



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 03:26 PM UTC

PDB ID : 8QSL / pdb_00008qsl
EMDB ID : EMD-18635
Title : Cryo-EM structure of human SLC15A4 dimer in outward open state in LMNG
Authors : Rehan, S.; Matsuoka, R.; Jazayeri, A.; Duerr, K.L.
Deposited on : 2023-10-10
Resolution : 2.81 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

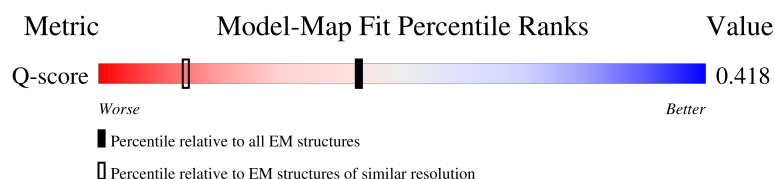
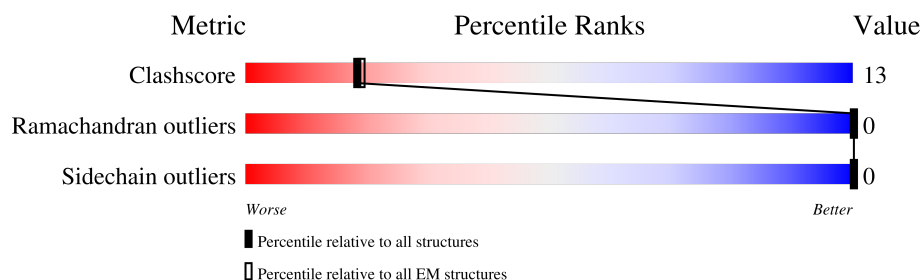
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 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	11740 (2.31 - 3.31)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	577	44% 65% 25% 9%
1	C	577	45% 65% 25% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8506 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.

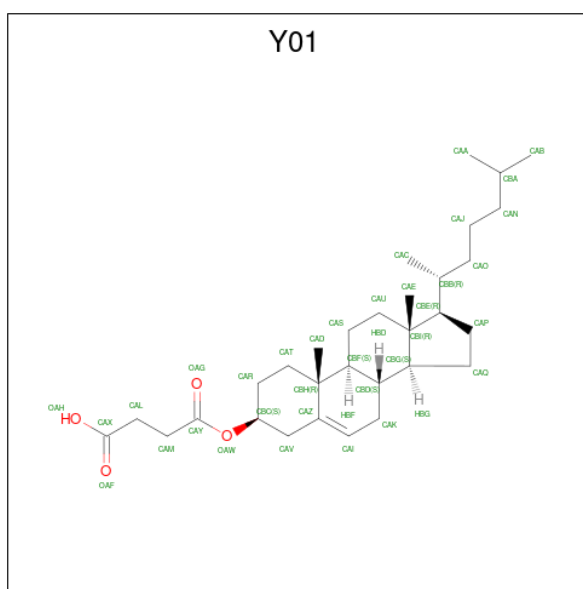
- Molecule 1 is a protein called Solute carrier family 15 member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	523	Total	C	N	O	S	0	0
			3978	2617	654	683	24		
1	C	523	Total	C	N	O	S	0	0
			3978	2617	654	683	24		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ALA	LEU	engineered mutation	UNP Q8N697
A	15	ALA	LEU	engineered mutation	UNP Q8N697
C	14	ALA	LEU	engineered mutation	UNP Q8N697
C	15	ALA	LEU	engineered mutation	UNP Q8N697

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



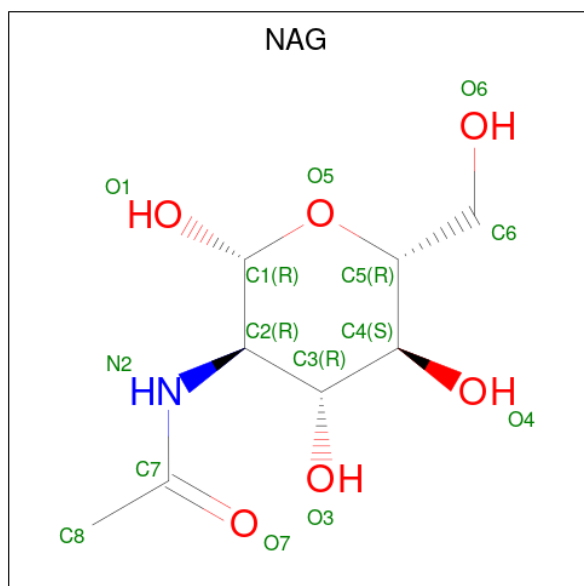
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	

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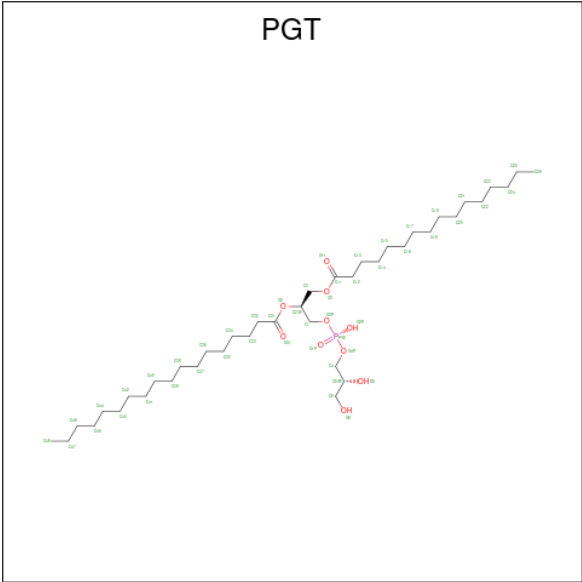
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).

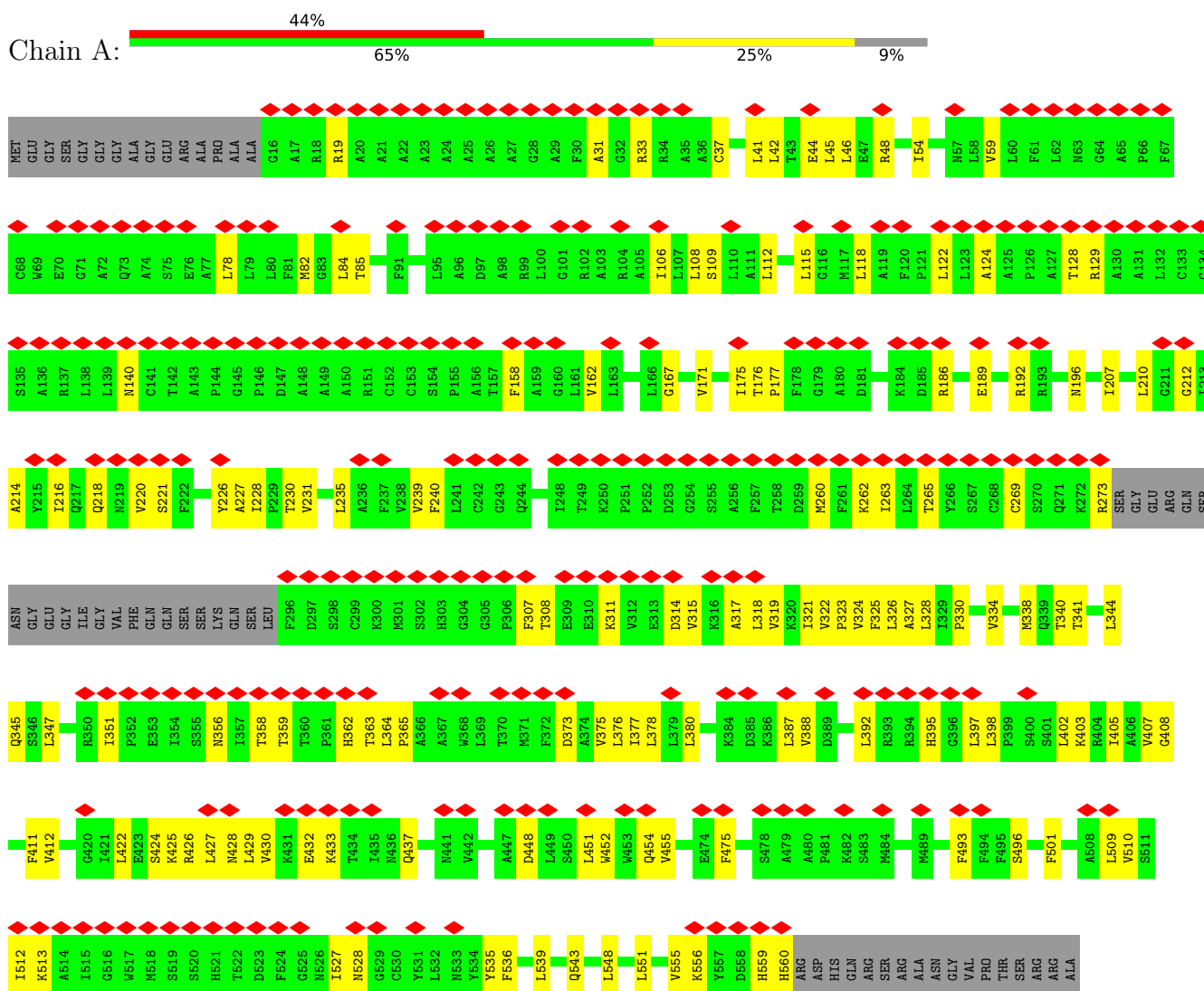


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			51	40	10	1	
4	C	1	Total	C	O	P	0
			51	40	10	1	

3 Residue-property plots

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: Solute carrier family 15 member 4



• Molecule 1: Solute carrier family 15 member 4



ILE										MET									
GLY										GLU									
VAL										GLY									
PHE										SER									
GLN										GLY									
GLN										GLY									
SER										ALA									
SER										GLY									
LYS										GLU									
GLN										ARG									
SER										ALA									
LEU										ALA									
F296										G16									
D297										A17									
S298										R18									
C299										R19									
K300										A20									
M301										A21									
S302										A22									
H303										A23									
G304										A24									
G305										A25									
P306										A26									
F307										A27									
T308										G28									
E309										A29									
E310										F30									
K311										A31									
V312										G32									
E313										R33									
D314										R34									
V315										A35									
K316										A36									
A317										C37									
L318										L41									
I321										L42									
V322										T43									
P323										E44									
V324										E45									
F325										L46									
L326										E47									
A327										R48									
L328										N57									
I329										L58									
P330										V59									
V334										L60									
H338										F61									
Q339										L62									
S400										N63									
S401										G64									
L402										A65									
K403										P66									
R404										F67									
I405										C68									
A406										W69									
V407																			
L347																			
H348																			
L349																			
R350										Q217									
I351										Q218									
P352										N219									
E353										V220									
I354										S221									
S355										F222									
N356																			
I357										Y226									
T358										A227									
T359										T230									
T360										V231									
P361										L235									
H362										A236									
T363										F237									
L364										V238									
P365										V239									
A366										F240									
A367										C153									
W368										L241									
L369										C242									
T370										G243									
M371										A156									
F372										T157									
D373										F158									
A374										A159									
V375										G160									
L376										L161									
I377										V162									
W453										L163									
Q454										A103									
V455										R104									
P456										A105									
Q457										I106									
I461										L107									
E474										L108									
F475										S109									
S478										L110									
A479										A111									
A480										L112									
P481																			
K482										L115									
S483										G116									
W484										M117									
I488										L118									
W489										A119									
F493										F120									
F494										P121									
F495										L122									
S496										L123									
F501										A124									
A508										A125									
L509										P126									
										A127									
										T128									
										R129									
										A130									
										A131									
										L132									
										C133									
										G134									
										Y215									
										I216									
										A136									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	438976	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.593	Depositor
Minimum map value	-0.332	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.207	Depositor
Map size ($\text{\AA}$)	250.79999, 250.79999, 250.79999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, NAG, PGT

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	0/4079	0.36	0/5549
1	C	0.17	0/4079	0.37	0/5549
All	All	0.17	0/8158	0.37	0/11098

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	3978	0	4062	105	0
1	C	3978	0	4062	107	0
2	A	210	0	294	11	0
2	C	210	0	294	10	0
3	A	14	0	13	1	0
3	C	14	0	13	1	0
4	A	51	0	78	1	0
4	C	51	0	78	1	0
All	All	8506	0	8894	227	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 13.

