



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 03:43 PM EDT

PDB ID : 6BWD
EMDB ID : EMD-7297
Title : 3.7 angstrom cryoEM structure of truncated mouse TRPM7
Authors : Zhang, J.; Li, Z.; Duan, J.; Li, J.; Hulse, R.E.; Santa-Cruz, A.; Abiria, S.A.; Krapivinsky, G.; Clapham, D.E.
Deposited on : 2017-12-14
Resolution : 3.70 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

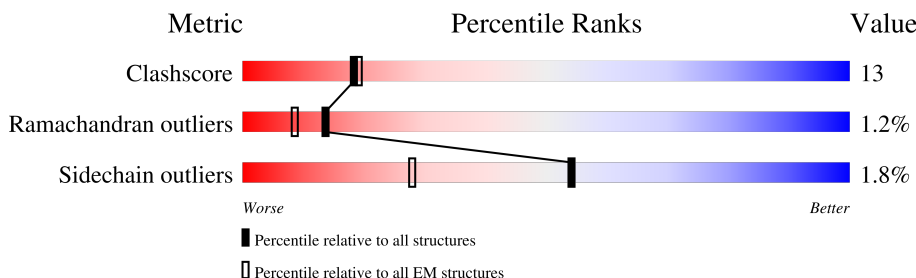
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	955	
1	B	955	
1	C	955	
1	D	955	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Y01	D	1203	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23187 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 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	771	Total	C	N	O	S	0	0
			5613	3636	954	992	31		
1	B	771	Total	C	N	O	S	0	0
			5618	3636	957	995	30		
1	C	771	Total	C	N	O	S	0	0
			5628	3640	957	1000	31		
1	D	771	Total	C	N	O	S	0	0
			5593	3624	954	985	30		

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



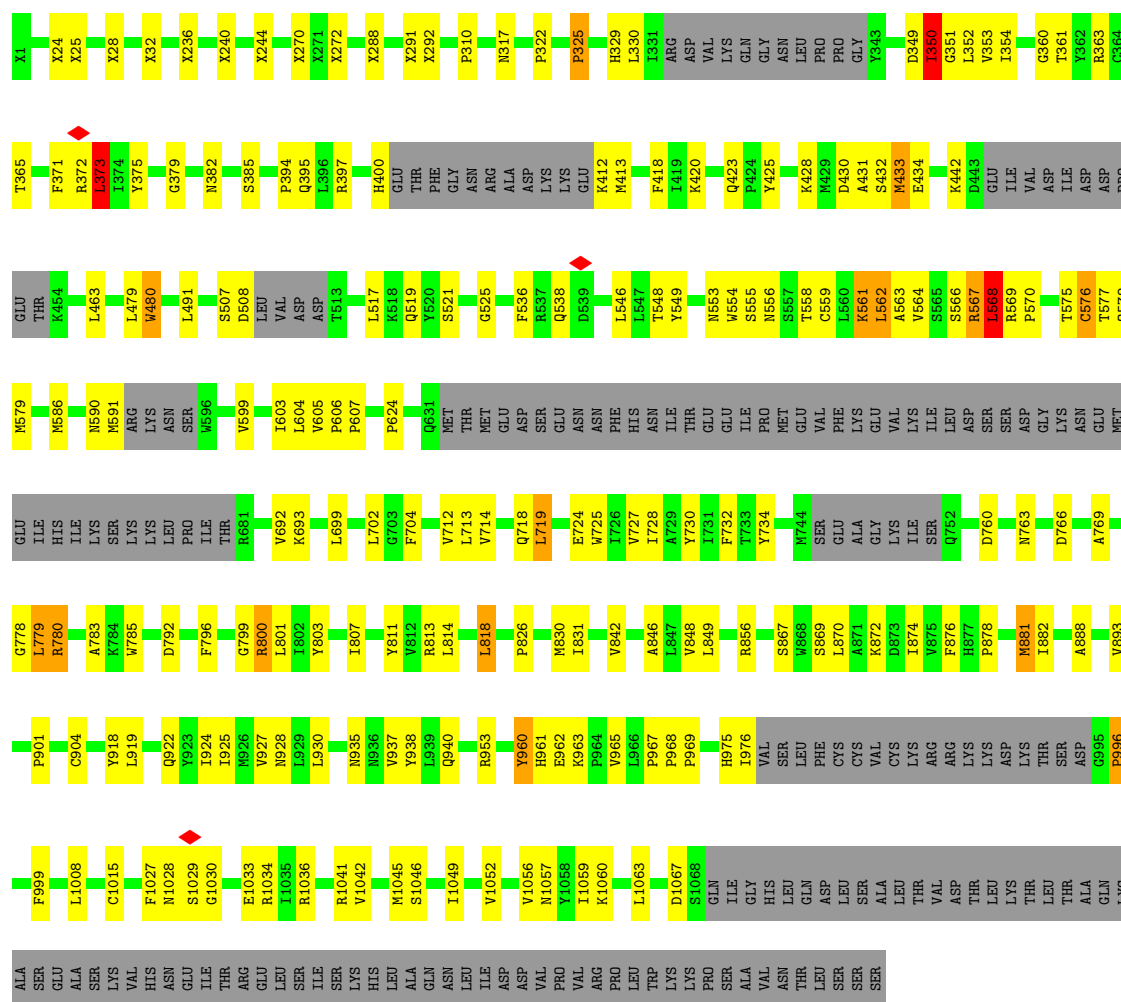
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Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total	C	O	0
			35	31	4	
3	C	1	Total	C	O	0
			35	31	4	
3	C	1	Total	C	O	0
			35	31	4	
3	C	1	Total	C	O	0
			35	31	4	
3	D	1	Total	C	O	0
			35	31	4	
3	D	1	Total	C	O	0
			35	31	4	

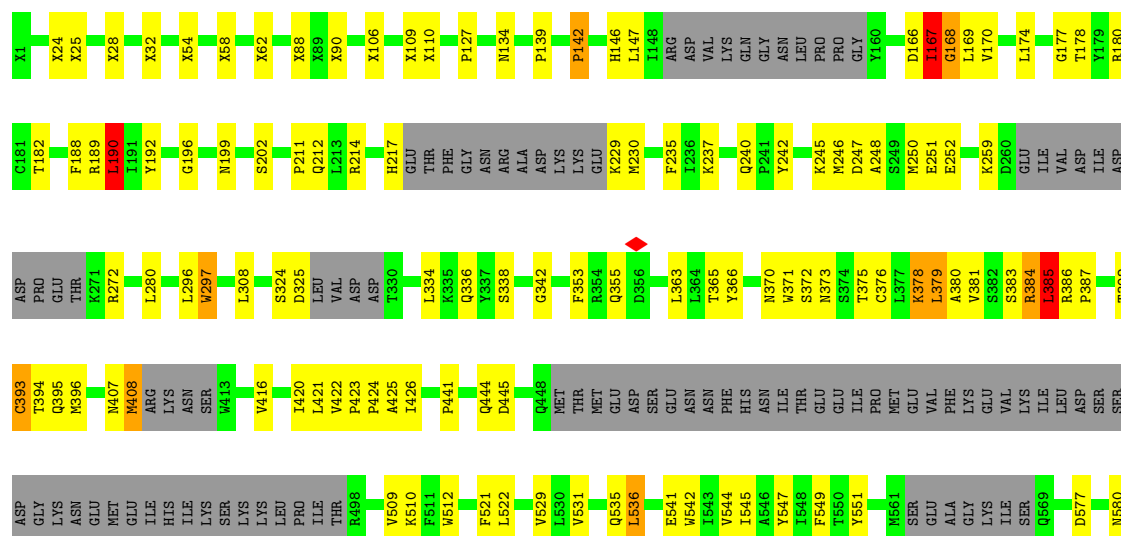
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	7	Total	O	0
			7	7	
4	B	6	Total	O	0
			6	6	
4	C	8	Total	O	0
			8	8	
4	D	9	Total	O	0
			9	9	



- Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain C: 59% 20% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232930	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.238	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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, MG

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	0.48	0/5124	0.79	20/6947 (0.3%)
1	B	0.48	0/5129	0.79	19/6954 (0.3%)
1	C	0.49	0/5139	0.79	19/6967 (0.3%)
1	D	0.48	0/5105	0.79	20/6925 (0.3%)
All	All	0.48	0/20497	0.79	78/27793 (0.3%)

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	26
1	B	0	26
1	C	0	27
1	D	0	26
All	All	0	105

There are no bond length outliers.

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ILE	C-N-CA	8.81	140.79	122.30
1	C	385	LEU	CA-CB-CG	7.84	133.33	115.30
1	B	568	LEU	CA-CB-CG	7.83	133.31	115.30
1	A	568	LEU	CA-CB-CG	7.82	133.29	115.30
1	D	568	LEU	CA-CB-CG	7.82	133.27	115.30

There are no chirality outliers.

5 of 105 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	UNK	Peptide
1	A	272	UNK	Peptide
1	A	350	ILE	Peptide
1	A	353	VAL	Peptide
1	A	361	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5613	0	4850	150	0
1	B	5618	0	4852	125	0
1	C	5628	0	4860	127	0
1	D	5593	0	4822	132	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	1	0	0	1	0
3	A	210	0	294	20	0
3	B	140	0	196	9	0
3	C	280	0	392	19	0
3	D	70	0	98	24	0
4	A	7	0	0	0	0
4	B	6	0	0	0	0
4	C	8	0	0	0	0
4	D	9	0	0	1	0
All	All	23187	0	20364	561	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 561 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:LYS:CE	1:D:431:ALA:HB2	1.37	1.52
1:D:428:LYS:CE	1:D:431:ALA:CB	2.25	1.14
1:A:412:LYS:HD2	1:A:413:MET:CB	1.77	1.14
1:C:407:ASN:HB3	1:C:408:MET:HG2	1.28	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ASN:HB3	1:B:591:MET:HG2	1.12	1.10

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	632/955 (66%)	544 (86%)	79 (12%)	9 (1%)	9	39
1	B	632/955 (66%)	546 (86%)	79 (12%)	7 (1%)	12	43
1	C	632/955 (66%)	544 (86%)	79 (12%)	9 (1%)	9	39
1	D	632/955 (66%)	548 (87%)	79 (12%)	5 (1%)	16	49
All	All	2528/3820 (66%)	2182 (86%)	316 (12%)	30 (1%)	14	41

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ILE
1	A	996	PRO
1	B	996	PRO
1	C	142	PRO
1	C	168	GLY

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	481/758 (64%)	472 (98%)	9 (2%)	52	70
1	B	482/758 (64%)	474 (98%)	8 (2%)	56	73
1	C	485/758 (64%)	476 (98%)	9 (2%)	52	70
1	D	476/758 (63%)	467 (98%)	9 (2%)	52	70
All	All	1924/3032 (64%)	1889 (98%)	35 (2%)	54	71

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	567	ARG
1	D	576	CYS
1	D	856	ARG
1	B	780	ARG
1	B	567	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	370	ASN
1	D	395	GLN
1	C	757	GLN
1	D	538	GLN
1	B	395	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

Of 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 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	1203	-	38,38,38	1.89	5 (13%)	57,57,57	1.71	13 (22%)
3	Y01	C	1307	-	38,38,38	1.95	6 (15%)	57,57,57	2.35	14 (24%)
3	Y01	C	1301	-	38,38,38	1.83	4 (10%)	57,57,57	1.97	14 (24%)
3	Y01	A	1205	-	38,38,38	2.02	8 (21%)	57,57,57	1.86	14 (24%)
3	Y01	C	1308	-	38,38,38	1.84	5 (13%)	57,57,57	2.12	16 (28%)
3	Y01	A	1203	-	38,38,38	1.98	6 (15%)	57,57,57	1.58	10 (17%)
3	Y01	A	1204	-	38,38,38	1.84	5 (13%)	57,57,57	1.76	11 (19%)
3	Y01	B	1205	-	38,38,38	1.92	6 (15%)	57,57,57	2.07	18 (31%)
3	Y01	C	1302	-	38,38,38	2.13	9 (23%)	57,57,57	2.05	13 (22%)
3	Y01	A	1206	-	38,38,38	2.04	8 (21%)	57,57,57	2.22	19 (33%)
3	Y01	A	1207	-	38,38,38	1.85	5 (13%)	57,57,57	1.79	13 (22%)
3	Y01	A	1208	-	38,38,38	2.02	8 (21%)	57,57,57	2.25	14 (24%)
3	Y01	B	1204	-	38,38,38	1.93	7 (18%)	57,57,57	1.51	9 (15%)
3	Y01	D	1203	-	38,38,38	1.88	6 (15%)	57,57,57	1.69	16 (28%)
3	Y01	C	1305	-	38,38,38	1.91	4 (10%)	57,57,57	1.80	12 (21%)
3	Y01	B	1206	-	38,38,38	1.87	6 (15%)	57,57,57	1.82	11 (19%)
3	Y01	C	1304	-	38,38,38	1.93	8 (21%)	57,57,57	2.08	14 (24%)
3	Y01	C	1303	-	38,38,38	2.16	5 (13%)	57,57,57	2.04	16 (28%)
3	Y01	C	1306	-	38,38,38	2.09	7 (18%)	57,57,57	1.89	18 (31%)
3	Y01	D	1202	-	38,38,38	1.85	6 (15%)	57,57,57	1.81	13 (22%)

