



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 09:45 AM UTC

PDB ID : 6TBU / pdb_00006tbu
EMDB ID : EMD-10452
Title : Structure of Drosophila melanogaster Dispatched
Authors : Korkhov, V.M.; Cannac, F.
Deposited on : 2019-11-04
Resolution : 3.16 Å(reported)

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

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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

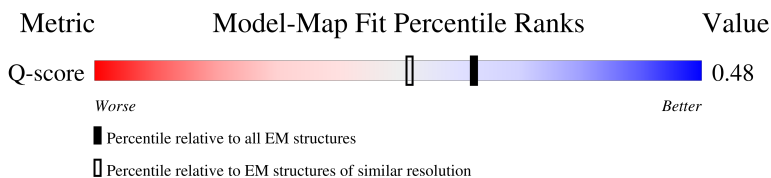
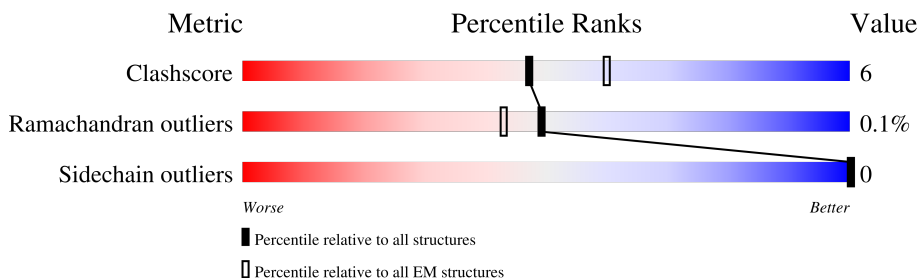
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 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	14474 (2.66 - 3.66)

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	1218	
2	B	2	

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
2	NAG	B	2	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14212 atoms, of which 7124 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.

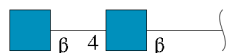
- Molecule 1 is a protein called Protein dispatched.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	842	13376	4440	6645	1055	1186	50	0	0

There is a discrepancy between the modelled and reference sequences:

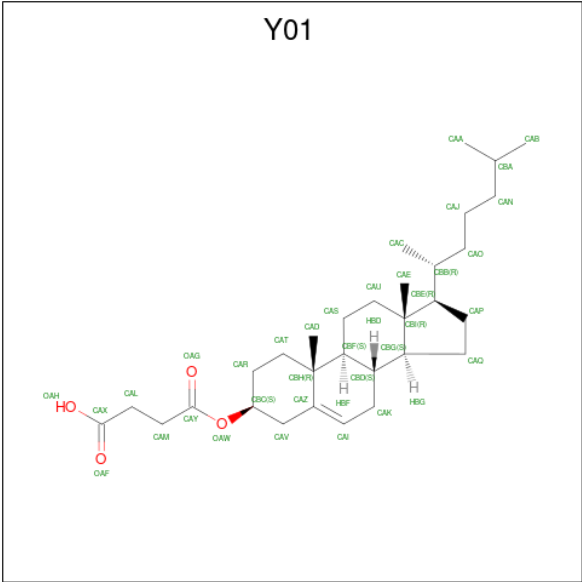
Chain	Residue	Modelled	Actual	Comment	Reference
A	731	TYR	GLU	conflict	UNP Q9VNIJ5

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
2	B	2	53	16	25	2	10	0	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).

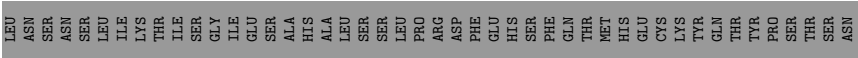
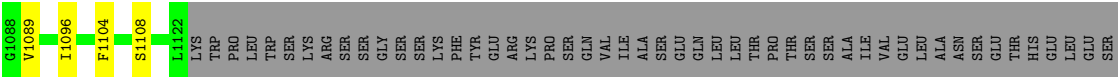


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
4	A	1	27	8	13	1	5	0



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	286136	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	246.24, 246.24, 246.24	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.81, 0.81, 0.81	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, NAG

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	0.28	0/6915	0.49	1/9413 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	45	PRO	CB-CG-CD	-5.25	89.31	106.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	LEU	Peptide
1	A	422	ILE	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	6731	6645	6637	73	0
2	B	28	25	25	0	0
3	A	315	441	439	18	0
4	A	14	13	13	0	0
All	All	7088	7124	7114	85	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 6.