The worst 5 of 227 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:218:GLN:O	1:C:218:GLN:NE2	2.04	0.90
1:A:227:ALA:O	1:A:230:THR:OG1	1.97	0.83
1:C:227:ALA:O	1:C:230:THR:OG1	1.97	0.81
1:C:425:LYS:NZ	2:C:602:Y01:OAG	2.13	0.81
1:C:433:LYS:NZ	1:C:448:ASP:OD2	2.17	0.78

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	519/577 (90%)	476 (92%)	43 (8%)	0	100	100
1	C	519/577 (90%)	472 (91%)	47 (9%)	0	100	100
All	All	1038/1154 (90%)	948 (91%)	90 (9%)	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	410/448 (92%)	410 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	410/448 (92%)	410 (100%)	0	100	100
All	All	820/896 (92%)	820 (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	A	174	ASN
1	A	437	GLN
1	C	174	ASN
1	C	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	Y01	C	601	-	38,38,38	0.57	0	57,57,57	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y01	C	605	-	38,38,38	0.55	0	57,57,57	0.87	1 (1%)
4	PGT	A	608	-	50,50,50	0.50	0	53,56,56	0.45	0
2	Y01	A	607	-	38,38,38	0.56	0	57,57,57	0.67	0
2	Y01	A	605	-	38,38,38	0.55	0	57,57,57	0.90	1 (1%)
2	Y01	A	603	-	38,38,38	0.60	0	57,57,57	1.16	4 (7%)
2	Y01	A	606	-	38,38,38	0.55	0	57,57,57	0.59	0
2	Y01	A	601	-	38,38,38	0.57	0	57,57,57	0.55	0
2	Y01	C	602	-	38,38,38	0.56	0	57,57,57	0.83	2 (3%)
2	Y01	C	607	-	38,38,38	0.56	0	57,57,57	0.67	0
3	NAG	C	604	1	14,14,15	0.77	0	17,19,21	0.86	0
2	Y01	C	603	-	38,38,38	0.61	0	57,57,57	1.16	4 (7%)
4	PGT	C	608	-	50,50,50	0.50	0	53,56,56	0.45	0
2	Y01	C	606	-	38,38,38	0.55	0	57,57,57	0.59	0
3	NAG	A	604	1	14,14,15	0.77	0	17,19,21	0.86	0
2	Y01	A	602	-	38,38,38	0.57	0	57,57,57	0.79	1 (1%)

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	Y01	C	601	-	-	4/19/77/77	0/4/4/4
2	Y01	C	605	-	-	7/19/77/77	0/4/4/4
4	PGT	A	608	-	-	25/55/55/55	-
2	Y01	A	607	-	-	8/19/77/77	0/4/4/4
2	Y01	A	605	-	-	7/19/77/77	0/4/4/4
2	Y01	A	603	-	-	4/19/77/77	0/4/4/4
2	Y01	A	606	-	-	8/19/77/77	0/4/4/4
2	Y01	A	601	-	-	4/19/77/77	0/4/4/4
2	Y01	C	602	-	-	8/19/77/77	0/4/4/4
2	Y01	C	607	-	-	8/19/77/77	0/4/4/4
3	NAG	C	604	1	-	0/6/23/26	0/1/1/1
2	Y01	C	603	-	-	4/19/77/77	0/4/4/4
4	PGT	C	608	-	-	25/55/55/55	-
2	Y01	C	606	-	-	8/19/77/77	0/4/4/4
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	Y01	A	602	-	-	7/19/77/77	0/4/4/4

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	Y01	CAR-CBC-CAV	4.27	116.90	110.97
2	C	603	Y01	CAR-CBC-CAV	4.25	116.88	110.97
2	C	603	Y01	CBC-CAV-CAZ	4.04	117.42	111.45
2	A	603	Y01	CBC-CAV-CAZ	4.03	117.40	111.45
2	C	603	Y01	CAT-CBH-CAZ	-2.98	103.61	108.74

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	Y01	CAM-CAY-OAW-CBC
2	A	607	Y01	OAG-CAY-OAW-CBC
2	C	603	Y01	CAM-CAY-OAW-CBC
2	C	607	Y01	OAG-CAY-OAW-CBC
4	A	608	PGT	C1-O3P-P-O4P

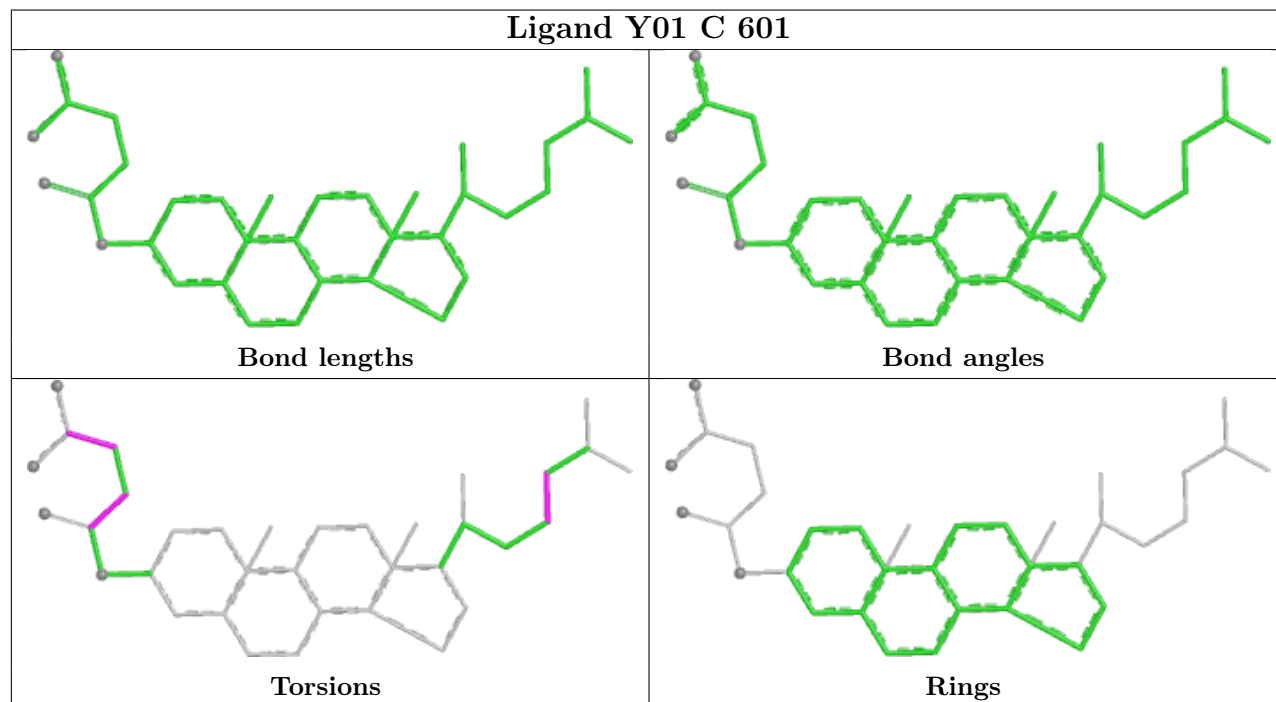
There are no ring outliers.

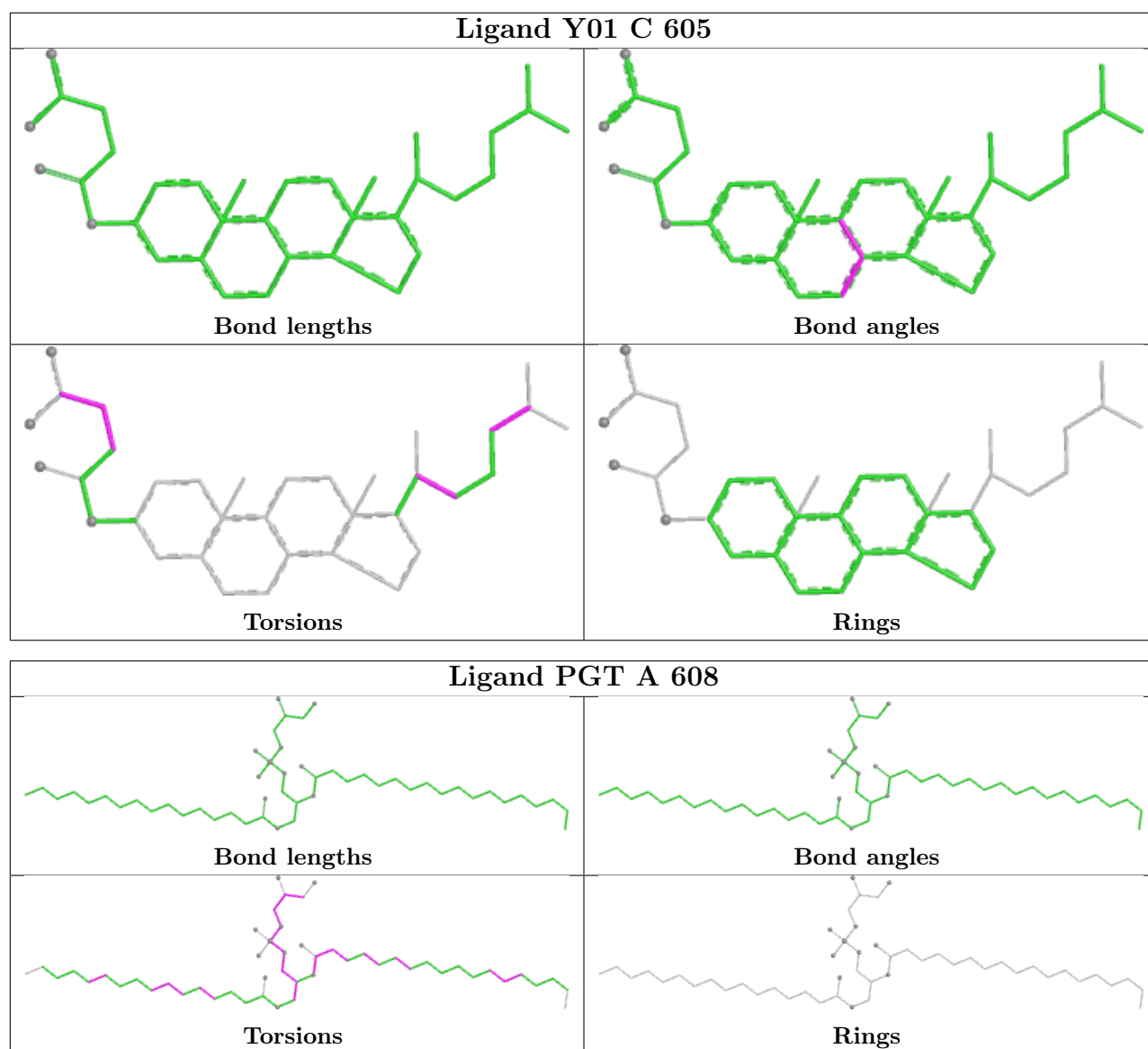
16 monomers are involved in 25 short contacts:

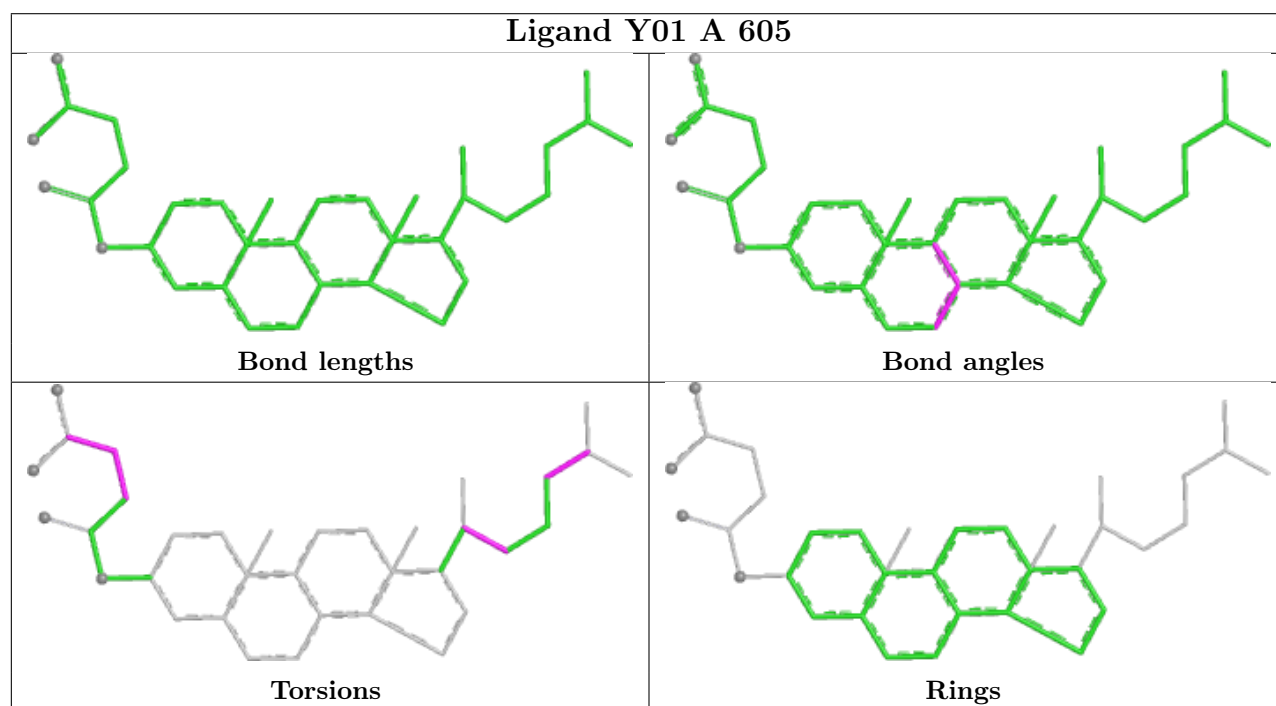
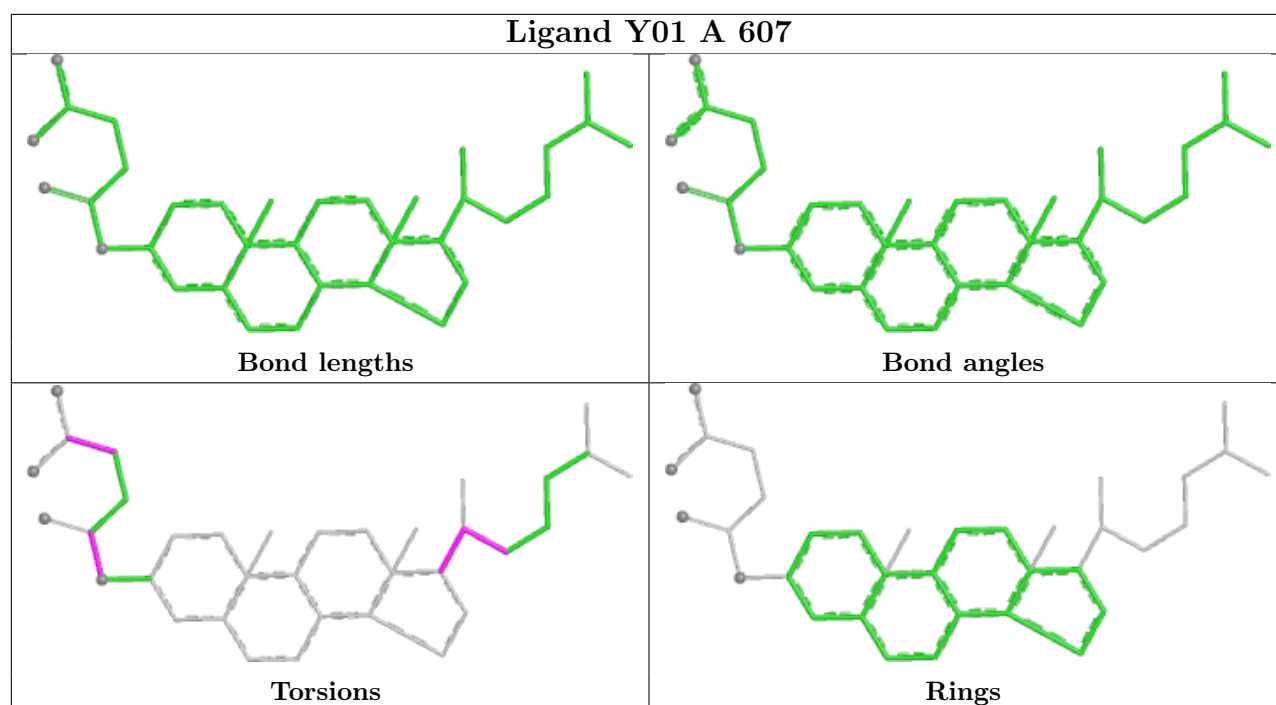
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	Y01	4	0
2	C	605	Y01	1	0
4	A	608	PGT	1	0
2	A	607	Y01	1	0
2	A	605	Y01	1	0
2	A	603	Y01	2	0
2	A	606	Y01	1	0
2	A	601	Y01	5	0
2	C	602	Y01	3	0
2	C	607	Y01	1	0
3	C	604	NAG	1	0
2	C	603	Y01	2	0
4	C	608	PGT	1	0
2	C	606	Y01	1	0
3	A	604	NAG	1	0
2	A	602	Y01	3	0

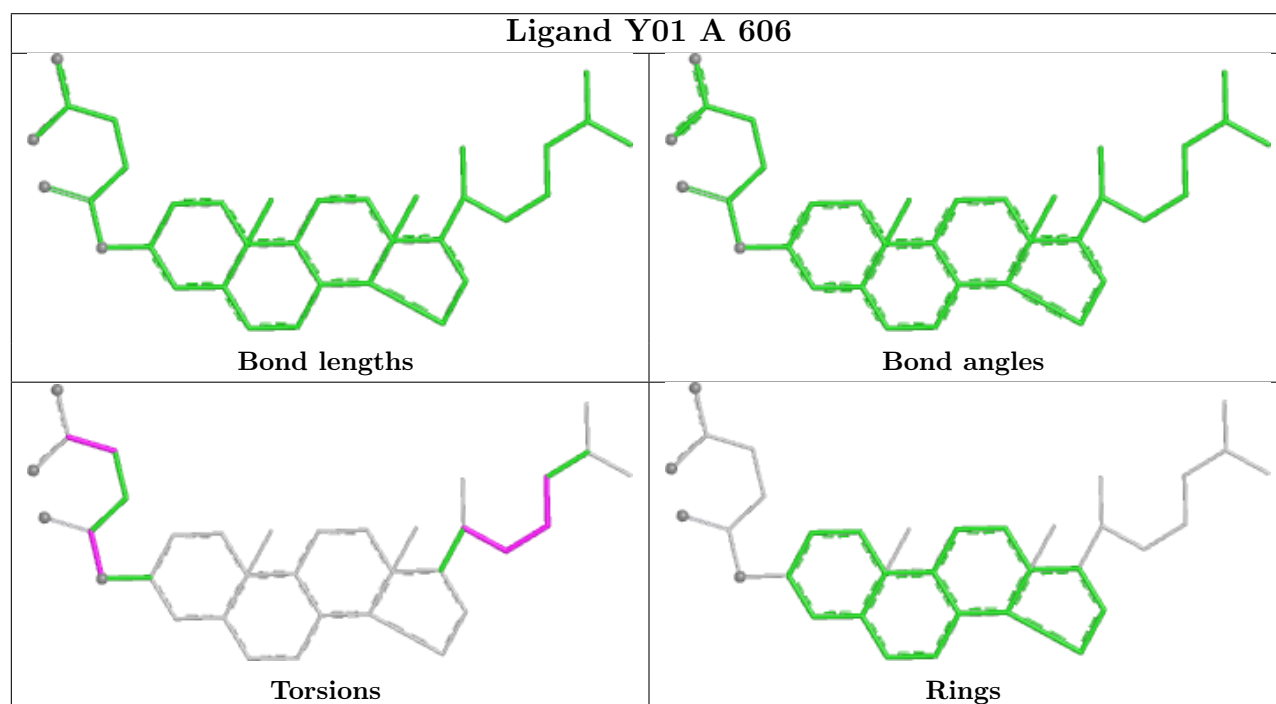
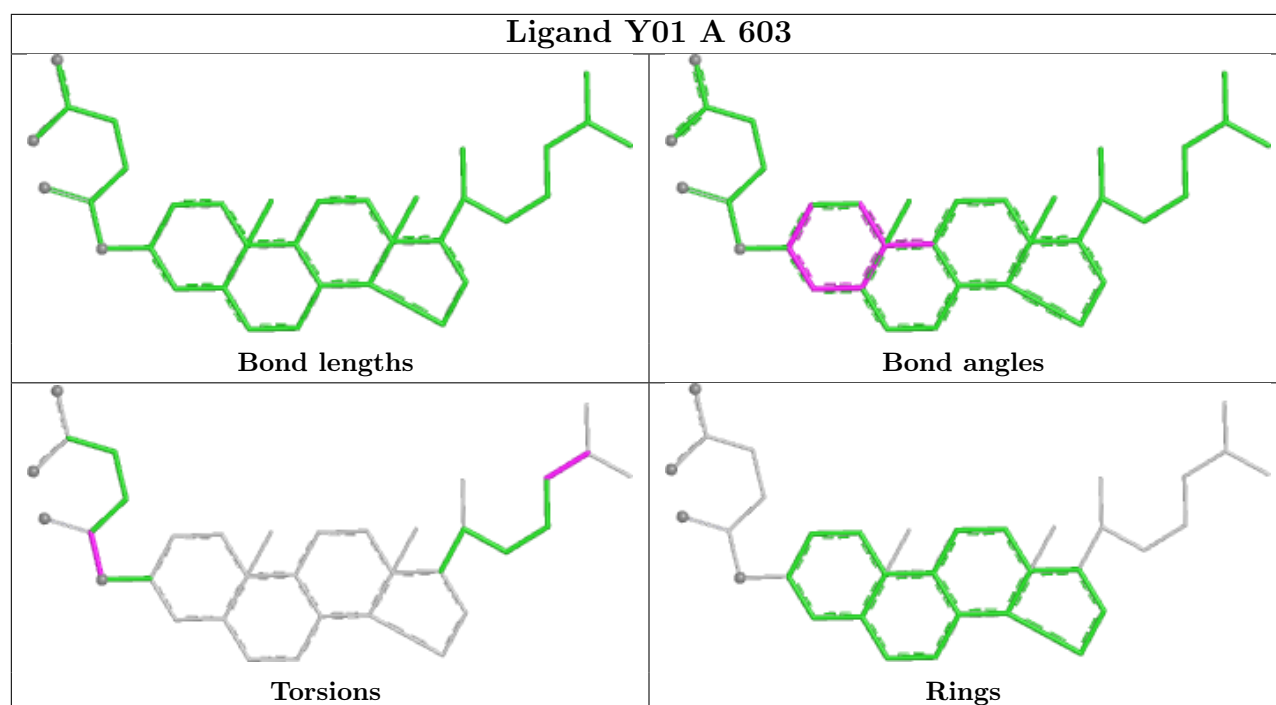
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