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	1203	-	-	11/19/77/77	0/4/4/4
3	Y01	C	1307	-	-	12/19/77/77	0/4/4/4
3	Y01	C	1301	-	-	9/19/77/77	0/4/4/4
3	Y01	A	1205	-	-	11/19/77/77	0/4/4/4
3	Y01	C	1308	-	-	11/19/77/77	0/4/4/4
3	Y01	A	1203	-	-	11/19/77/77	0/4/4/4
3	Y01	A	1204	-	-	6/19/77/77	0/4/4/4
3	Y01	B	1205	-	-	14/19/77/77	0/4/4/4
3	Y01	C	1302	-	-	12/19/77/77	0/4/4/4
3	Y01	A	1206	-	-	13/19/77/77	0/4/4/4
3	Y01	A	1207	-	-	9/19/77/77	0/4/4/4
3	Y01	A	1208	-	-	8/19/77/77	0/4/4/4
3	Y01	B	1204	-	-	12/19/77/77	0/4/4/4
3	Y01	D	1203	-	-	11/19/77/77	0/4/4/4
3	Y01	C	1305	-	-	6/19/77/77	0/4/4/4
3	Y01	B	1206	-	-	6/19/77/77	0/4/4/4
3	Y01	C	1304	-	-	13/19/77/77	0/4/4/4
3	Y01	C	1303	-	-	7/19/77/77	0/4/4/4
3	Y01	C	1306	-	-	8/19/77/77	0/4/4/4
3	Y01	D	1202	-	-	11/19/77/77	0/4/4/4

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	Y01	CAV-CAZ	-7.52	1.36	1.51
3	B	1204	Y01	CBH-CAZ	-6.80	1.39	1.52
3	A	1203	Y01	CBH-CAZ	-6.80	1.39	1.52
3	C	1306	Y01	CAV-CAZ	-6.73	1.38	1.51
3	C	1303	Y01	CBH-CAZ	-6.36	1.40	1.52

The worst 5 of 278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1307	Y01	CAV-CAZ-CBH	7.05	125.45	116.42
3	A	1206	Y01	CBH-CBF-CBD	-6.04	103.88	112.71
3	A	1206	Y01	CAQ-CBG-CBD	-5.98	109.56	119.10
3	A	1208	Y01	CAV-CAZ-CBH	5.87	123.94	116.42
3	A	1208	Y01	CAQ-CBG-CBD	-5.82	109.81	119.10

There are no chirality outliers.

5 of 201 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	Y01	CAM-CAY-OAW-CBC
3	A	1206	Y01	CAO-CBB-CBE-CBI
3	A	1207	Y01	CAM-CAY-OAW-CBC
3	A	1208	Y01	CAO-CBB-CBE-CBI
3	B	1204	Y01	CAM-CAY-OAW-CBC

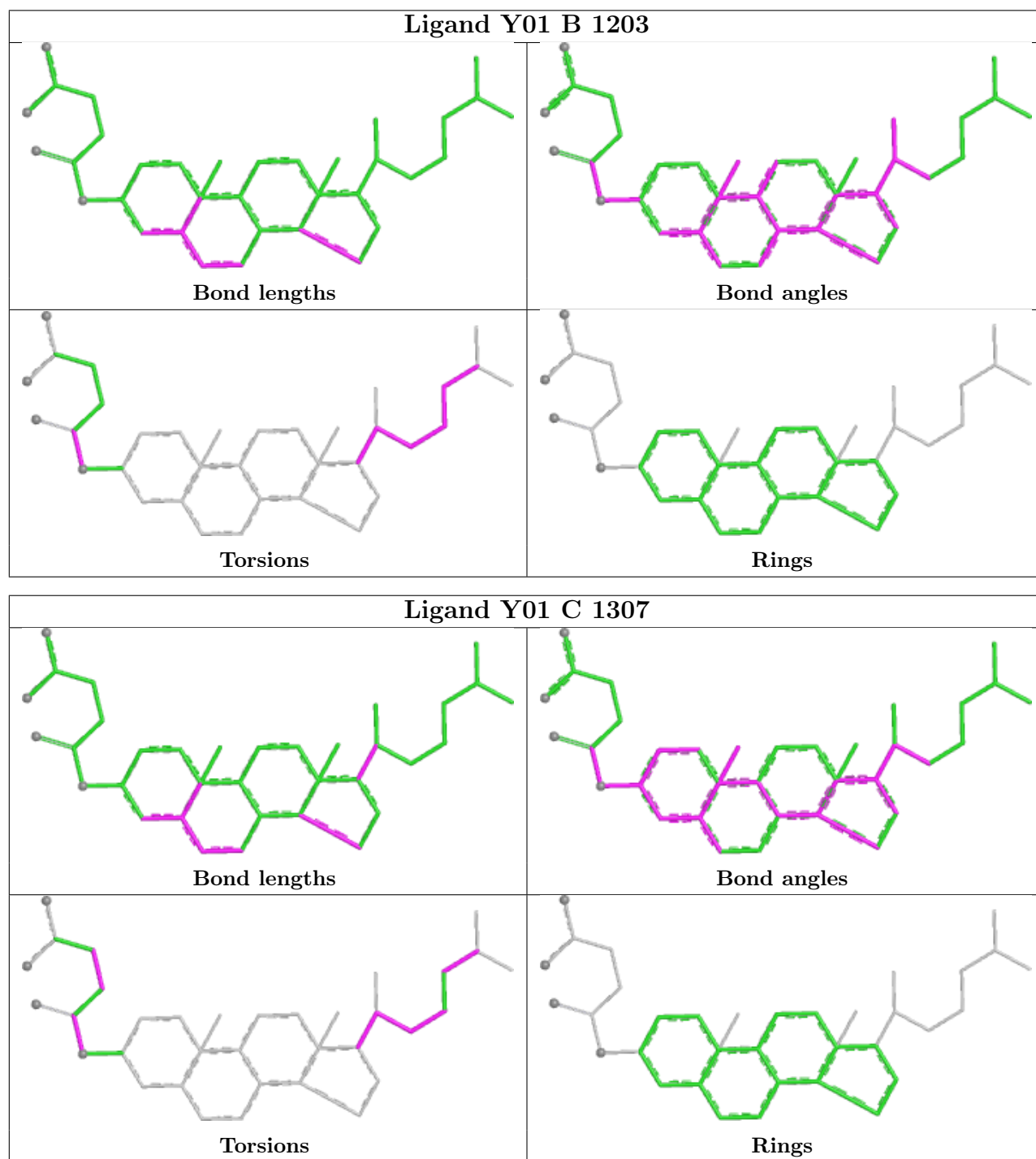
There are no ring outliers.

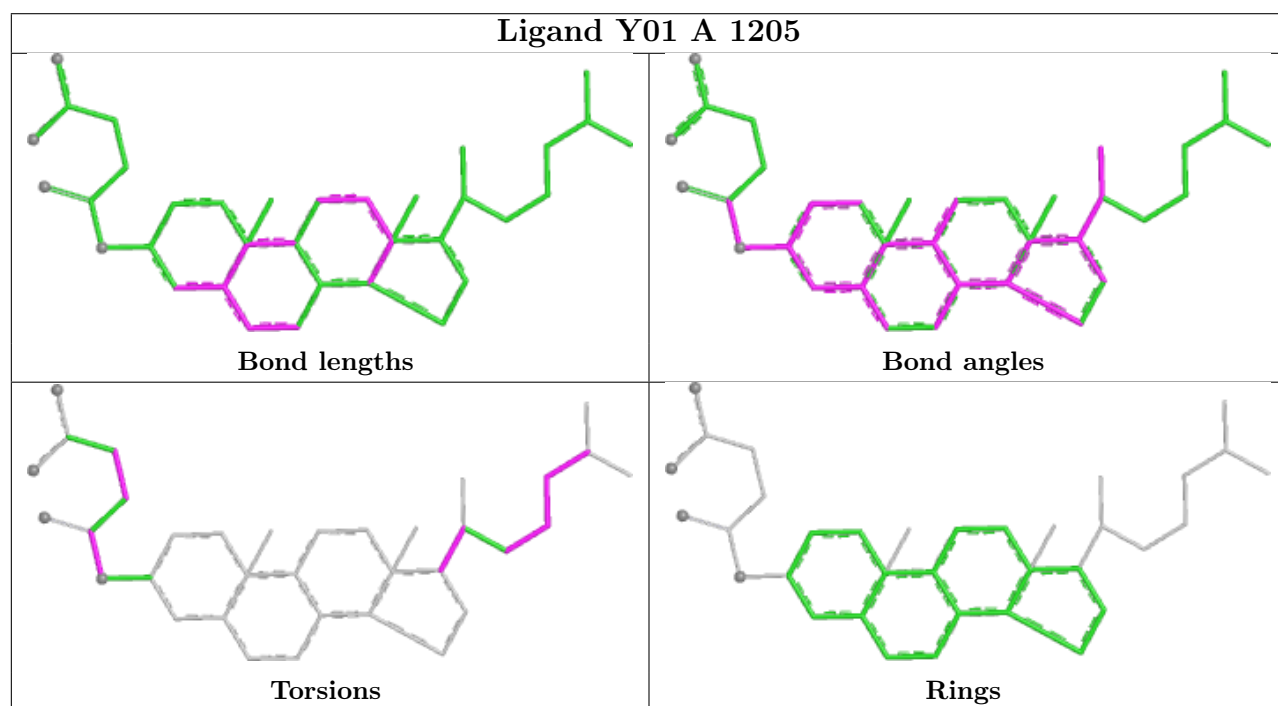
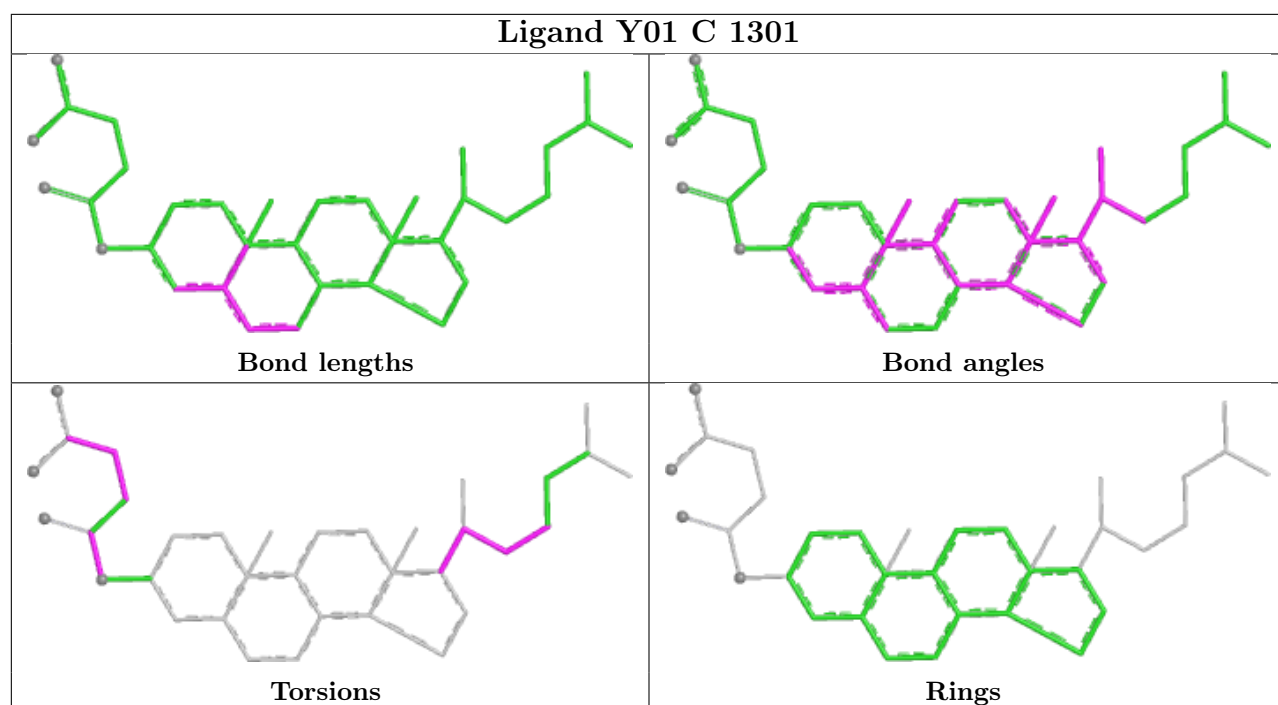
19 monomers are involved in 68 short contacts:

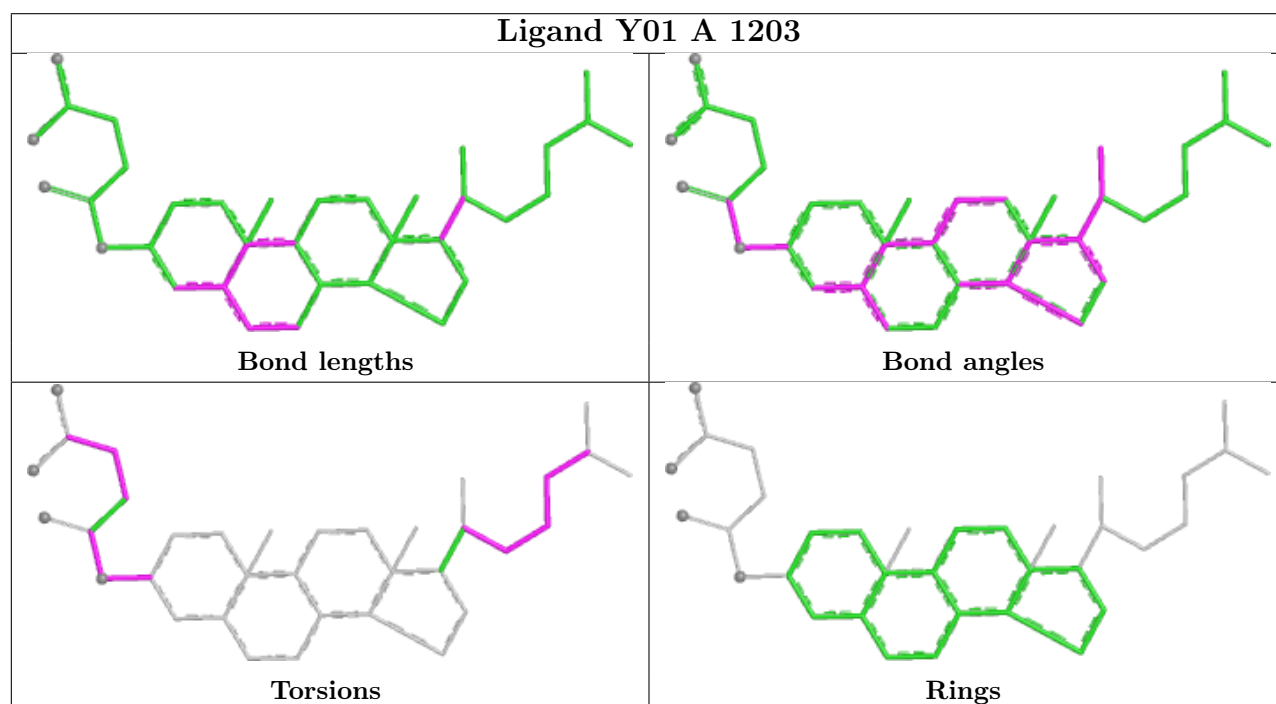
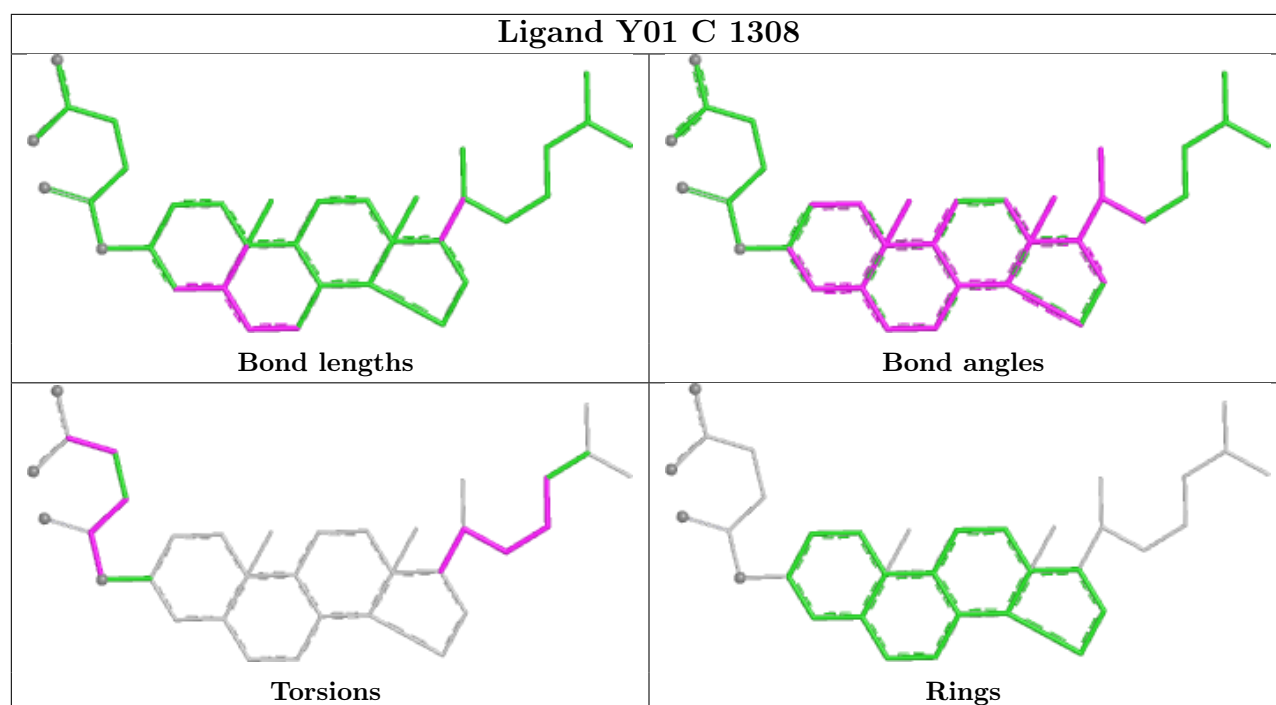
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1203	Y01	1	0
3	C	1307	Y01	2	0
3	C	1301	Y01	1	0
3	A	1205	Y01	5	0
3	C	1308	Y01	8	0
3	A	1203	Y01	3	0
3	B	1205	Y01	2	0
3	C	1302	Y01	3	0
3	A	1206	Y01	4	0
3	A	1207	Y01	3	0
3	A	1208	Y01	6	0
3	B	1204	Y01	4	0
3	D	1203	Y01	22	0
3	C	1305	Y01	1	0
3	B	1206	Y01	3	0
3	C	1304	Y01	2	0
3	C	1303	Y01	2	0
3	C	1306	Y01	1	0
3	D	1202	Y01	2	0

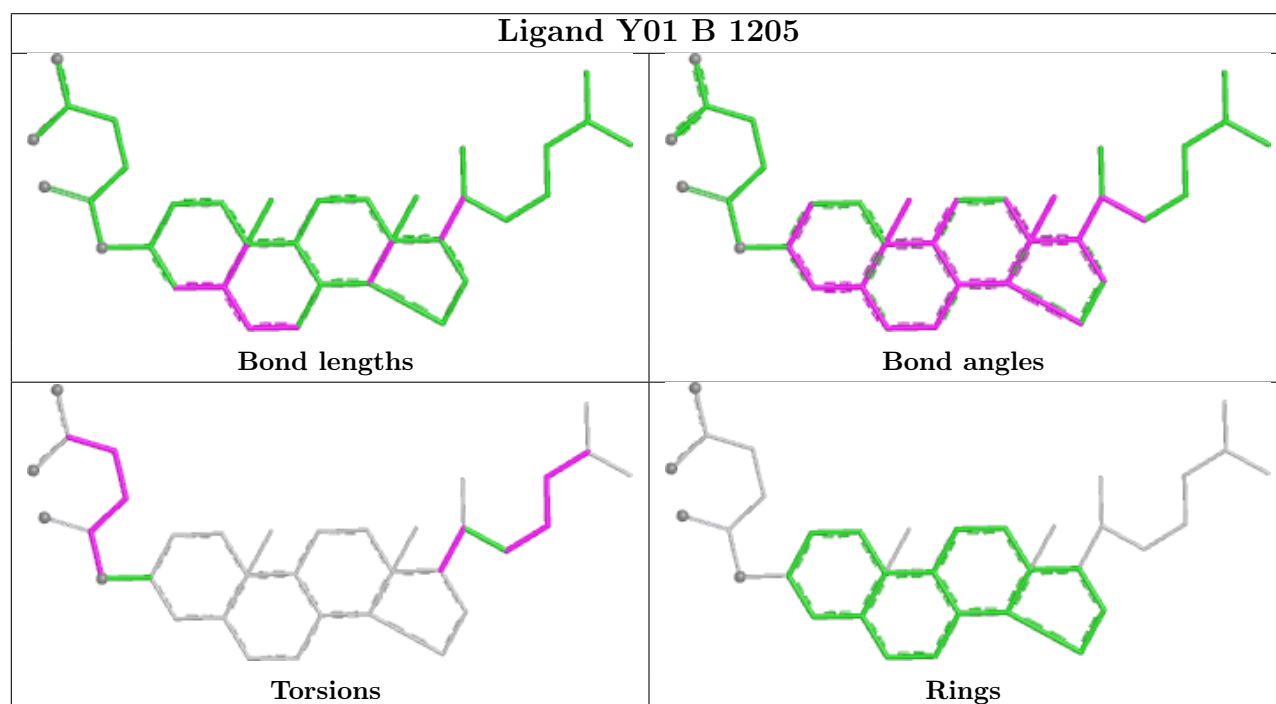
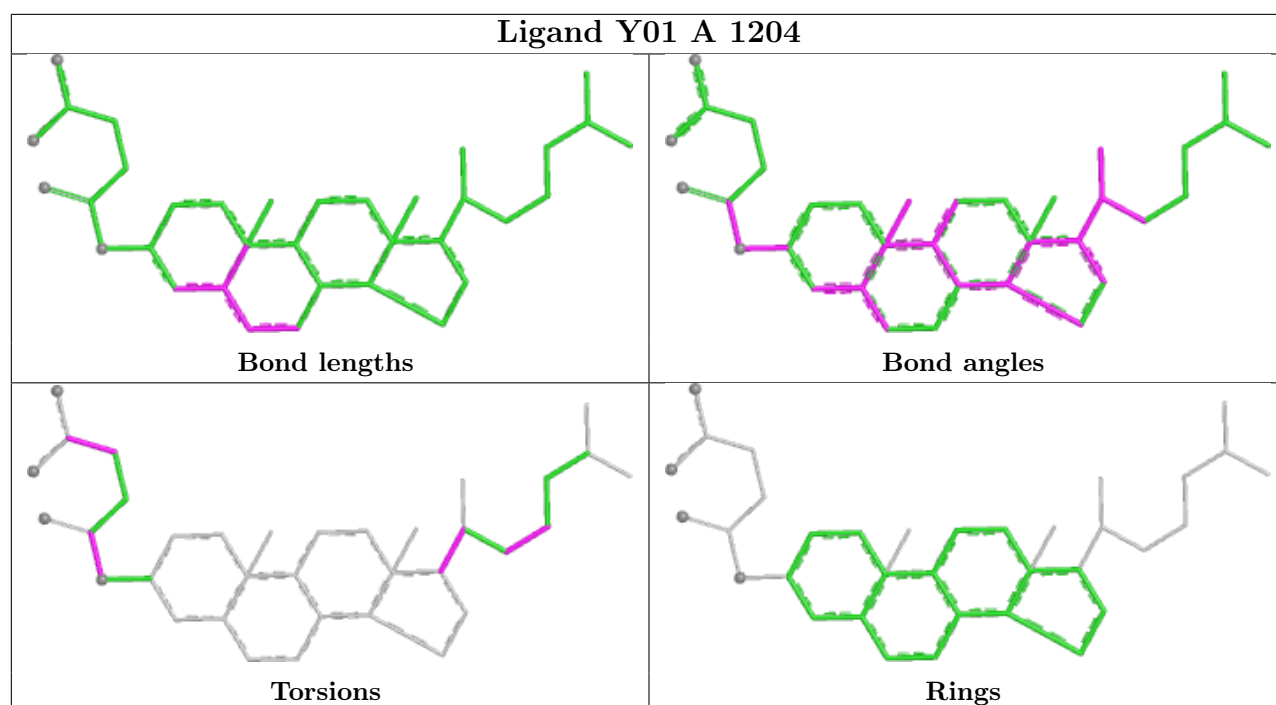
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

