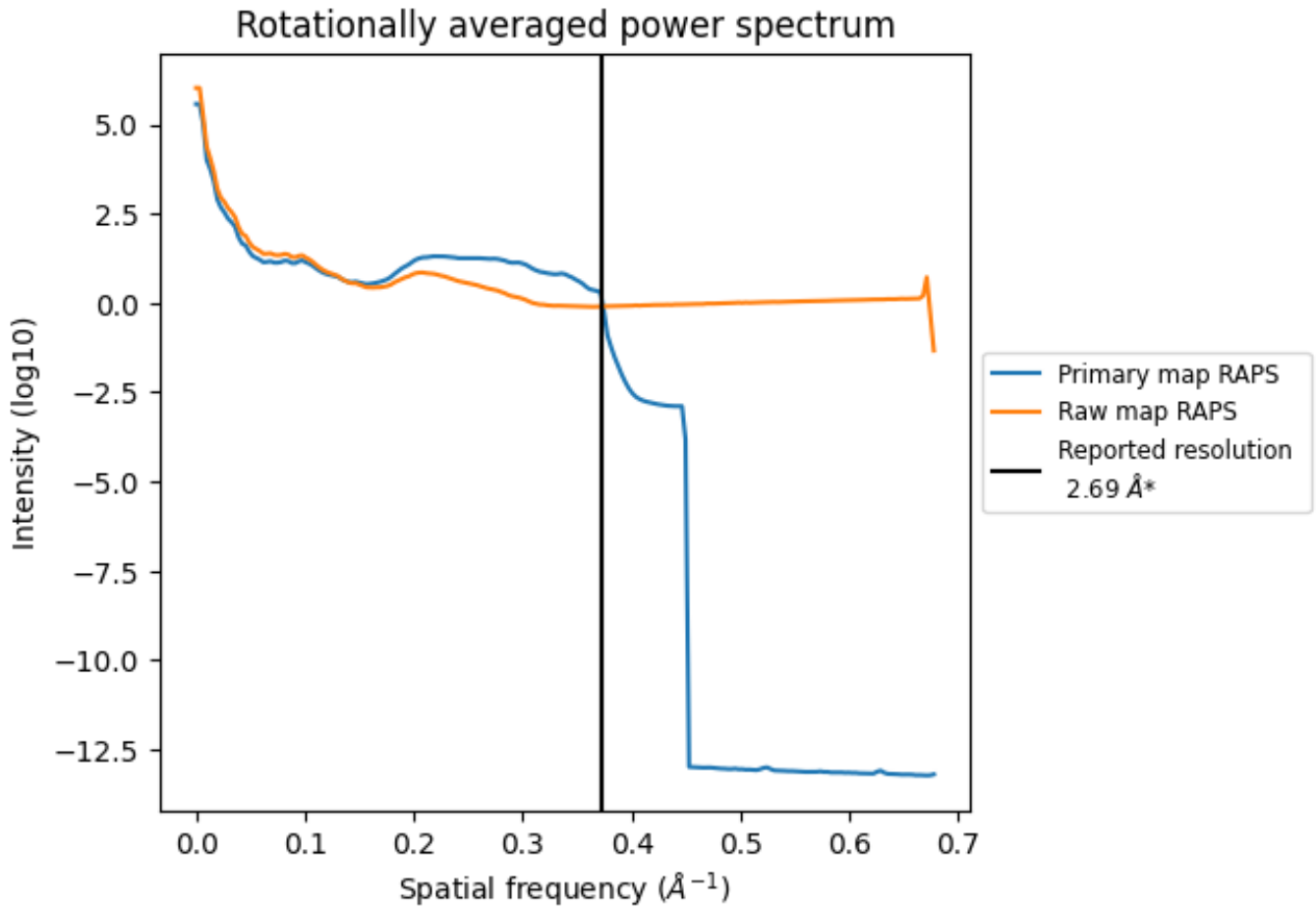
7.2 Volume estimate (i)



The volume at the recommended contour level is 127 nm^3; this corresponds to an approximate mass of 115 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)

