wwPDB EM Validation Summary Report (i)

Aug 8, 2026 – 02:17 PM EDT

PDB ID	:	9YVM / pdb_00009yvm
EMDB ID	:	EMD-73528
Title	:	Cryo-EM structure of the human TRPM4 channel in an open state bound to NC1 and PI(4,5)P2 in the presence of EGTA.
Authors	:	Teixeira-Duarte, C.M.; Jiang, Y.
Deposited on	:	2025-10-23
Resolution	:	2.73 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 (i) 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 (i)) were used in the production of this report:

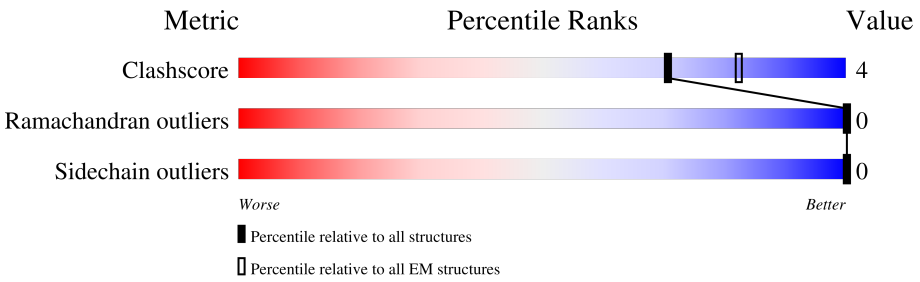
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

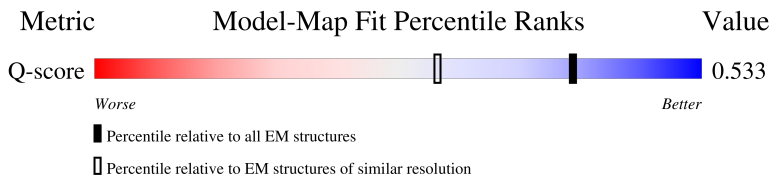
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.73 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	10432 (2.23 - 3.23)

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	25% 70% 7% 23%
1	B	1231	25% 70% 7% 23%
1	C	1231	25% 71% 7% 23%
1	D	1231	25% 70% 7% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30708 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
			Total	C	N	O	S		
1	A	951	7581	4891	1340	1309	41	0	0
1	B	951	7581	4891	1340	1309	41	0	0
1	C	951	7581	4891	1340	1309	41	0	0
1	D	951	7581	4891	1340	1309	41	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q8TD43
A	-15	ASP	-	expression tag	UNP Q8TD43
A	-14	TYR	-	expression tag	UNP Q8TD43
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

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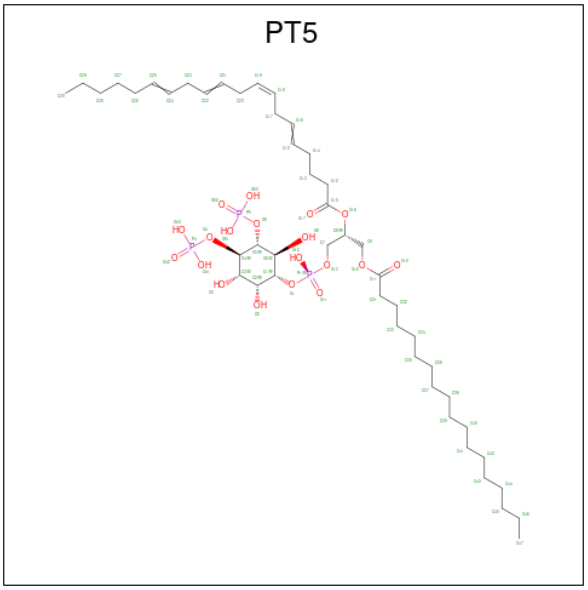
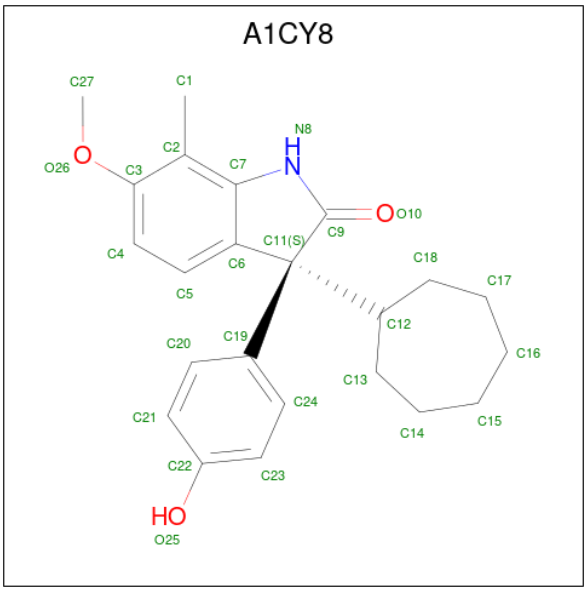
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	GLY	-	expression tag	UNP Q8TD43
D	-6	SER	-	expression tag	UNP Q8TD43
D	-5	GLY	-	expression tag	UNP Q8TD43
D	-4	LEU	-	expression tag	UNP Q8TD43
D	-3	VAL	-	expression tag	UNP Q8TD43
D	-2	PRO	-	expression tag	UNP Q8TD43
D	-1	ARG	-	expression tag	UNP Q8TD43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

- Molecule 2 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	A	1	69	47	19	3	0
2	B	1	69	47	19	3	0
2	C	1	69	47	19	3	0
2	D	1	69	47	19	3	0

- Molecule 3 is Necrocide 1 (CCD ID: A1CY8) (formula: $C_{23}H_{27}NO_3$).



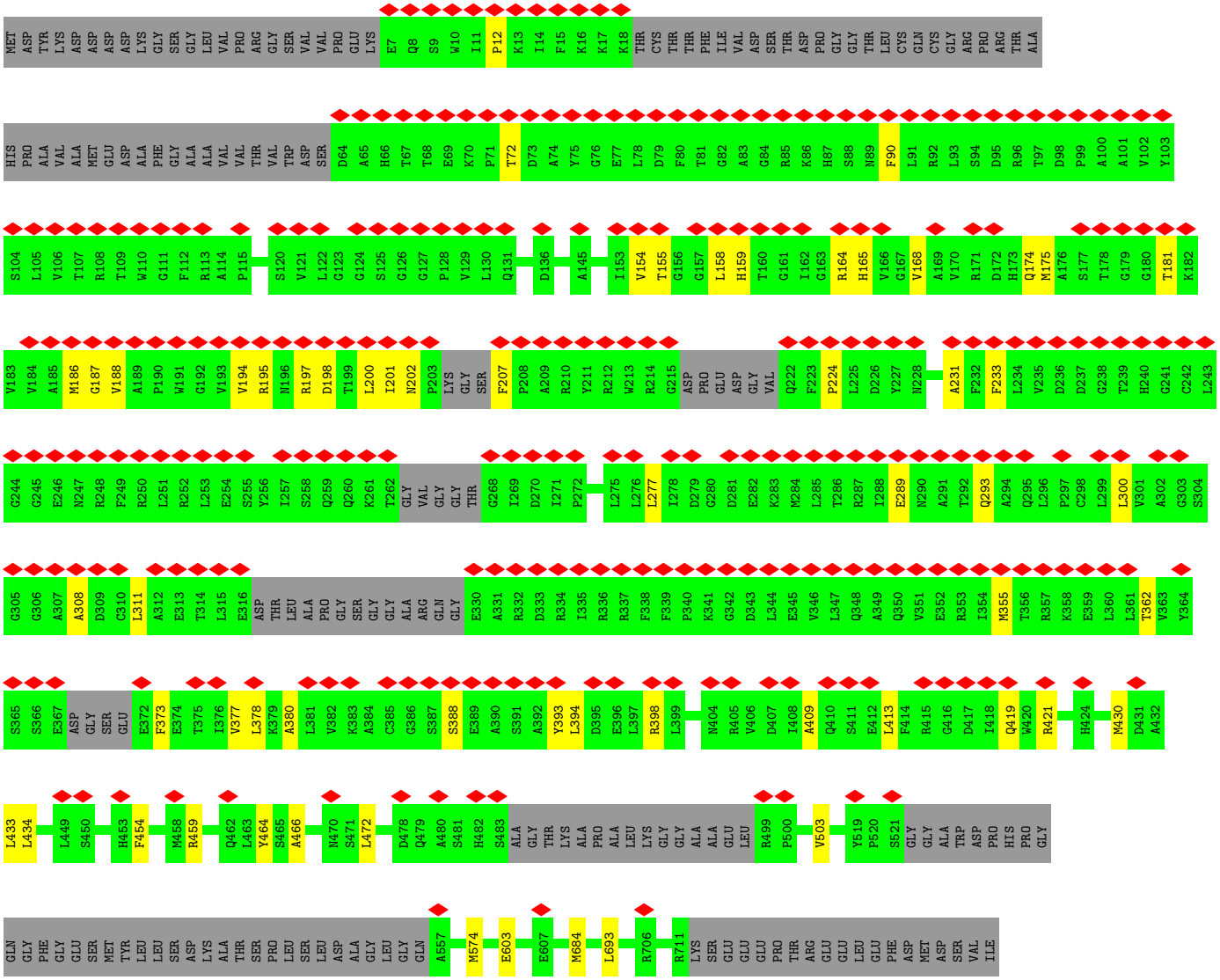
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	27	23	1	3	0
3	B	1	27	23	1	3	0
3	C	1	27	23	1	3	0
3	D	1	27	23	1	3	0

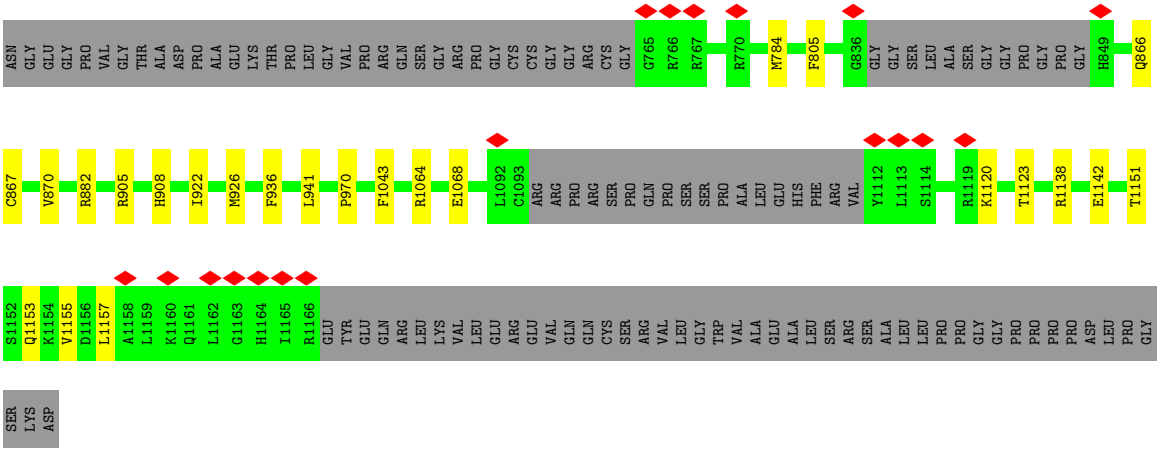
3 Residue-property plots (i)