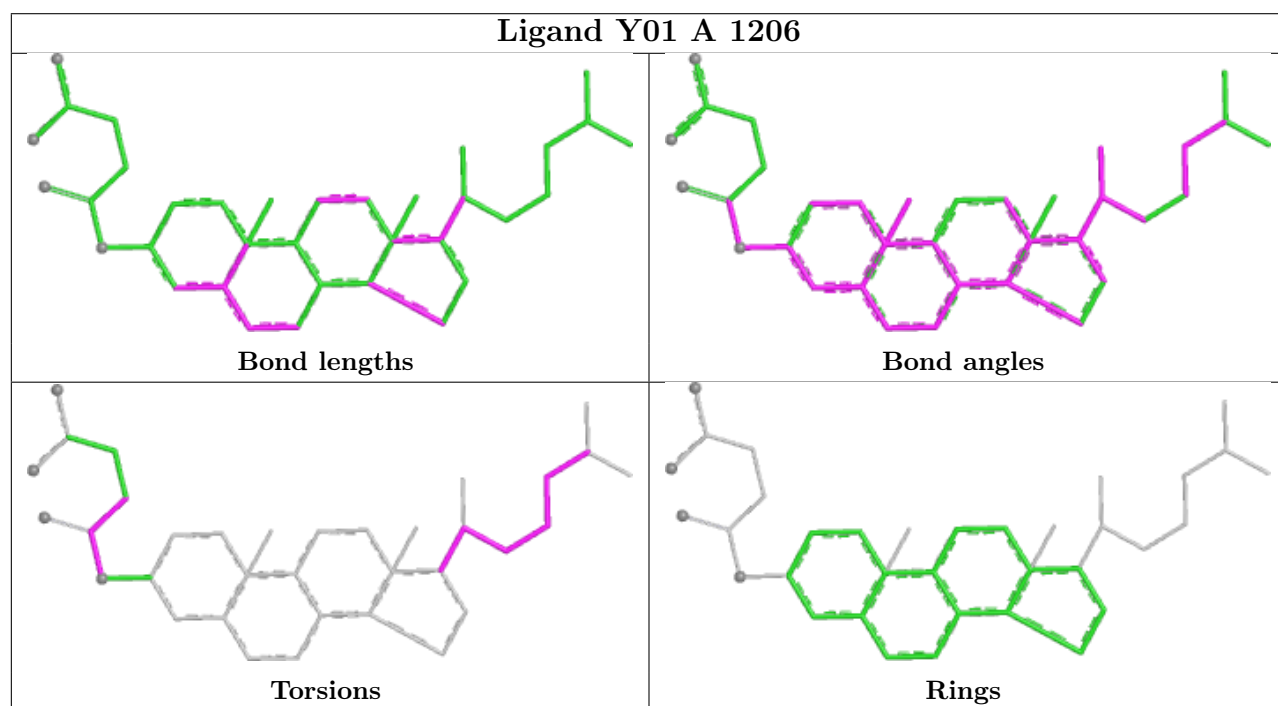
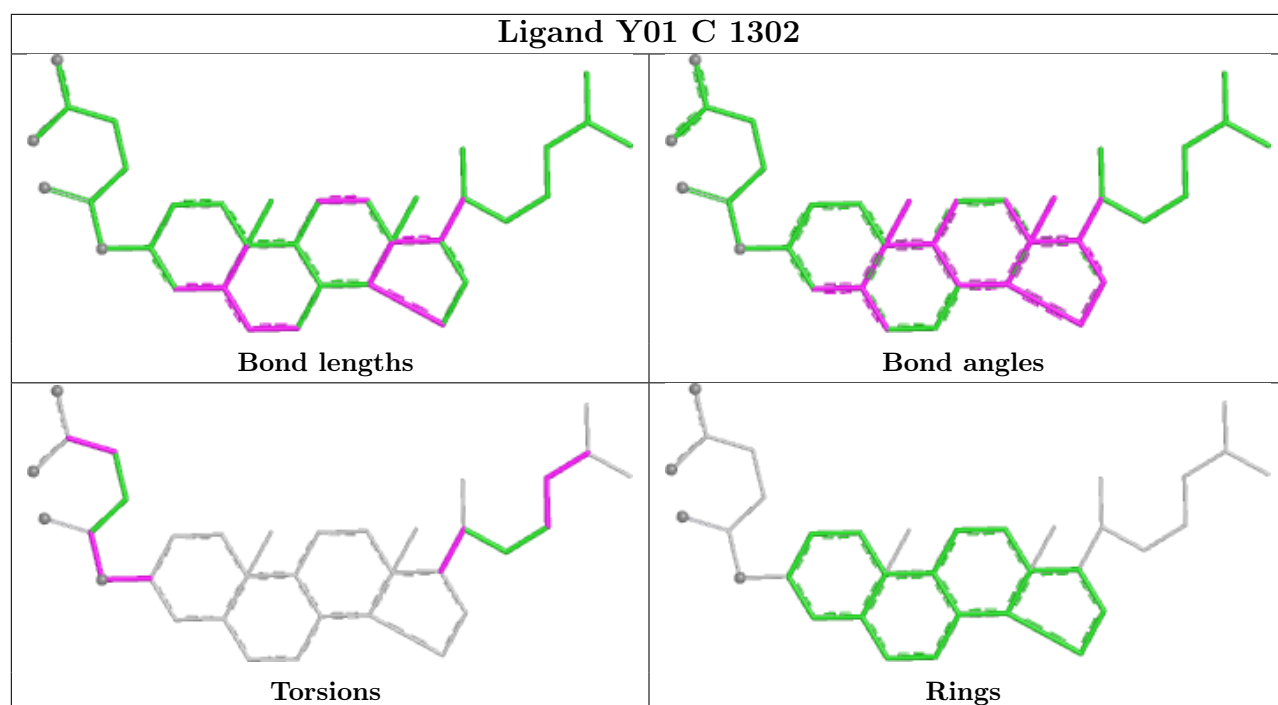
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

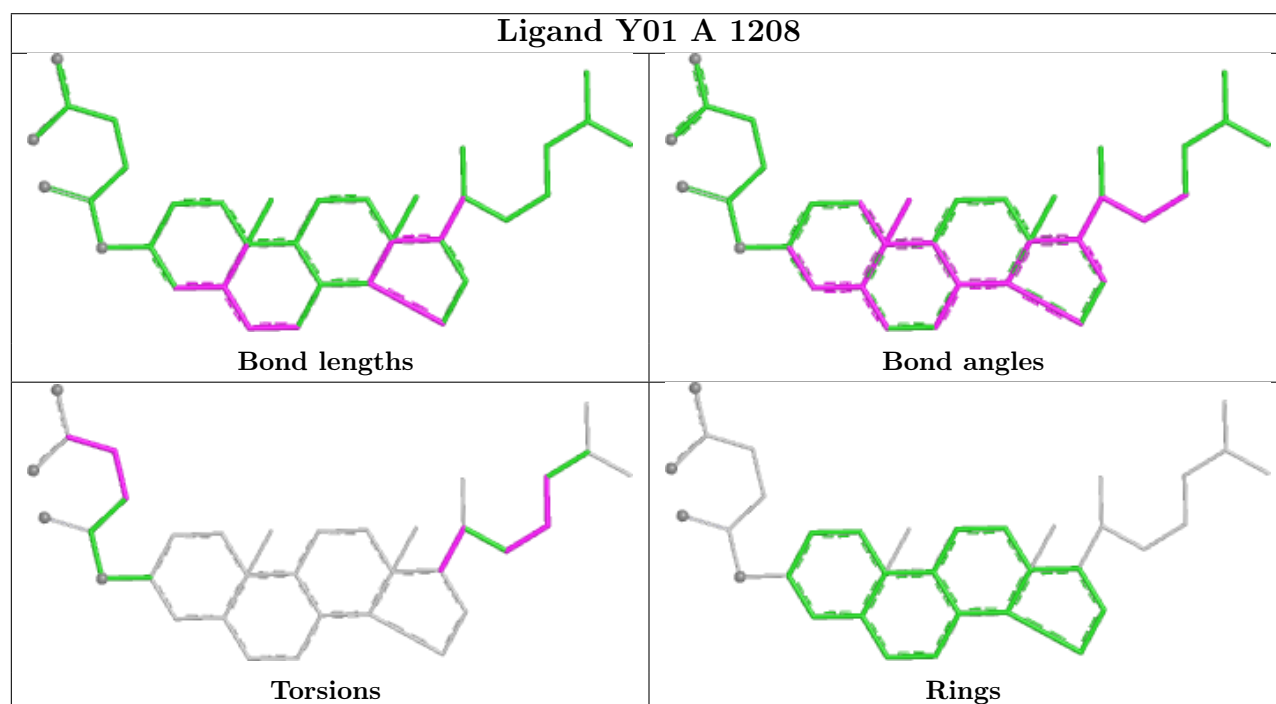
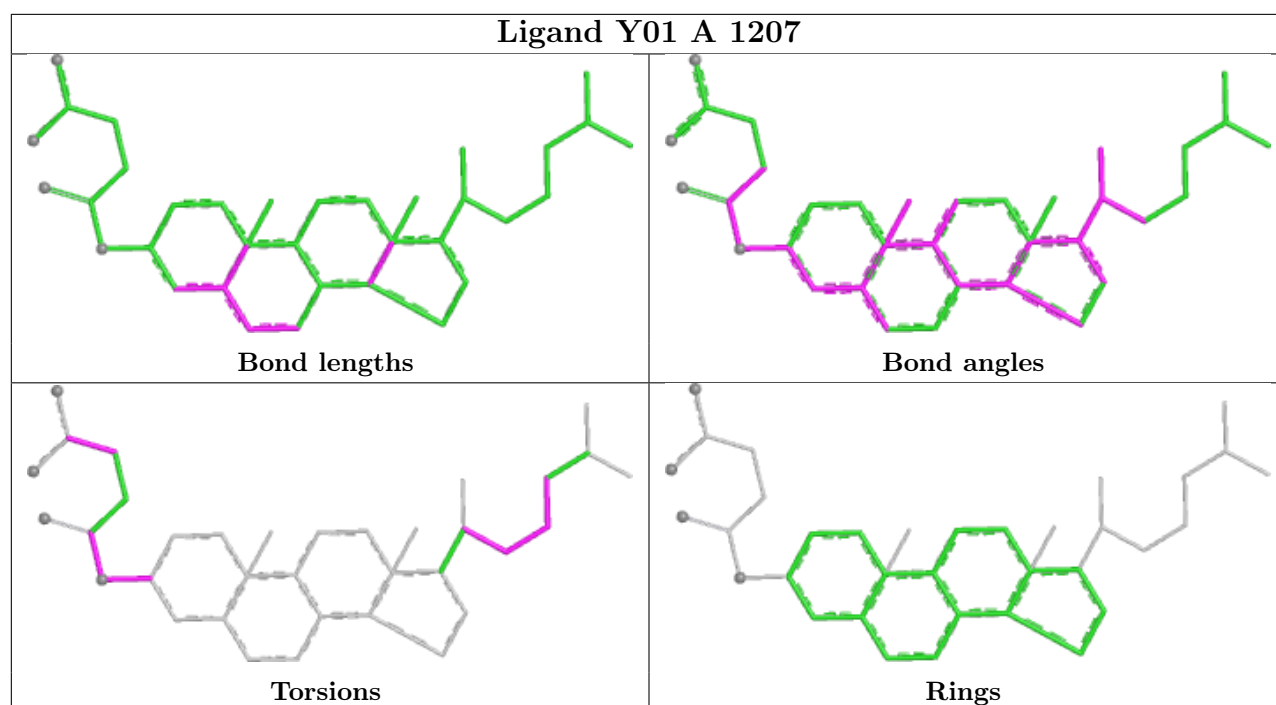