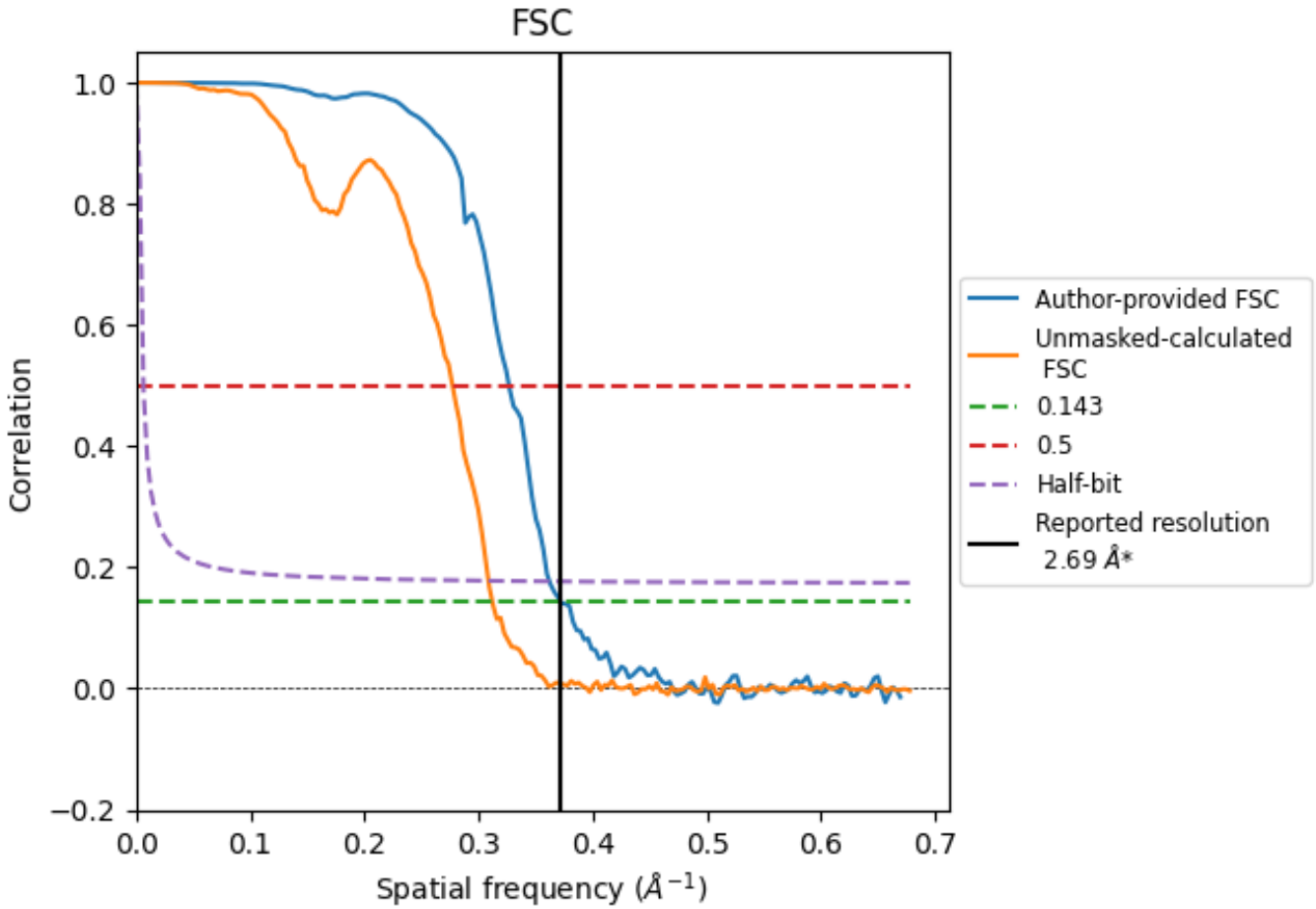


*Reported resolution corresponds to spatial frequency of 0.372 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.372 Å^{-1}

8.2 Resolution estimates (i)

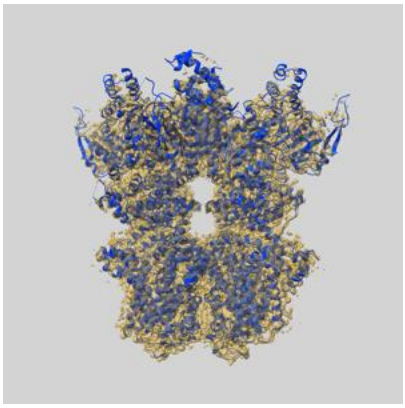
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	3.06	2.76
Unmasked-calculated*	3.21	3.61	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.21 differs from the reported value 2.69 by more than 10 %