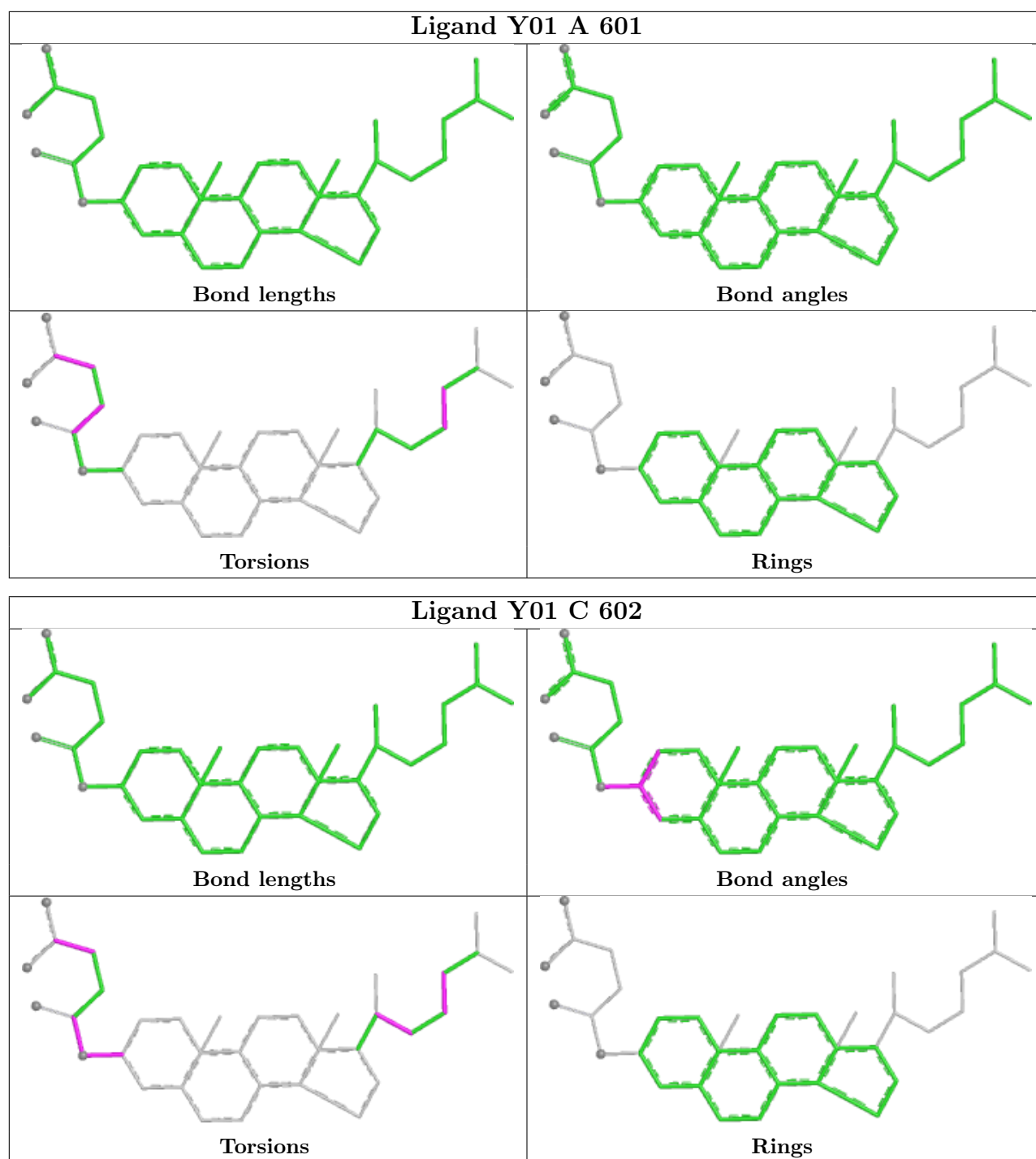
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

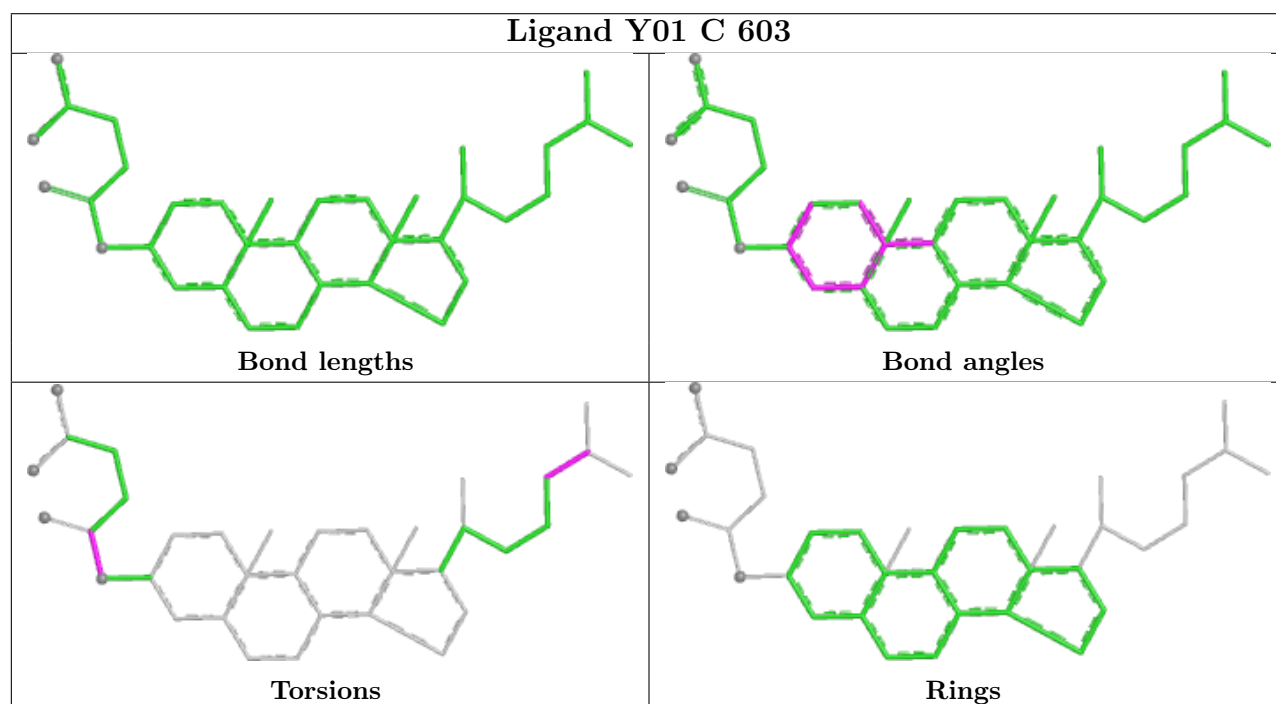
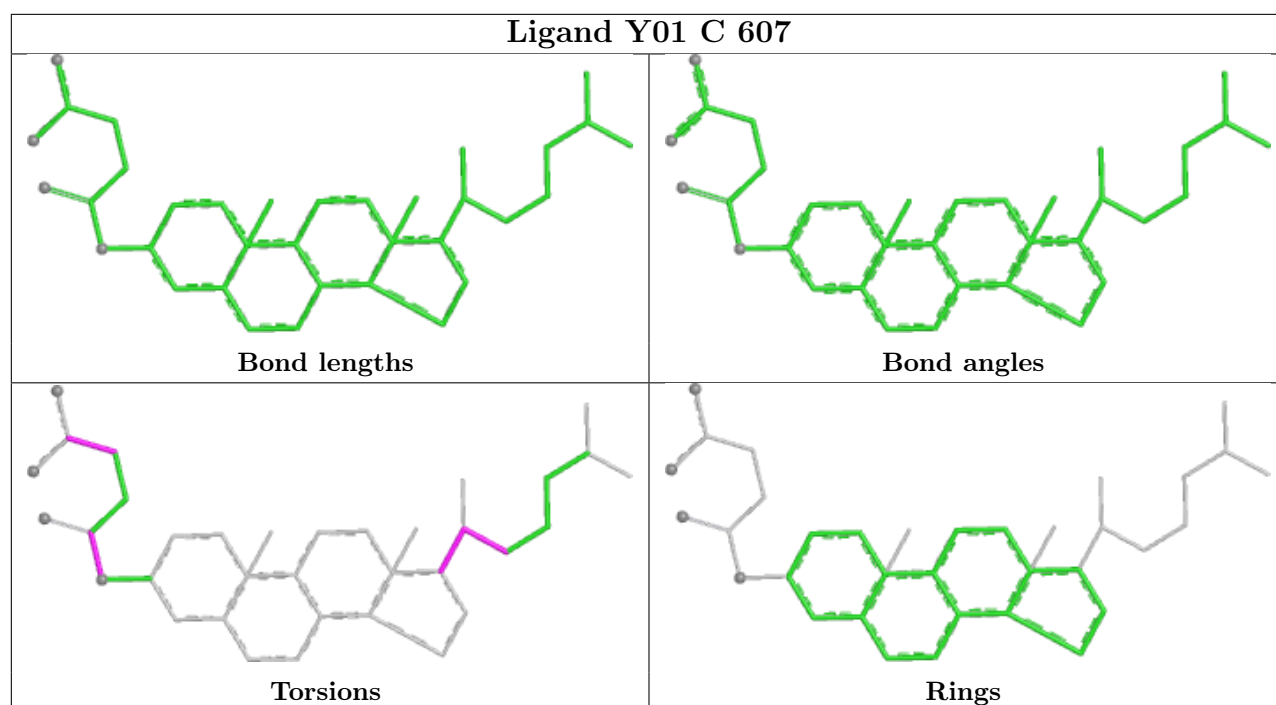


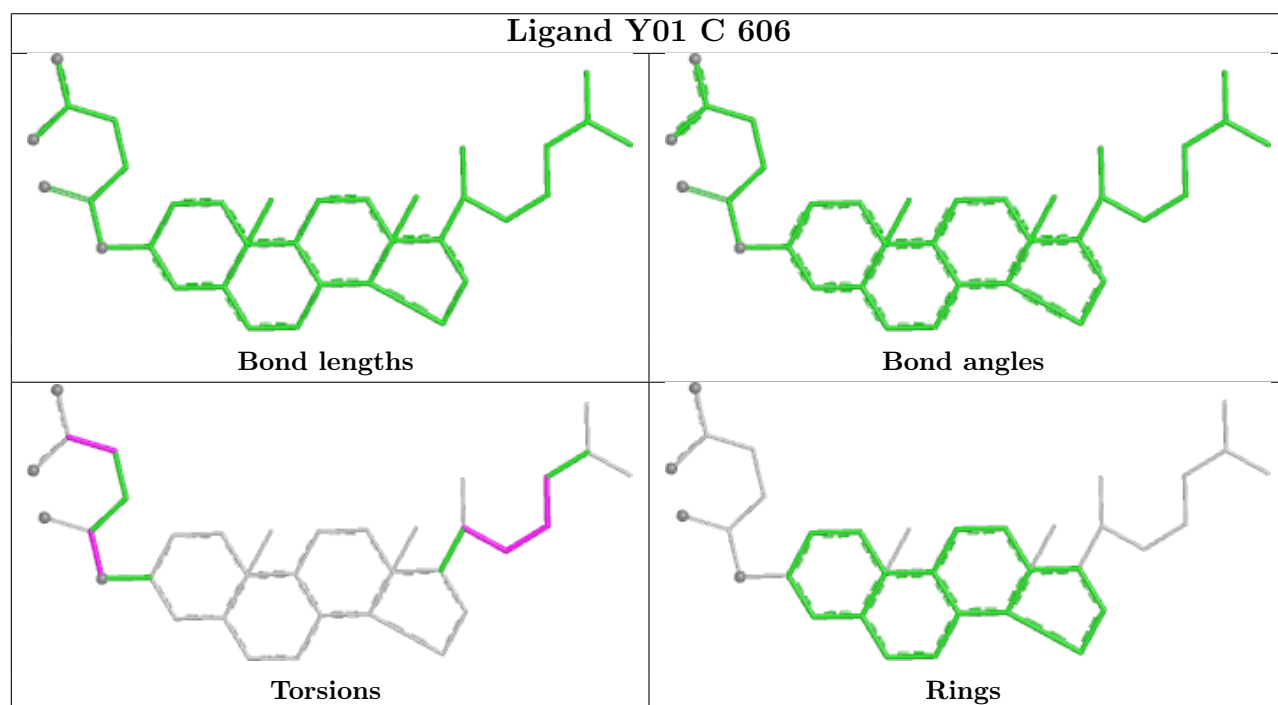
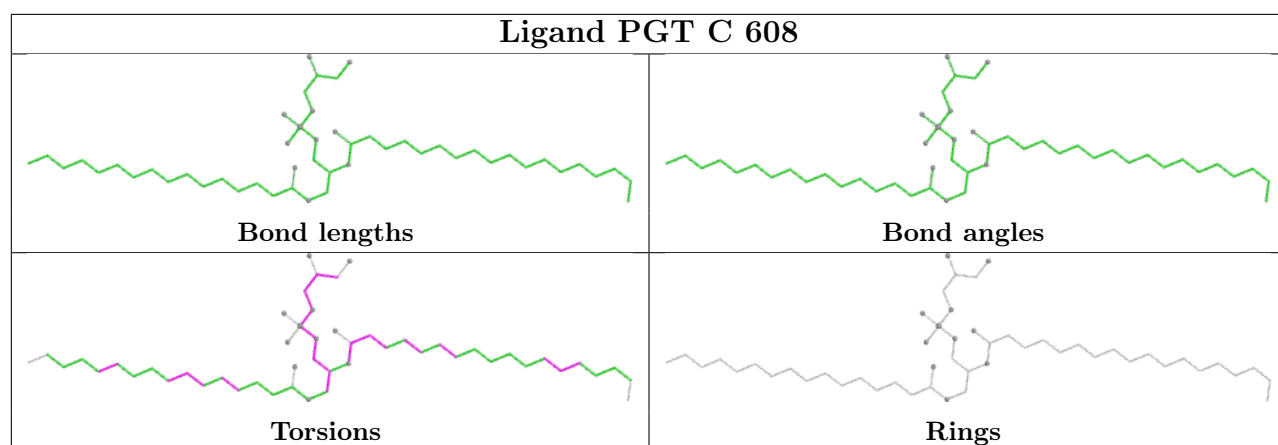