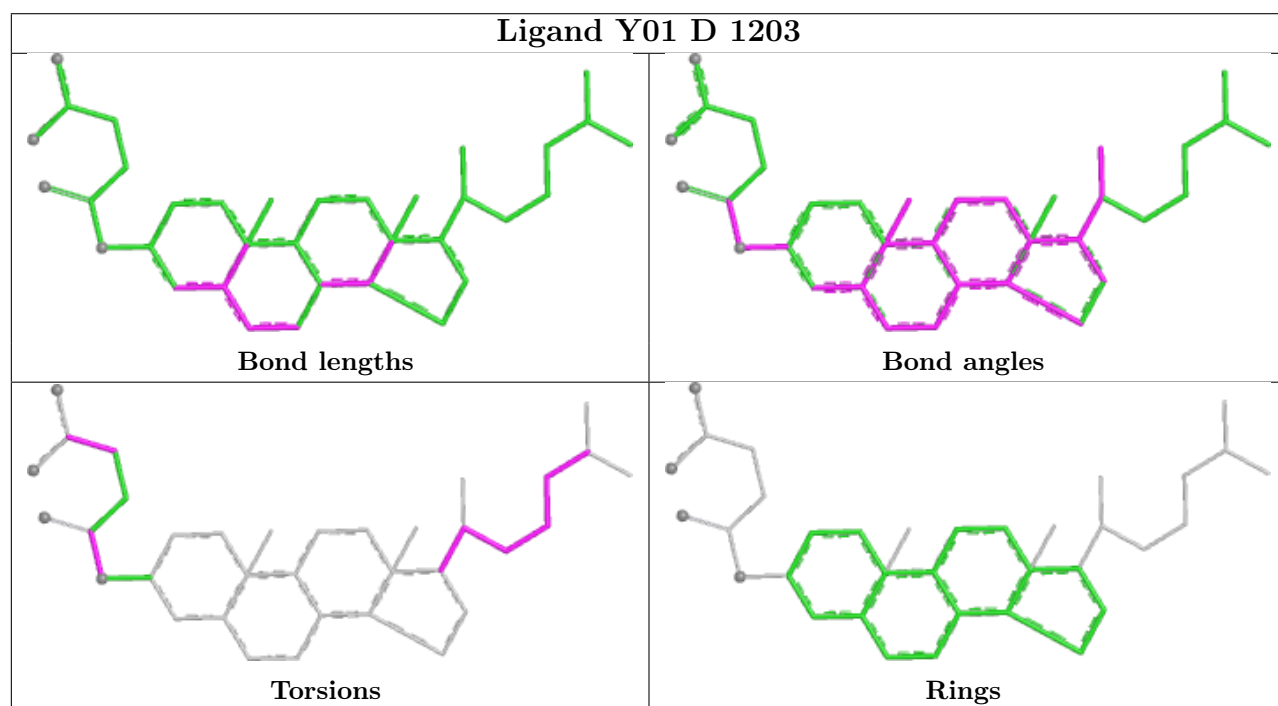
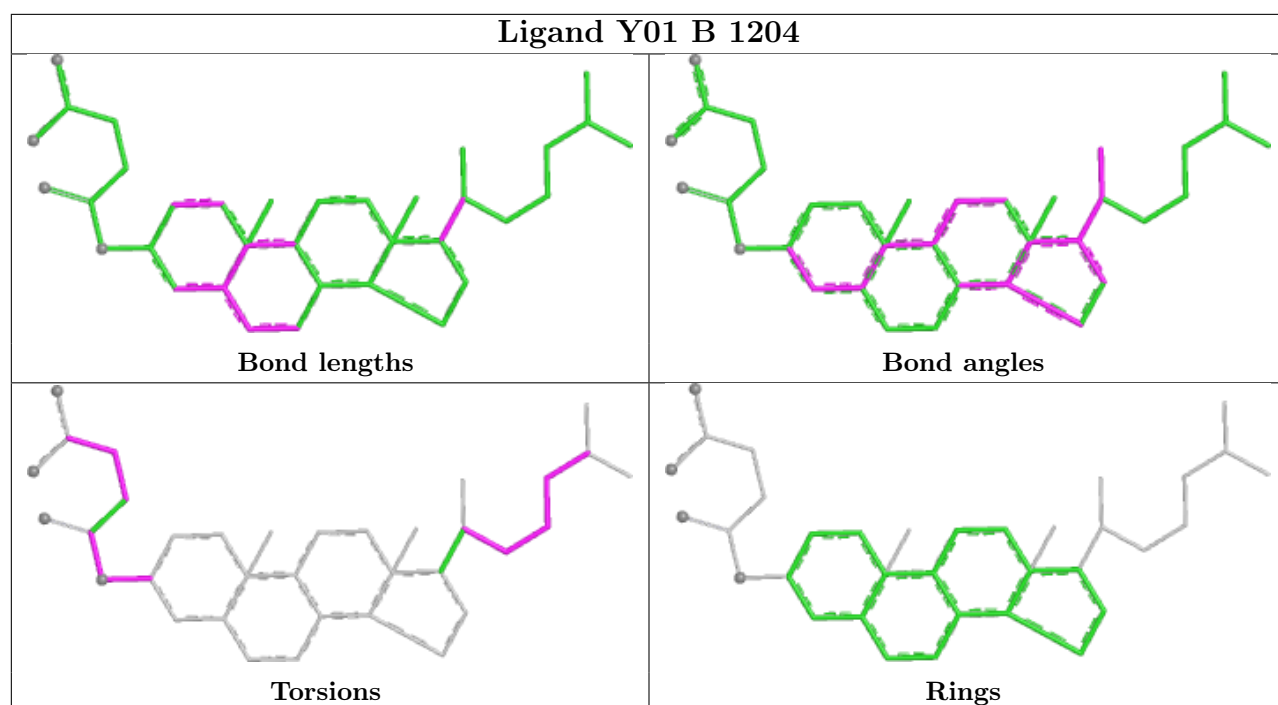


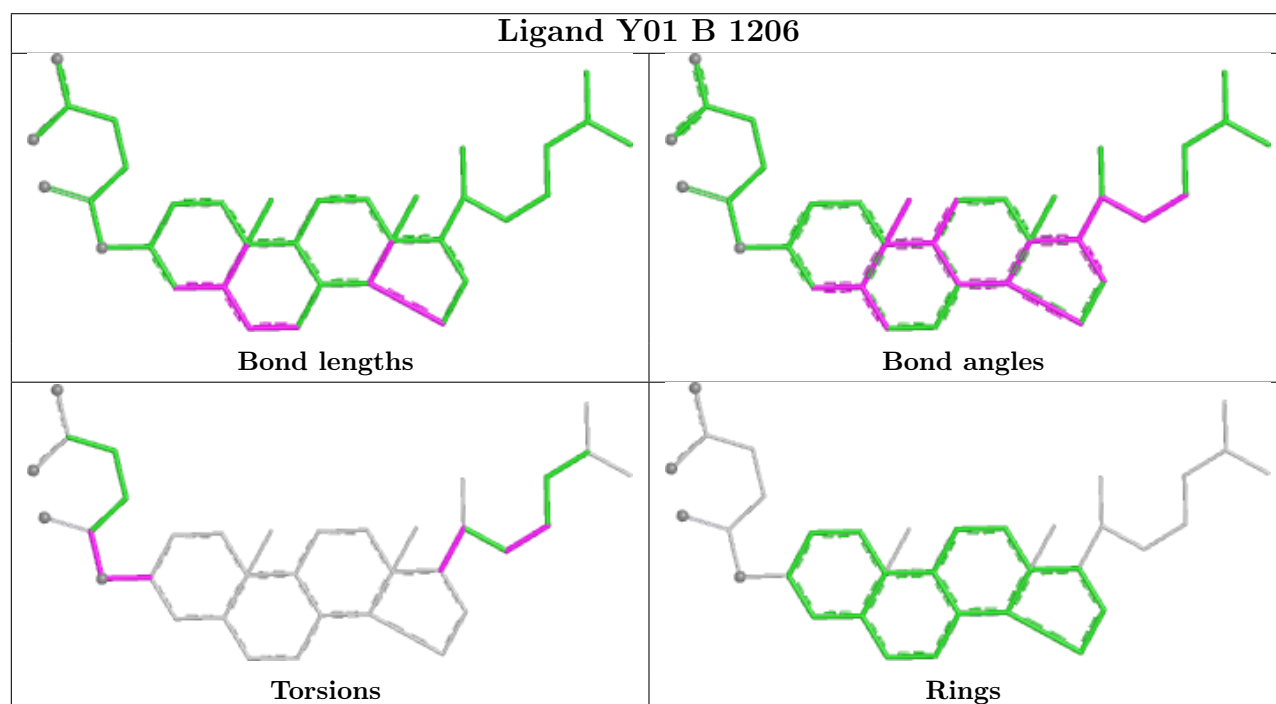
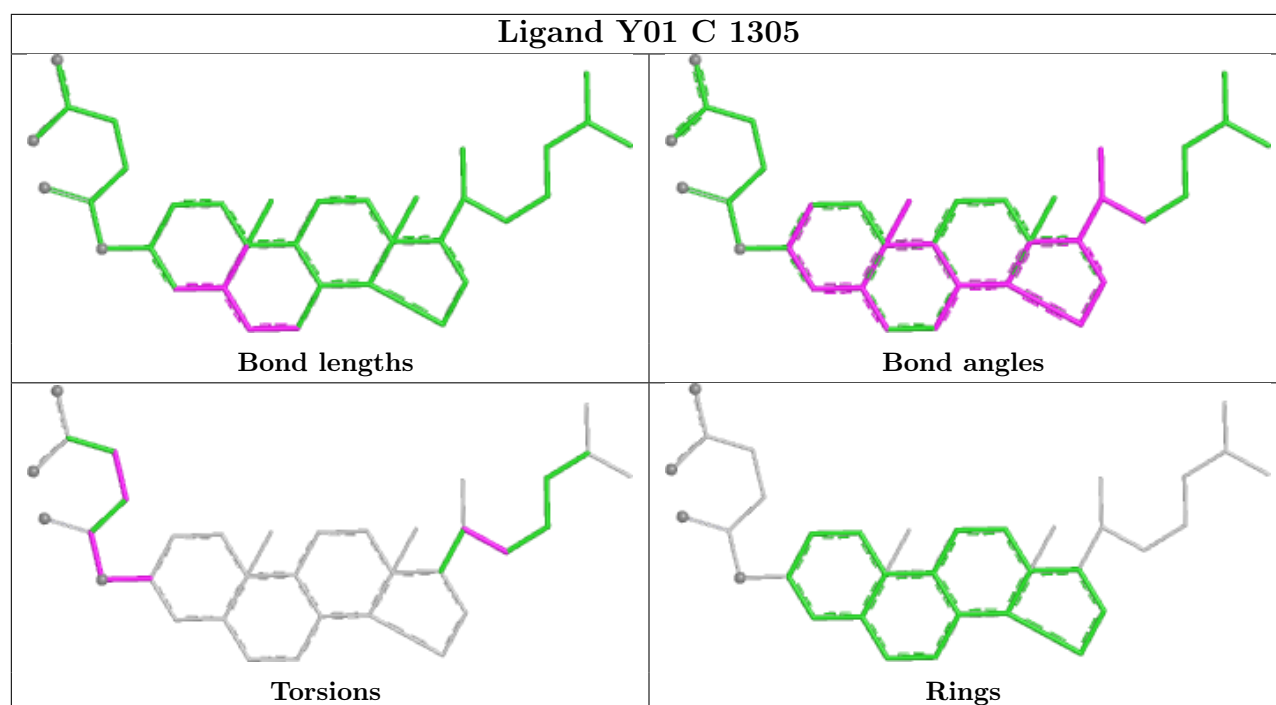


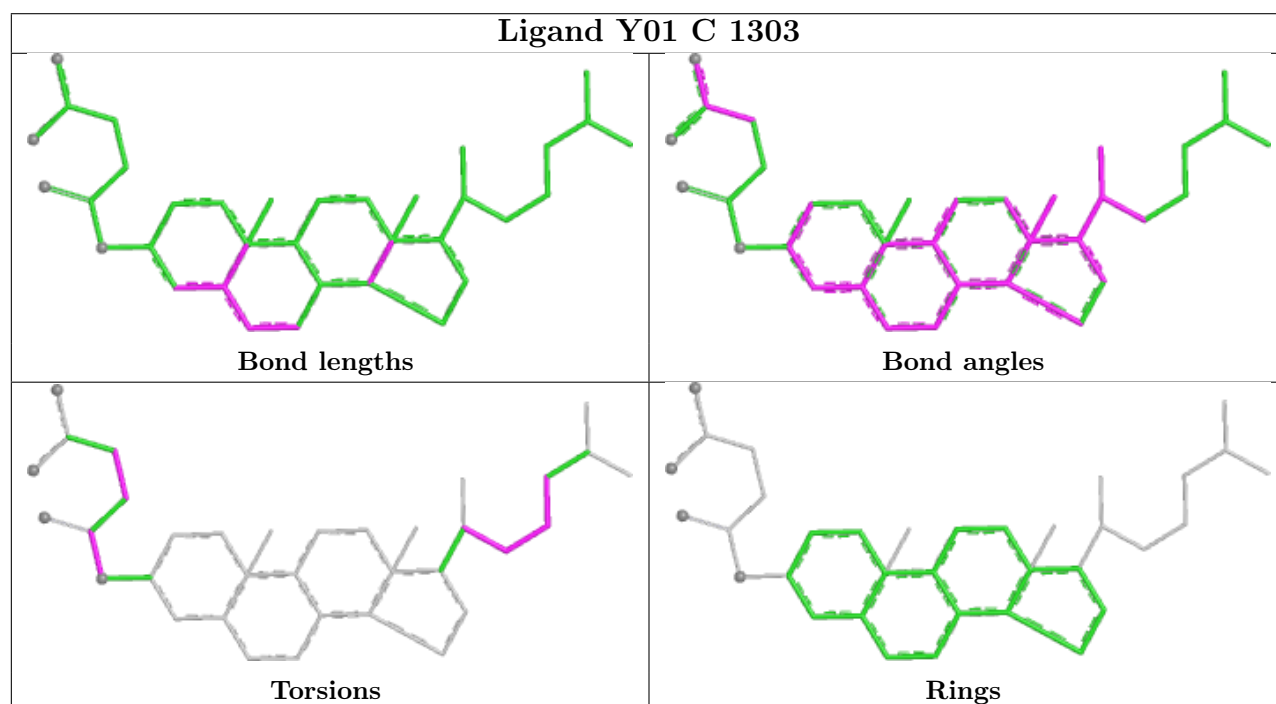
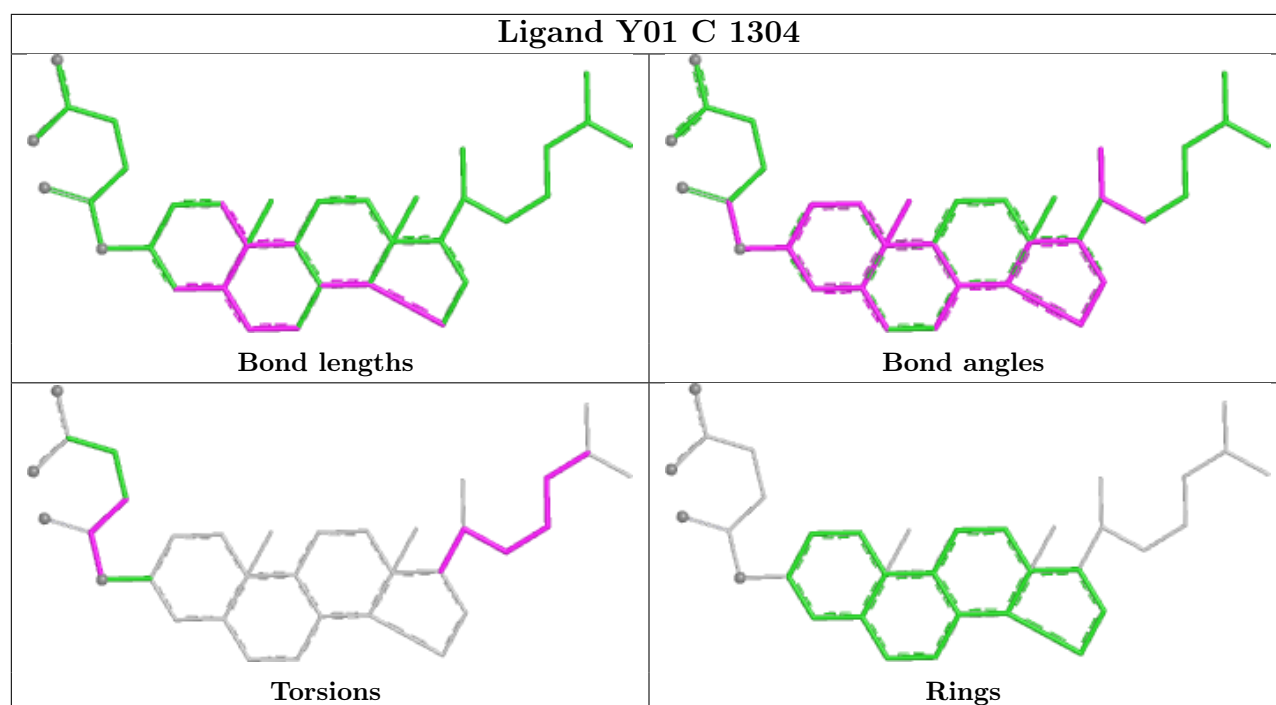


