wwPDB EM Validation Summary Report (i)

Mar 3, 2024 – 08:05 AM EST

PDB ID	:	6BQV
EMDB ID	:	EMD-7133
Title	:	Human TRPM4 ion channel in lipid nanodiscs in a calcium-bound state
Authors	:	Autzen, H.E.; Myasnikov, A.G.; Campbell, M.G.; Asarnow, D.; Julius, D.; Cheng, Y.
Deposited on	:	2017-11-28
Resolution	:	3.10 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 (1)) were used in the production of this report:

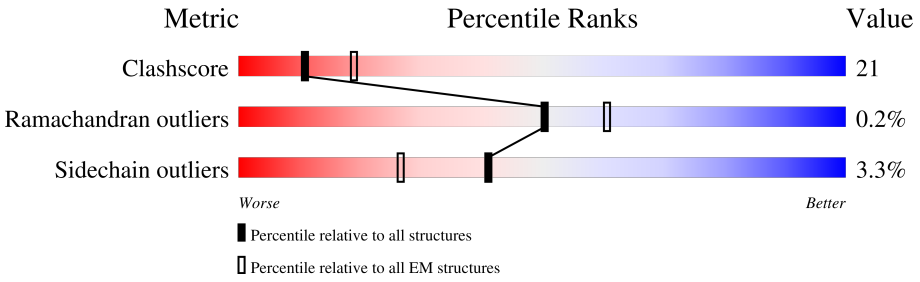
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1218	17% 57% 18% • 23%
1	B	1218	17% 57% 18% • 23%
1	C	1218	17% 57% 18% • 23%
1	D	1218	17% 57% 18% • 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29716 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	932	7323	4724	1287	1274	38	0	0
1	B	932	7323	4724	1287	1274	38	0	0
1	C	932	7323	4724	1287	1274	38	0	0
1	D	932	7323	4724	1287	1274	38	0	0

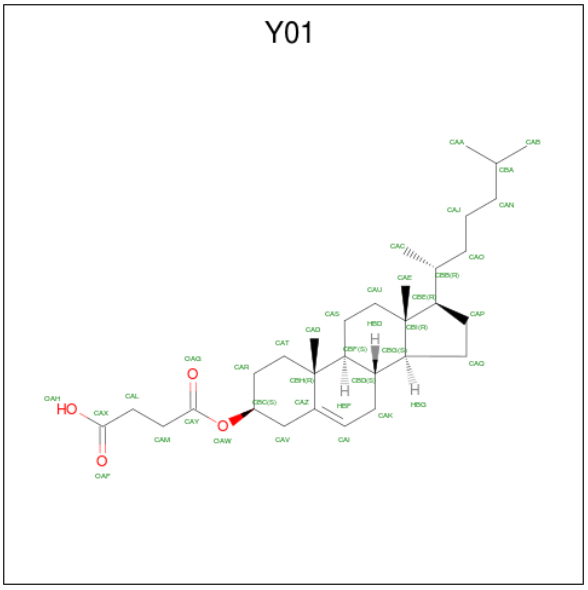
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP Q8TD43
A	-2	GLY	-	expression tag	UNP Q8TD43
A	-1	ARG	-	expression tag	UNP Q8TD43
A	0	SER	-	expression tag	UNP Q8TD43
A	1	GLY	-	expression tag	UNP Q8TD43
B	-3	SER	-	expression tag	UNP Q8TD43
B	-2	GLY	-	expression tag	UNP Q8TD43
B	-1	ARG	-	expression tag	UNP Q8TD43
B	0	SER	-	expression tag	UNP Q8TD43
B	1	GLY	-	expression tag	UNP Q8TD43
C	-3	SER	-	expression tag	UNP Q8TD43
C	-2	GLY	-	expression tag	UNP Q8TD43
C	-1	ARG	-	expression tag	UNP Q8TD43
C	0	SER	-	expression tag	UNP Q8TD43
C	1	GLY	-	expression tag	UNP Q8TD43
D	-3	SER	-	expression tag	UNP Q8TD43
D	-2	GLY	-	expression tag	UNP Q8TD43
D	-1	ARG	-	expression tag	UNP Q8TD43
D	0	SER	-	expression tag	UNP Q8TD43
D	1	GLY	-	expression tag	UNP Q8TD43

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	A	1	1	1	0
2	B	1	1	1	0
2	C	1	1	1	0
2	D	1	1	1	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	35	31	4	0
3	A	1	35	31	4	0
3	A	1	35	31	4	0
3	B	1	35	31	4	0
3	B	1	35	31	4	0
3	B	1	35	31	4	0
3	C	1	35	31	4	0

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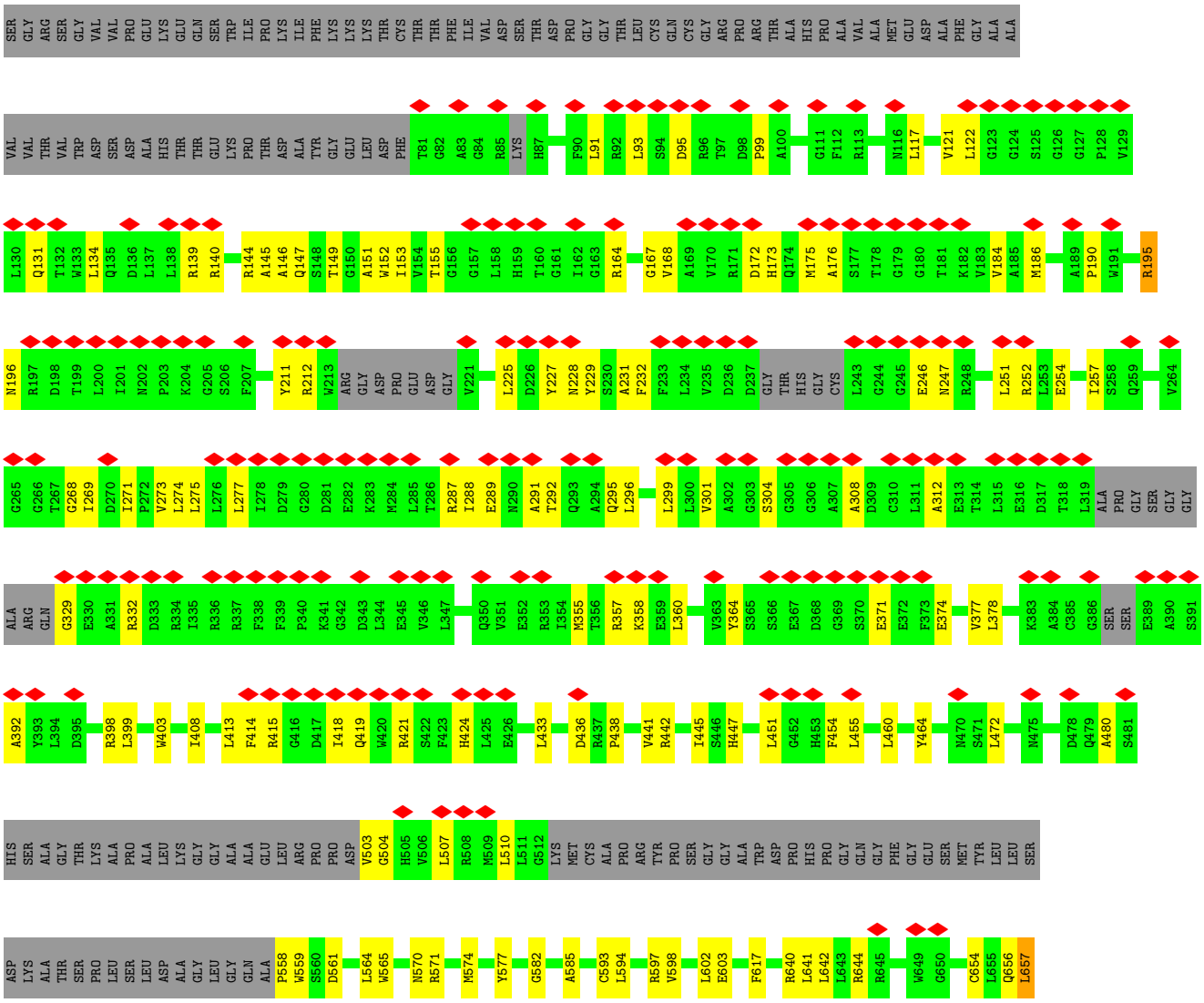
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	C	1	35	31	4	0
			Total	C	O	
3	C	1	35	31	4	0
			Total	C	O	
3	D	1	35	31	4	0
			Total	C	O	
3	D	1	35	31	4	0
			Total	C	O	
3	D	1	35	31	4	0

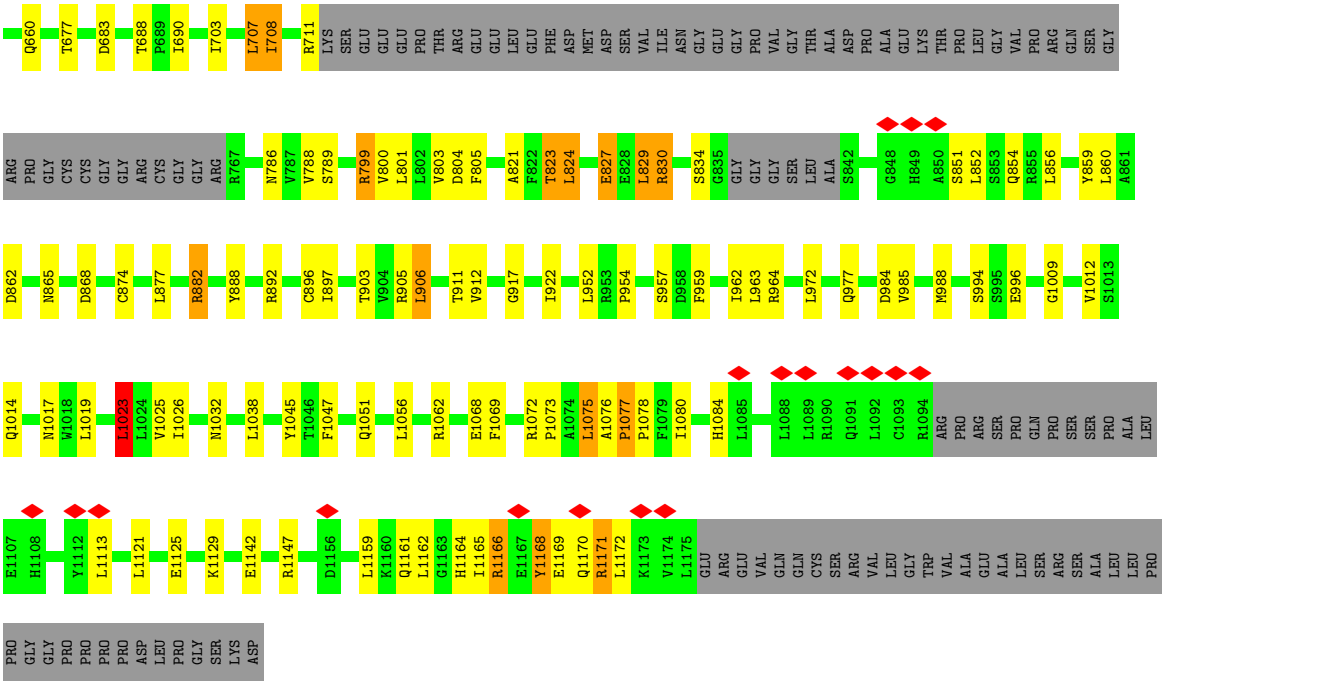
3 Residue-property plots (i)