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

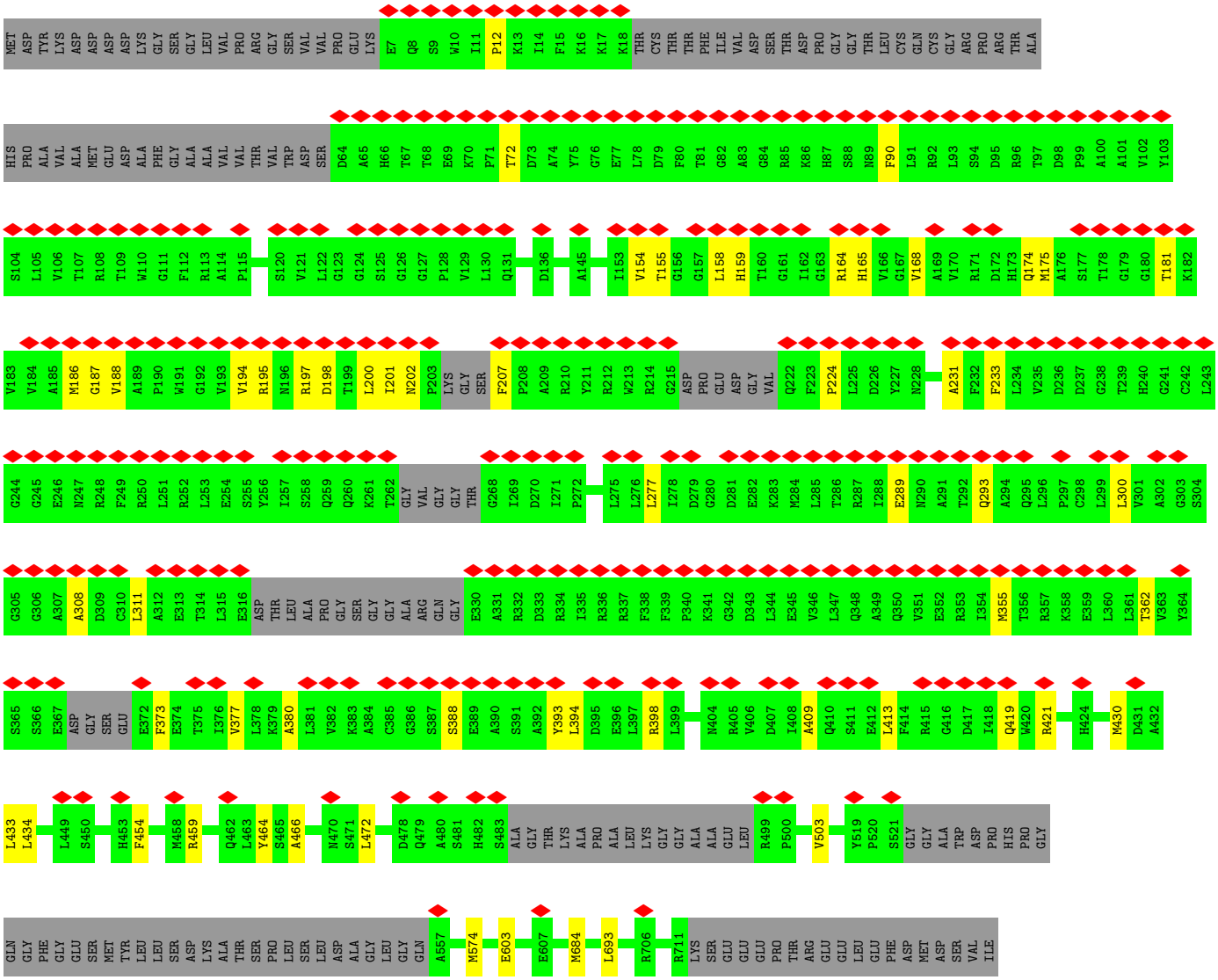
Chain A:

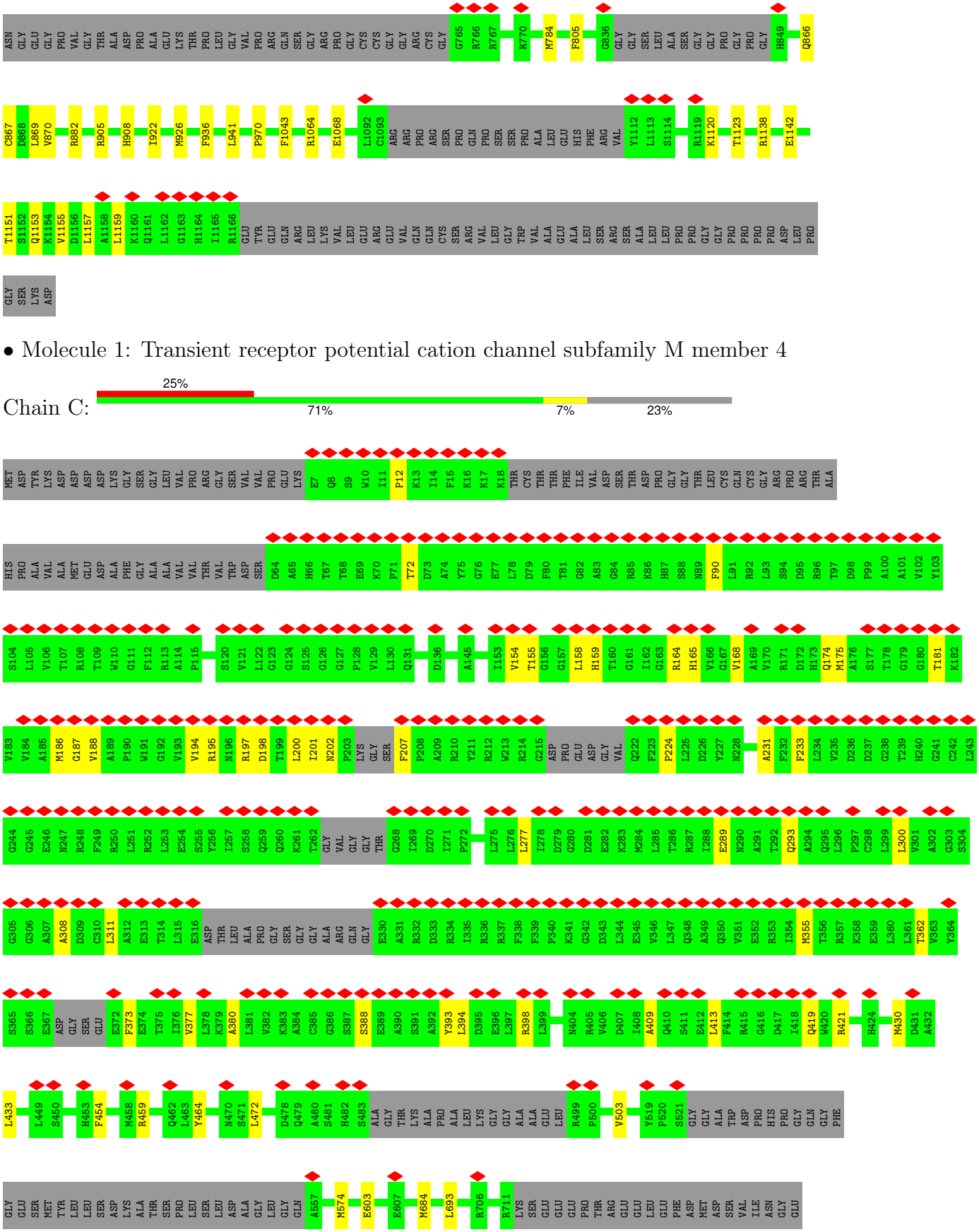


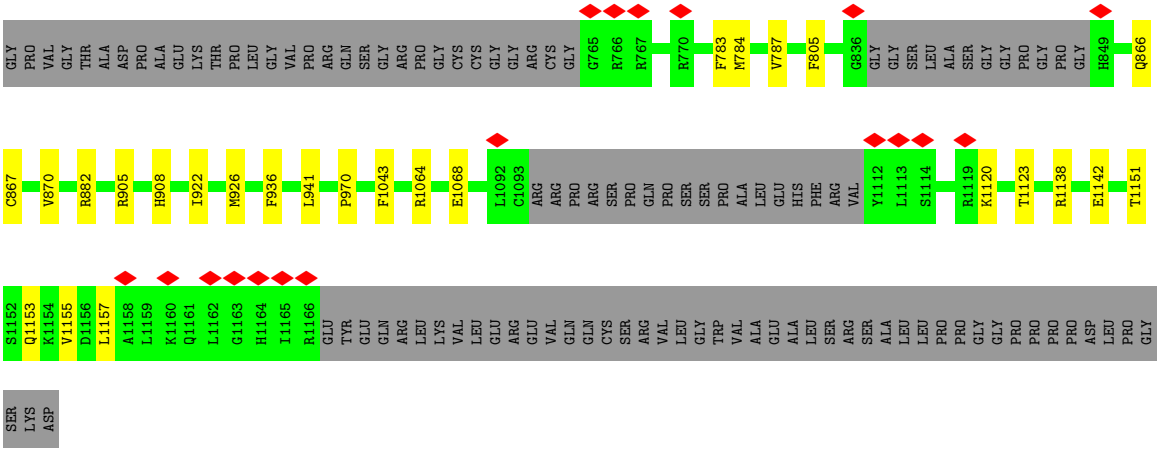


- Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain B:

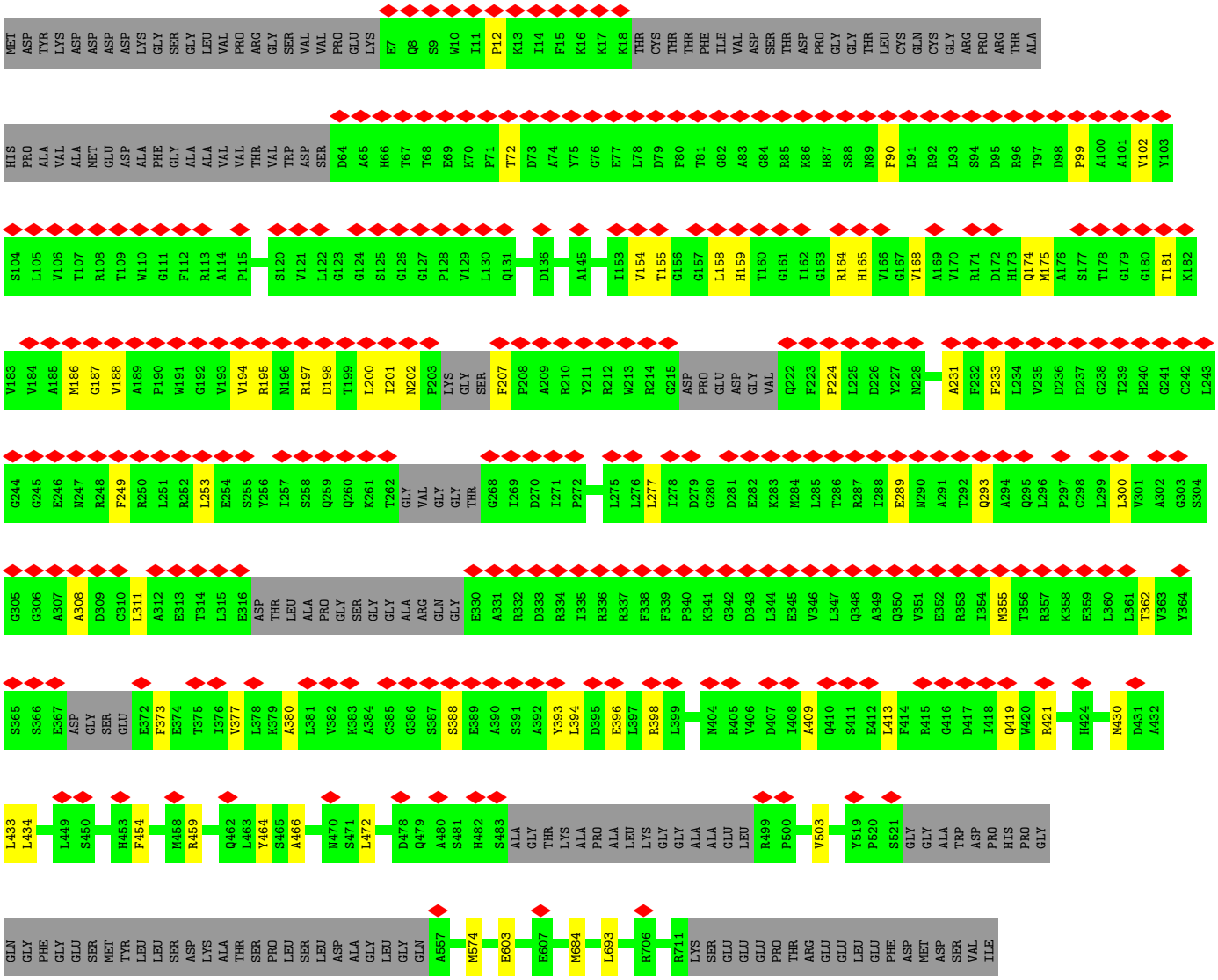


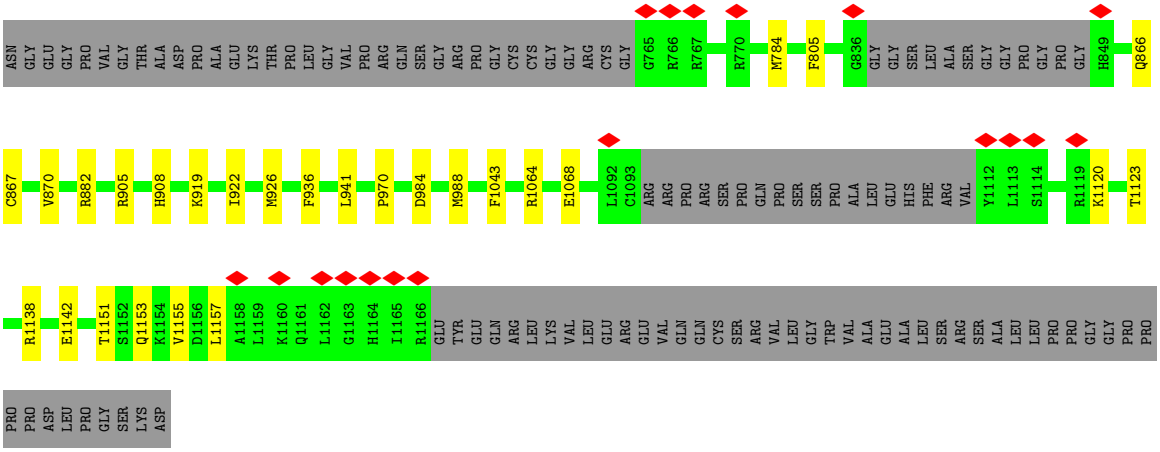

ASN GLY GLU GLY PRO VAL GLY THR ALA ASP PRO ALA GLU LYS THR PRO LEU GLY VAL PRO ARG GLN SER GLY ARG PRO GLY CYS CYS GLY GLY ARG CYS GLY G765 R766 R767 R770 M784 F805 G836 GLY GLY SER LEU ALA SER GLY GLY PRO GLY PRO GLY H849 Q866
C867 D868 L869 V870 R882 R905 H908 I922 M926 F936 L941 P970 F1043 R1064 E1068 L1092 C1093 ARG ARG PRO ARG SER PRO GLN PRO SER SER PRO ALA LEU GLU HIS PHE ARG VAL Y1112 L1113 S1114 R1119 K1120 T1123 R1138 E1142
T1151 S1152 Q1153 K1154 V1155 D1156 L1157 A1158 L1159 K1160 Q1161 L1162 G1163 H1164 I1165 R1166 GLU TYR GLU GLN ARG LEU LYS VAL LEU GLU ARG GLU VAL GLN GLN CYS SER ARG VAL LEU GLY TRP VAL ALA GLU ALA LEU SER ARG SER ALA LEU LEU PRO PRO PRO GLY GLY PRO PRO PRO PRO PRO ASP LEU PRO
GLY SER LYS ASP
• Molecule 1: Transient receptor potential cation channel subfamily M member 4
Chain C:
25%
71%
7%
23%
MET ASP TYR LYS ASP ASP ASP ASP LYS GLY SER GLY LEU VAL PRO ARG GLY SER VAL VAL PRO GLU LYS E7 Q8 S9 W10 I11 P12 K13 I14 F15 K16 K17 K18 THR CYS THR THR PHE ILE VAL ASP SER THR ASP PRO GLY GLY THR LEU CYS GLN CYS GLY ARG PRO ARG THR ALA
HIS PRO ALA VAL ALA MET GLU ASP ALA PHE GLY ALA ALA VAL VAL THR VAL TRP ASP SER D64 A65 H66 T67 T68 E69 K70 P71 T72 D73 A74 Y75 G76 E77 L78 D79 F80 T81 G82 A83 G84 R85 K86 H87 S88 M89 F90 L91 R92 L93 S94 D95 R96 T97 D98 P99 A100 A101 V102 Y103
S104 L105 V106 T107 R108 T109 W110 G111 F112 R113 A114 P115 S120 V121 L122 G123 G124 S125 G126 G127 P128 V129 L130 Q131 D136 A145 I153 V154 T155 G156 G157 L158 H159 T160 G161 I162 G163 R164 H165 V166 G167 V168 A169 V170 R171 D172 H173 Q174 M175 A176 S177 T178 G179 G180 T181 K182
V183 V184 A185 M186 G187 R248 V188 A189 P190 W191 G192 V193 V194 R195 N196 R197 D198 T199 L200 I201 N202 P203 LYS GLY SER F207 P208 A209 R210 Y211 R212 W213 R214 G215 ASP PRO GLU ASP GLY VAL Q222 F223 P224 L225 D226 Y227 N228 A231 F232 F233 L234 V235 D236 D237 G238 T239 H240 G241 C242 L243
G244 G245 E246 N247 R248 F249 R250 L251 R252 L253 E254 S255 Y256 I257 S258 Q259 Q260 K261 T262 GLY VAL GLY GLY THR G268 I269 D270 I271 P272 L275 L276 L277 I278 D279 G280 D281 E282 K283 M284 L285 T286 R287 I288 E289 N290 A291 T292 Q293 A294 Q295 L296 P297 C298 L299 L300 V301 A302 G303 S304
G305 G306 A307 A308 D309 C310 L311 A312 E313 T314 L315 E316 ASP THR LEU ALA PRO GLY SER GLY GLY ALA ARG GLN GLY E330 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 L361 T362 V363 Y364
S365 S366 E367 ASP GLY SER GLU E372 F373 E374 T375 I376 V377 L378 K379 A380 L381 V382 K383 A384 C385 G386 S387 S388 E389 A390 S391 A392 Y393 L394 D395 E396 L397 R398 L399 N404 R405 V406 D407 I408 A409 Q410 S411 E412 L413 F414 R415 G416 D417 I418 Q419 W420 R421 H424 M430 D431 A432
L433 L449 S450 H453 F454 M458 R459 Q462 L463 Y464 N470 S471 L472 D478 Q479 A480 S481 H482 S483 ALA GLY THR LYS ALA PRO ALA LEU LYS GLY GLY ALA ALA GLU LEU R499 P500 V503 Y519 P520 S521 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 E603 E607 M684 L693 R706 R711 LYS SER GLU GLU GLU PRO THR ARG GLU GLU LEU GLU PHE ASP MET ASP SER VAL ILE ASN GLY GLU



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

Chain D:




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
G765 R766 R767
R770
M784
F805
G836
GLY GLY SER LEU ALA SER GLY GLY PRO GLY PRO GLY
H849
Q866
C867 V870 R882 R905 H908 K919 I922 M926 F936 L941 P970 D984 M988 F1043 R1064 E1068
L1092 C1093
ARG ARG PRO ARG SER PRO GLN PRO SER SER PRO ALA LEU GLU HIS PHE ARG VAL
Y1112 L1113 S1114
R1119 K1120 T1123
R1138 E1142 T1151 S1152 Q1153 K1154 V1155 D1156 L1157 A1158 L1159 K1160 Q1161 L1162 G1163 H1164 I1165 R1166
GLU TYR GLU GLN ARG LEU LYS VAL LEU GLU ARG 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 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	79688	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	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.055	Depositor
Minimum map value	-1.535	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.266	Depositor
Map size (Å)	308.52, 308.52, 308.52	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.857, 0.857, 0.857	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: PT5, 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	0.24	0/7756	0.37	0/10501
1	B	0.24	0/7756	0.37	0/10501
1	C	0.24	0/7756	0.37	0/10501
1	D	0.24	0/7756	0.37	0/10501
All	All	0.24	0/31024	0.37	0/42004

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 (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	7581	0	7669	52	0
1	B	7581	0	7669	55	0
1	C	7581	0	7669	53	0
1	D	7581	0	7669	58	0
2	A	69	0	80	3	0
2	B	69	0	80	2	0
2	C	69	0	80	4	0
2	D	69	0	80	3	0
3	A	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	0	1	0
3	C	27	0	0	1	0
3	D	27	0	0	1	0
All	All	30708	0	30996	217	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 217 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:174:GLN:HE22	1:B:181:THR:HA	1.41	0.83
1:A:174:GLN:HE22	1:A:181:THR:HA	1.52	0.71
1:D:174:GLN:HE22	1:D:181:THR:HA	1.55	0.71
1:A:158:LEU:HD11	1:A:194:VAL:HG12	1.71	0.71
1:C:158:LEU:HD11	1:C:194:VAL:HG12	1.71	0.71

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	927/1231 (75%)	913 (98%)	14 (2%)	0	100	100
1	B	927/1231 (75%)	913 (98%)	14 (2%)	0	100	100
1	C	927/1231 (75%)	913 (98%)	14 (2%)	0	100	100
1	D	927/1231 (75%)	913 (98%)	14 (2%)	0	100	100
All	All	3708/4924 (75%)	3652 (98%)	56 (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	803/1014 (79%)	803 (100%)	0	100	100
1	B	803/1014 (79%)	803 (100%)	0	100	100
1	C	803/1014 (79%)	803 (100%)	0	100	100
1	D	803/1014 (79%)	803 (100%)	0	100	100
All	All	3212/4056 (79%)	3212 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
1	C	908	HIS
1	D	908	HIS
1	D	147	GLN
1	B	147	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	PT5	A	2001	-	69,69,69	0.49	0	84,87,87	0.55	1 (1%)
3	A1CY8	A	2002	-	29,30,30	0.36	0	36,44,44	0.62	0
3	A1CY8	B	2002	-	29,30,30	0.36	0	36,44,44	0.62	0
3	A1CY8	D	1301	-	29,30,30	0.36	0	36,44,44	0.62	0
2	PT5	C	2001	-	69,69,69	0.50	0	84,87,87	0.54	1 (1%)
2	PT5	B	2001	-	69,69,69	0.49	0	84,87,87	0.55	1 (1%)
2	PT5	D	1302	-	69,69,69	0.50	0	84,87,87	0.53	1 (1%)
3	A1CY8	C	2002	-	29,30,30	0.36	0	36,44,44	0.62	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	PT5	A	2001	-	-	25/66/90/90	0/1/1/1
3	A1CY8	A	2002	-	-	2/8/39/39	0/4/4/4
3	A1CY8	B	2002	-	-	2/8/39/39	0/4/4/4
3	A1CY8	D	1301	-	-	2/8/39/39	0/4/4/4
2	PT5	C	2001	-	-	27/66/90/90	0/1/1/1
2	PT5	B	2001	-	-	25/66/90/90	0/1/1/1
2	PT5	D	1302	-	-	25/66/90/90	0/1/1/1
3	A1CY8	C	2002	-	-	2/8/39/39	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2001	PT5	P5-O5-C5	2.22	129.36	123.43
2	D	1302	PT5	P5-O5-C5	2.22	129.35	123.43
2	B	2001	PT5	P5-O5-C5	2.21	129.33	123.43
2	A	2001	PT5	P5-O5-C5	2.19	129.28	123.43

There are no chirality outliers.

5 of 110 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	PT5	C7-O13-P1-O11
2	A	2001	PT5	C7-O13-P1-O1
2	A	2001	PT5	C1-O1-P1-O13
2	A	2001	PT5	C1-O1-P1-O11
2	B	2001	PT5	C7-O13-P1-O11

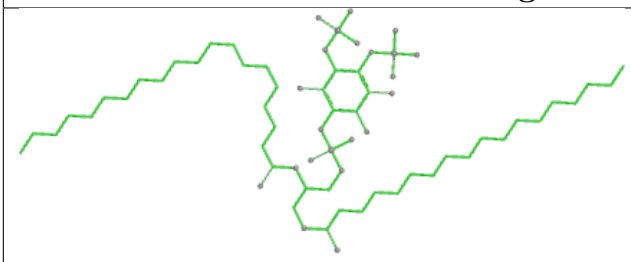
There are no ring outliers.

8 monomers are involved in 16 short contacts:

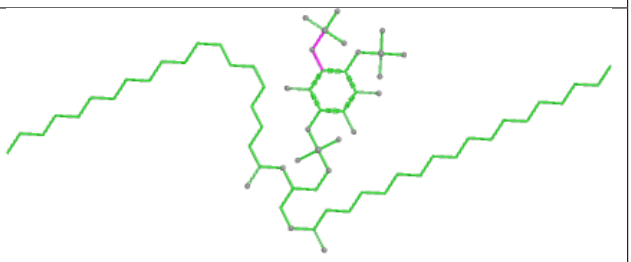
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	PT5	3	0
3	A	2002	A1CY8	1	0
3	B	2002	A1CY8	1	0
3	D	1301	A1CY8	1	0
2	C	2001	PT5	4	0
2	B	2001	PT5	2	0
2	D	1302	PT5	3	0
3	C	2002	A1CY8	1	0

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 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.