All (85) 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:A:17:ALA:O	1:A:627:ARG:NH2	2.21	0.74
1:A:1017:GLU:OE2	1:A:1086:GLN:NE2	2.21	0.74
1:A:698:GLU:O	1:A:914:THR:OG1	2.06	0.71
1:A:576:VAL:HG12	1:A:1033:LEU:HD13	1.74	0.70
1:A:842:TYR:O	1:A:846:GLN:NE2	2.26	0.69
1:A:591:SER:O	1:A:597:LYS:NZ	2.28	0.67
1:A:1025:ILE:O	1:A:1029:VAL:HG23	1.94	0.67
1:A:384:PHE:O	1:A:392:VAL:N	2.28	0.67
1:A:611:TYR:CZ	1:A:615:ILE:HD11	2.30	0.67
1:A:861:VAL:HG12	1:A:903:VAL:HG21	1.81	0.63
1:A:520:LEU:HD21	1:A:573:SER:OG	1.99	0.62
1:A:444:LEU:HD12	1:A:1081:ILE:HD13	1.81	0.61
1:A:780:PHE:O	1:A:784:VAL:HG23	2.00	0.61
1:A:734:LYS:NZ	1:A:909:ASN:O	2.23	0.60
1:A:737:MET:HE1	1:A:789:PHE:CD1	2.37	0.60
1:A:525:TRP:NE1	1:A:626:GLU:OE2	2.35	0.59
1:A:525:TRP:HE3	1:A:566:THR:HG21	1.66	0.59
1:A:1079:SER:O	1:A:1085:ILE:HD11	2.04	0.58
3:A:1506:Y01:HAC1	3:A:1506:Y01:HAU2	1.87	0.57
1:A:505:LEU:HD22	1:A:1087:ILE:CD1	2.34	0.57
1:A:327:THR:O	1:A:331:VAL:N	2.39	0.55
1:A:784:VAL:HG22	1:A:929:TRP:HH2	1.71	0.55
1:A:1104:PHE:O	1:A:1108:SER:OG	2.16	0.55
1:A:575:PHE:CZ	1:A:579:LEU:HD12	2.42	0.55
1:A:520:LEU:HD13	1:A:1058:ILE:HD11	1.90	0.54
1:A:576:VAL:CG1	1:A:1033:LEU:HD13	2.38	0.53
1:A:272:LEU:HD13	1:A:327:THR:CB	2.39	0.52
3:A:1509:Y01:HAC1	3:A:1509:Y01:HAU2	1.91	0.52
1:A:784:VAL:HG22	1:A:929:TRP:CH2	2.45	0.52
1:A:576:VAL:HG13	1:A:977:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:TRP:CE3	1:A:566:THR:HG21	2.44	0.51
1:A:999:ILE:O	1:A:1003:VAL:HG23	2.10	0.51
3:A:1503:Y01:HAC1	3:A:1503:Y01:HAU2	1.93	0.51
1:A:1017:GLU:N	1:A:1017:GLU:OE1	2.44	0.51
1:A:432:ASP:O	1:A:433:LEU:HD23	2.10	0.50
1:A:700:SER:OG	1:A:701:HIS:N	2.45	0.50
3:A:1501:Y01:HAC1	3:A:1501:Y01:HAU2	1.94	0.50
1:A:1019:ILE:O	1:A:1023:THR:HG23	2.12	0.50
1:A:451:VAL:HG22	1:A:1076:MET:SD	2.52	0.50
1:A:505:LEU:HD13	1:A:1087:ILE:HD11	1.94	0.49
1:A:490:TYR:OH	1:A:498:PHE:O	2.29	0.49
1:A:562:ILE:O	1:A:566:THR:HG22	2.12	0.49
1:A:56:THR:OG1	1:A:954:ASN:ND2	2.46	0.49
3:A:1501:Y01:HAC1	3:A:1501:Y01:CAU	2.43	0.49
3:A:1507:Y01:HAC1	3:A:1507:Y01:HAU2	1.93	0.48
1:A:282:GLN:NE2	1:A:312:ASN:OD1	2.46	0.48
1:A:449:TRP:O	1:A:452:SER:OG	2.15	0.48
1:A:430:ALA:HB1	1:A:714:TYR:HB2	1.95	0.48
1:A:56:THR:HG21	1:A:958:THR:OG1	2.14	0.47
1:A:257:VAL:HB	1:A:430:ALA:HB3	1.94	0.47
1:A:436:GLU:OE1	1:A:436:GLU:N	2.47	0.47
1:A:698:GLU:HB3	1:A:915:ILE:HG22	1.96	0.47