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

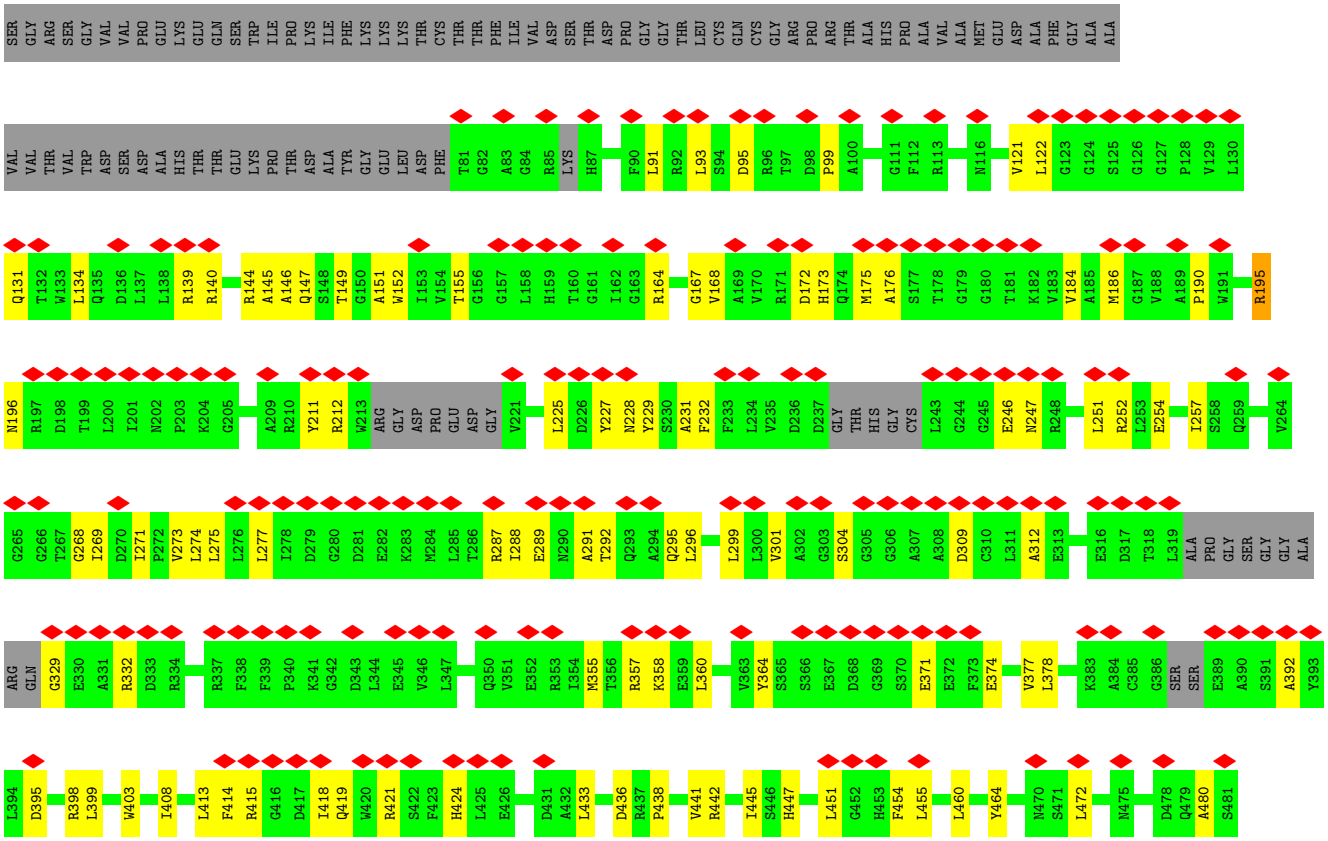
Chain A: 17% 57% 18% 23%

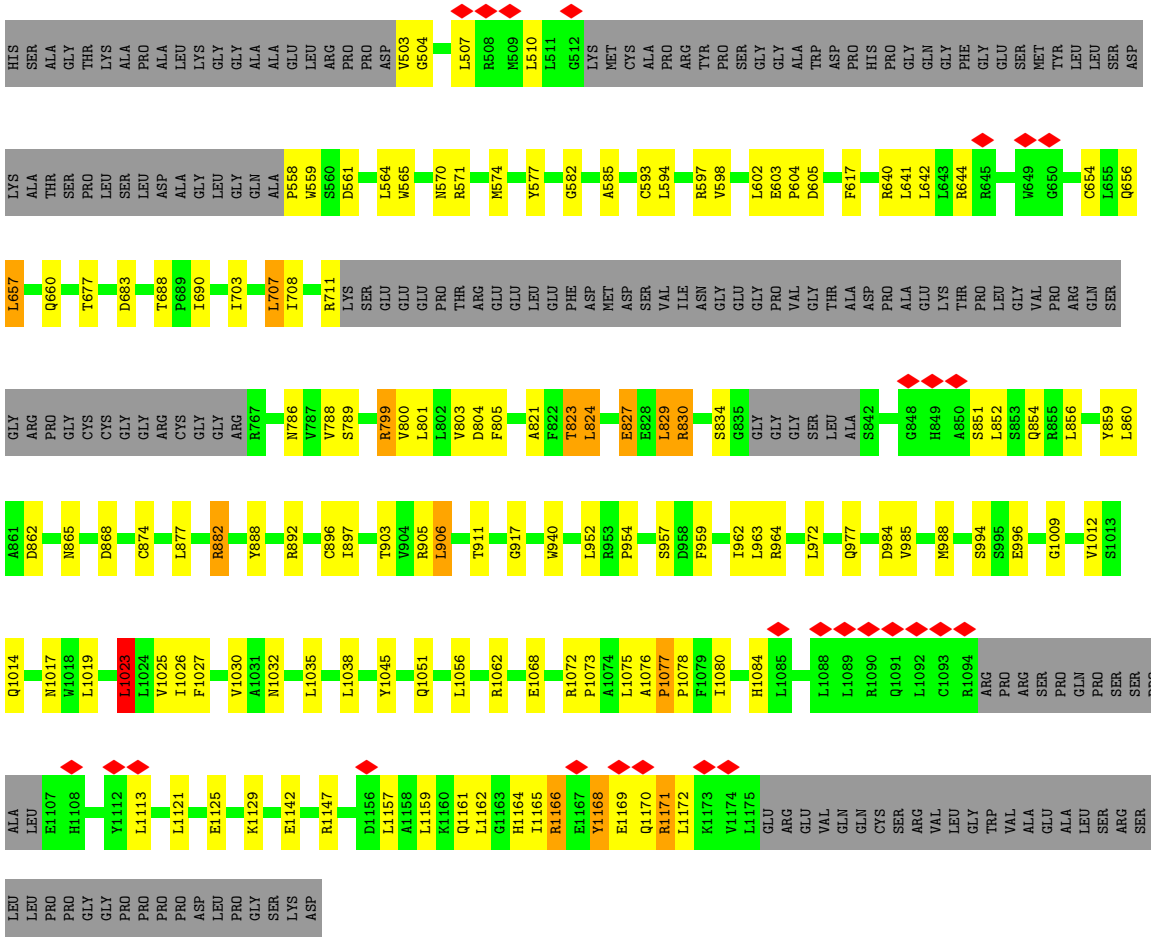




• Molecule 1: Transient receptor potential cation channel subfamily M member 4

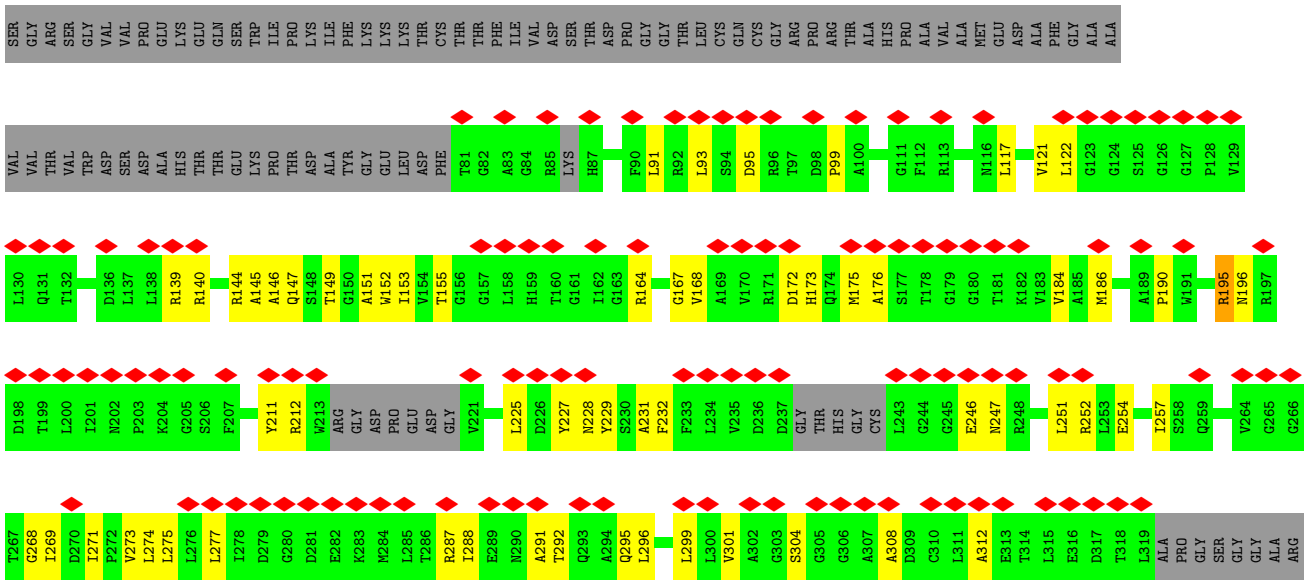
Chain B: 17% 57% 18% • 23%

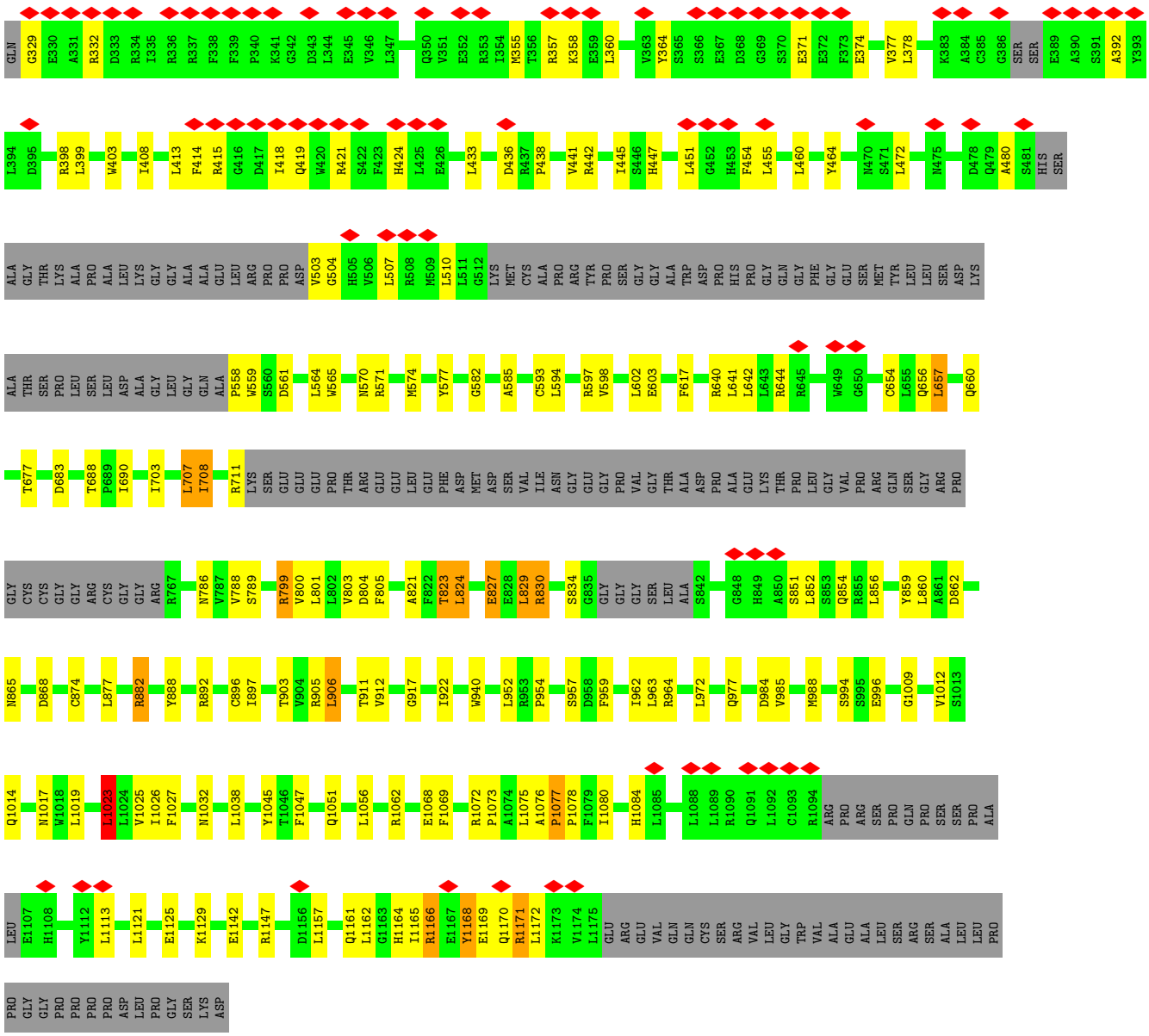




- Molecule 1: Transient receptor potential cation channel subfamily M member 4

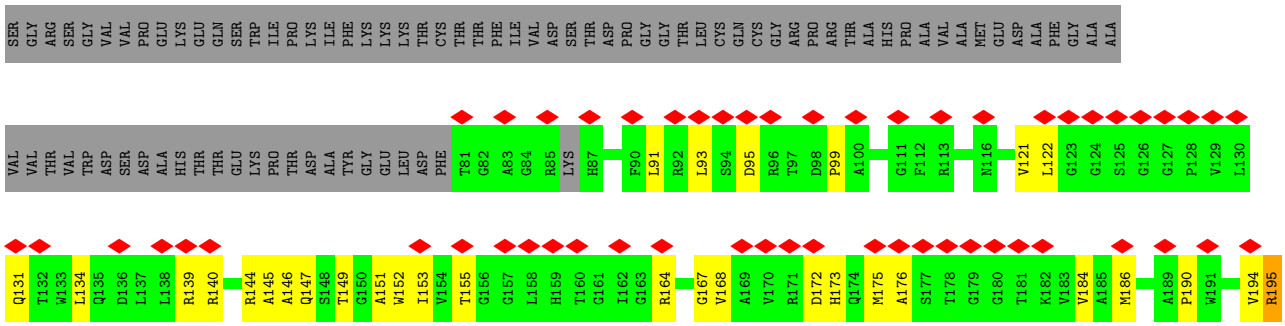
Chain C:





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

Chain D:



N196 R197 D198 T199 L200 I201 N202 P203 K204 G205 S206 F207 Y211 R212 W213 ARG GLY ASP PRO GLU ASP GLY V221 L225 D226 Y227 N228 Y229 S230 A231 F232 F233 L234 V235 D236 D237 GLY THR HIS GLY CYS L243 G244 G245 E246 N247 R248 L251 R252 L253 E254 I257 S258 Q259 V264
G265 G266 T267 G268 I269 D270 I271 P272 V273 L274 L275 L276 L277 I278 D279 G280 D281 E282 K283 M284 L285 T286 R287 I288 E289 N290 A291 T292 Q293 A294 Q295 L296 L299 L300 V301 A302 G303 S304 G305 G306 A307 A308 D309 C310 L311 A312 E313 T314 L315 E316 D317 T318 L319 ALA PRO GLY SER GLY GLY
ALA ARG GLN G329 E330 A331 R332 D333 R334 I335 R336 R337 F338 F339 P340 K341 G342 D343 L344 E345 V346 L347 Q350 V351 E352 R353 I354 M355 T356 R357 K358 E359 L360 L361 T362 V363 Y364 S365 S366 E367 D368 G369 S370 E371 E372 F373 E374 V377 L378 K383 A384 C385 G386 SER SER E389 A390
S391 A392 Y393 L394 D395 R398 L399 W403 I408 L413 F414 R415 G416 D417 I418 Q419 W420 R421 S422 F423 H424 L425 E426 L433 D436 R437 P438 V441 R442 I445 S446 H447 L451 G452 H453 F454 L455 L460 Y464 N470 S471 L472 N475 D478 Q479 A480
S481 HIS SER ALA GLY THR LYS ALA PRO ALA LEU LYS GLY GLY ALA ALA GLU LEU ARG PRO PRO ASP V503 G504 H505 V506 L507 R508 M509 L510 L511 G512 LYS MET CYS ALA PRO 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 ALA P558 W559 S560 D561 L564 W565 N570 R571 M574 Y577 G582 A585 C593 L594 R597 V598 L602 E603 P604 F617 R640 L641 L642 L643 R644 R645 W649 G650 C654 L655
Q656 L657 Q660 T677 D683 T688 P689 I690 I703 L707 I708 R711 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 R767 N786 V787 V788 S789 R799 V800 L801 L802 V803 D804 F805 A821 F822 T823 L824 E827 E828 L829 R830 S834 G835 GLY GLY GLY SER LEU ALA S842 G848 H849 A850 S851 L852 S853 Q854 R855 L856 Y859
L860 A861 D862 N865 D868 C874 L877 R882 Y888 R892 C896 I897 T903 V904 R905 L906 T911 G917 I922 W940 L952 R953 P954 S957 D958 F959 I962 L963 R964 L972 Q977 D984 V985 M988 S994 S995 E996 G1009
V1012 S1013 Q1014 N1017 W1018 L1019 L1023 L1024 V1025 I1026 F1027 N1032 L1038 Y1045 T1046 F1047 Q1051 L1056 R1062 I1066 R1067 E1068 R1072 P1073 A1074 L1075 A1076 P1077 P1078 F1079 I1080 H1084 L1085 L1088 L1089 R1090 Q1091 L1092 C1093 R1094 ARG PRO ARG SER PRO GLN PRO
SER SER PRO ALA LEU E1107 Y1112 L1113 L1121 E1125 K1129 E1142 R1147 D1156 L1157 A1158 L1159 K1160 Q1161 L1162 G1163 H1164 I1165 R1166 E1167 Y1168 E1169 Q1170 R1171 L1172 K1173 V1174 L1175 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	45346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	47.156	Depositor
Minimum map value	-30.481	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	334.72, 334.72, 334.72	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.046, 1.046, 1.046	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: Y01, CA

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	0.45	0/7484	0.66	5/10138 (0.0%)
1	B	0.45	0/7484	0.66	5/10138 (0.0%)
1	C	0.45	0/7484	0.66	5/10138 (0.0%)
1	D	0.45	0/7484	0.66	5/10138 (0.0%)
All	All	0.45	0/29936	0.66	20/40552 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1023	LEU	CA-CB-CG	8.77	135.46	115.30
1	B	1023	LEU	CA-CB-CG	8.76	135.44	115.30
1	C	1023	LEU	CA-CB-CG	8.75	135.43	115.30
1	A	1023	LEU	CA-CB-CG	8.75	135.43	115.30
1	A	1038	LEU	CA-CB-CG	7.13	131.70	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	392	ALA	Peptide
1	A	707	LEU	Peptide
1	B	392	ALA	Peptide
1	B	707	LEU	Peptide
1	C	392	ALA	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	7323	0	7341	379	0
1	B	7323	0	7341	385	0
1	C	7323	0	7341	374	0
1	D	7323	0	7341	385	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	105	0	145	6	0
3	B	105	0	145	8	0
3	C	105	0	145	8	0
3	D	105	0	145	8	0
All	All	29716	0	29944	1229	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 21.

The worst 5 of 1229 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:C:503:VAL:CG2	1:C:598:VAL:HG11	1.22	1.68
1:B:503:VAL:CG2	1:B:598:VAL:HG11	1.22	1.68
1:A:503:VAL:CG2	1:A:598:VAL:HG11	1.22	1.66
1:D:503:VAL:CG2	1:D:598:VAL:HG11	1.22	1.63
1:A:464:TYR:CE1	1:A:565:TRP:HD1	1.19	1.60

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	910/1218 (75%)	830 (91%)	78 (9%)	2 (0%)	47	79
1	B	910/1218 (75%)	830 (91%)	78 (9%)	2 (0%)	47	79
1	C	910/1218 (75%)	830 (91%)	78 (9%)	2 (0%)	47	79
1	D	910/1218 (75%)	830 (91%)	78 (9%)	2 (0%)	47	79
All	All	3640/4872 (75%)	3320 (91%)	312 (9%)	8 (0%)	50	79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1077	PRO
1	B	1077	PRO
1	C	1077	PRO
1	D	1077	PRO
1	A	708	ILE

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	763/1002 (76%)	738 (97%)	25 (3%)	38	69
1	B	763/1002 (76%)	738 (97%)	25 (3%)	38	69
1	C	763/1002 (76%)	738 (97%)	25 (3%)	38	69
1	D	763/1002 (76%)	738 (97%)	25 (3%)	38	69
All	All	3052/4008 (76%)	2952 (97%)	100 (3%)	41	69

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	703	ILE
1	C	1166	ARG
1	D	1171	ARG
1	C	789	SER
1	C	830	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	228	ASN
1	C	1017	ASN
1	D	1037	ASN
1	C	348	GLN
1	C	660	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	Y01	B	1303	-	38,38,38	3.94	11 (28%)	57,57,57	2.13	17 (29%)
3	Y01	A	1301	-	38,38,38	3.95	12 (31%)	57,57,57	2.37	20 (35%)
3	Y01	D	1301	-	38,38,38	3.94	11 (28%)	57,57,57	2.38	20 (35%)
3	Y01	A	1303	-	38,38,38	3.94	11 (28%)	57,57,57	2.13	17 (29%)
3	Y01	C	1302	-	38,38,38	3.97	11 (28%)	57,57,57	2.04	20 (35%)
3	Y01	A	1302	-	38,38,38	3.97	11 (28%)	57,57,57	2.04	20 (35%)
3	Y01	D	1303	-	38,38,38	3.94	11 (28%)	57,57,57	2.13	17 (29%)
3	Y01	B	1302	-	38,38,38	3.97	11 (28%)	57,57,57	2.04	20 (35%)
3	Y01	B	1301	-	38,38,38	3.94	12 (31%)	57,57,57	2.37	20 (35%)
3	Y01	C	1301	-	38,38,38	3.95	12 (31%)	57,57,57	2.37	20 (35%)
3	Y01	C	1303	-	38,38,38	3.94	11 (28%)	57,57,57	2.13	17 (29%)
3	Y01	D	1302	-	38,38,38	3.97	11 (28%)	57,57,57	2.04	20 (35%)

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
3	Y01	B	1303	-	-	7/19/77/77	0/4/4/4
3	Y01	A	1301	-	-	14/19/77/77	0/4/4/4
3	Y01	D	1301	-	-	14/19/77/77	0/4/4/4
3	Y01	A	1303	-	-	7/19/77/77	0/4/4/4
3	Y01	C	1302	-	-	10/19/77/77	0/4/4/4
3	Y01	A	1302	-	-	10/19/77/77	0/4/4/4
3	Y01	D	1303	-	-	7/19/77/77	0/4/4/4
3	Y01	B	1302	-	-	10/19/77/77	0/4/4/4
3	Y01	B	1301	-	-	14/19/77/77	0/4/4/4
3	Y01	C	1301	-	-	14/19/77/77	0/4/4/4
3	Y01	C	1303	-	-	7/19/77/77	0/4/4/4
3	Y01	D	1302	-	-	10/19/77/77	0/4/4/4

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	Y01	CAI-CAZ	16.07	1.68	1.33
3	D	1302	Y01	CAI-CAZ	16.04	1.68	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	Y01	CAI-CAZ	16.03	1.68	1.33
3	C	1302	Y01	CAI-CAZ	16.01	1.68	1.33
3	D	1301	Y01	CAI-CAZ	15.87	1.67	1.33

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1301	Y01	CAU-CBI-CBG	6.17	116.85	107.27
3	B	1301	Y01	CAU-CBI-CBG	6.16	116.83	107.27
3	A	1301	Y01	CAU-CBI-CBG	6.16	116.82	107.27
3	C	1301	Y01	CAU-CBI-CBG	6.13	116.78	107.27
3	C	1303	Y01	CAK-CAI-CAZ	-5.82	114.33	125.06

There are no chirality outliers.

5 of 124 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1302	Y01	OAG-CAY-OAW-CBC
3	A	1303	Y01	CAC-CBB-CBE-CBI
3	B	1302	Y01	OAG-CAY-OAW-CBC
3	B	1303	Y01	CAC-CBB-CBE-CBI
3	C	1302	Y01	OAG-CAY-OAW-CBC

There are no ring outliers.

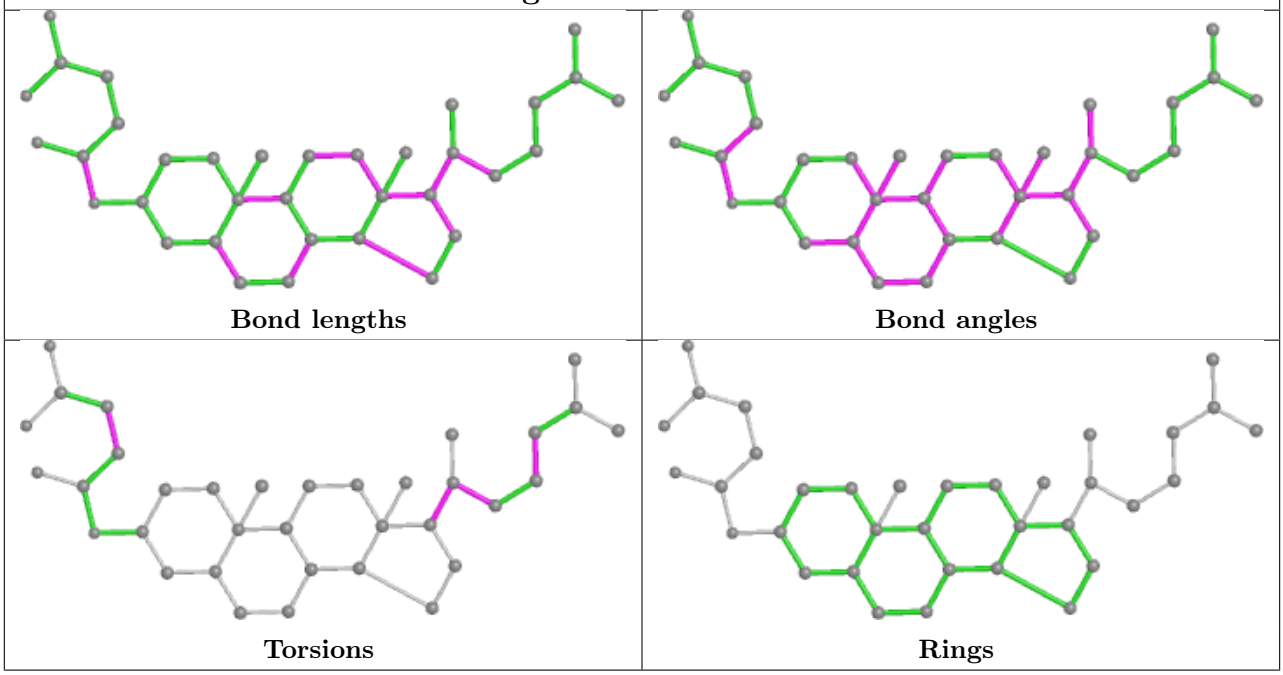
12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1303	Y01	3	0
3	A	1301	Y01	3	0
3	D	1301	Y01	2	0
3	A	1303	Y01	2	0
3	C	1302	Y01	3	0
3	A	1302	Y01	2	0
3	D	1303	Y01	3	0
3	B	1302	Y01	4	0
3	B	1301	Y01	2	0
3	C	1301	Y01	2	0
3	C	1303	Y01	4	0
3	D	1302	Y01	4	0

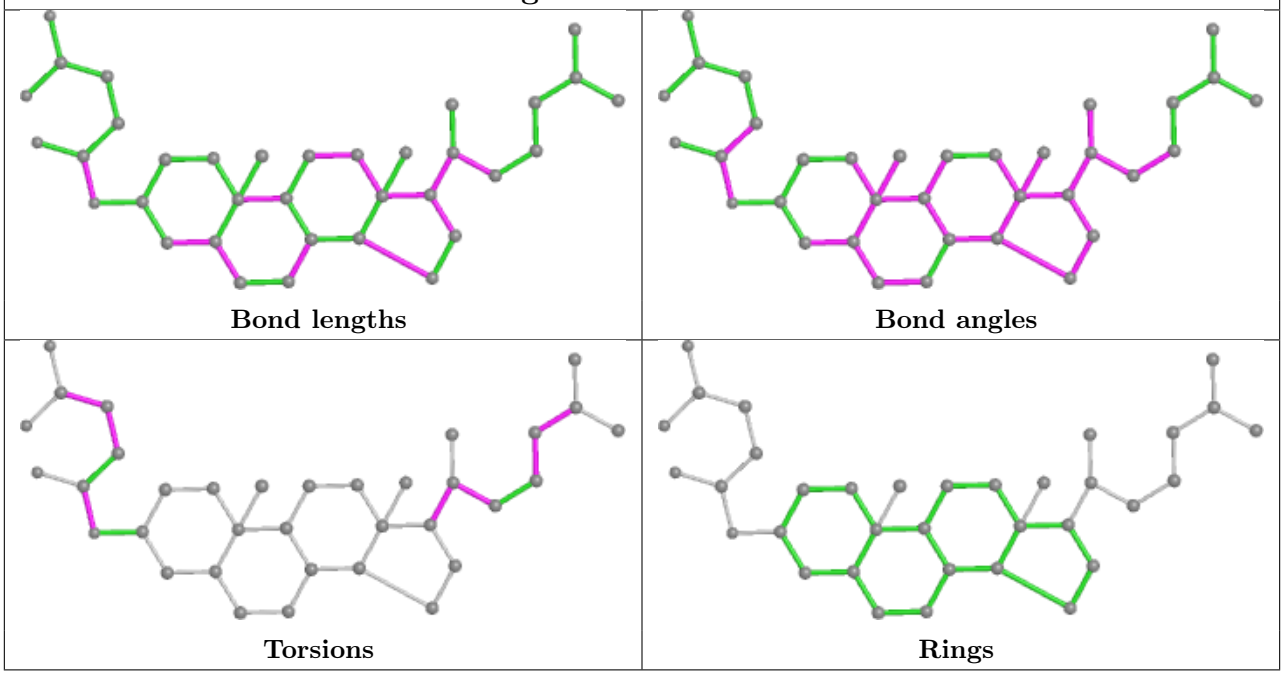
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