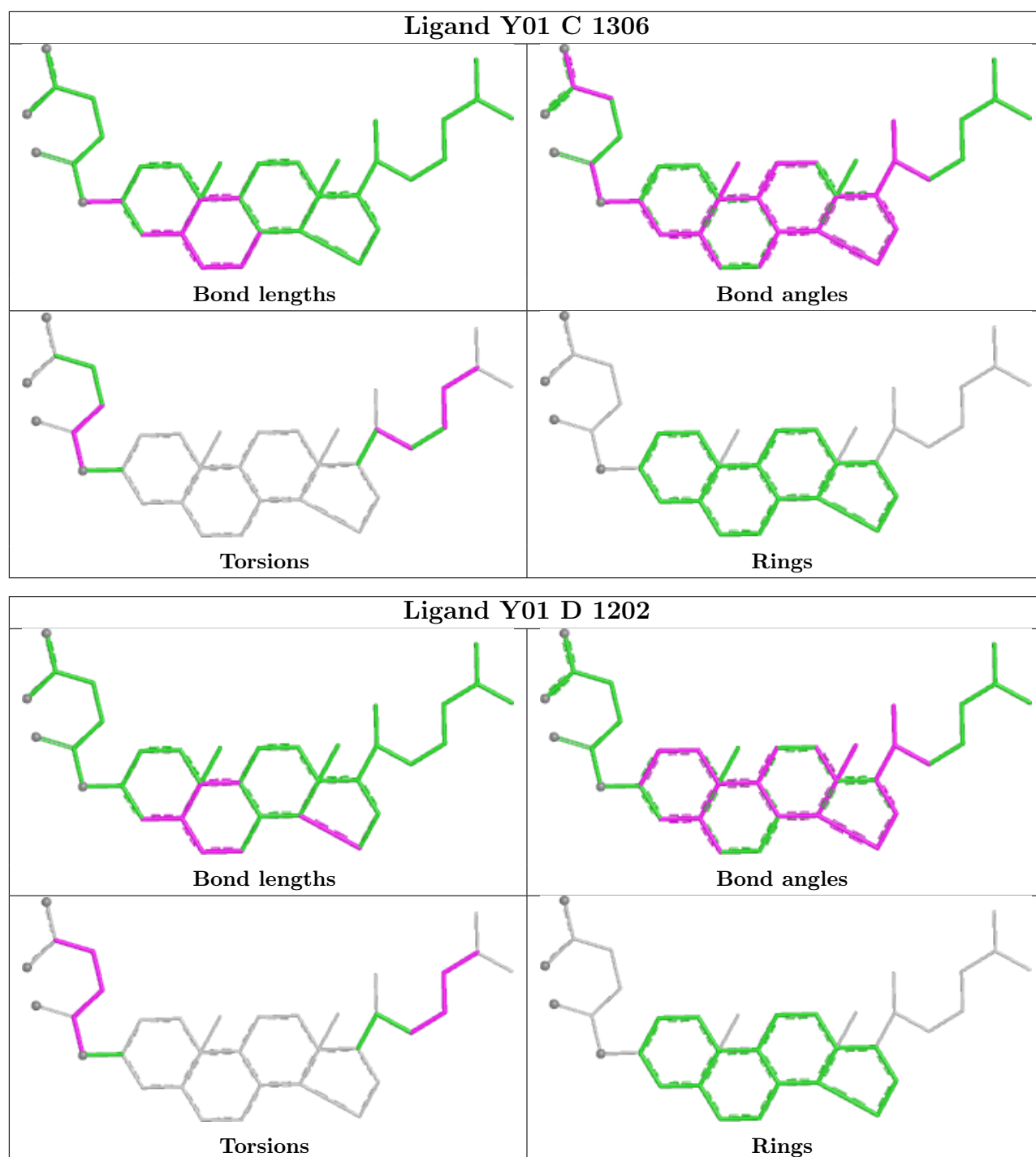












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7
1	B	7
1	C	7
1	D	7

The worst 5 of 28 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:UNK	C	159:UNK	N	27.67
1	B	36:UNK	C	159:UNK	N	27.67
1	C	36:UNK	C	37:UNK	N	27.67
1	D	36:UNK	C	159:UNK	N	27.67
1	A	303:UNK	C	305:LYS	N	27.63

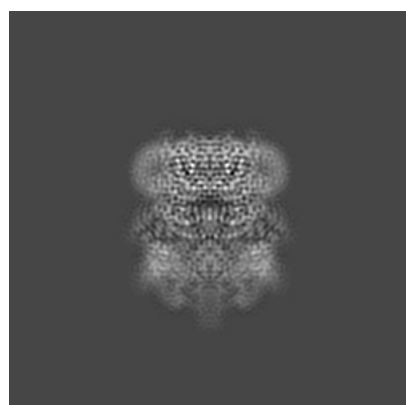
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7297. These allow visual inspection of the internal detail of the map and identification of artifacts.

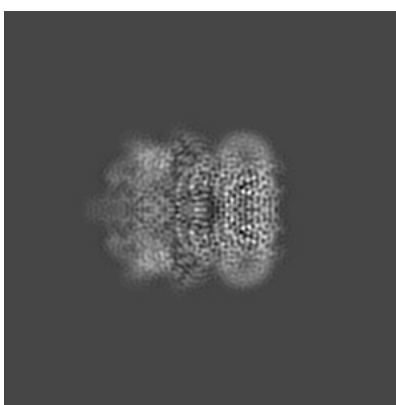
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

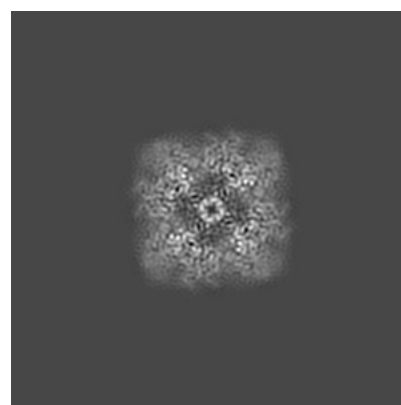
6.1.1 Primary map



X



Y



Z

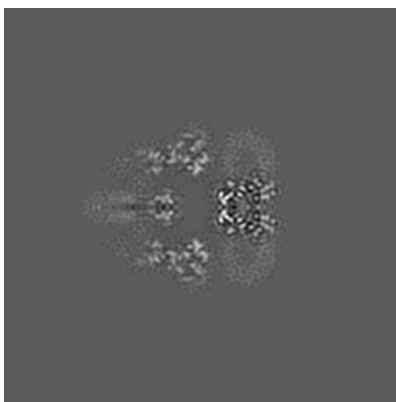
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

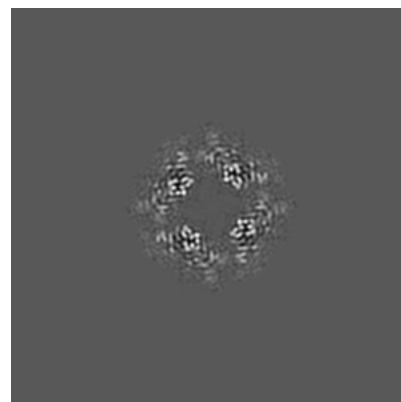
6.2.1 Primary map



X Index: 128



Y Index: 128

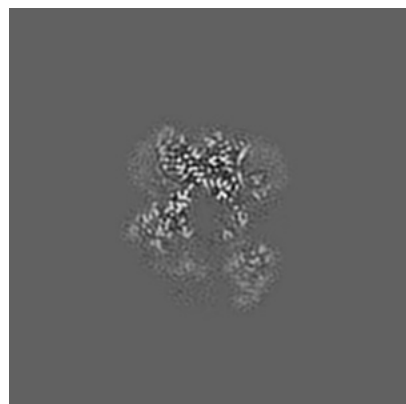


Z Index: 128

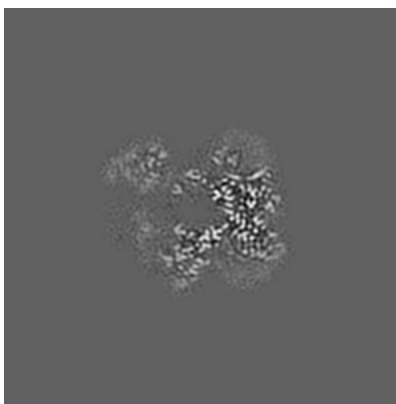
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

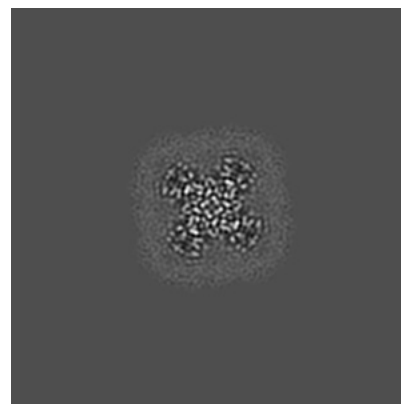
6.3.1 Primary map



X Index: 115



Y Index: 141

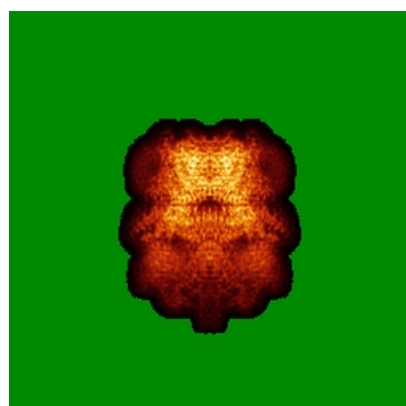


Z Index: 161

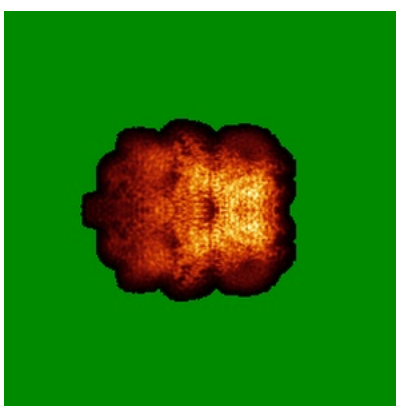
The images above show the largest variance slices of the map in three orthogonal directions.