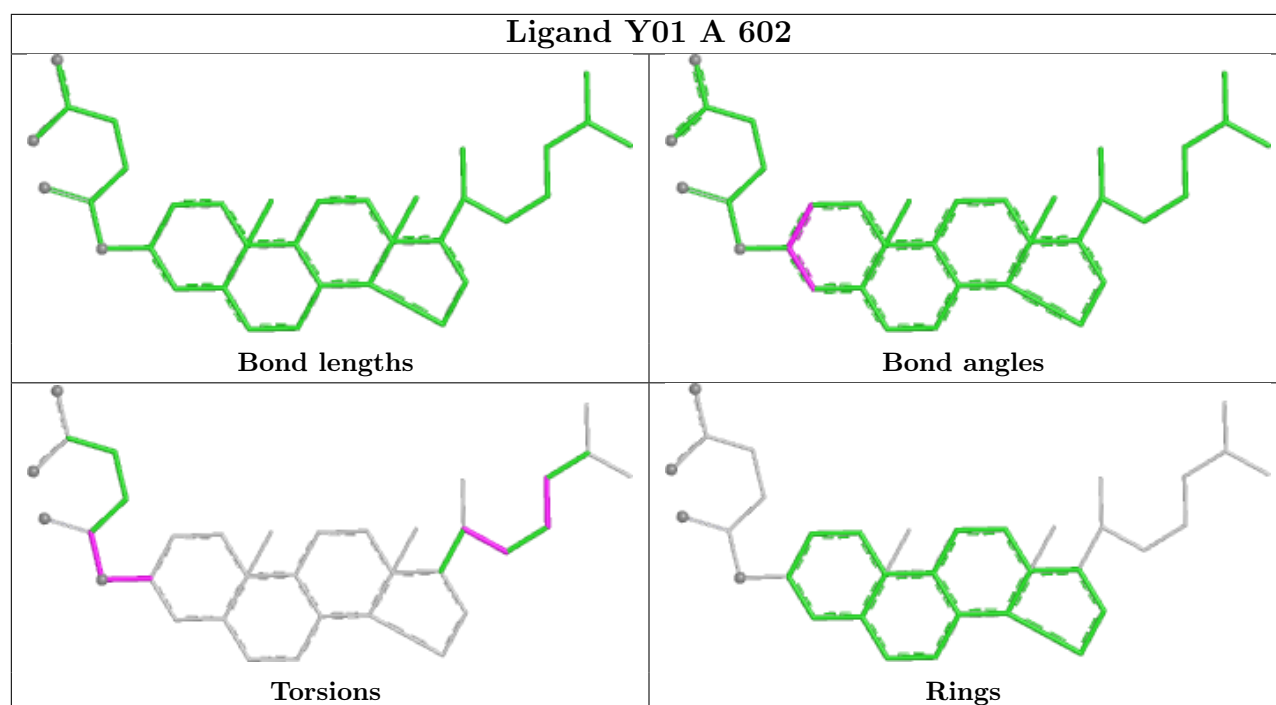












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

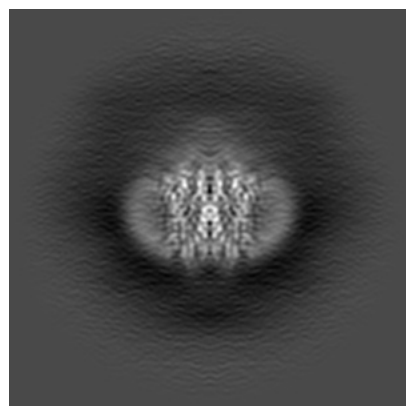
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18635. These allow visual inspection of the internal detail of the map and identification of artifacts.

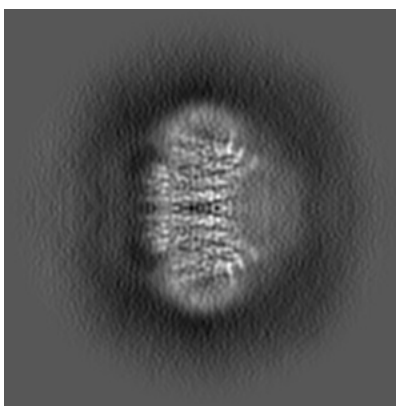
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

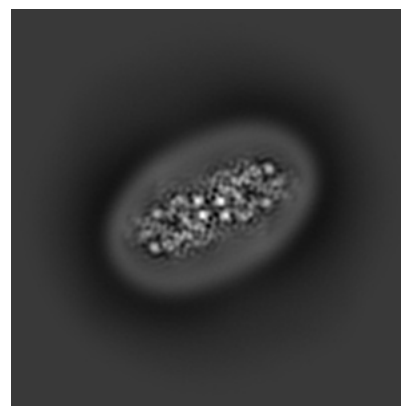
6.1.1 Primary map



X

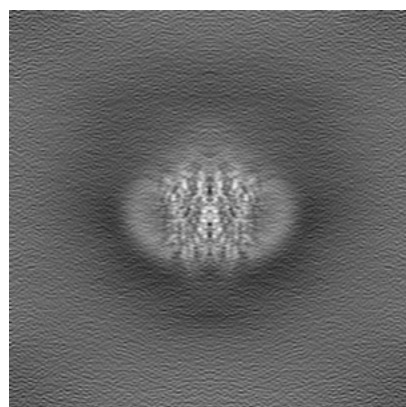


Y

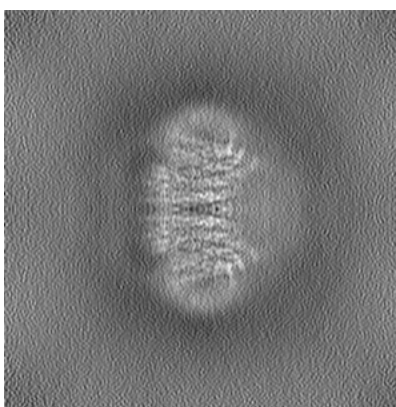


Z

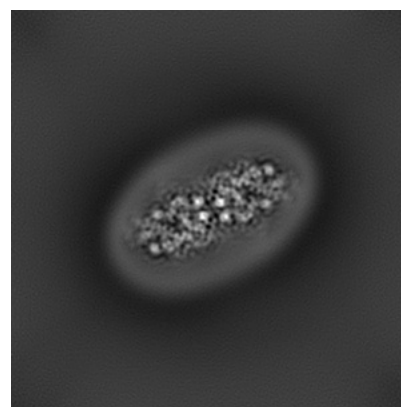
6.1.2 Raw map



X



Y

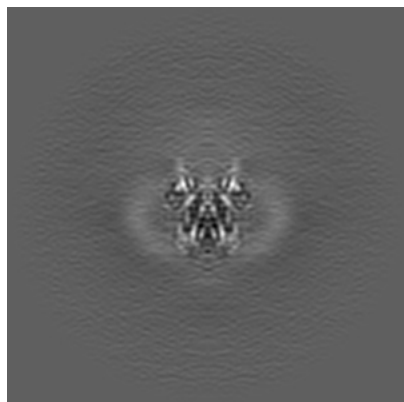


Z

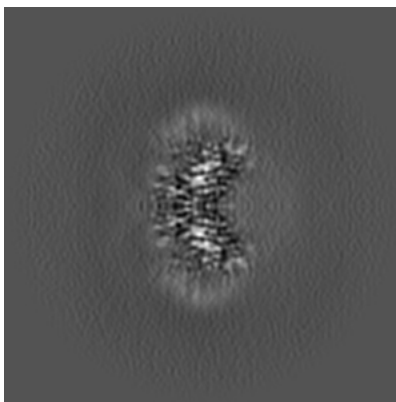
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

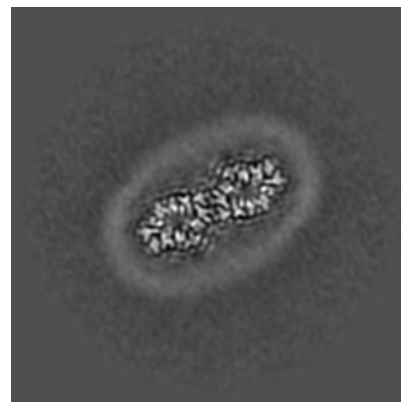
6.2.1 Primary map



X Index: 120

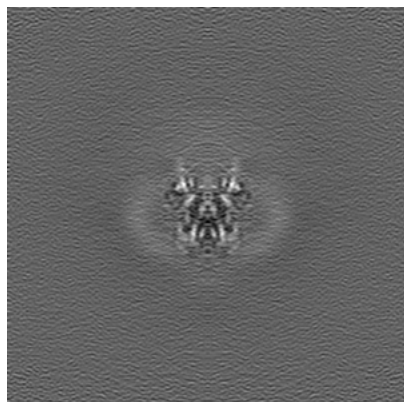


Y Index: 120

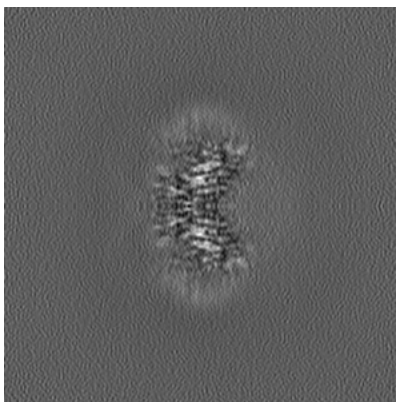


Z Index: 120

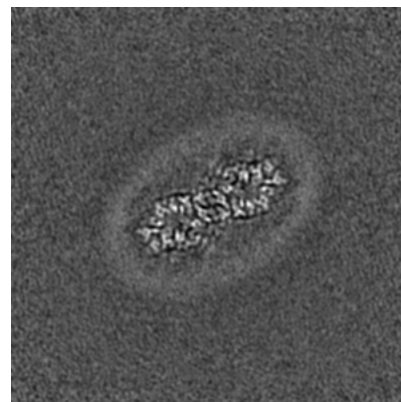
6.2.2 Raw map



X Index: 120



Y Index: 120

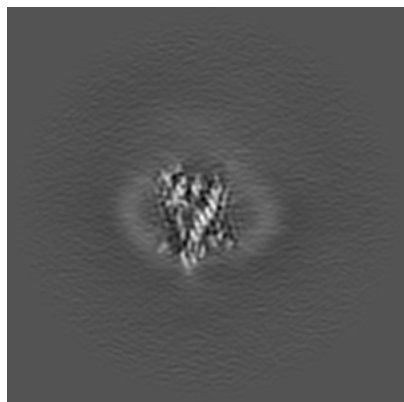


Z Index: 120

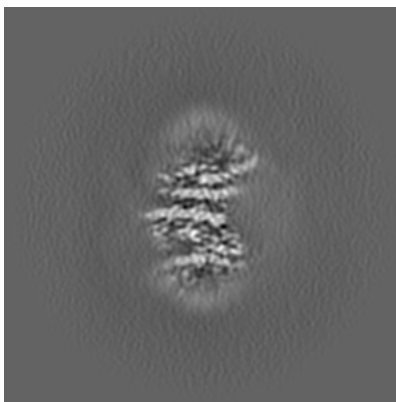
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