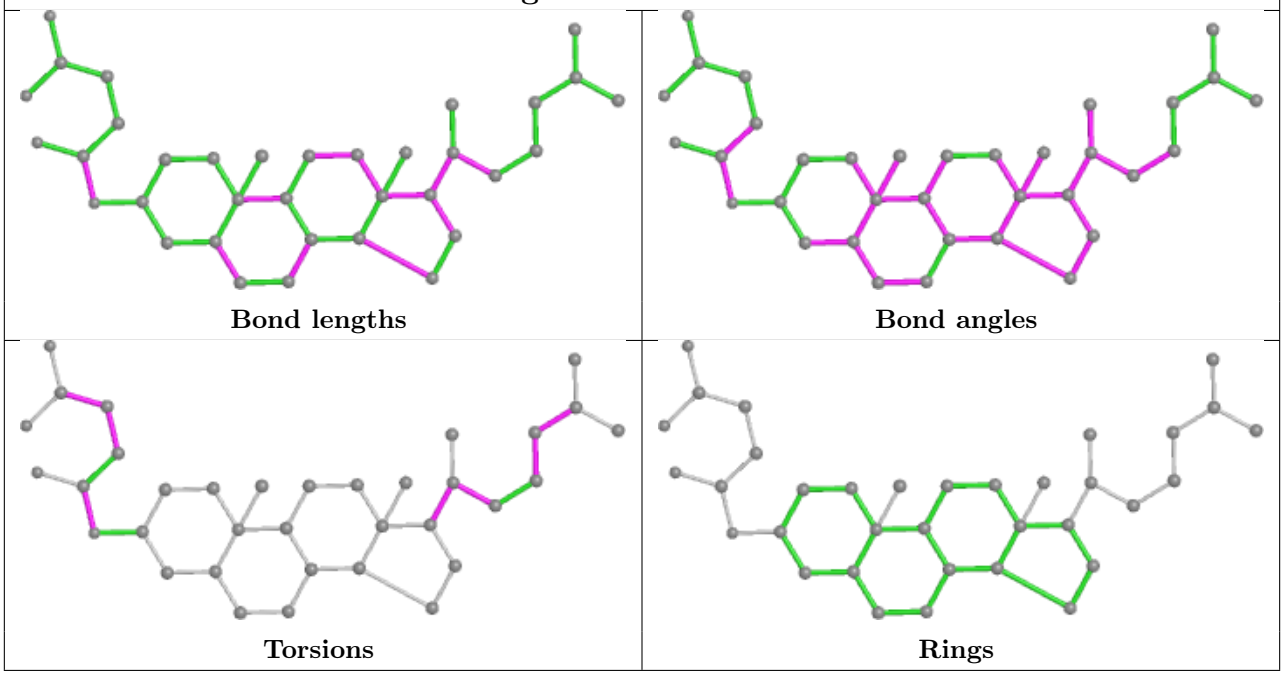
Ligand Y01 B 1303



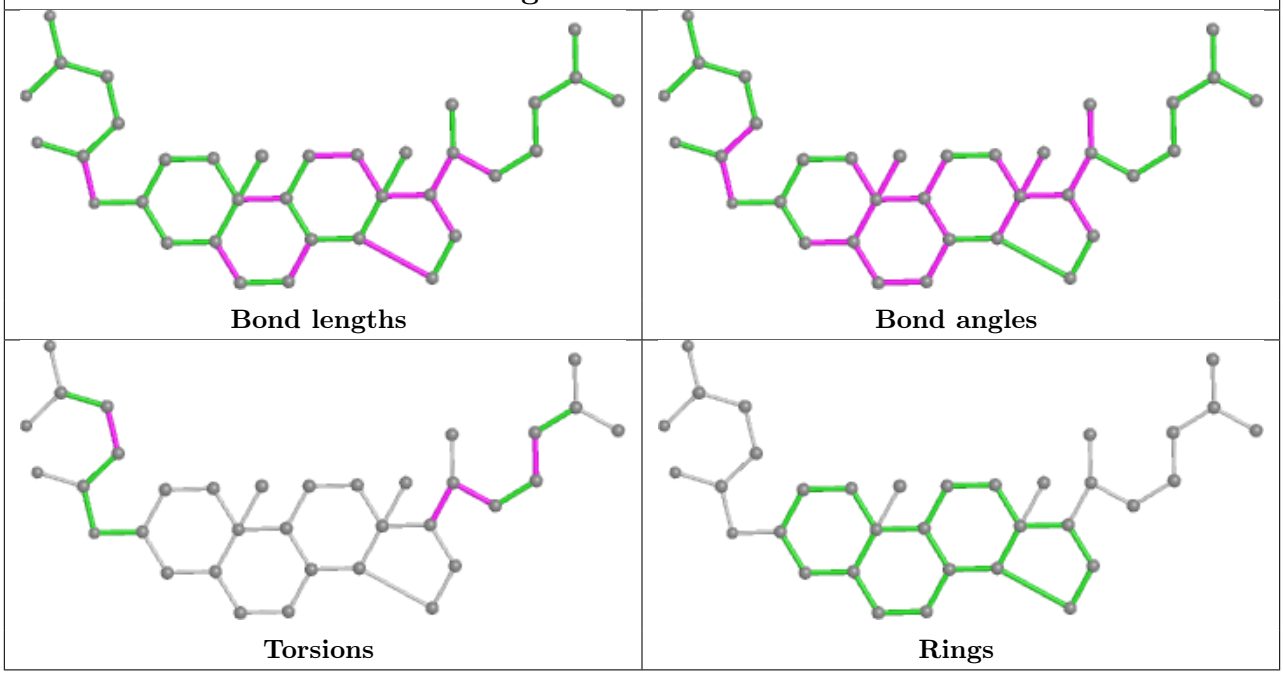
Ligand Y01 A 1301



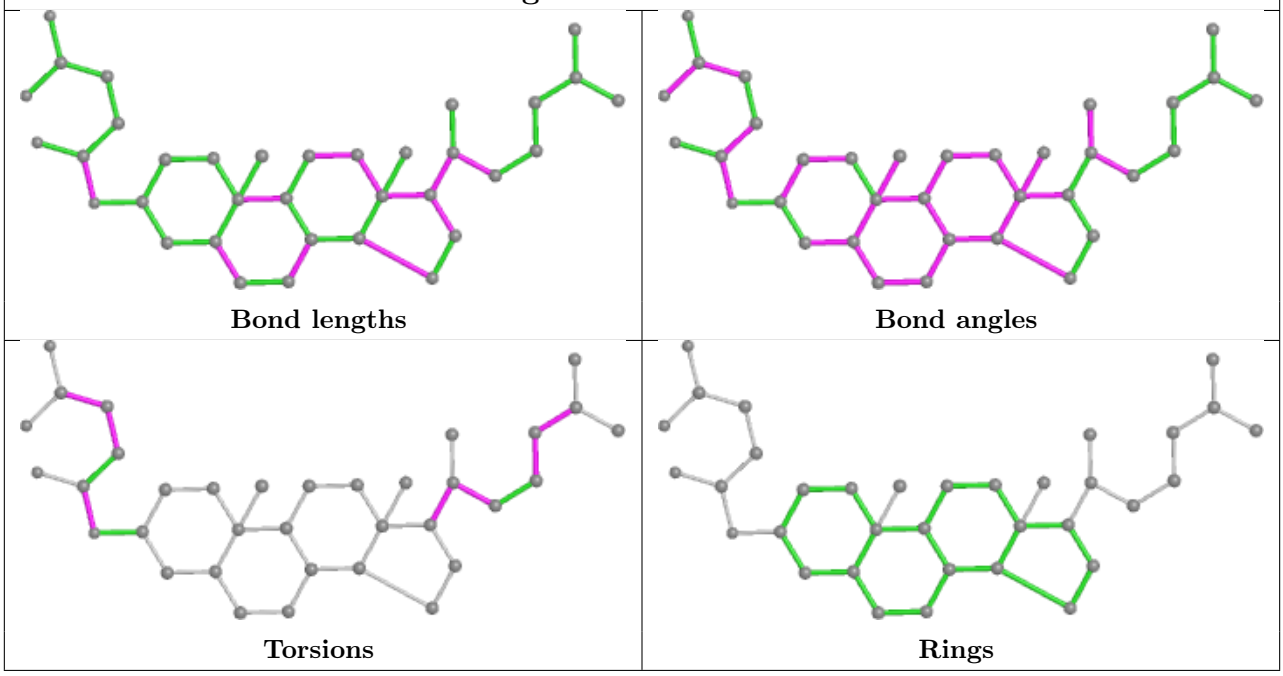
Ligand Y01 D 1301



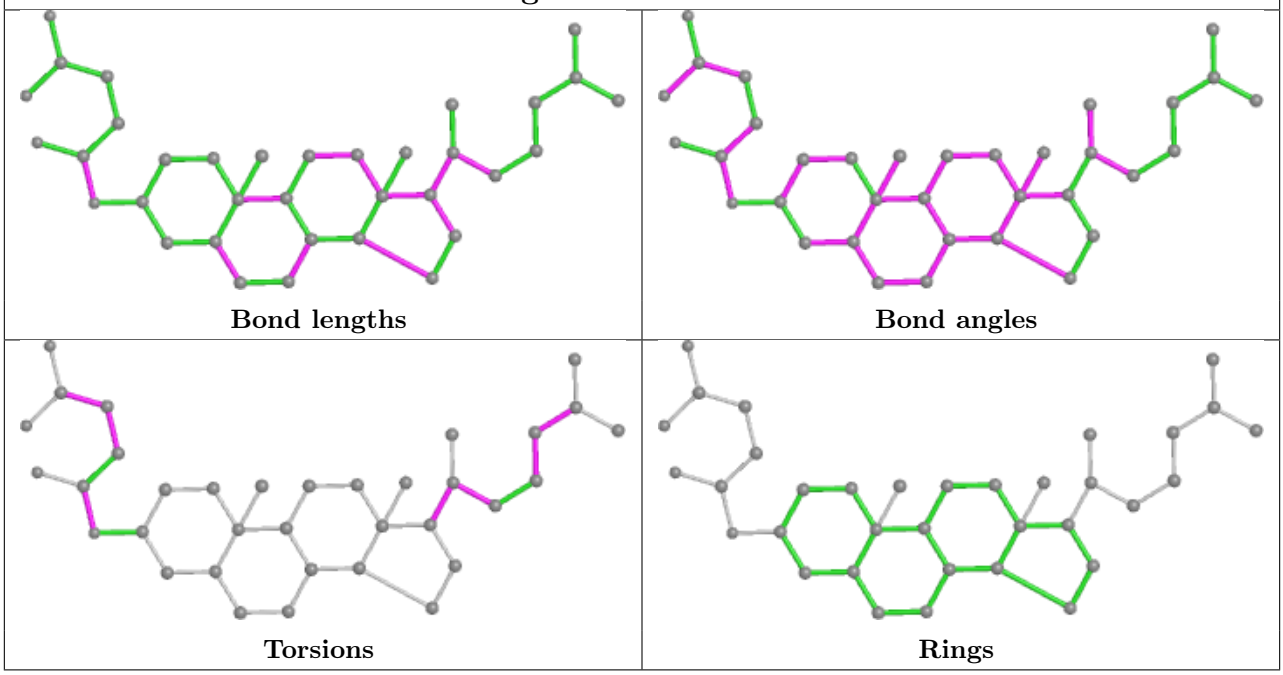
Ligand Y01 A 1303



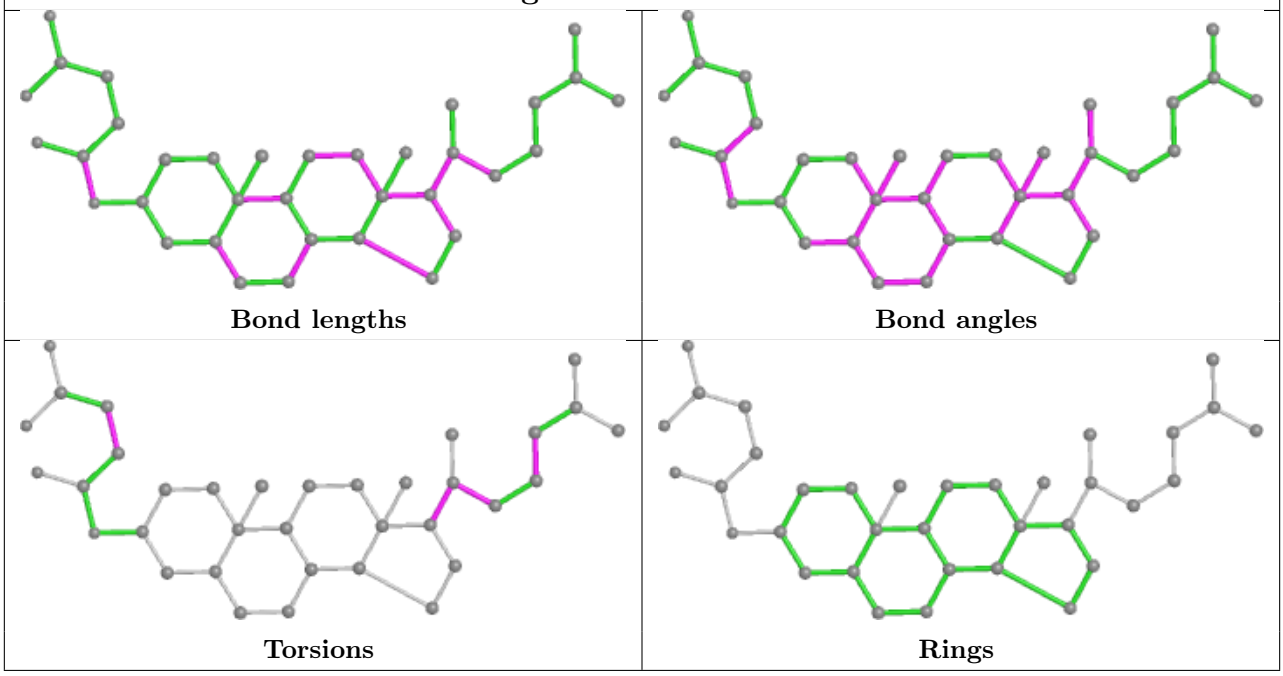
Ligand Y01 C 1302



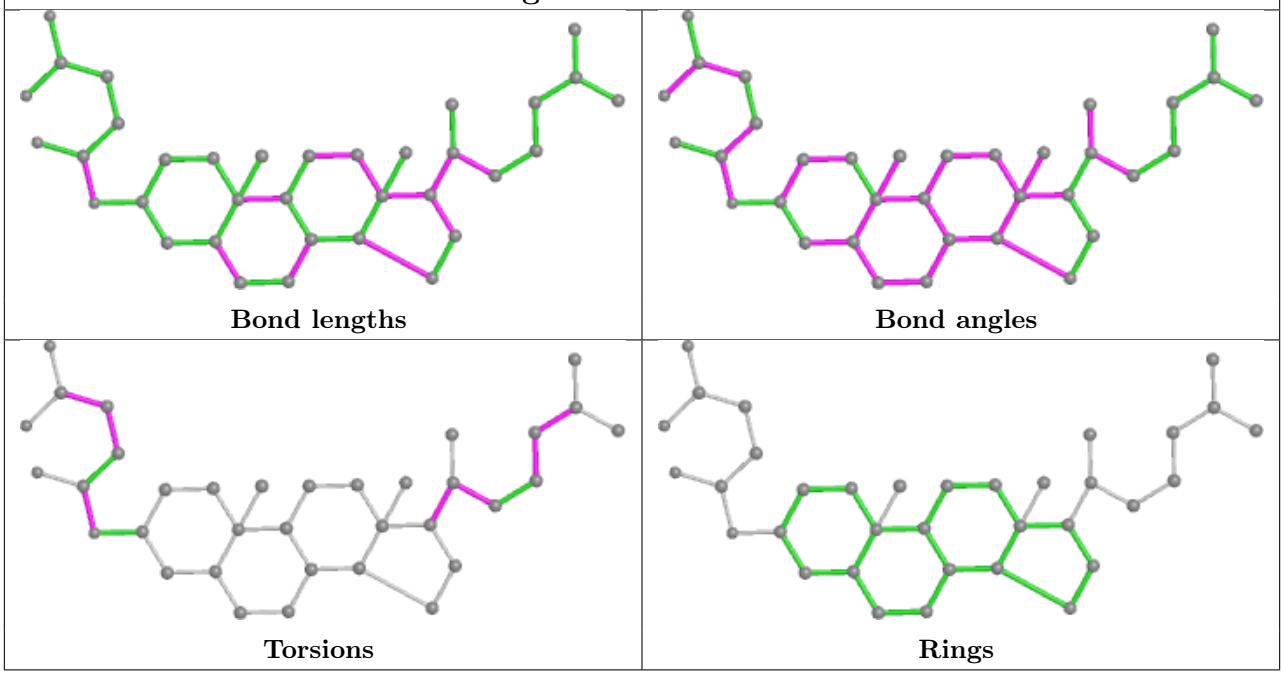
Ligand Y01 A 1302



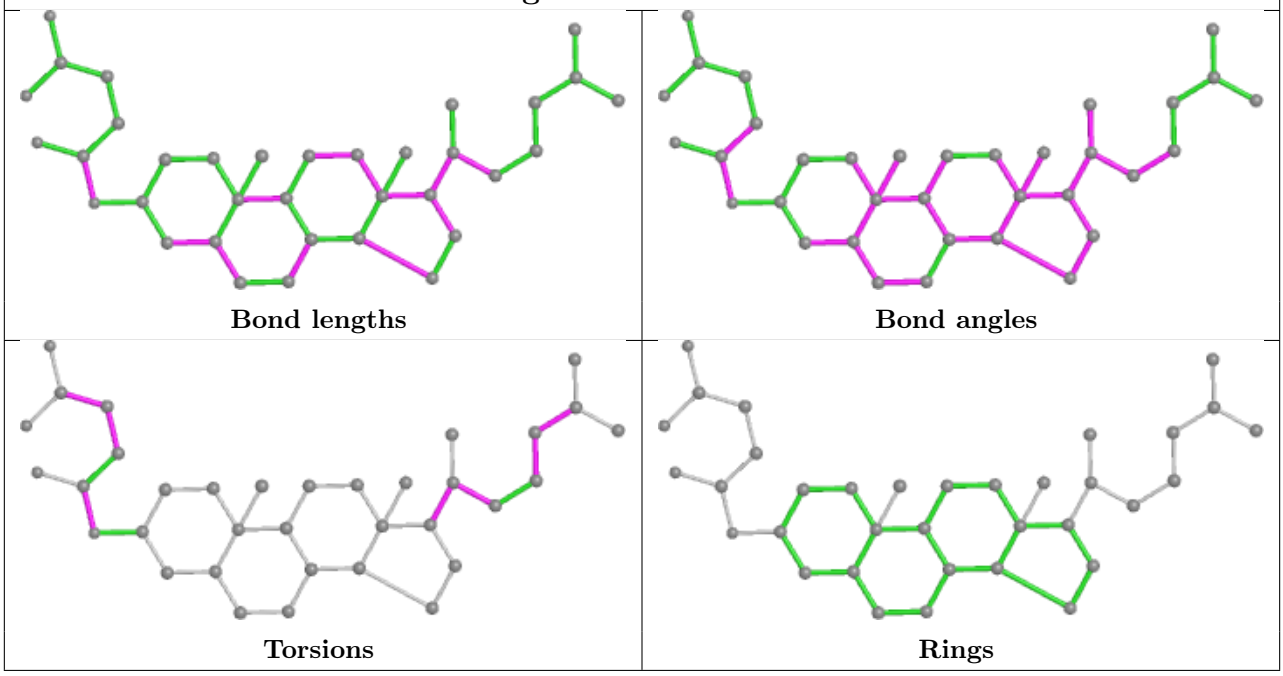
Ligand Y01 D 1303



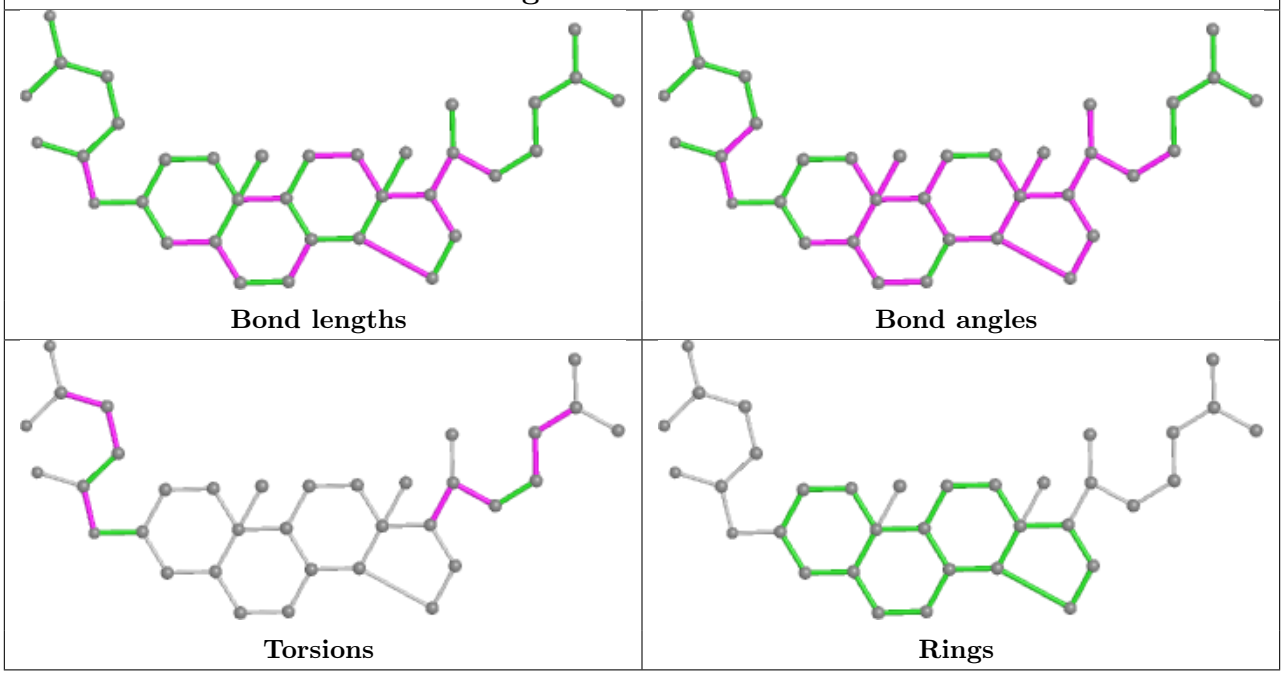
Ligand Y01 B 1302



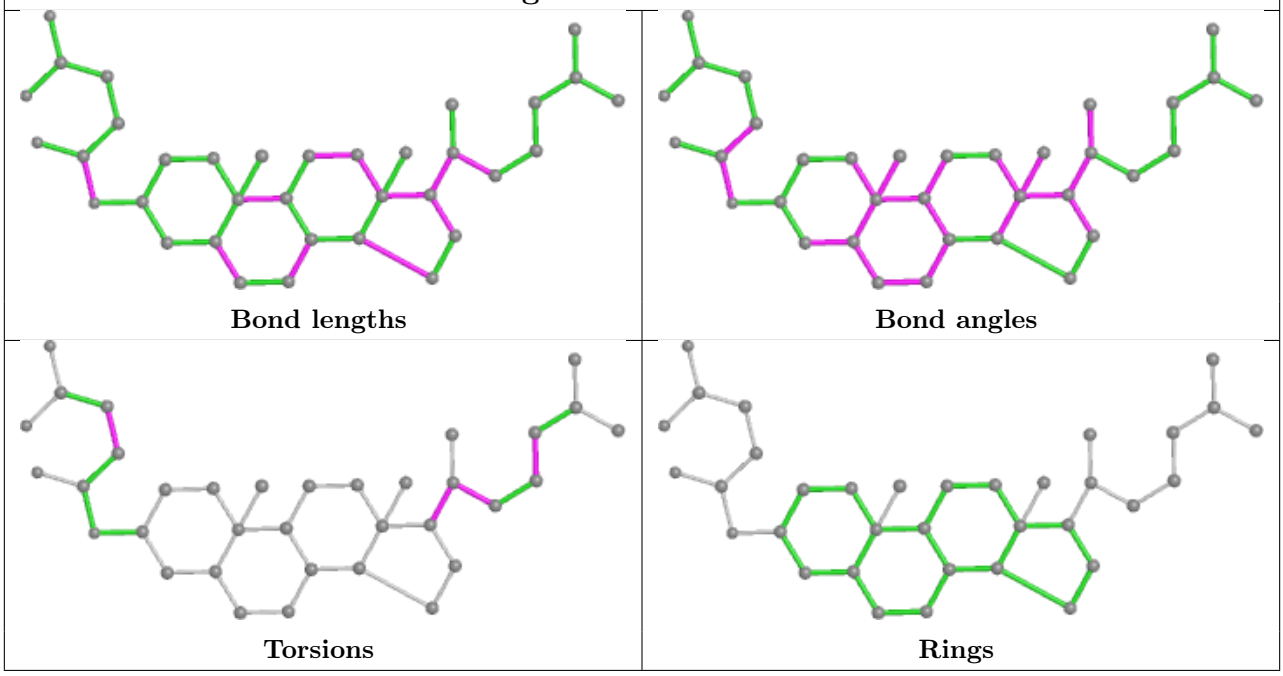
Ligand Y01 B 1301

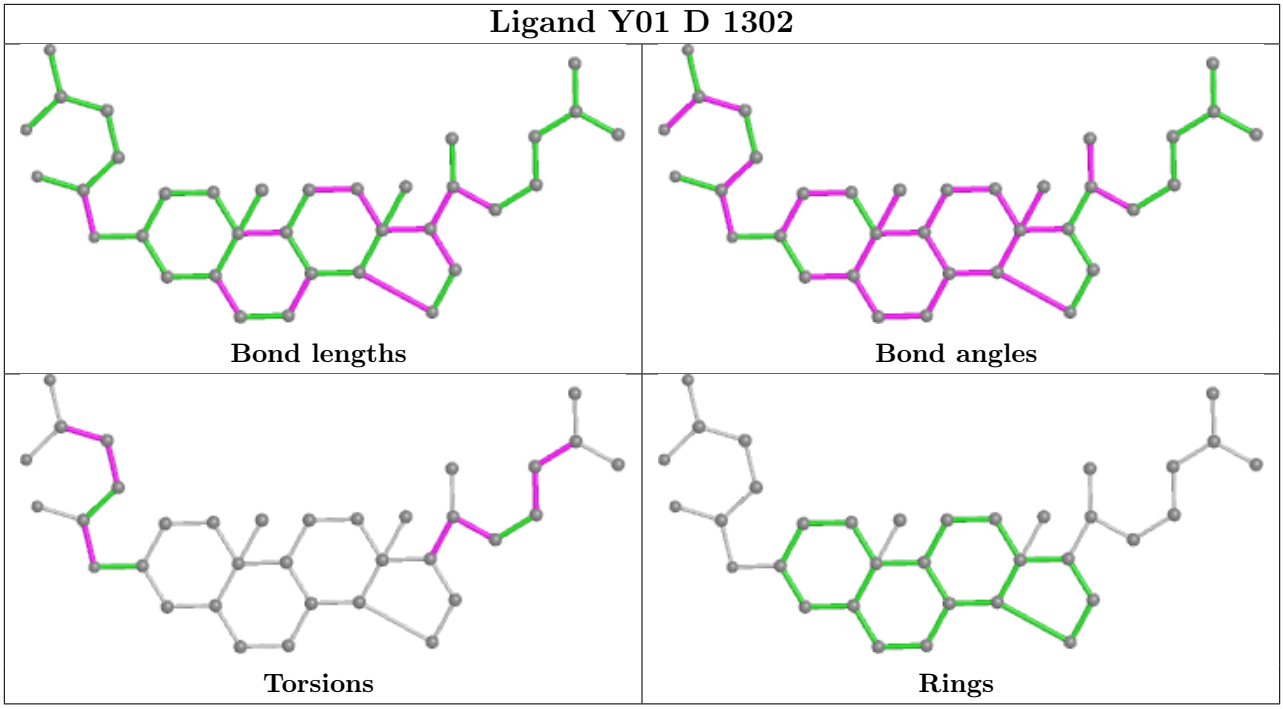


Ligand Y01 C 1301



Ligand Y01 C 1303





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.

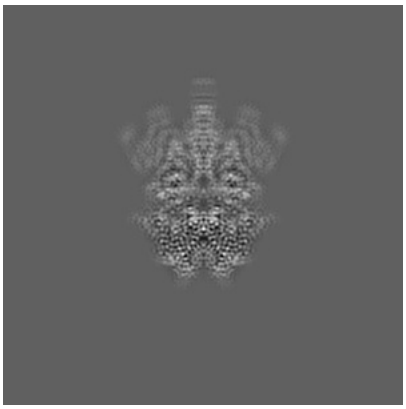