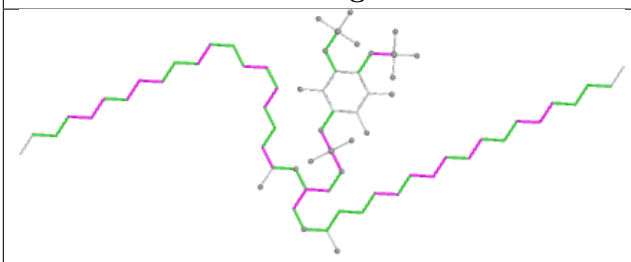
Ligand PT5 A 2001



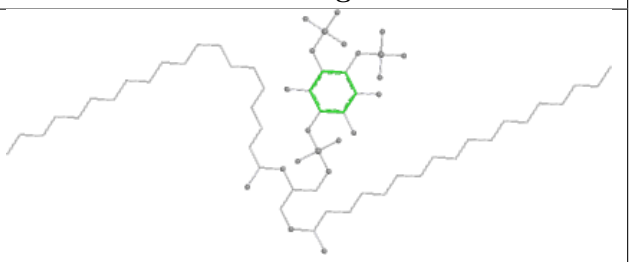
Bond lengths



Bond angles

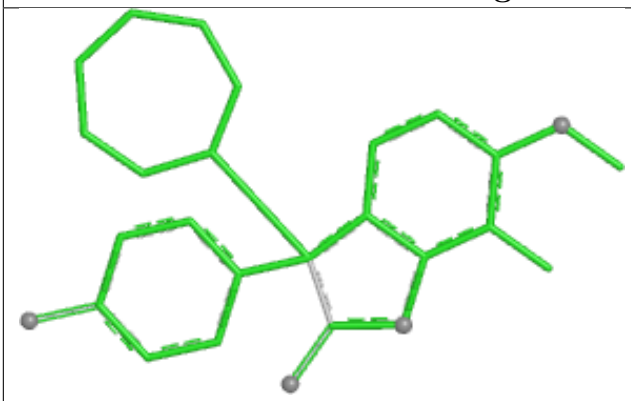


Torsions

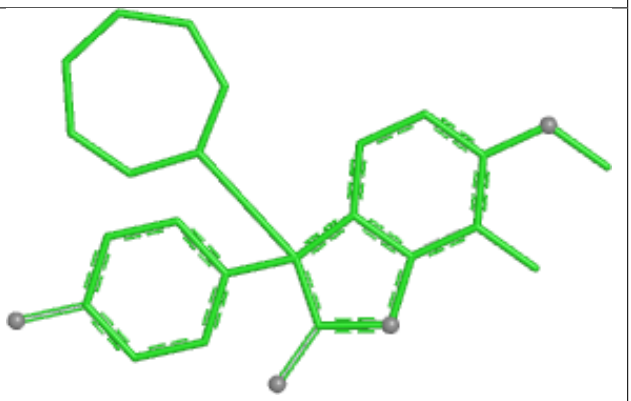


Rings

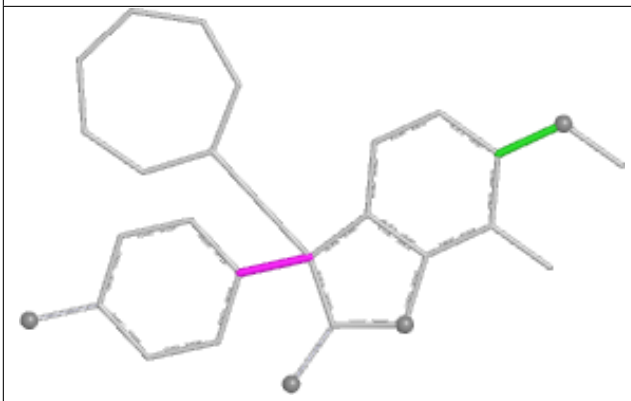
Ligand A1CY8 A 2002



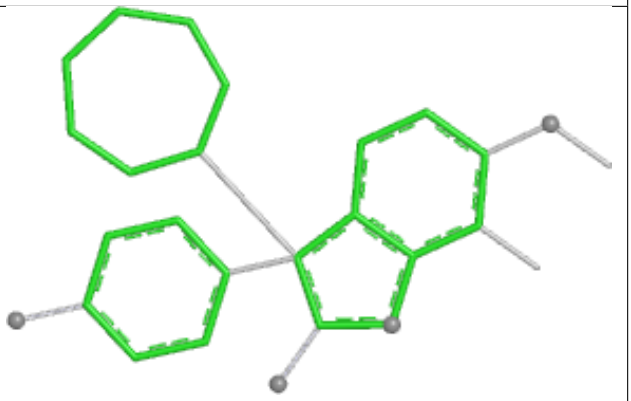
Bond lengths



Bond angles

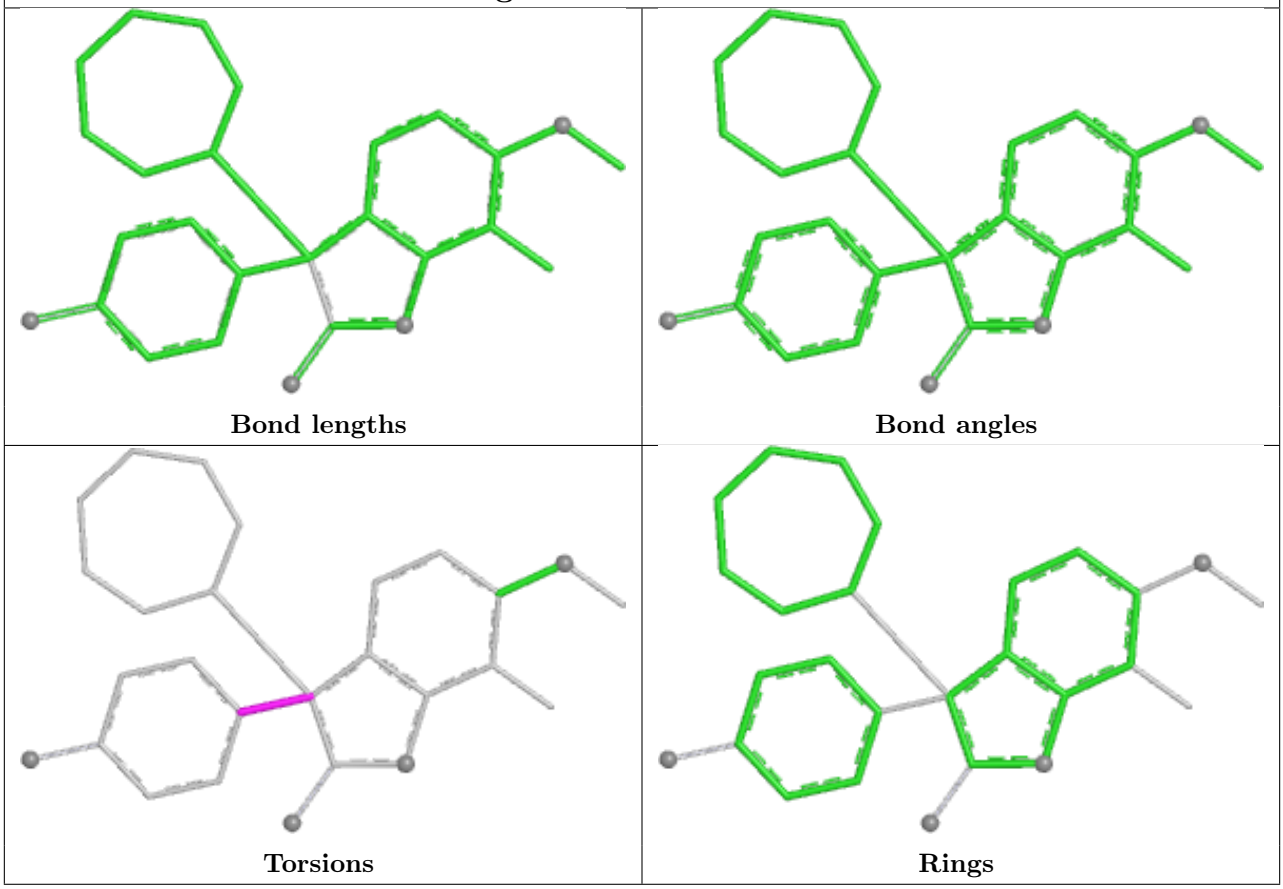


Torsions

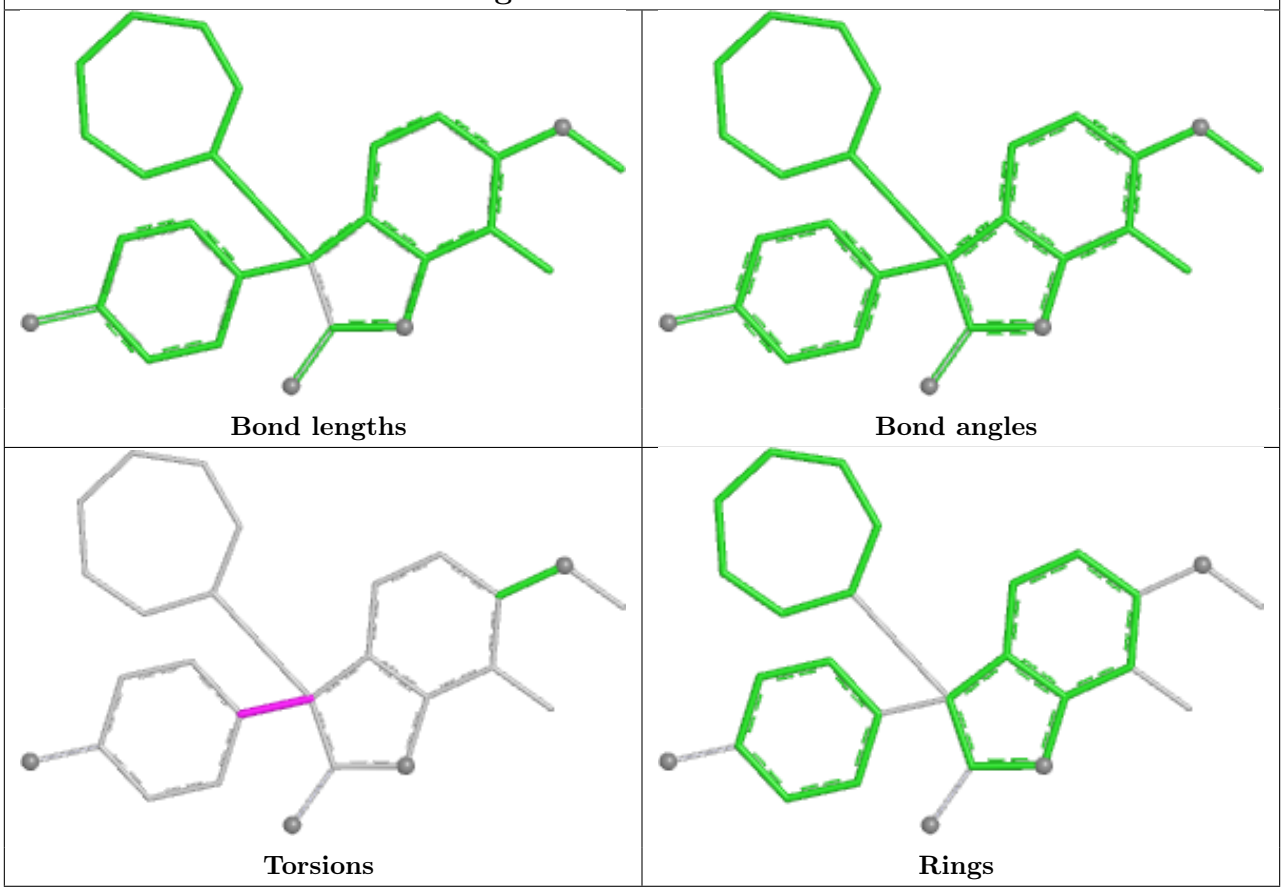


Rings

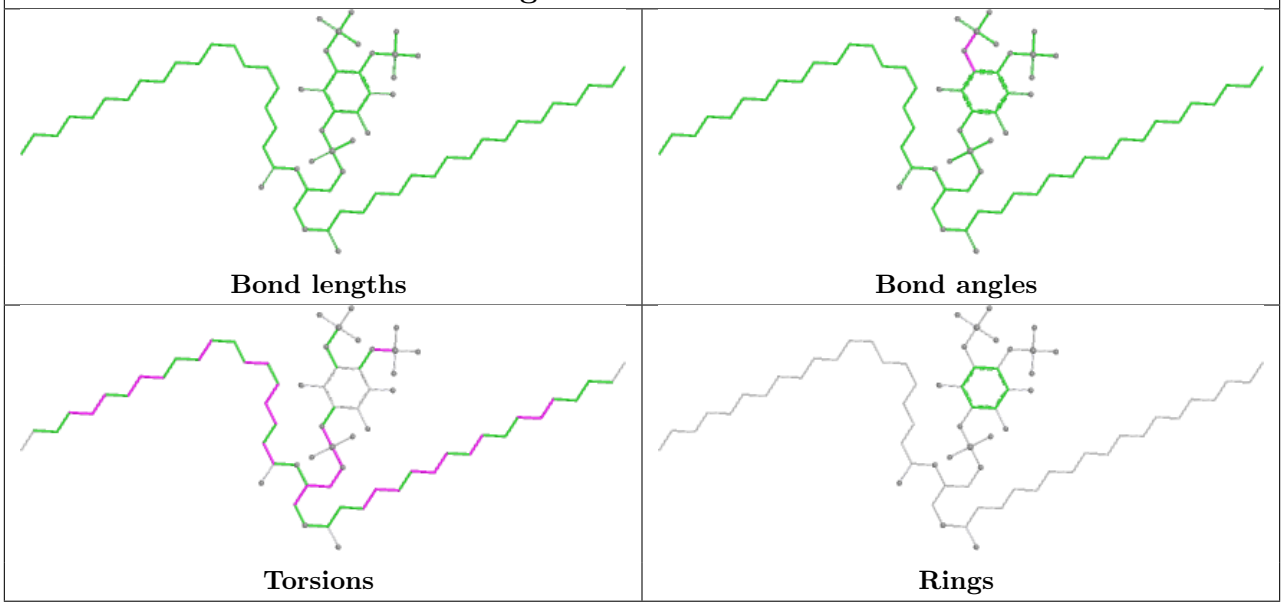
Ligand A1CY8 B 2002

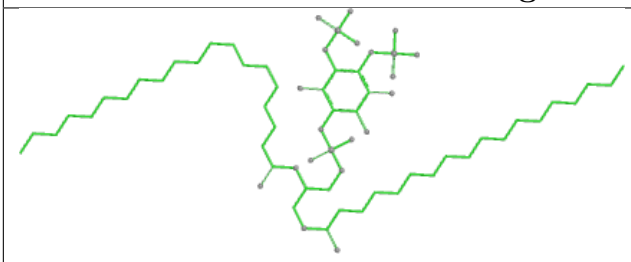
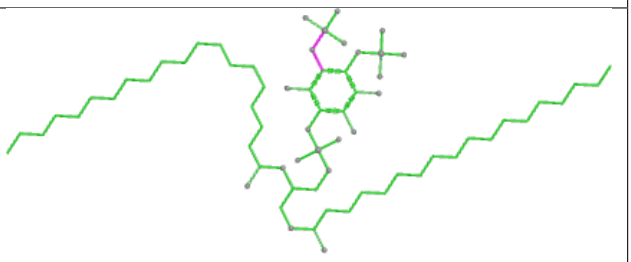
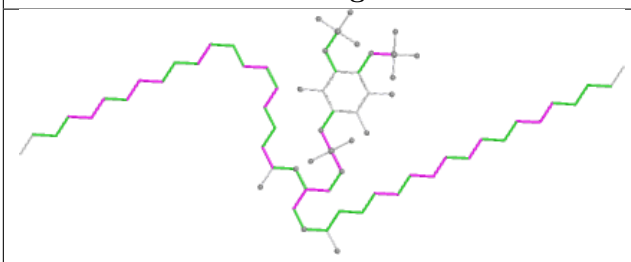