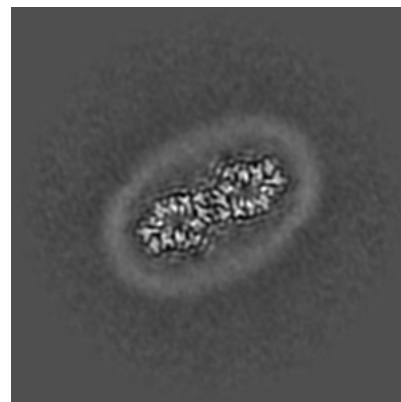
6.3.1 Primary map



X Index: 104

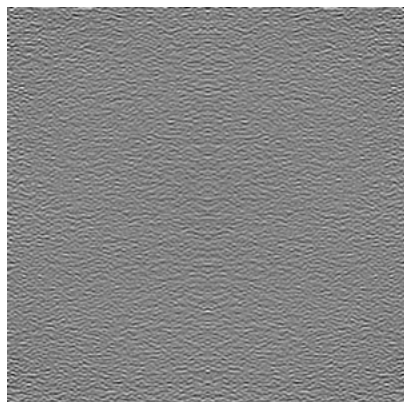


Y Index: 116

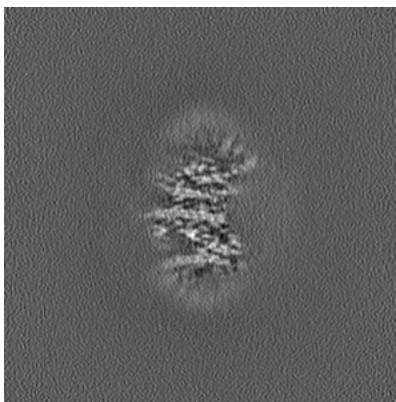


Z Index: 120

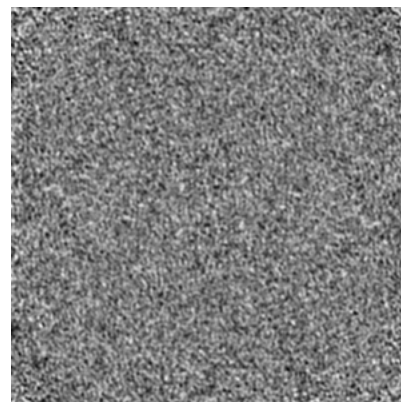
6.3.2 Raw map



X Index: 0



Y Index: 117

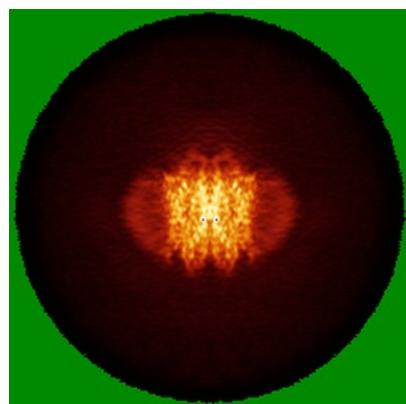


Z Index: 0

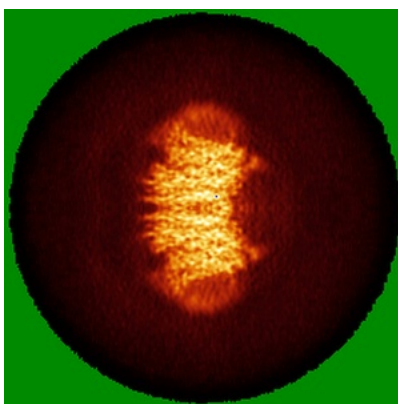
The images above show the largest variance slices of the map in three orthogonal directions.

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

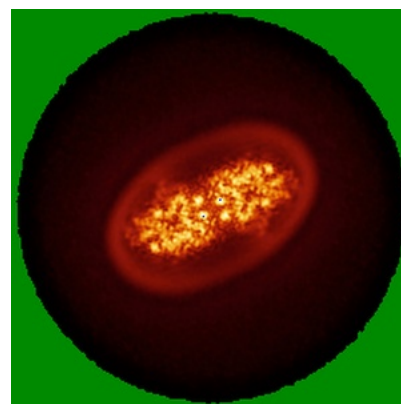
6.4.1 Primary map



X

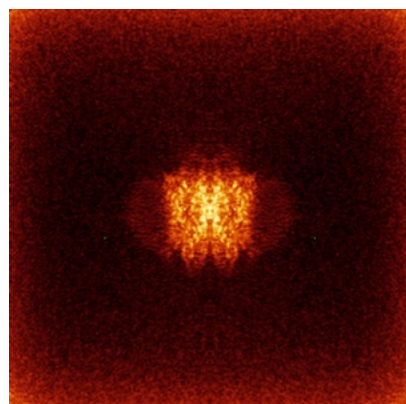


Y

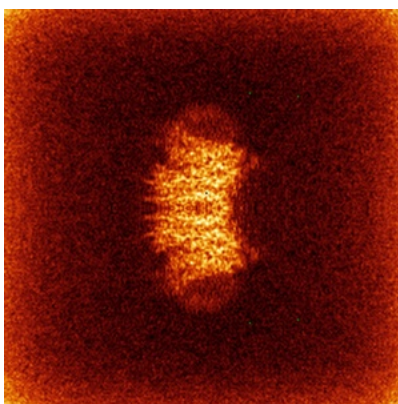


Z

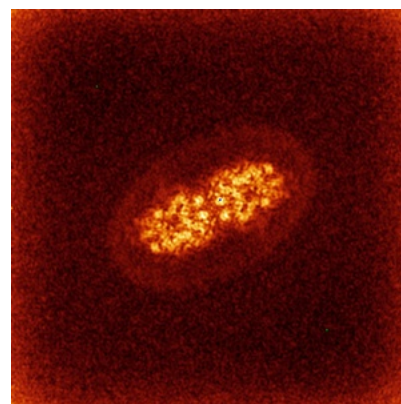
6.4.2 Raw map



X



Y

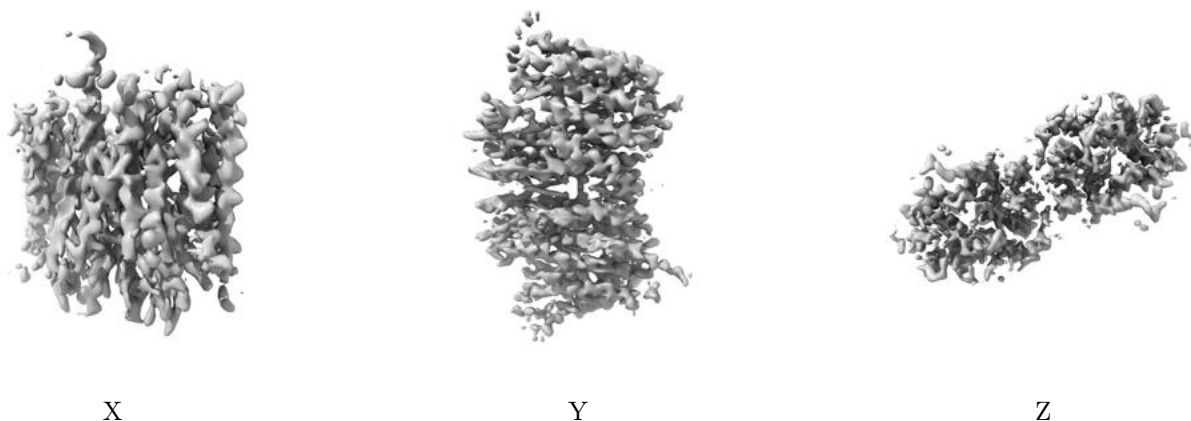


Z

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

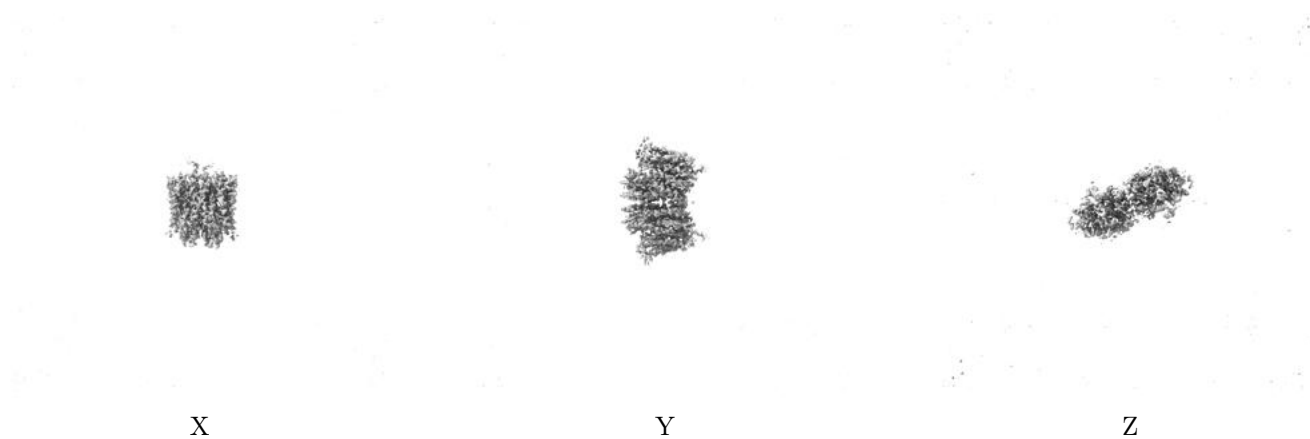
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.207. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

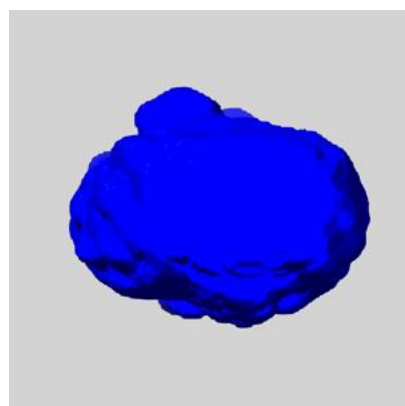
6.6 Mask visualisation [i](#)

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

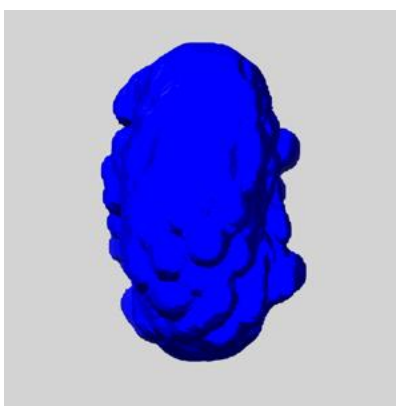
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

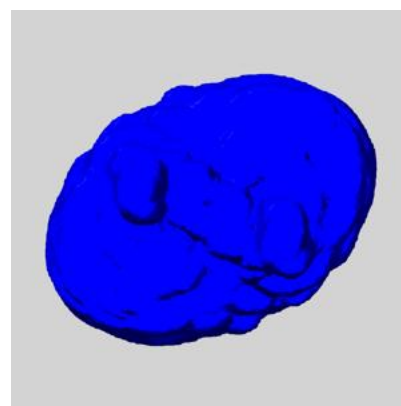
6.6.1 emd_18635_msk_1.map [i](#)