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7133. These allow visual inspection of the internal detail of the map and identification of artifacts.

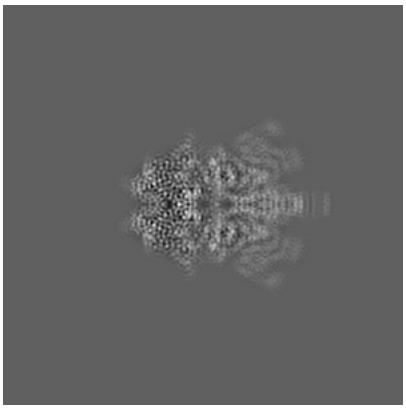
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

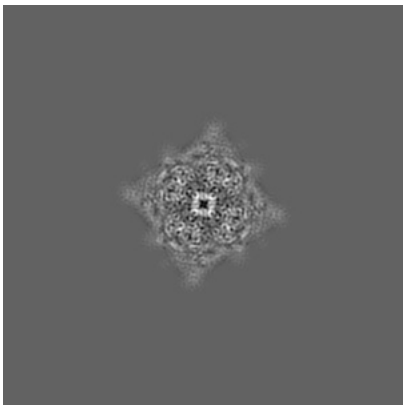
6.1.1 Primary map



X

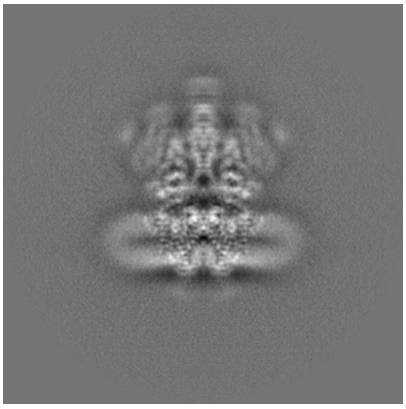


Y

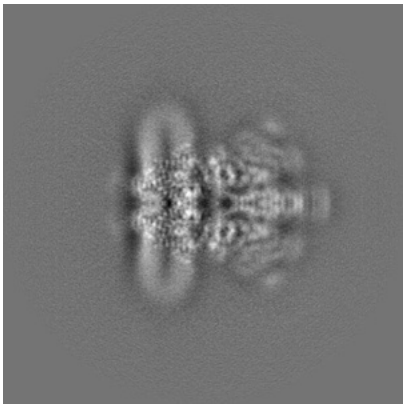


Z

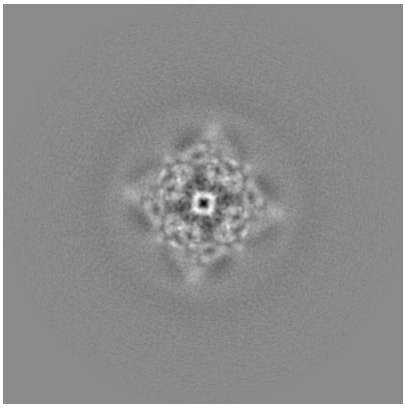
6.1.2 Raw map



X



Y

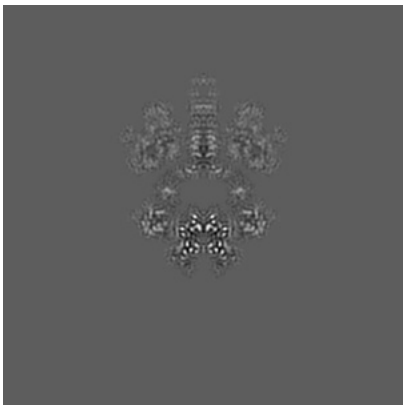


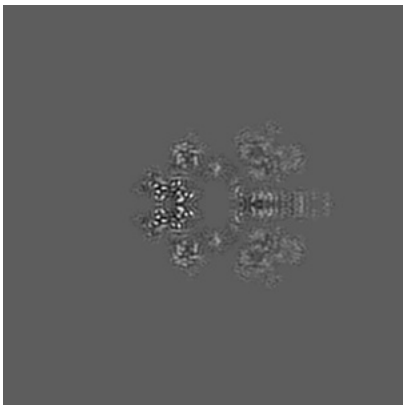
Z

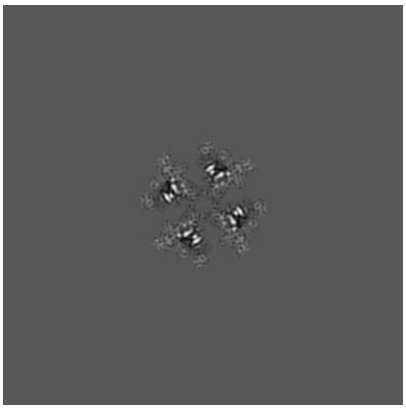
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

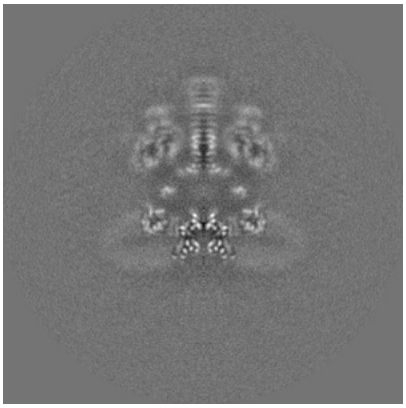
6.2.1 Primary map

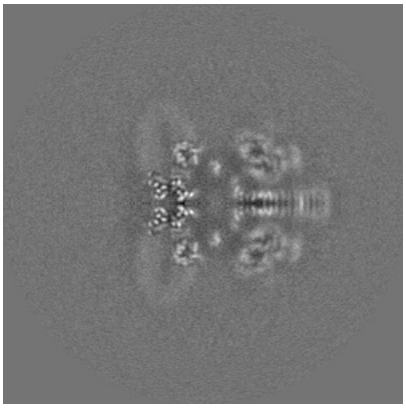

X Index: 160