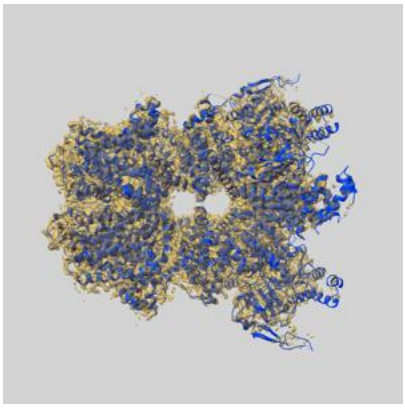
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73526 and PDB model 9YVK. Per-residue inclusion information can be found in section 3 on page 6.

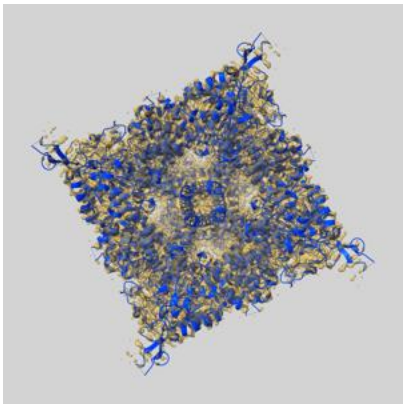
9.1 Map-model overlay



X



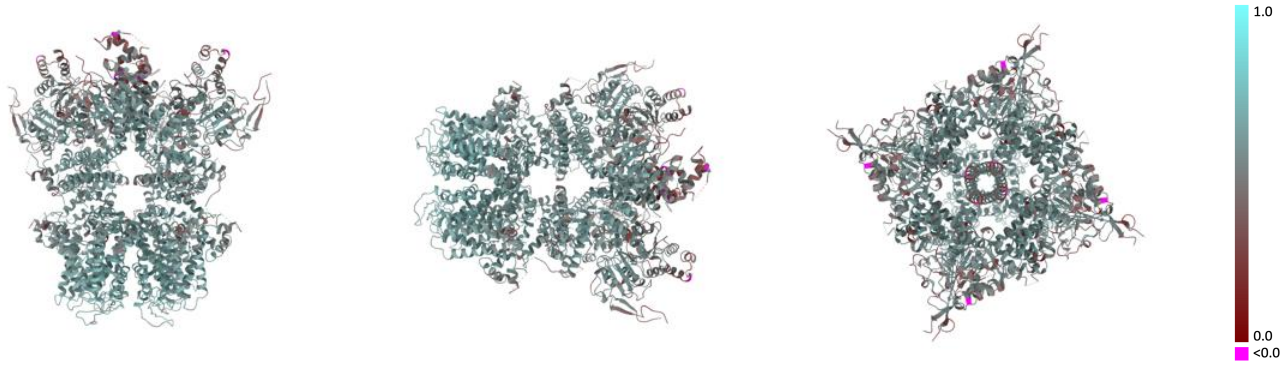
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

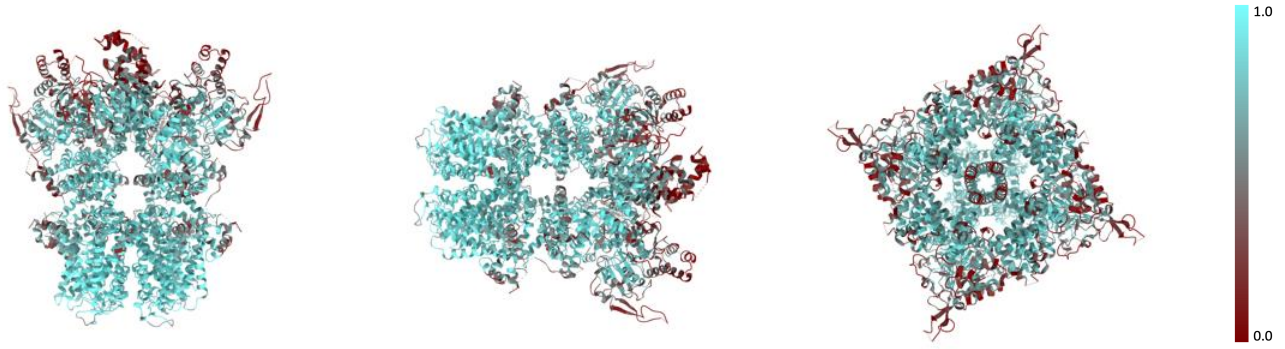
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