X



Y

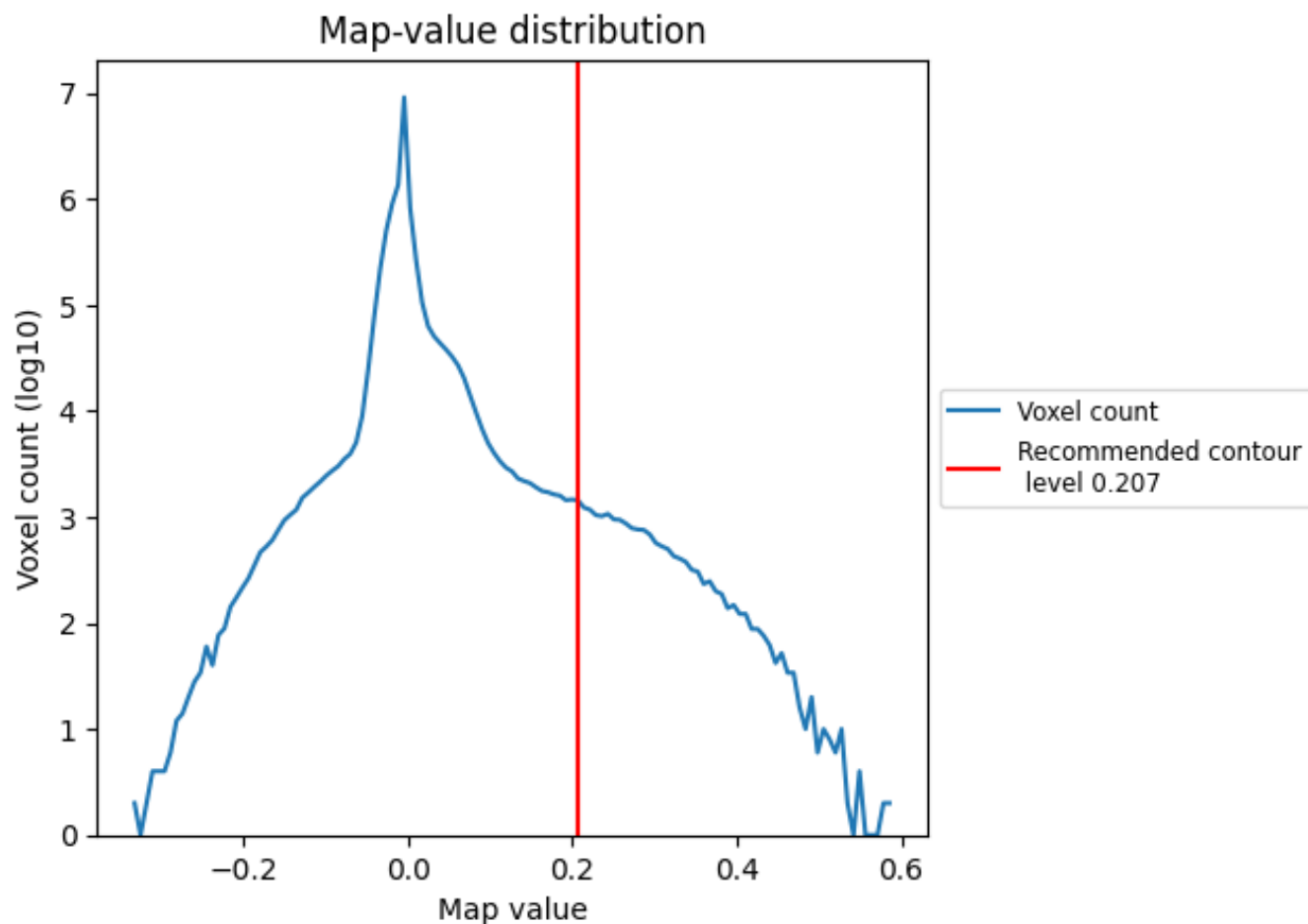


Z

7 Map analysis [i](#)

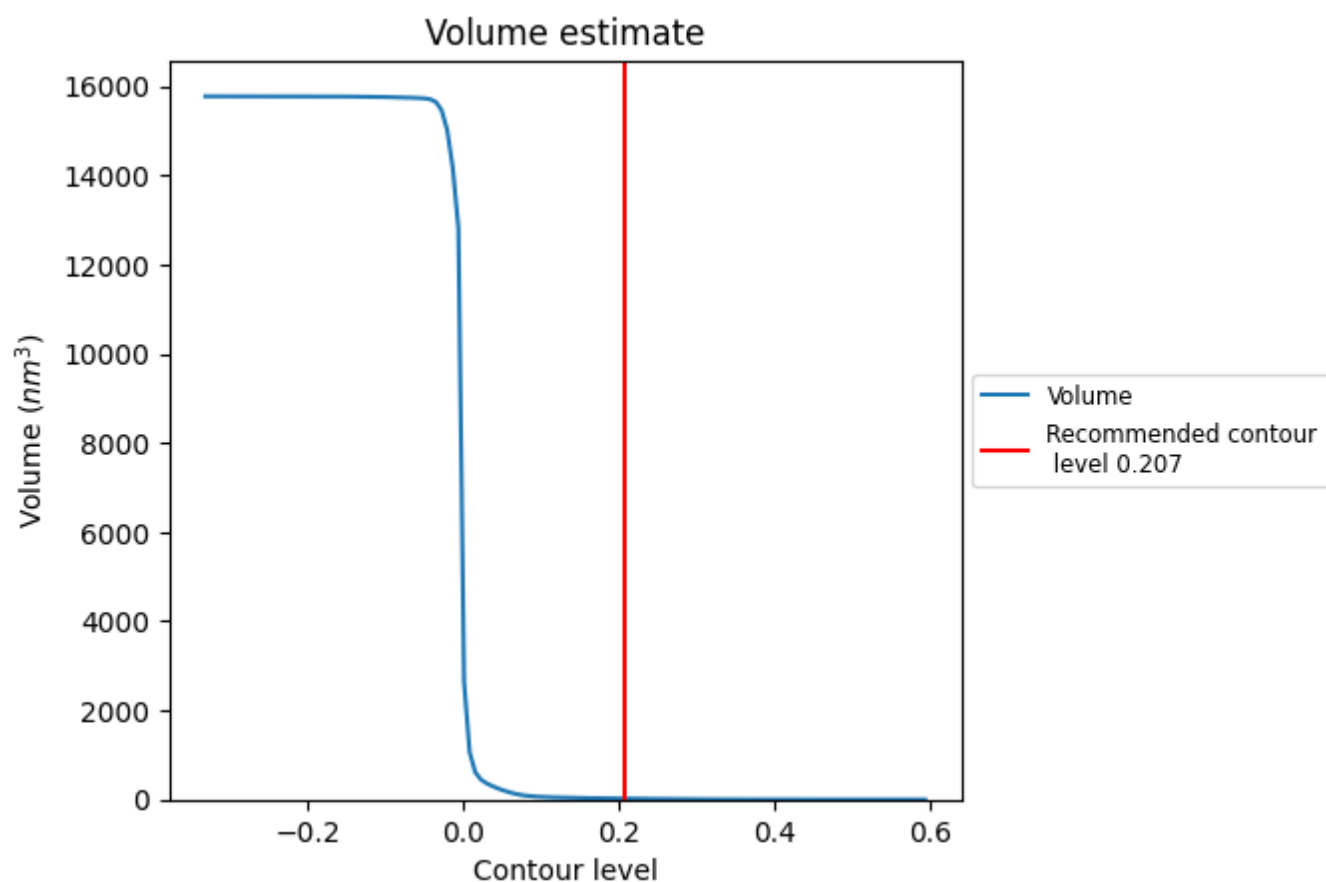
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

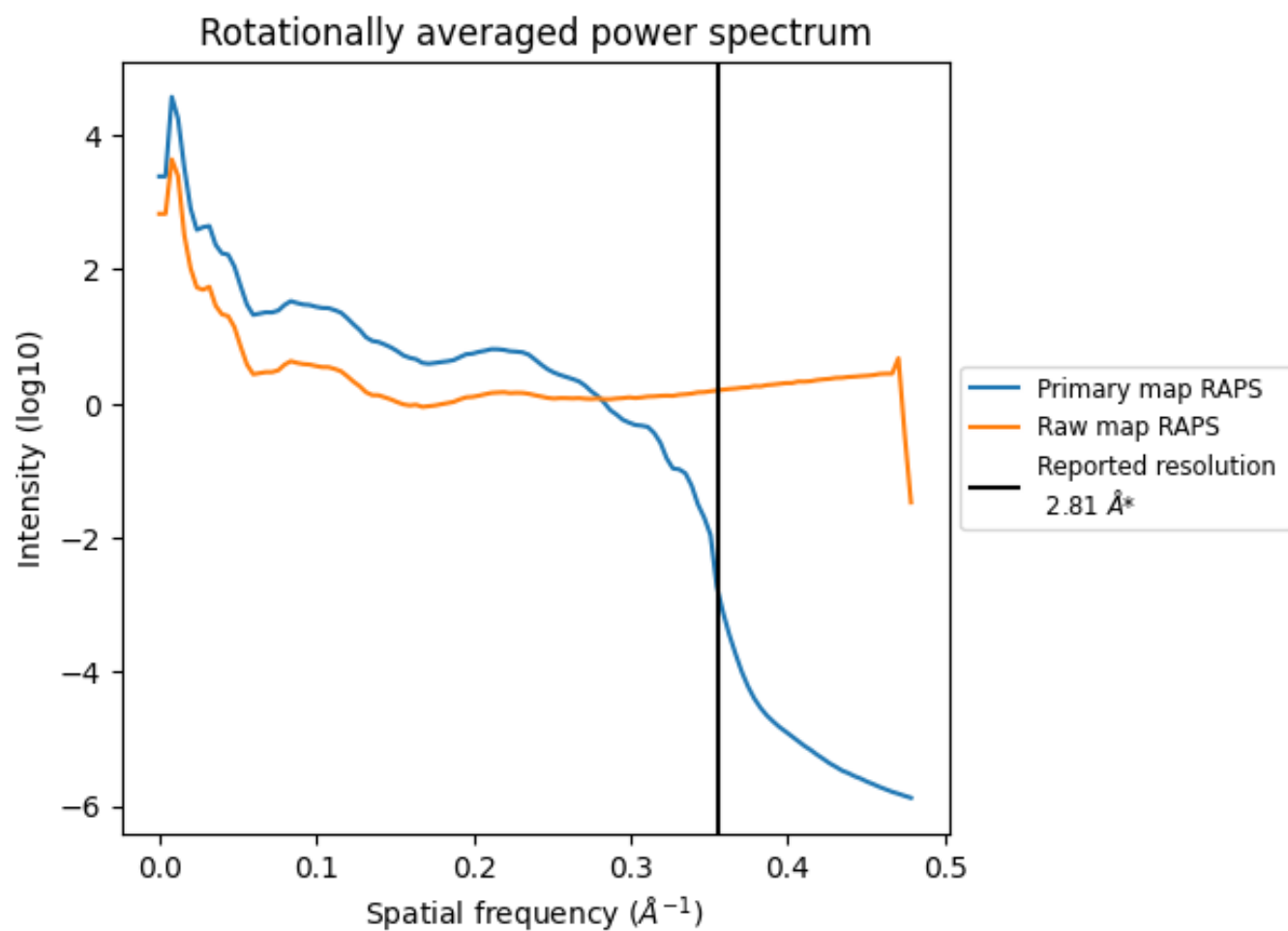
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21 nm³; this corresponds to an approximate mass of 19 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