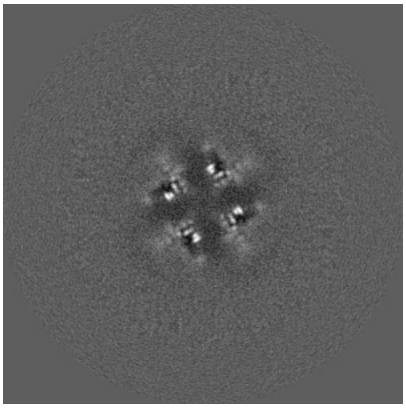

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160


Y Index: 160

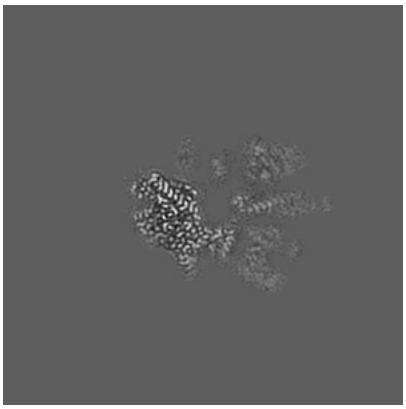

Z Index: 160

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

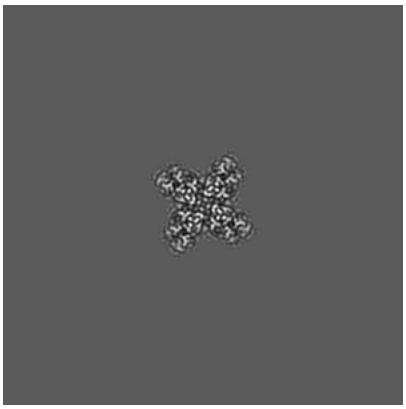
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 168

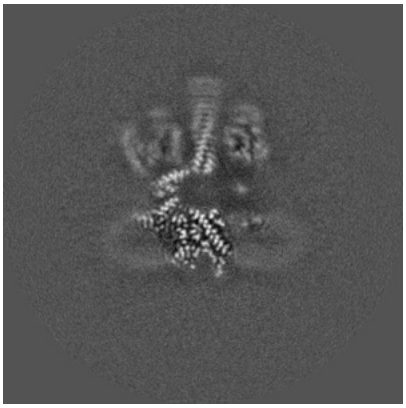


Y Index: 168

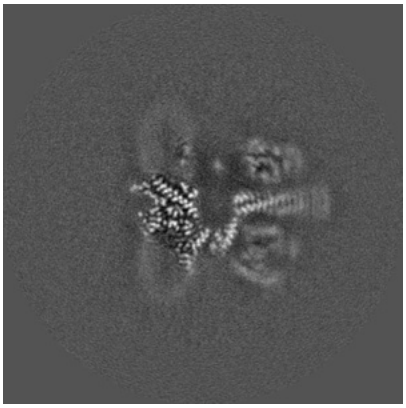


Z Index: 125

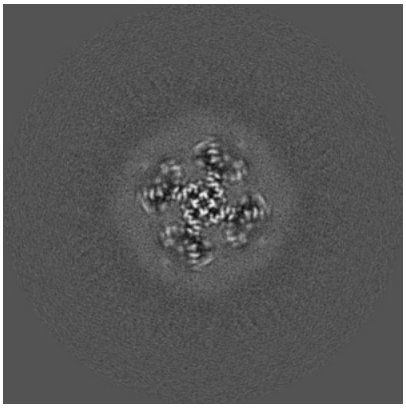
6.3.2 Raw map



X Index: 154



Y Index: 166

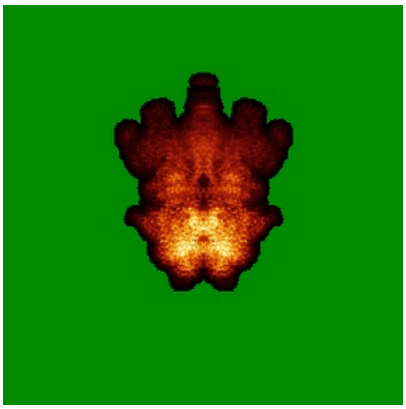


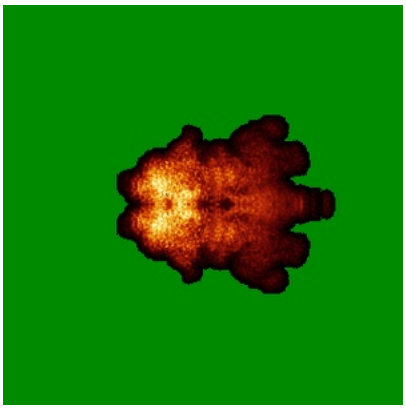
Z Index: 146

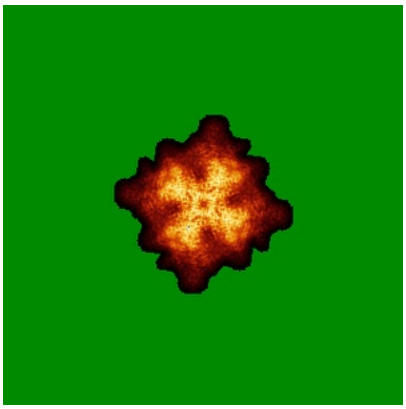
The images above show the largest variance slices of the map in three orthogonal directions.