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

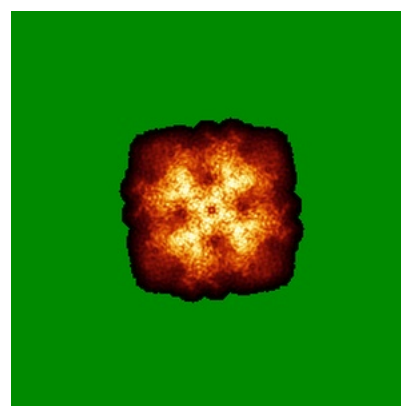
6.4.1 Primary map



X



Y

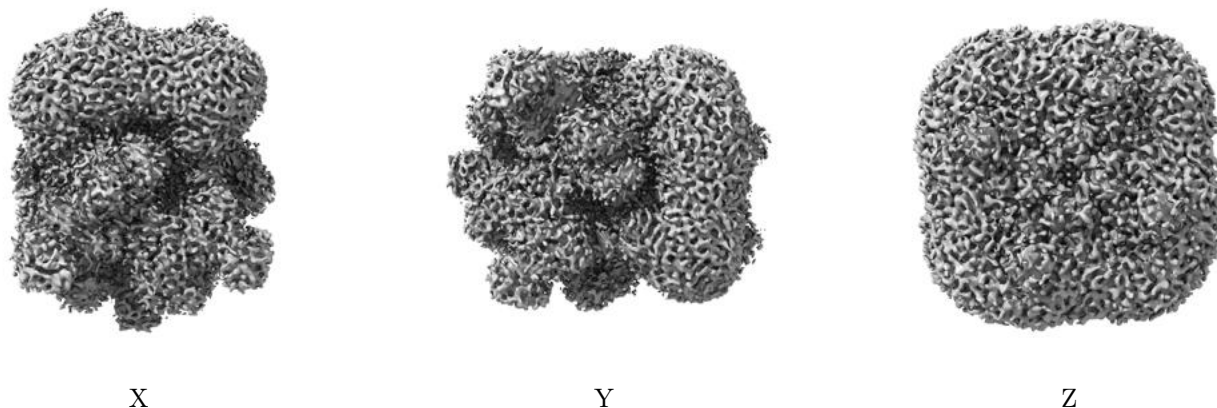


Z

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 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

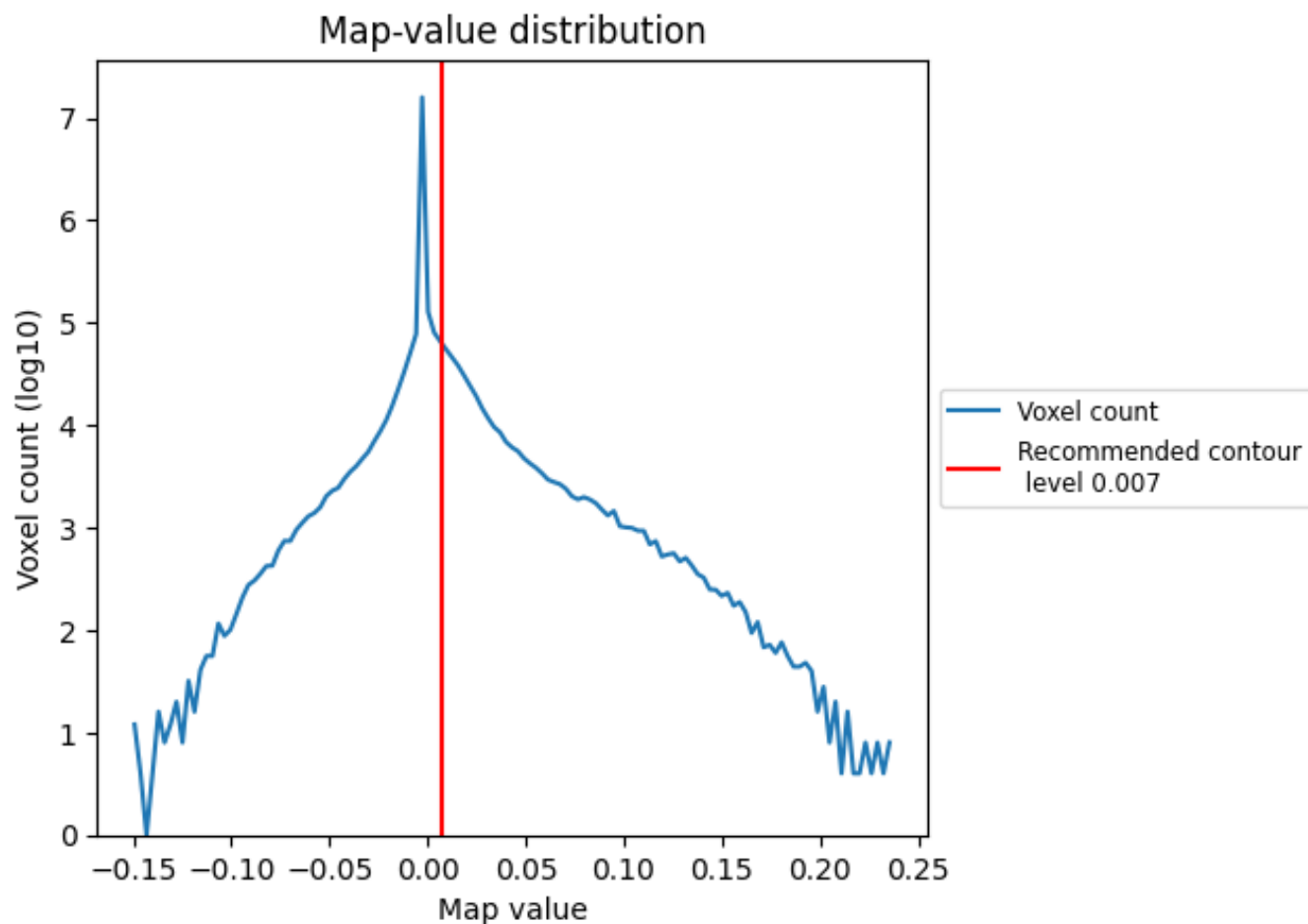
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

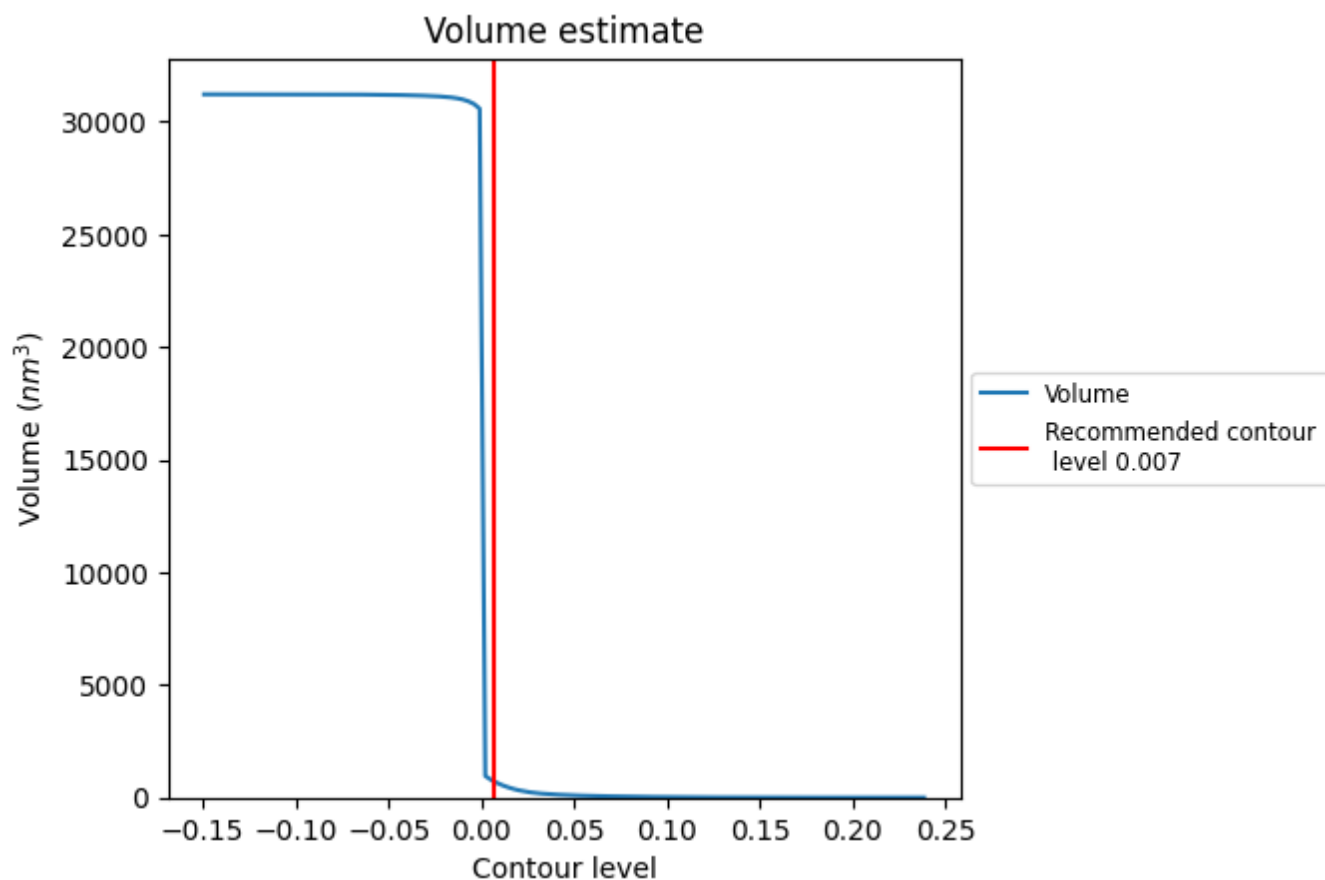
This section contains the results of statistical analysis of the map.

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.

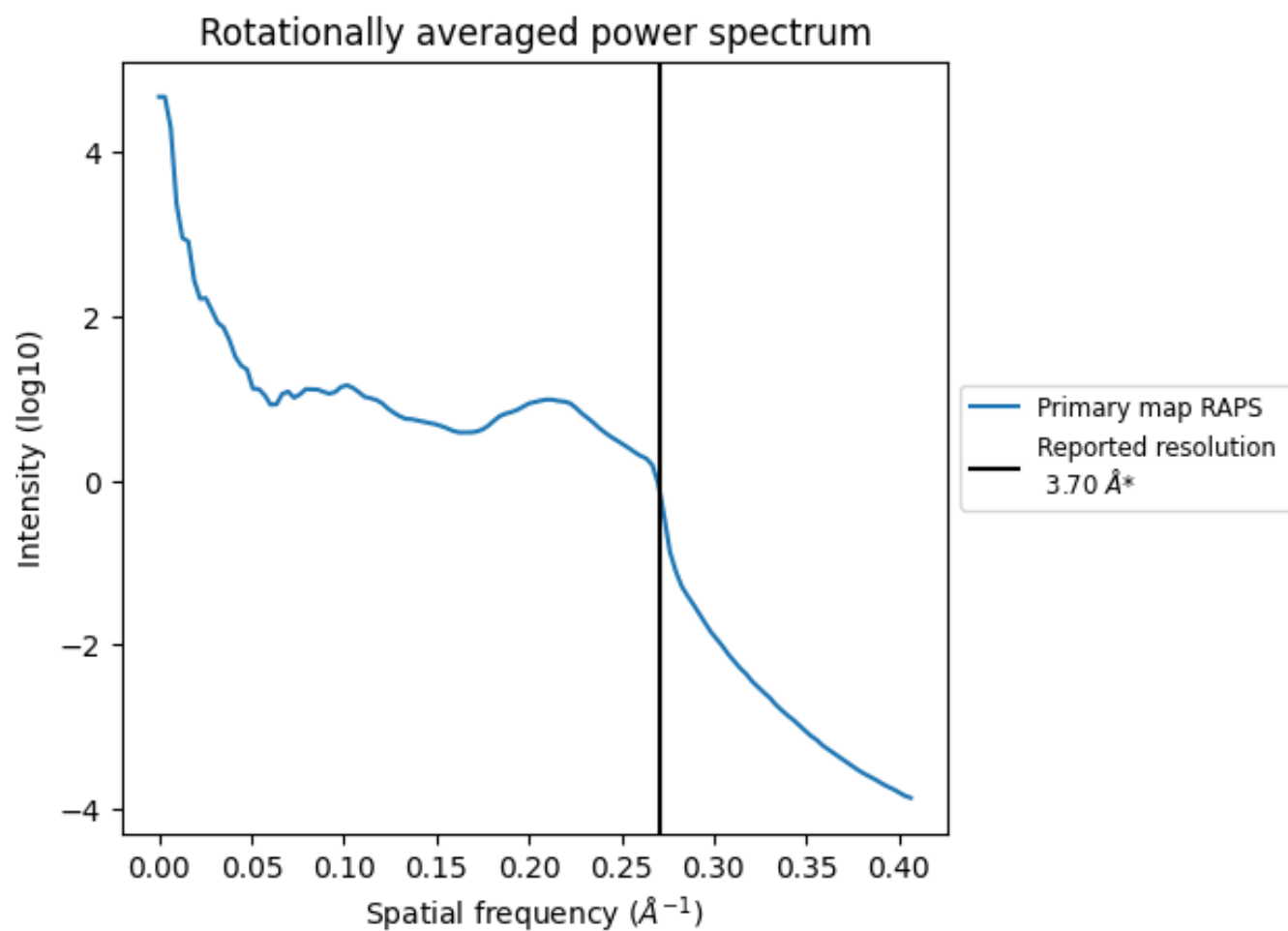
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 713 nm^3 ; this corresponds to an approximate mass of 644 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 ⓘ