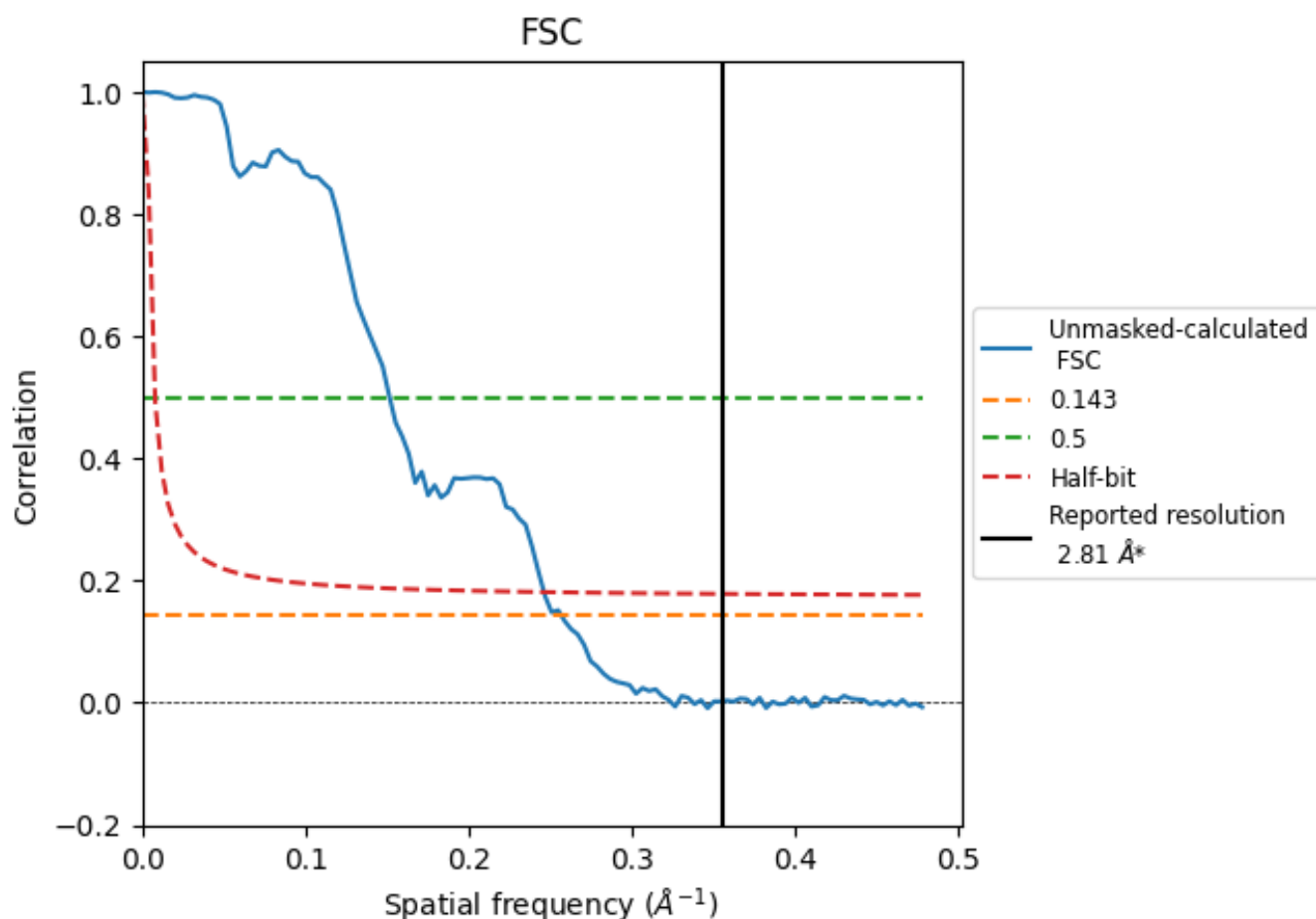


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

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 0.356 Å⁻¹

8.2 Resolution estimates [i](#)

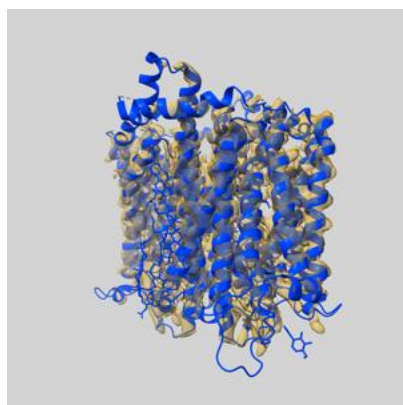
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	6.59	4.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 2.81 by more than 10 %

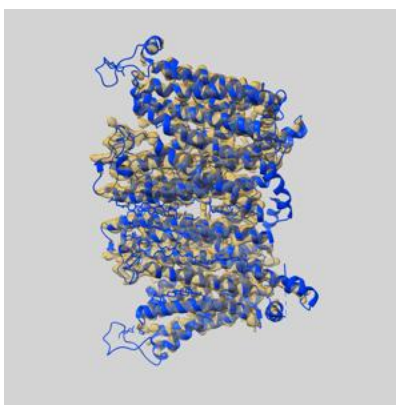
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18635 and PDB model 8QSL. Per-residue inclusion information can be found in section [3](#) on page [6](#).

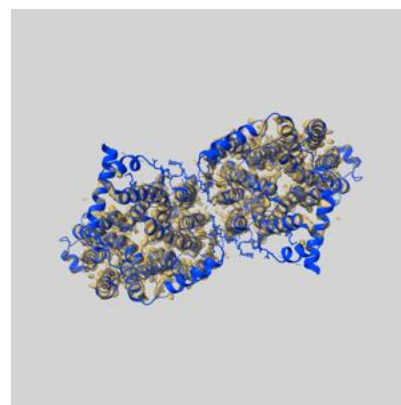
9.1 Map-model overlay [i](#)



X



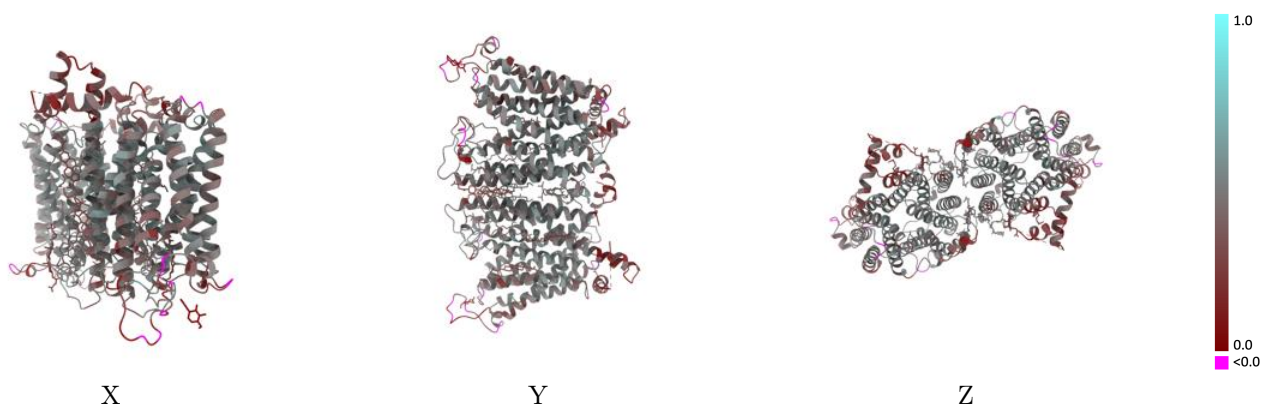
Y



Z

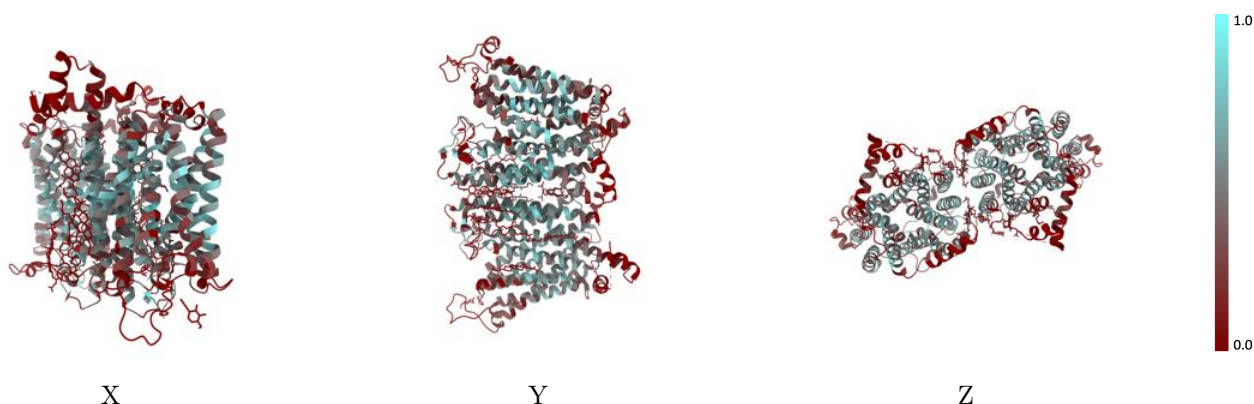
The images above show the 3D surface view of the map at the recommended contour level 0.207 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



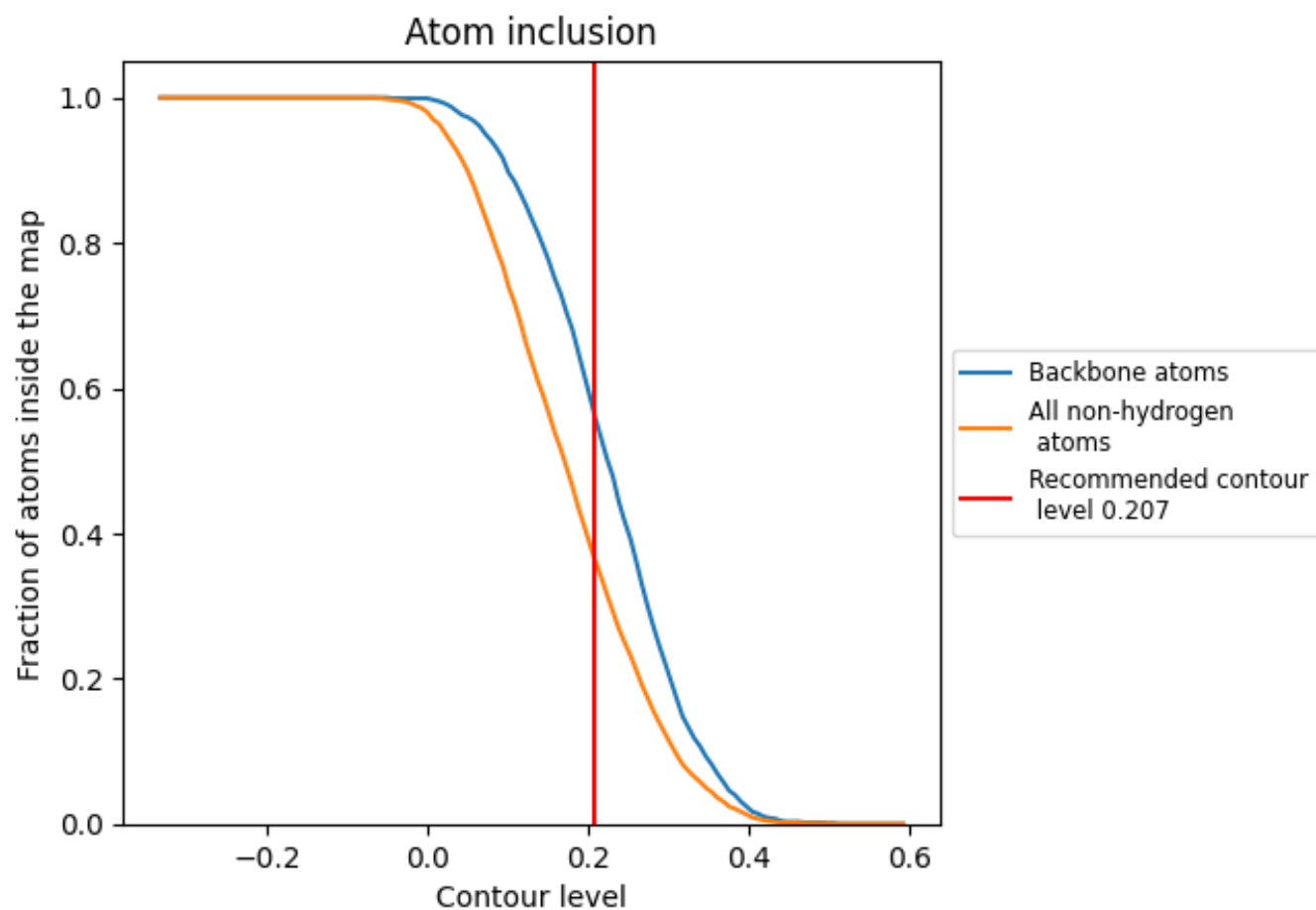
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.207).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 37% 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 (0.207) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3700	0.4180
A	0.3710	0.4180
C	0.3700	0.4170