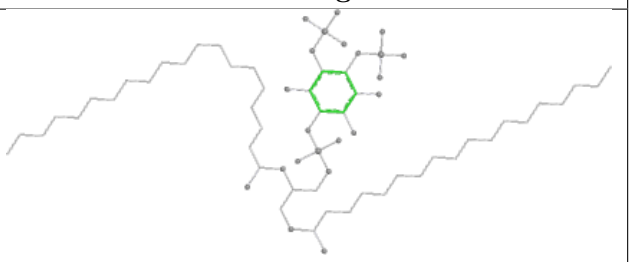


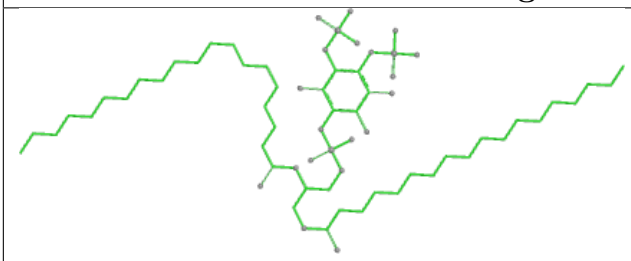
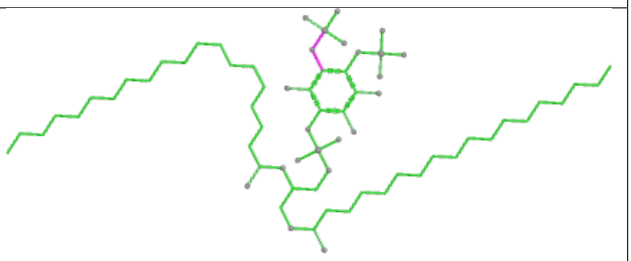
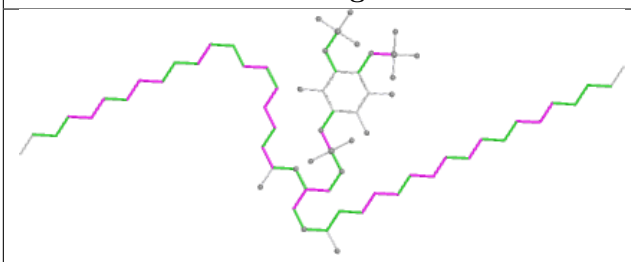
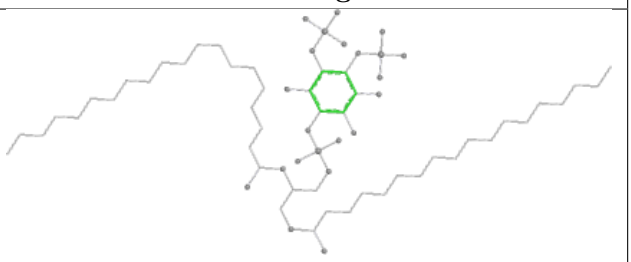
Ligand A1CY8 D 1301

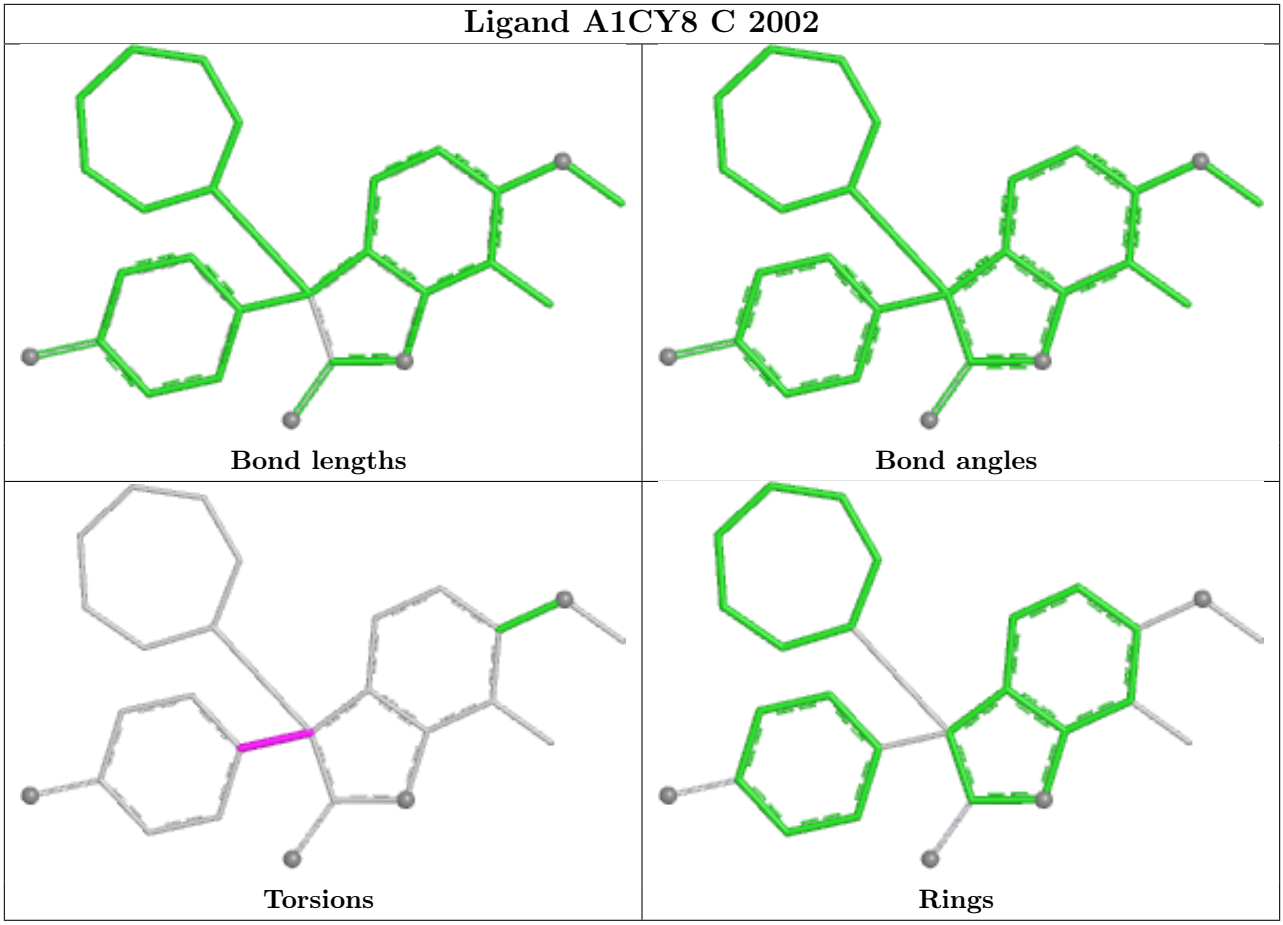


Ligand PT5 C 2001



Ligand PT5 B 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PT5 D 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings



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.

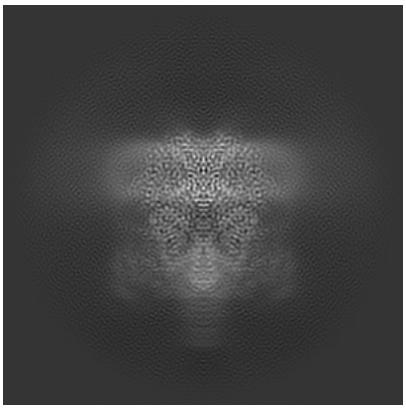
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-73528. These allow visual inspection of the internal detail of the map and identification of artifacts.