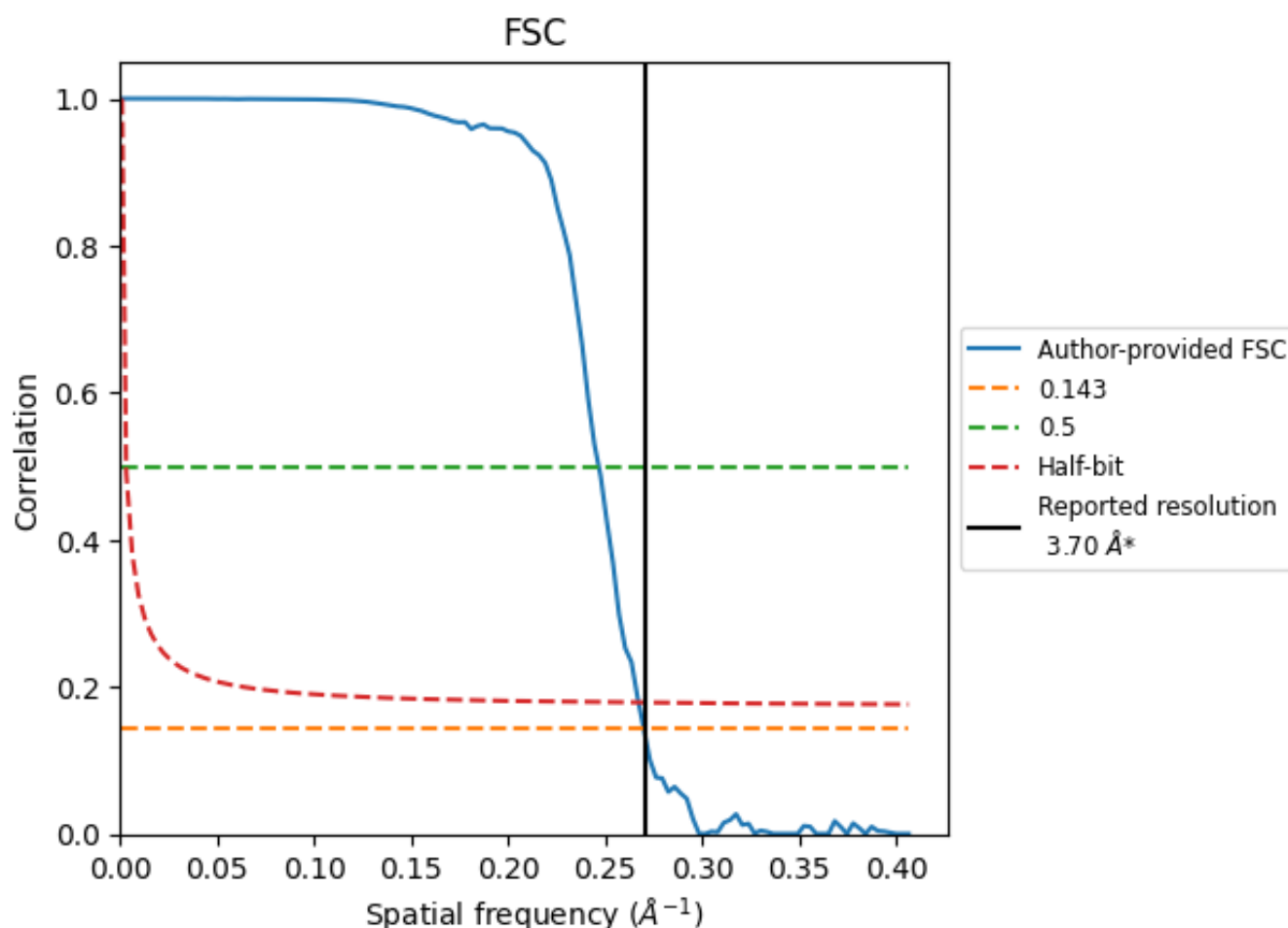


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

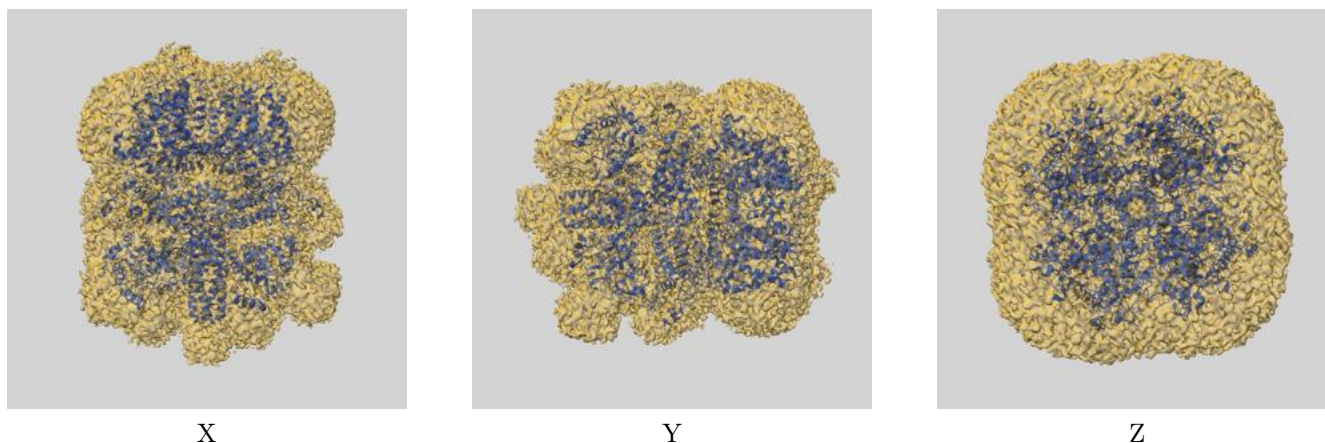
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.06	3.75
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

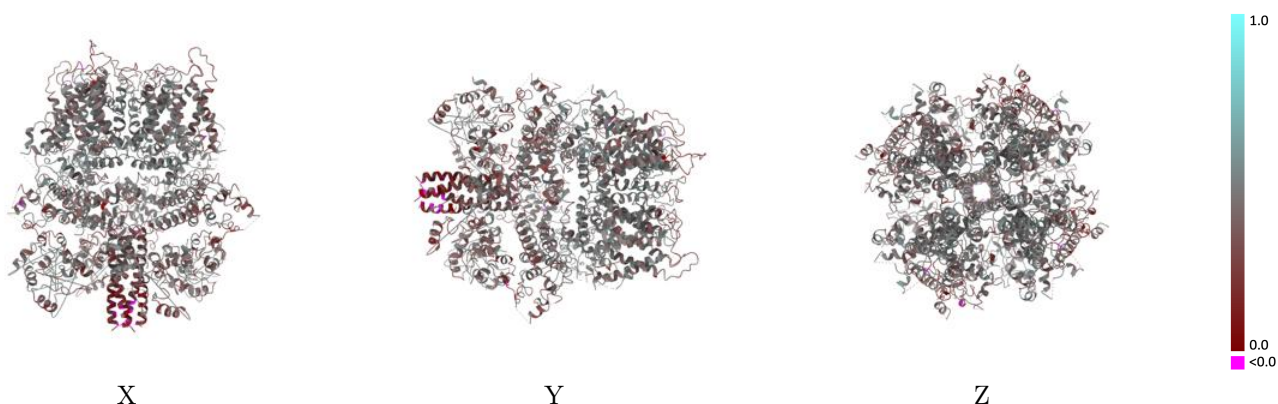
This section contains information regarding the fit between EMDB map EMD-7297 and PDB model 6BWD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



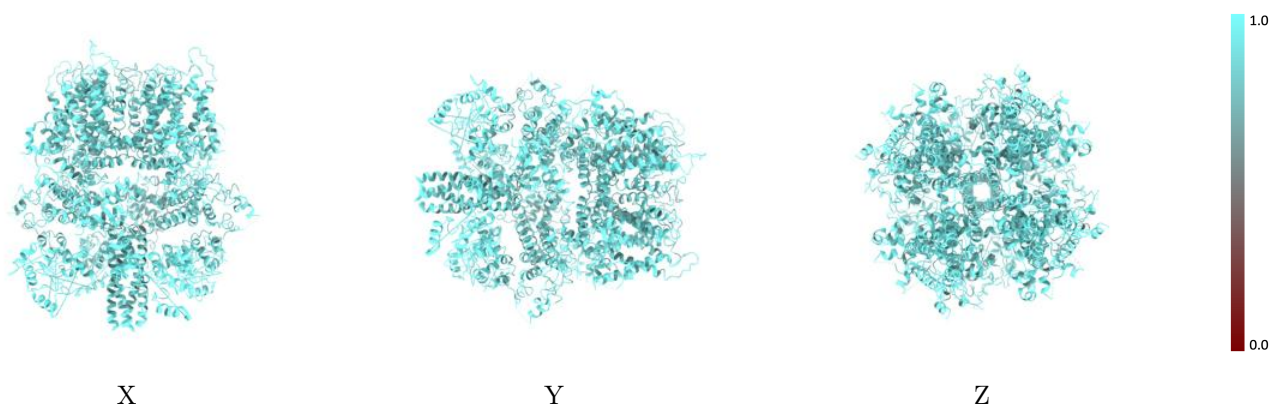
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



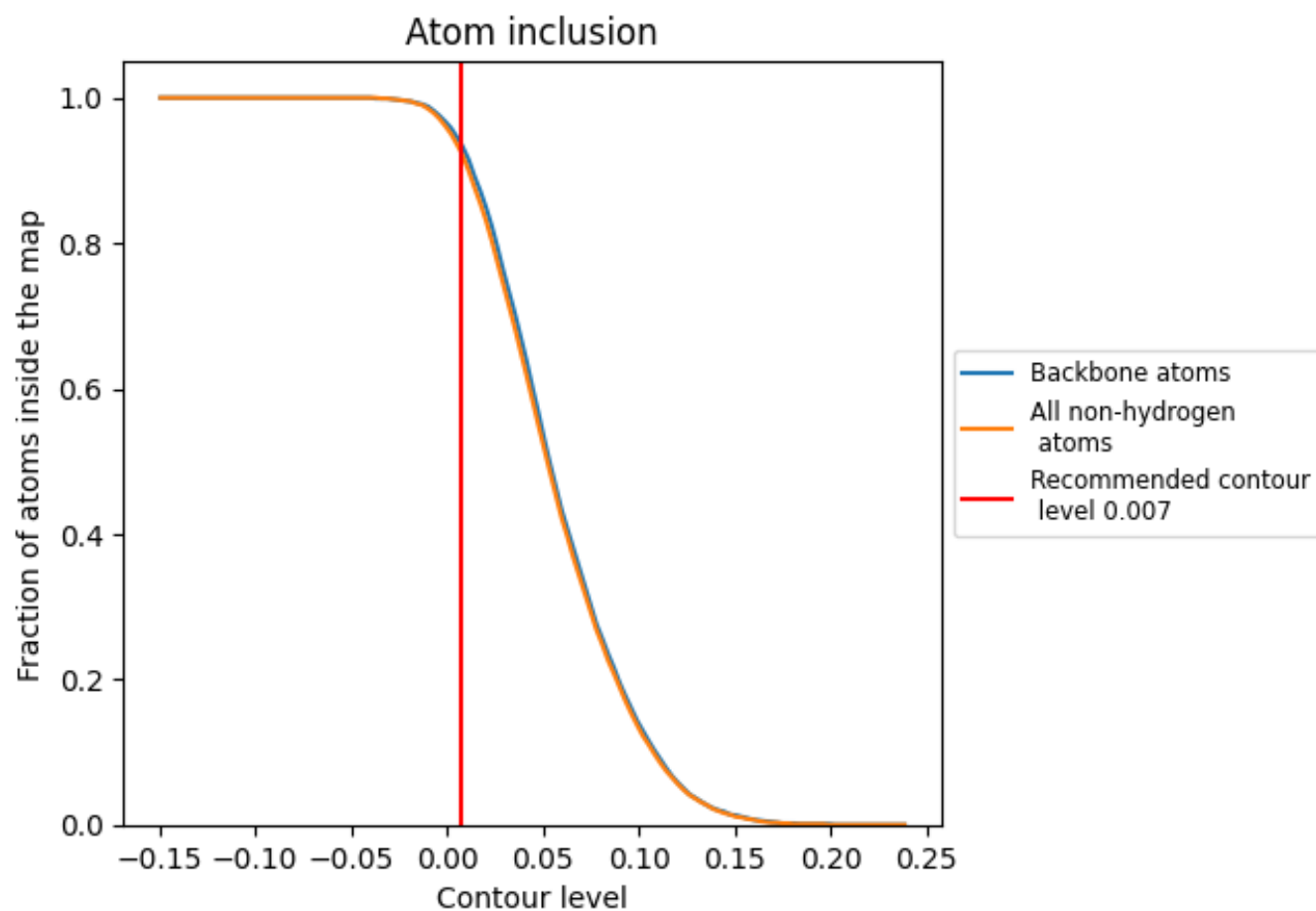
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9270	<div></div> 0.4180
A	<div></div> 0.9210	<div></div> 0.4030
B	<div></div> 0.9270	<div></div> 0.4230
C	<div></div> 0.9330	<div></div> 0.4270
D	<div></div> 0.9320	<div></div> 0.4200