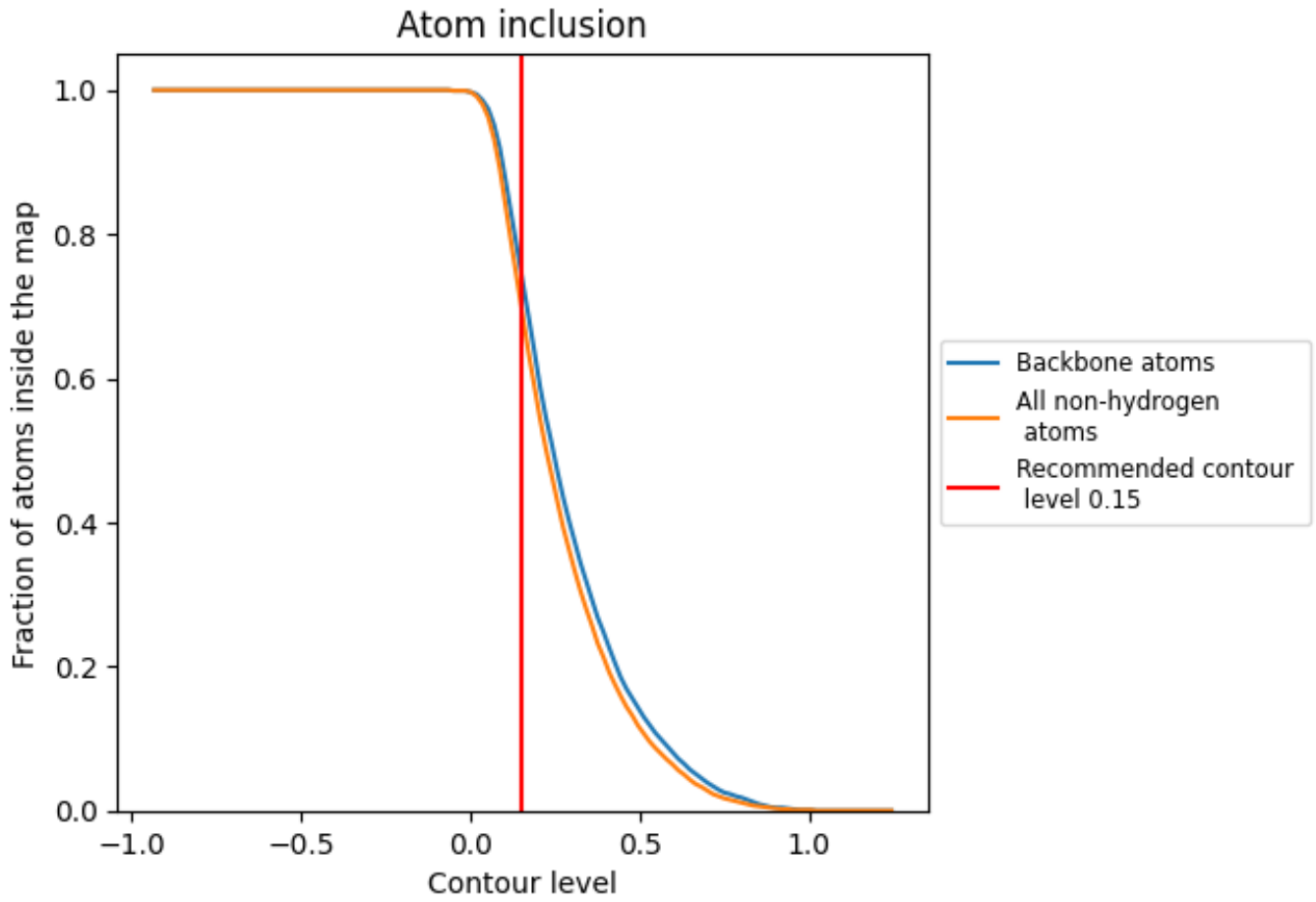
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.15) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7020	0.5580
A	0.7020	0.5580
B	0.7020	0.5590
C	0.7020	0.5580
D	0.7030	0.5590