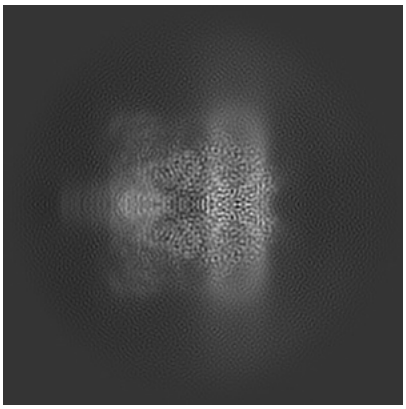
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

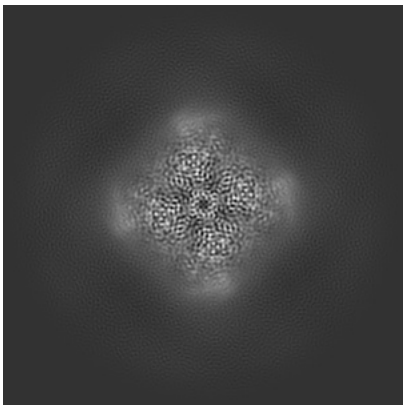
6.1.1 Primary map



X

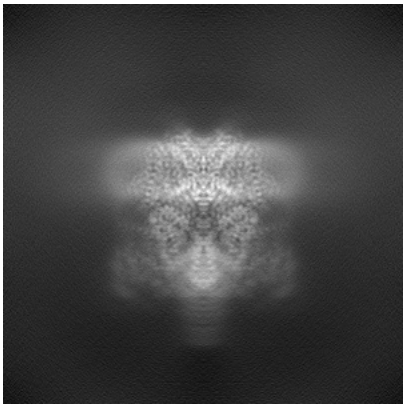


Y



Z

6.1.2 Raw map



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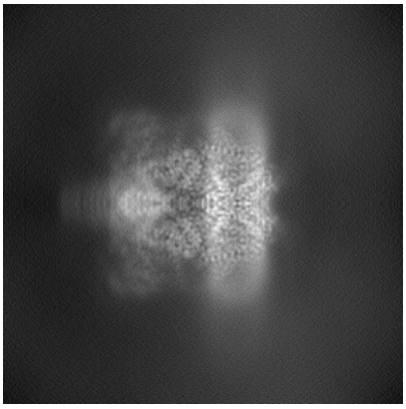
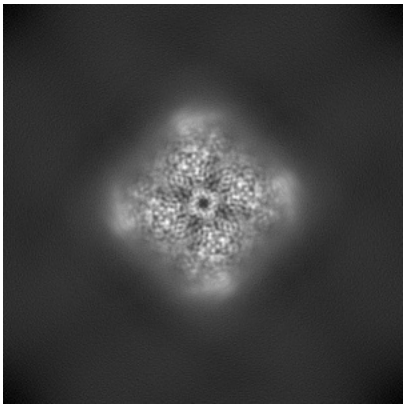


Y

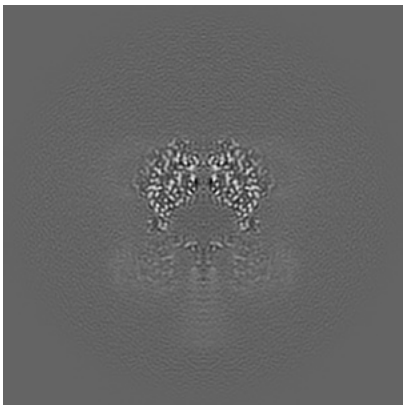


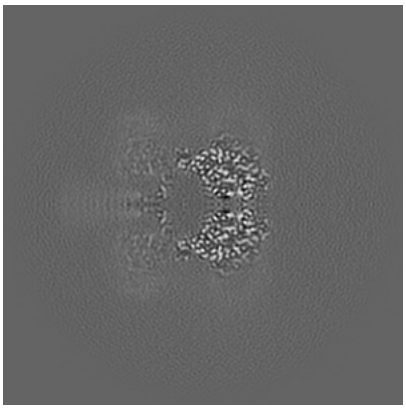
Z

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

6.2 Central slices (i)

6.2.1 Primary map


X Index: 180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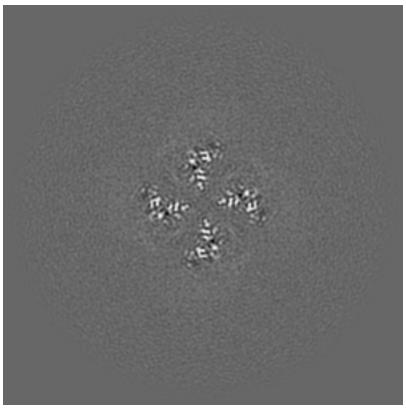
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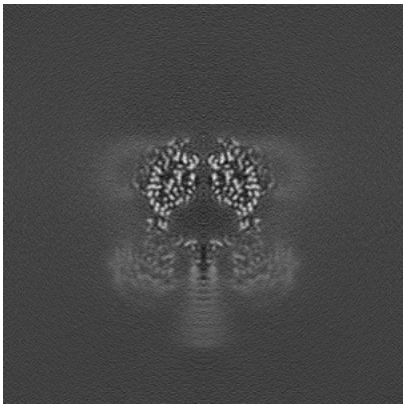
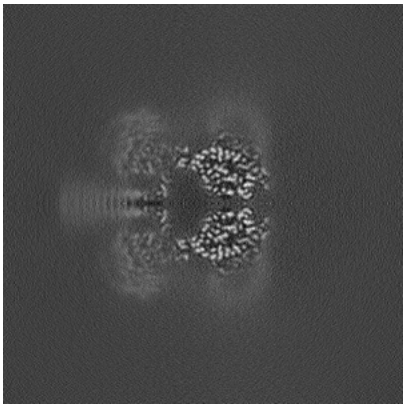
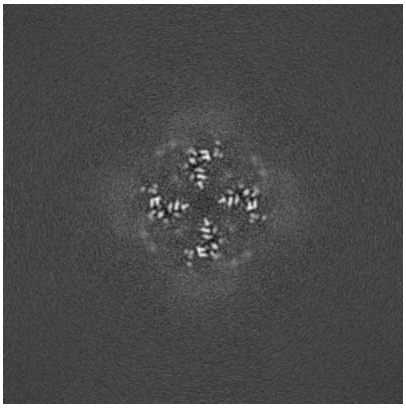
6.2.2 Raw map


X Index: 180

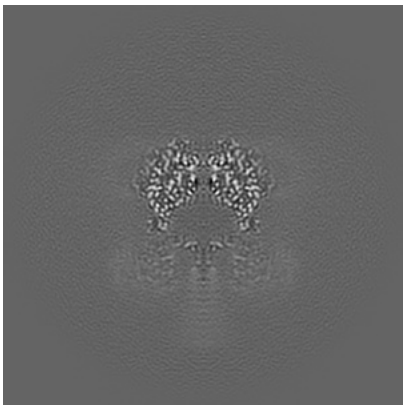

Y Index: 180

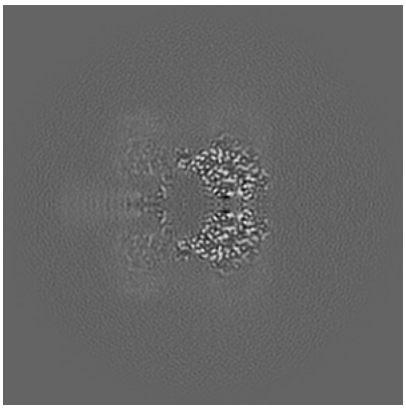

Z Index: 180

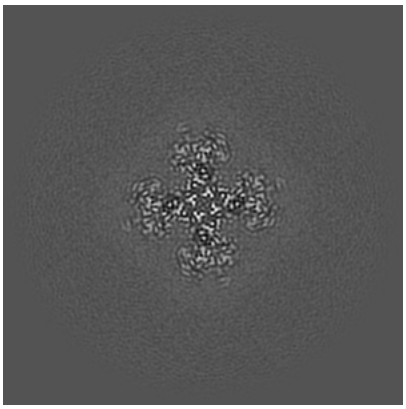
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

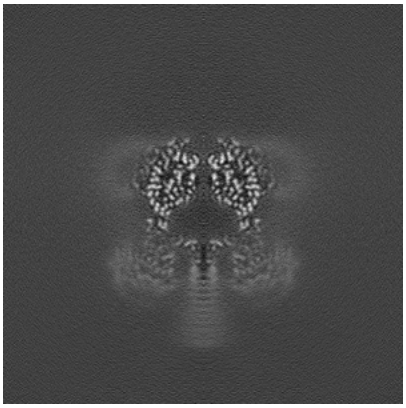
6.3.1 Primary map

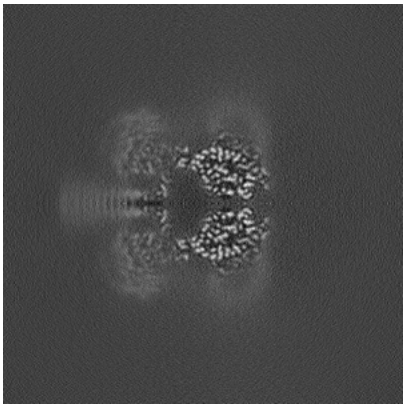

X Index: 180

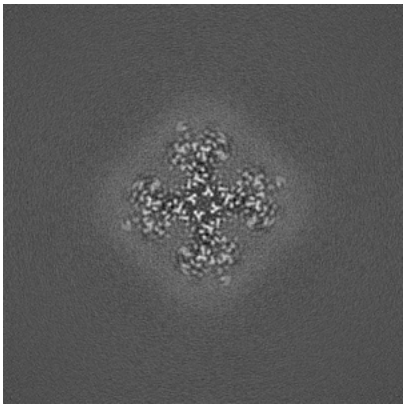

Y Index: 180


Z Index: 194

6.3.2 Raw map


X Index: 180

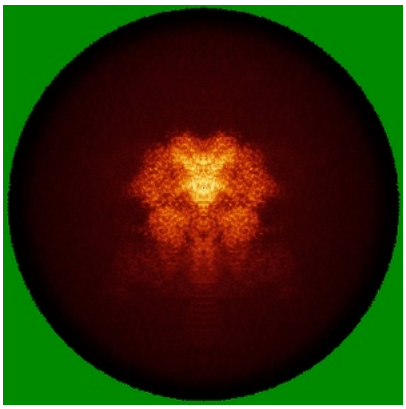

Y Index: 180

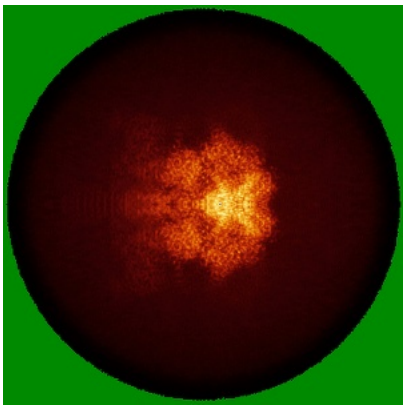

Z Index: 194

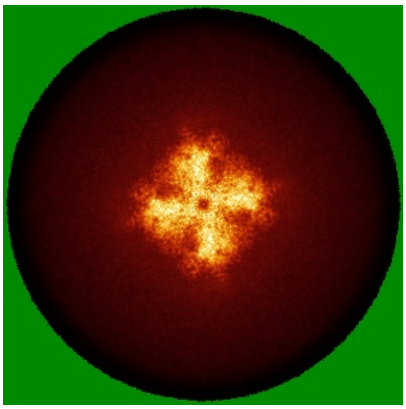
The images above show the largest variance slices of the map in three orthogonal directions.

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

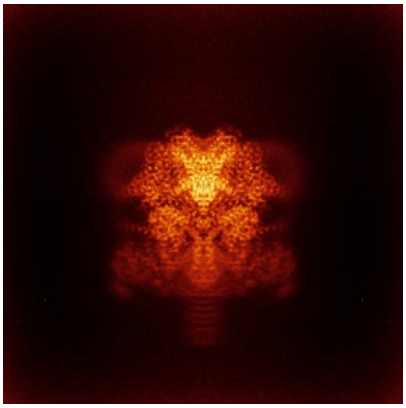
6.4.1 Primary map

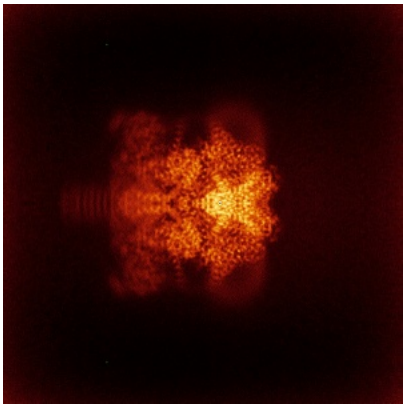

X

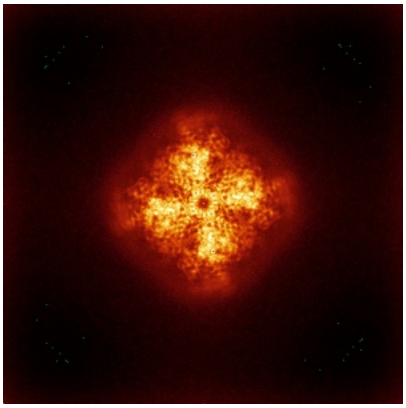

Y


Z

6.4.2 Raw map


X

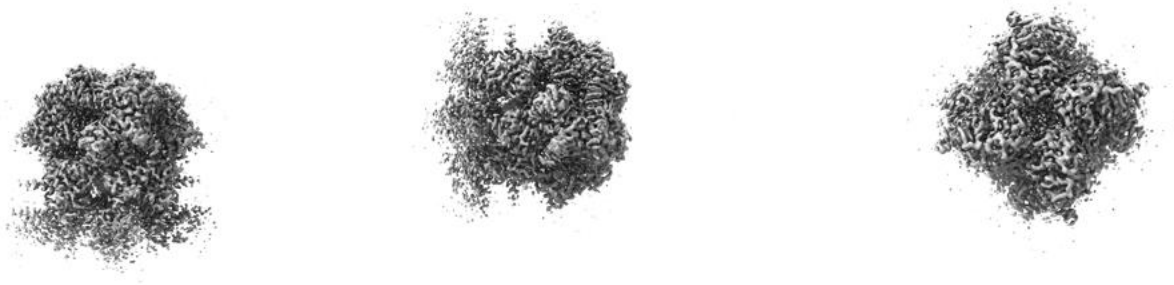

Y


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 0.266. 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.