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

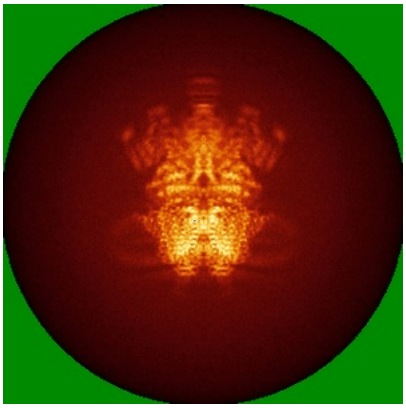
6.4.1 Primary map

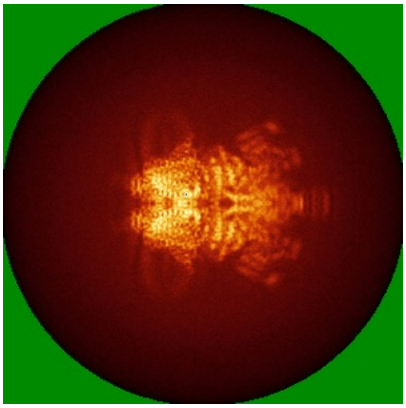

X

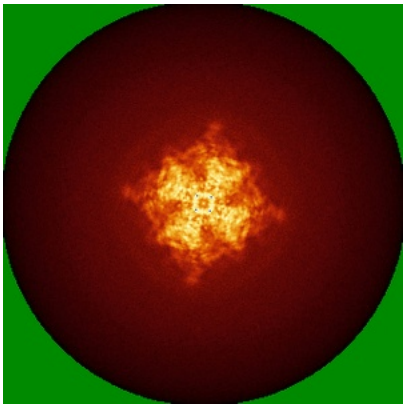

Y


Z

6.4.2 Raw map


X

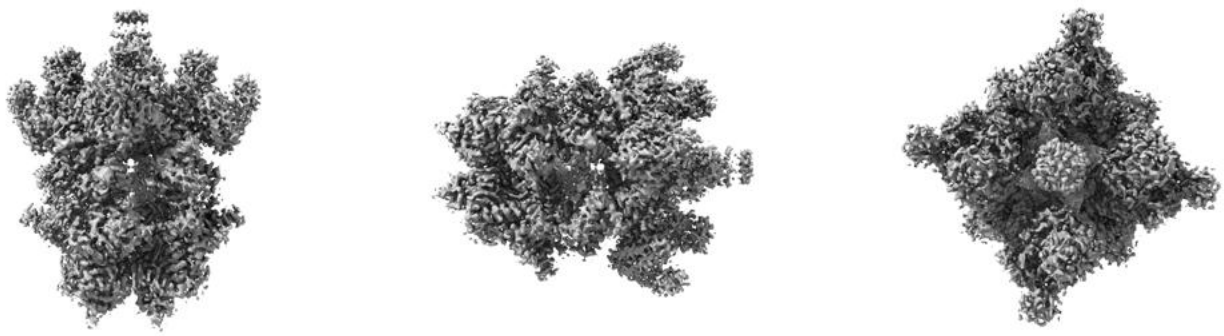

Y


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 4.0. 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.

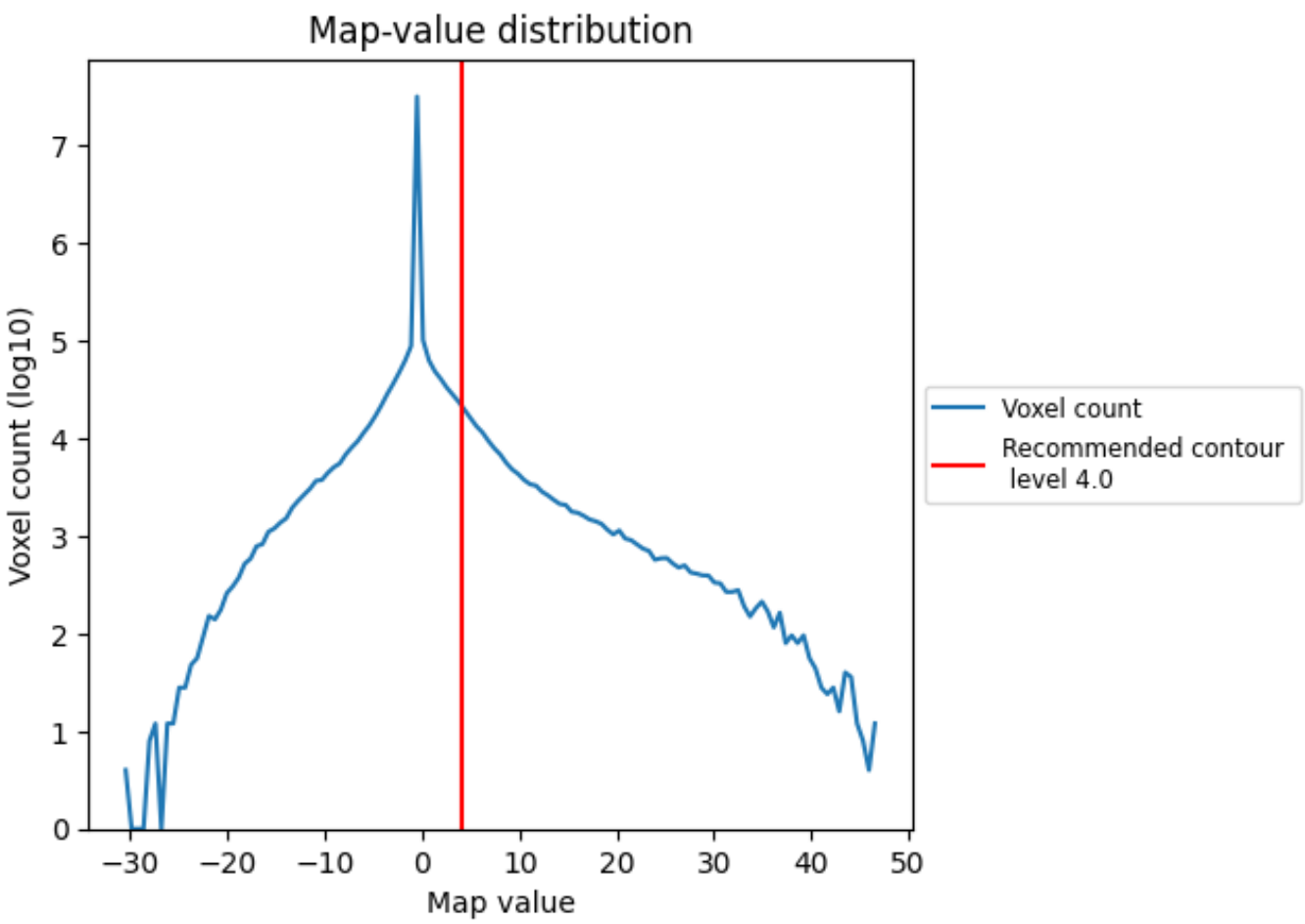
6.6 Mask visualisation (i)

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

7 Map analysis (i)

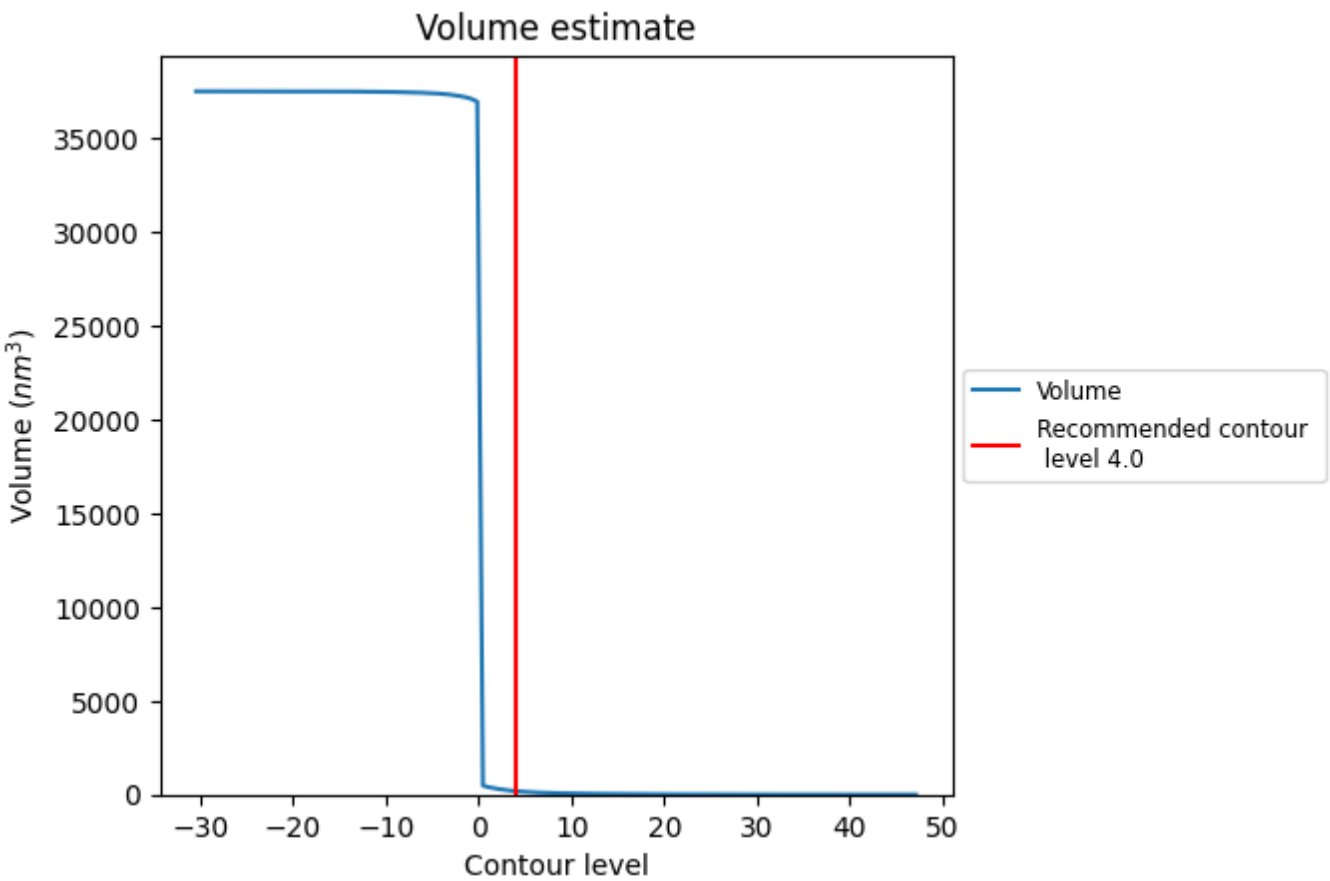
This section contains the results of statistical analysis of the map.

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.

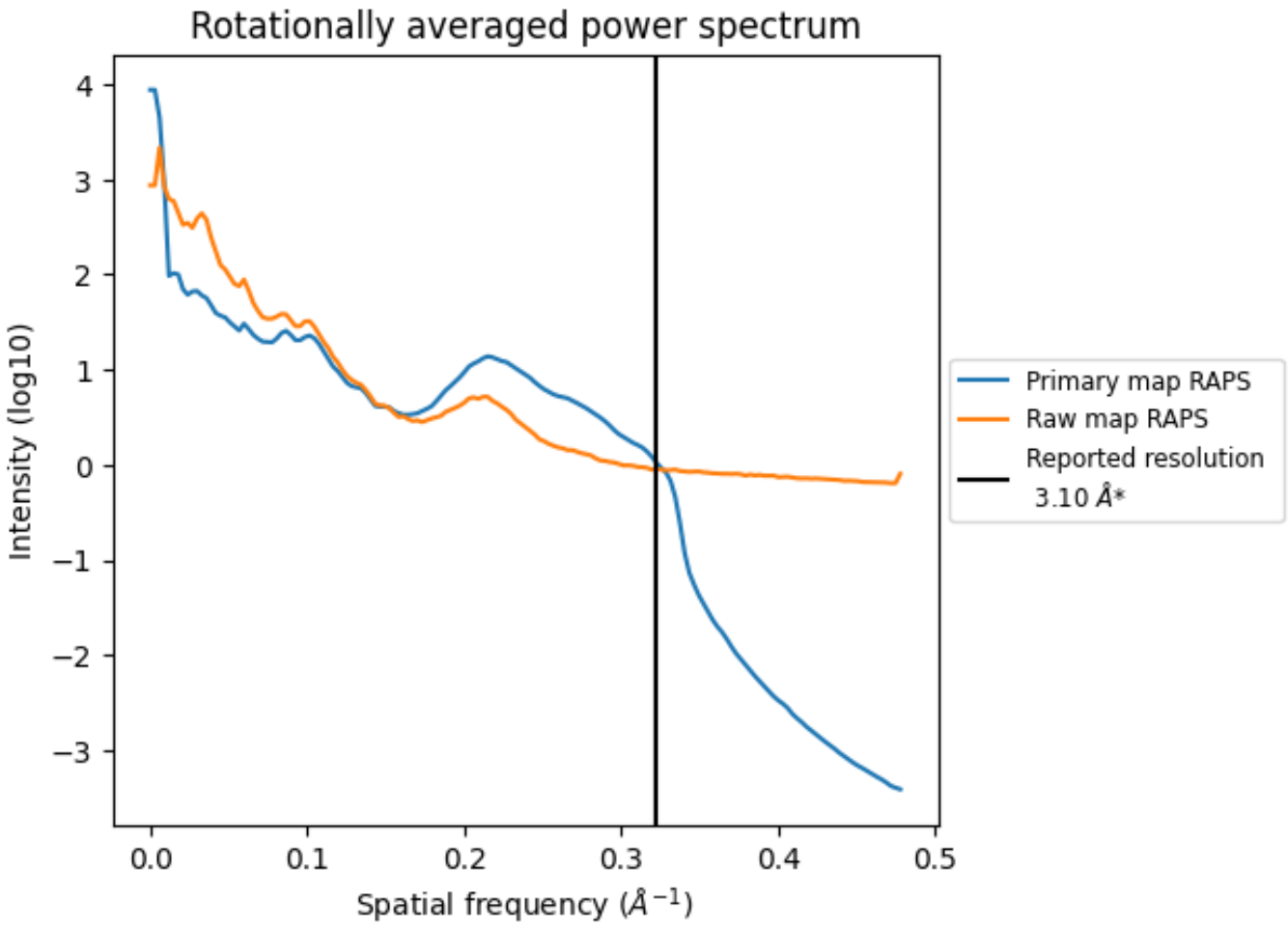
7.2 Volume estimate (i)