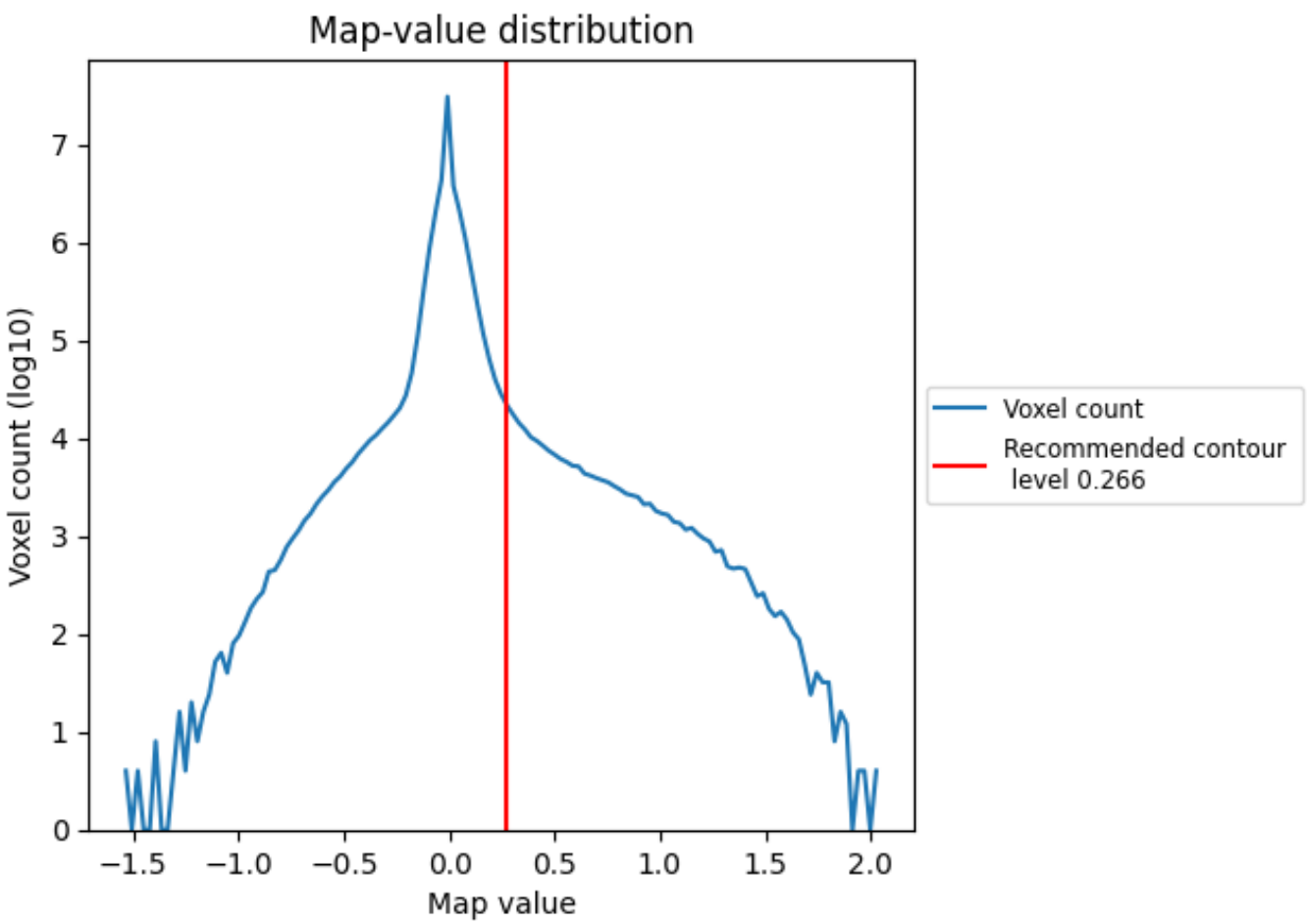
6.6 Mask visualisation (i)

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

7 Map analysis (i)

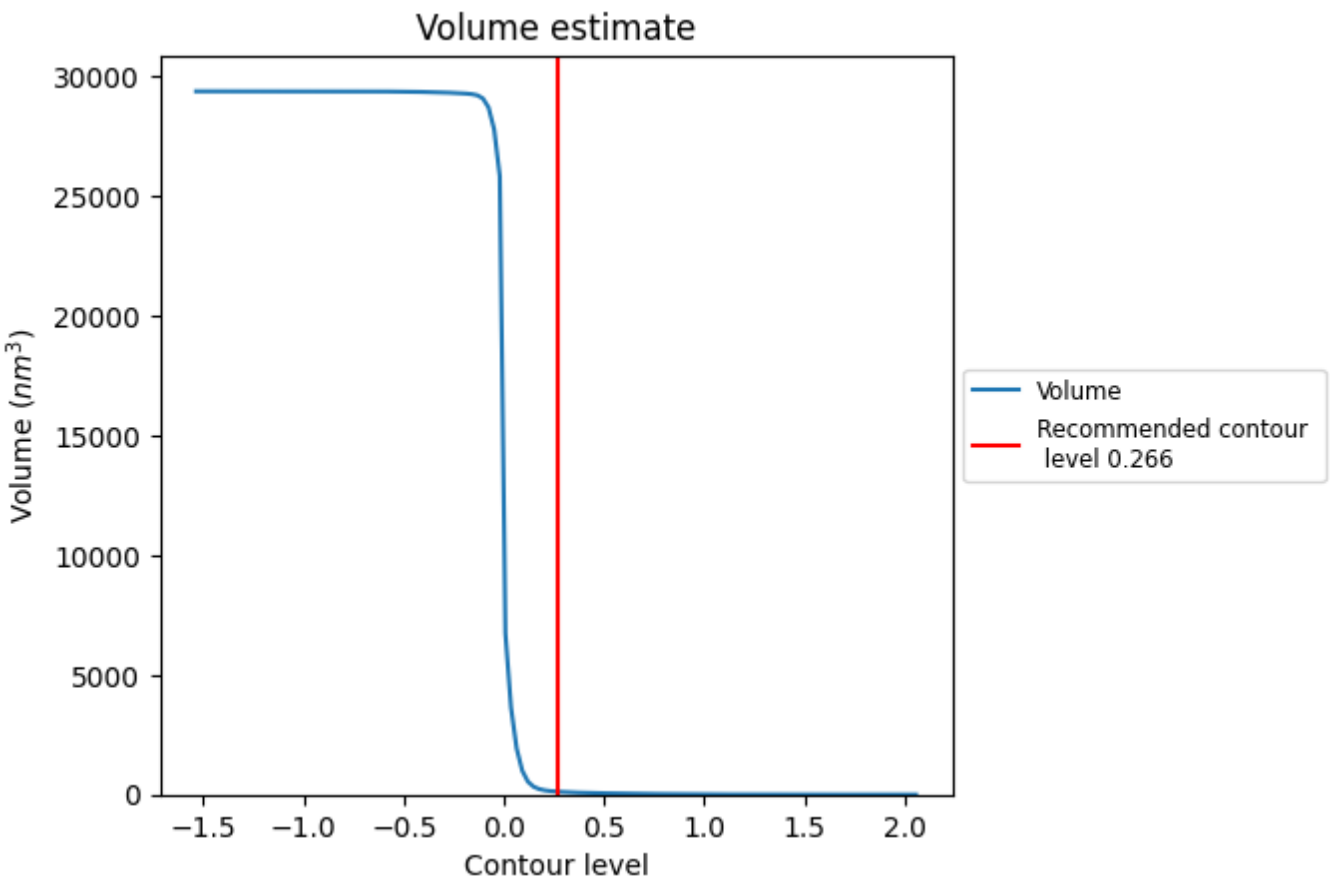
This section contains the results of statistical analysis of the map.

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.

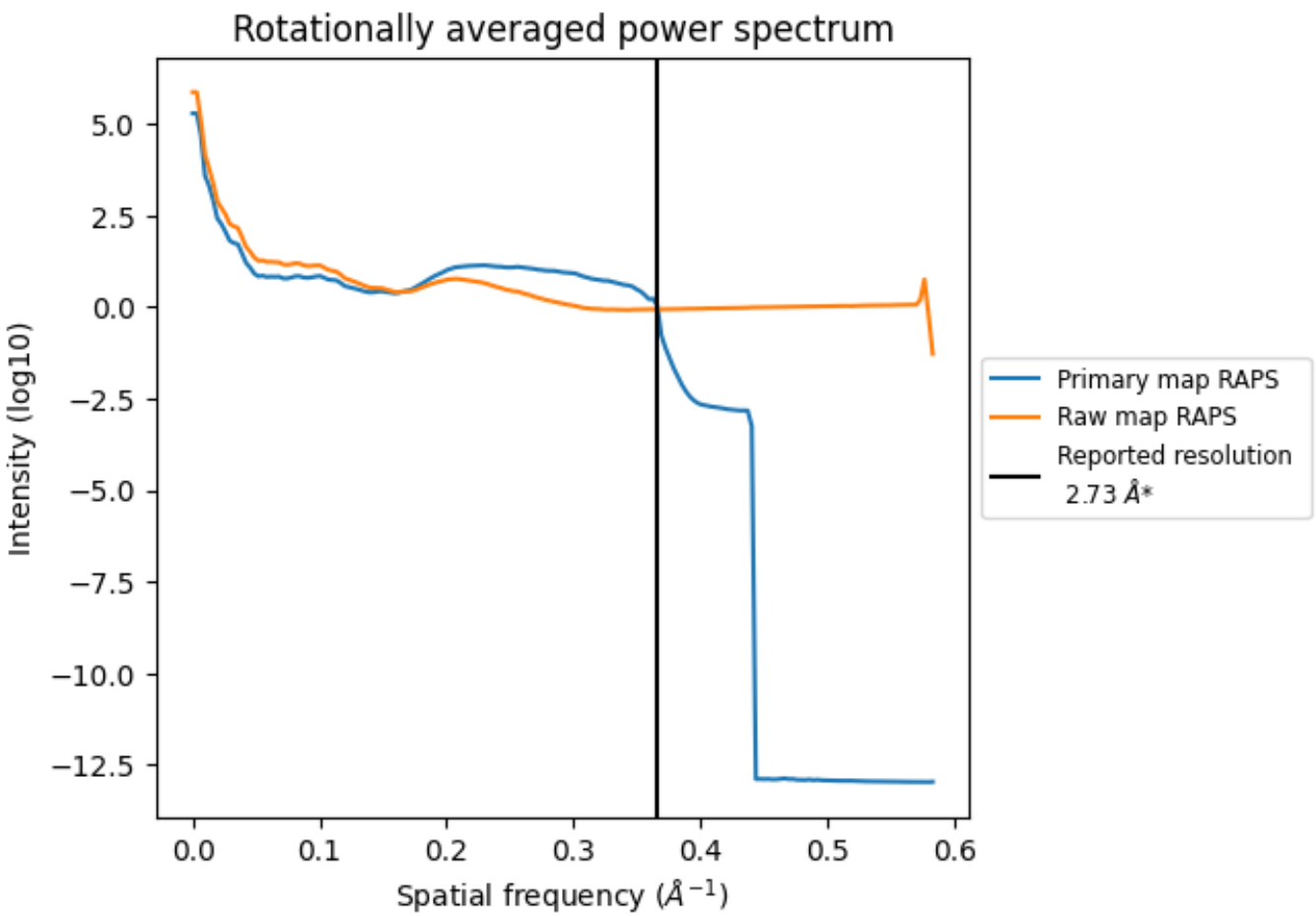
7.2 Volume estimate (i)



The volume at the recommended contour level is 122 nm^3; this corresponds to an approximate mass of 110 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)

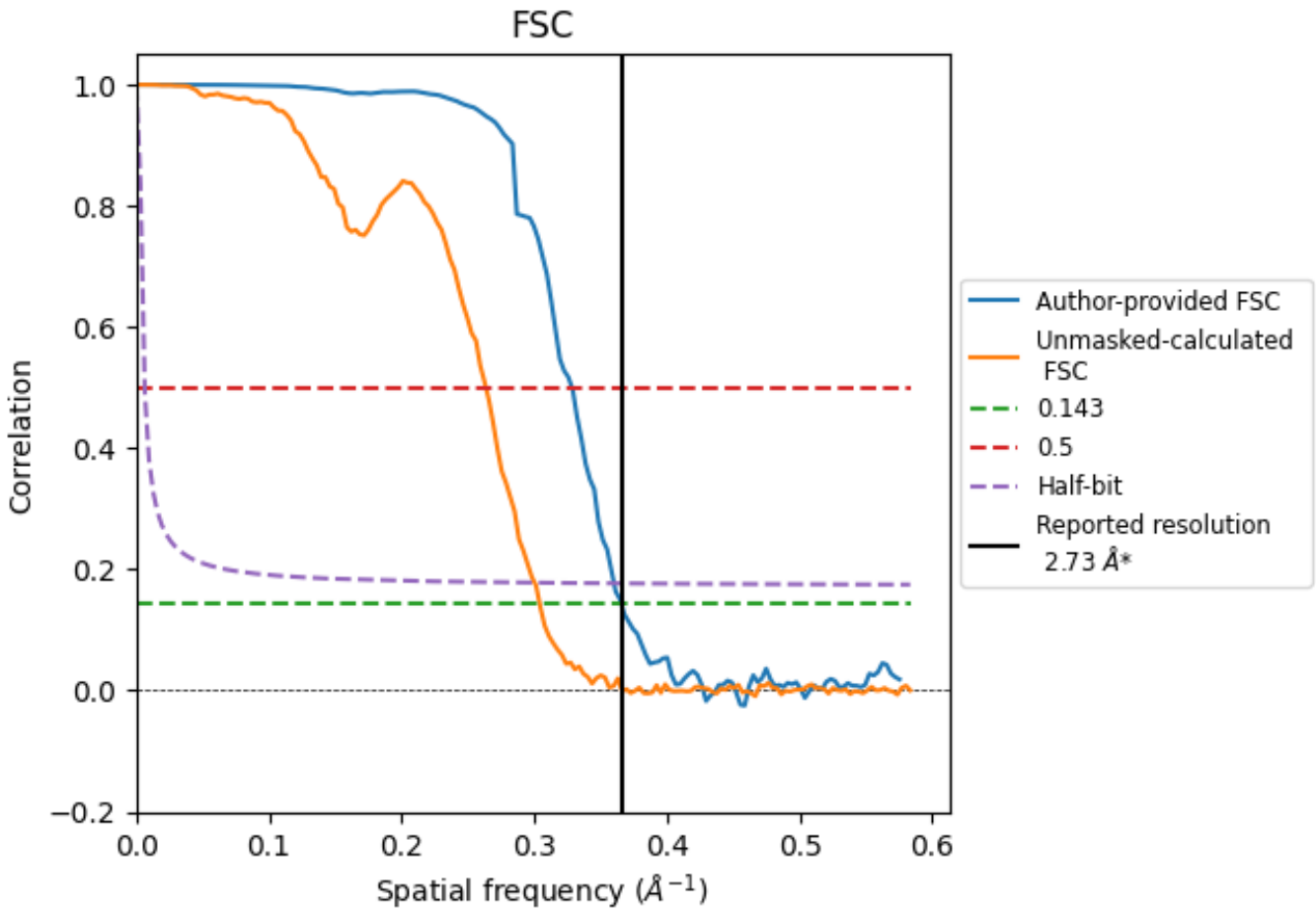


*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

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 0.366 Å^{-1}

8.2 Resolution estimates (i)

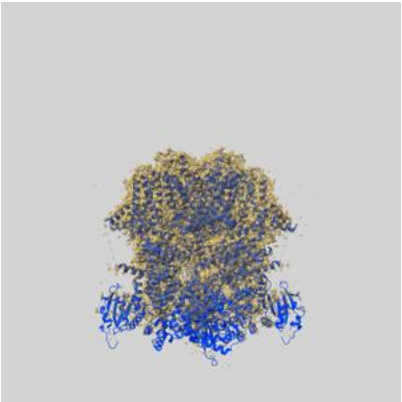
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.74	3.05	2.78
Unmasked-calculated*	3.29	3.79	3.33

*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 3.29 differs from the reported value 2.73 by more than 10 %

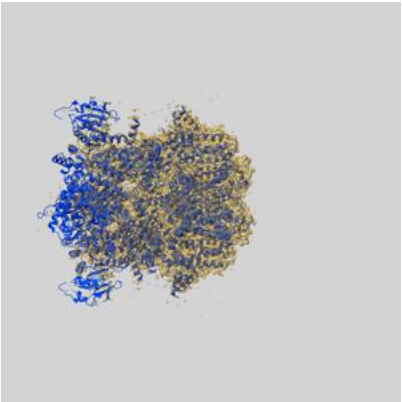
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-73528 and PDB model 9YVM. Per-residue inclusion information can be found in section 3 on page 7.

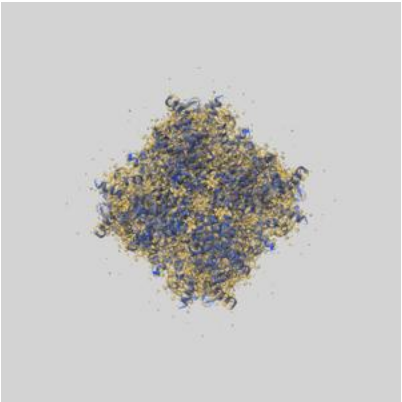
9.1 Map-model overlay (i)



X



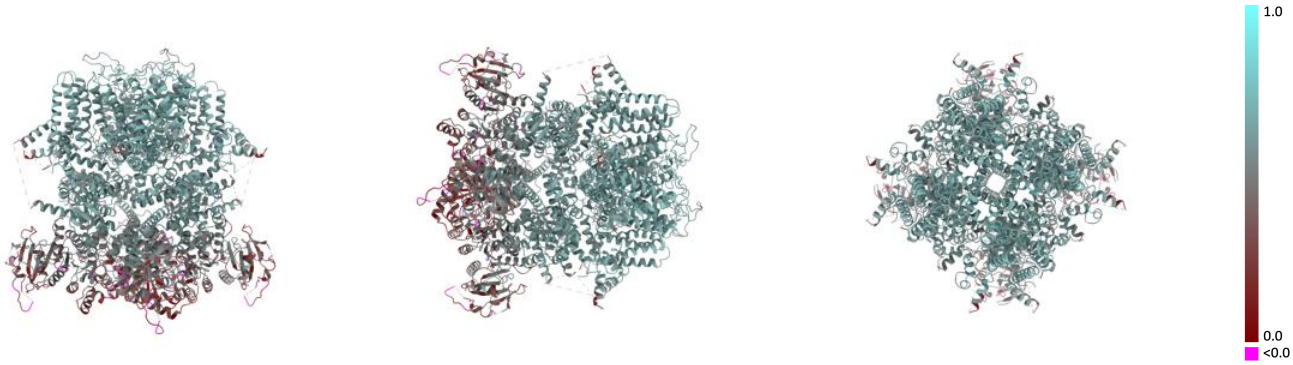
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.266 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.

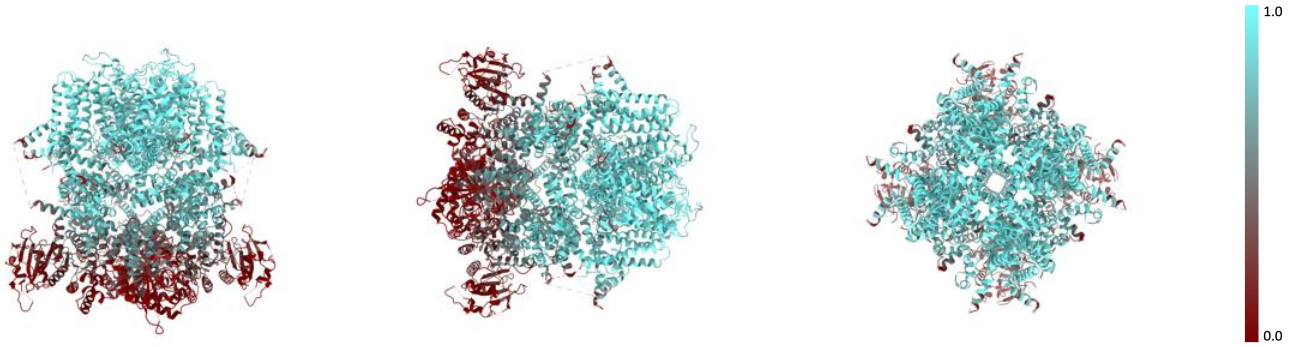
9.2 Q-score mapped to coordinate model (i)



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.

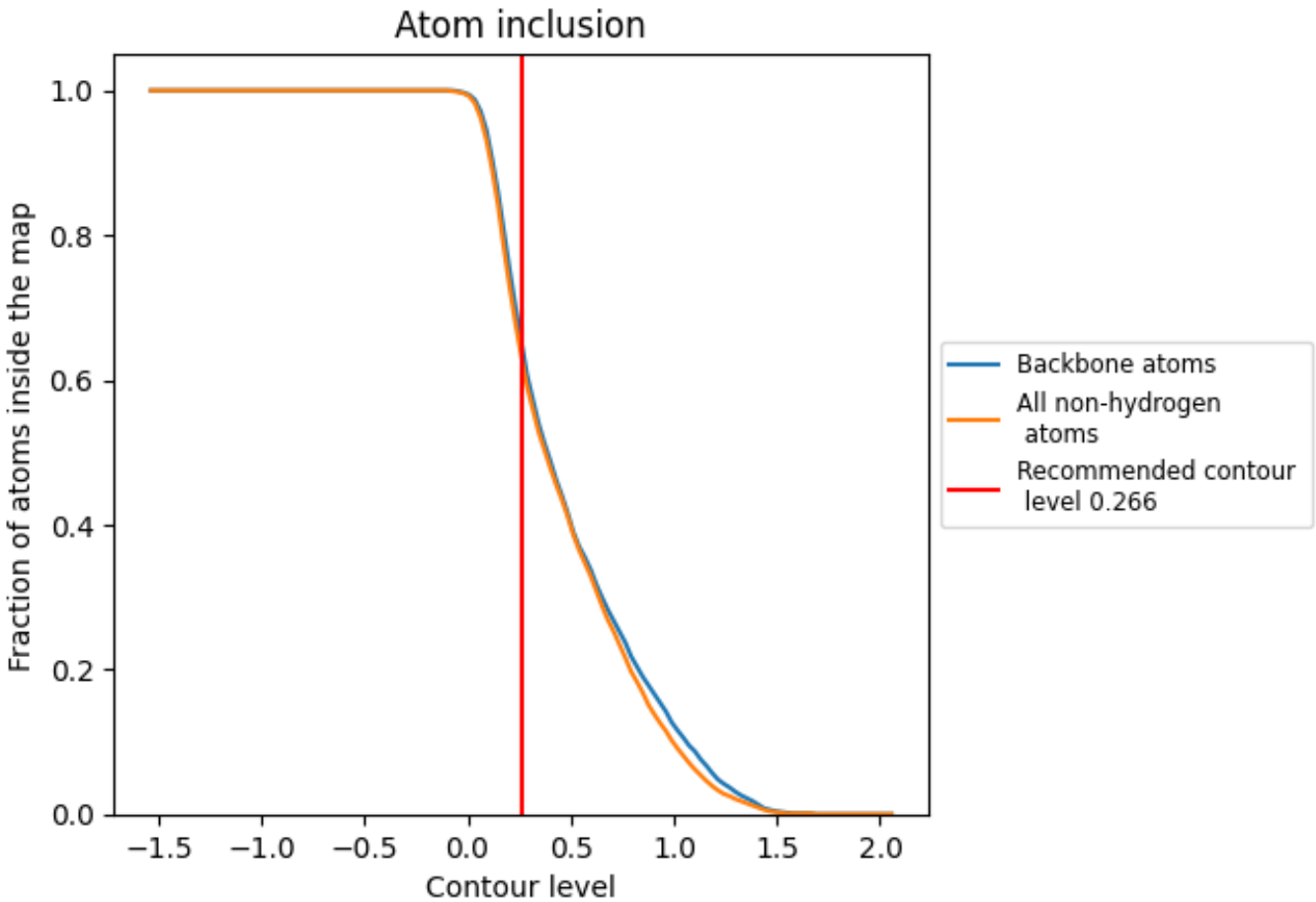
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.266).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6240	0.5330
A	0.6240	0.5330
B	0.6240	0.5330
C	0.6240	0.5320
D	0.6240	0.5320