The volume at the recommended contour level is 184 nm^3; this corresponds to an approximate mass of 166 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)

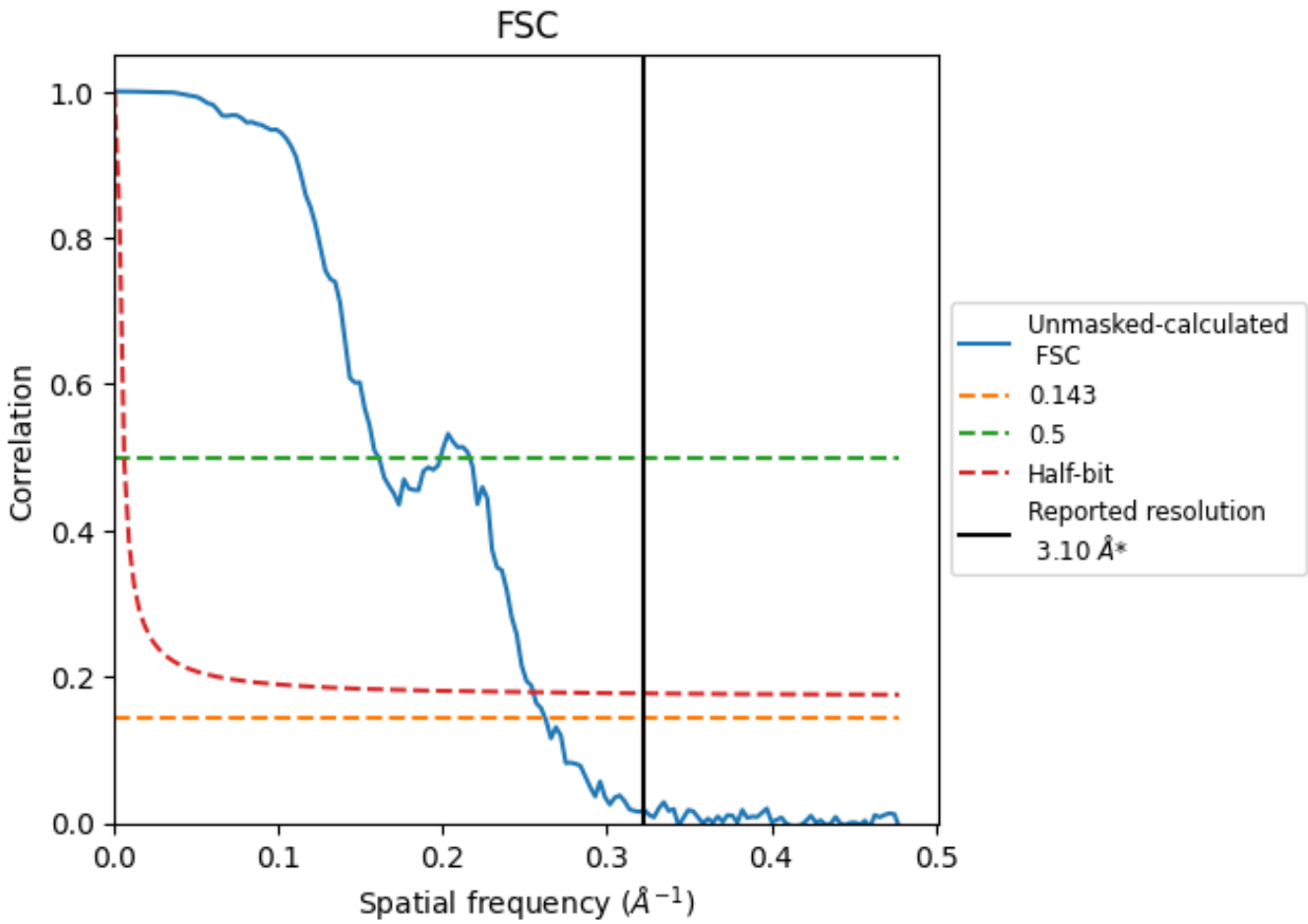


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

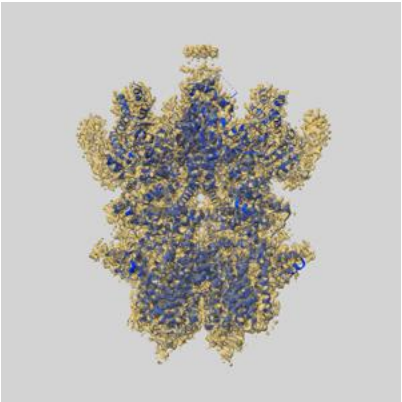
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	6.22	3.92

*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 3.81 differs from the reported value 3.1 by more than 10 %

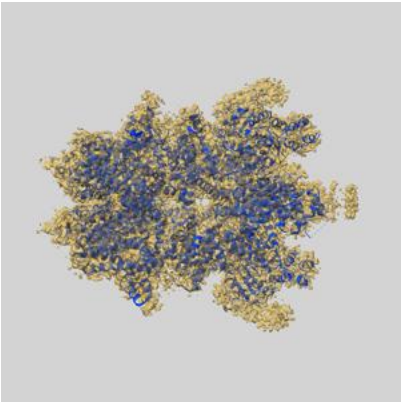
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7133 and PDB model 6BQV. Per-residue inclusion information can be found in section 3 on page 6.

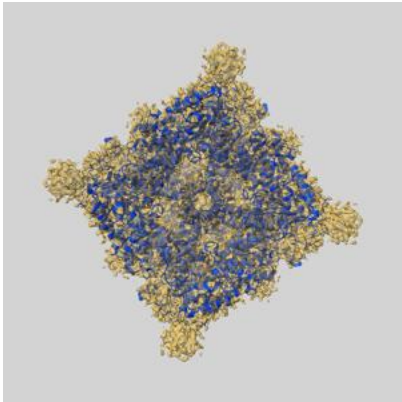
9.1 Map-model overlay (i)



X



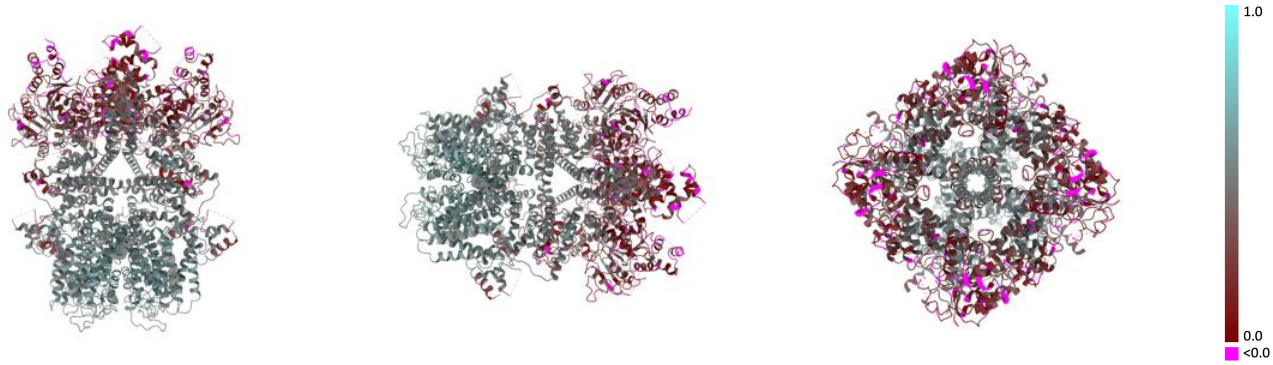
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

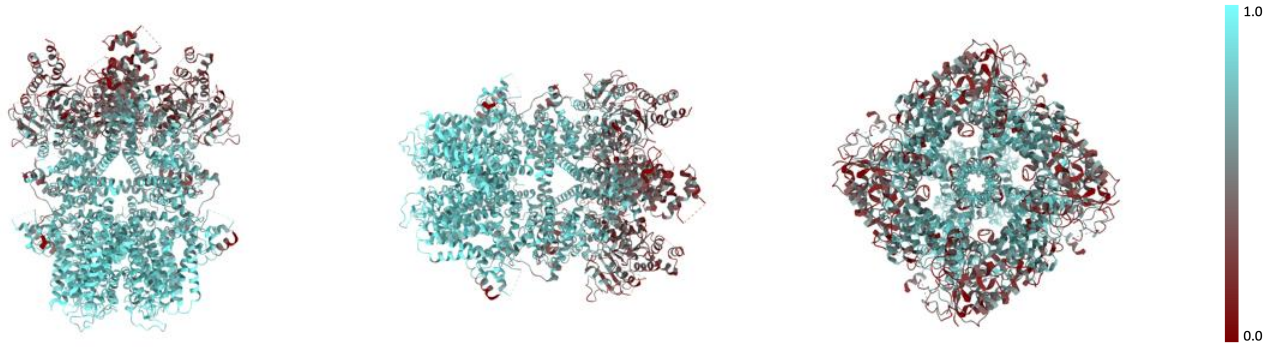
9.2 Q-score mapped to coordinate model (i)



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.

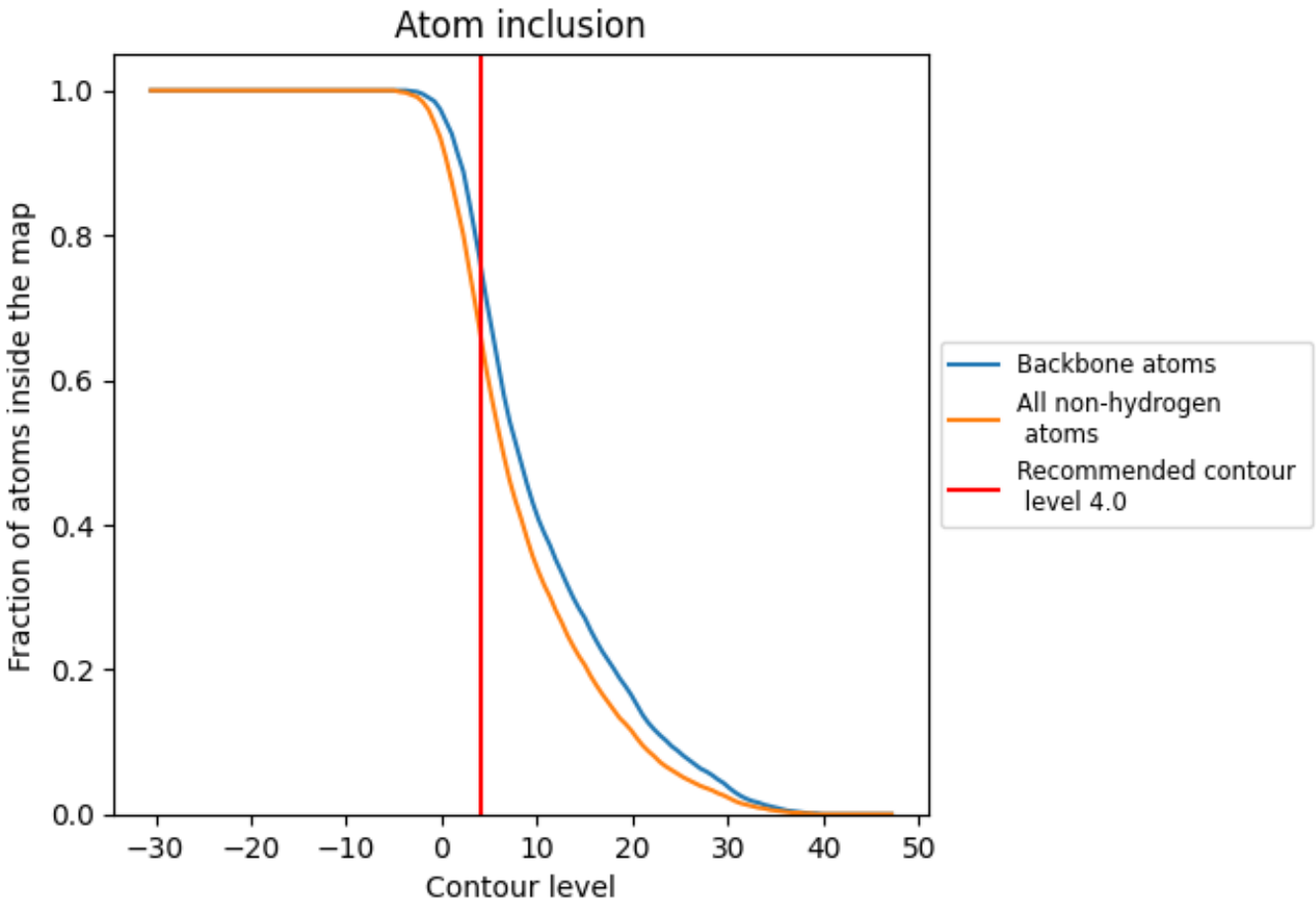
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6680	0.3990
A	0.6680	0.3980
B	0.6690	0.3990
C	0.6690	0.3990
D	0.6670	0.3980