3:A:1508:Y01:HAC1	3:A:1508:Y01:HAU2	1.95	0.47
1:A:967:ILE:HD11	1:A:1021:VAL:HG12	1.97	0.47
1:A:1096:ILE:HD11	3:A:1505:Y01:HAA2	1.97	0.47
1:A:740:VAL:HG22	1:A:903:VAL:HG12	1.98	0.46
1:A:471:ILE:HD13	1:A:522:LEU:HD11	1.98	0.46
1:A:317:LEU:HD11	1:A:372:VAL:HG11	1.98	0.45
1:A:338:LEU:HD21	1:A:376:LEU:HD22	1.98	0.45
1:A:959:LEU:HD21	1:A:1013:LEU:HD22	1.98	0.45
1:A:256:PHE:CE2	1:A:285:ILE:HD13	2.52	0.45
1:A:1009:LEU:HD21	3:A:1506:Y01:HAK1	1.99	0.44
1:A:1009:LEU:HD11	3:A:1506:Y01:HAK2	1.99	0.44
3:A:1505:Y01:HAU2	3:A:1505:Y01:HAC1	1.99	0.44
1:A:505:LEU:HD22	1:A:1087:ILE:HD11	2.00	0.44
1:A:683:SER:OG	3:A:1507:Y01:HAB2	2.18	0.44
1:A:466:THR:HG22	1:A:522:LEU:HD13	2.00	0.43
1:A:74:GLU:OE2	1:A:762:TYR:OH	2.36	0.43
1:A:1038:HIS:CE1	1:A:1058:ILE:HD13	2.54	0.43
3:A:1502:Y01:HAC1	3:A:1502:Y01:HAU2	2.00	0.43
1:A:667:MET:HE1	1:A:1048:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1506:Y01:HAD2	3:A:1506:Y01:HAS2	1.91	0.43
1:A:1009:LEU:HD11	3:A:1506:Y01:CAK	2.49	0.42
1:A:862:ALA:HA	1:A:903:VAL:HG23	2.02	0.42
1:A:665:SER:HB3	3:A:1504:Y01:HAE1	2.01	0.42
1:A:255:HIS:HB3	1:A:400:PHE:CD1	2.55	0.42
3:A:1505:Y01:HAC1	3:A:1505:Y01:CAU	2.50	0.41
1:A:369:LEU:HD23	1:A:370:ASN:H	1.84	0.41
1:A:1009:LEU:HD13	1:A:1089:VAL:HG11	2.02	0.41
1:A:419:VAL:O	1:A:419:VAL:HG23	2.20	0.41
1:A:47:PHE:O	1:A:441:ASN:ND2	2.53	0.41
3:A:1502:Y01:HAC1	3:A:1502:Y01:CAU	2.51	0.41
1:A:605:THR:O	1:A:609:THR:HG23	2.20	0.40
1:A:576:VAL:HG13	1:A:977:VAL:CG1	2.51	0.40
1:A:444:LEU:HD12	1:A:1081:ILE:CD1	2.48	0.40

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	820/1218 (67%)	778 (95%)	41 (5%)	1 (0%)	48 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	ASN

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	736/1087 (68%)	736 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	656	GLN
1	A	701	HIS

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 ⓘ

2 monosaccharides 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	NAG	B	1	1,2	14,14,15	0.24	0	17,19,21	0.50	0
2	NAG	B	2	2	14,14,15	0.28	0	17,19,21	1.04	2 (11%)

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	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/6/7	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	3.05	116.28	112.19
2	B	2	NAG	C2-N2-C7	2.22	125.88	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	NAG	C1

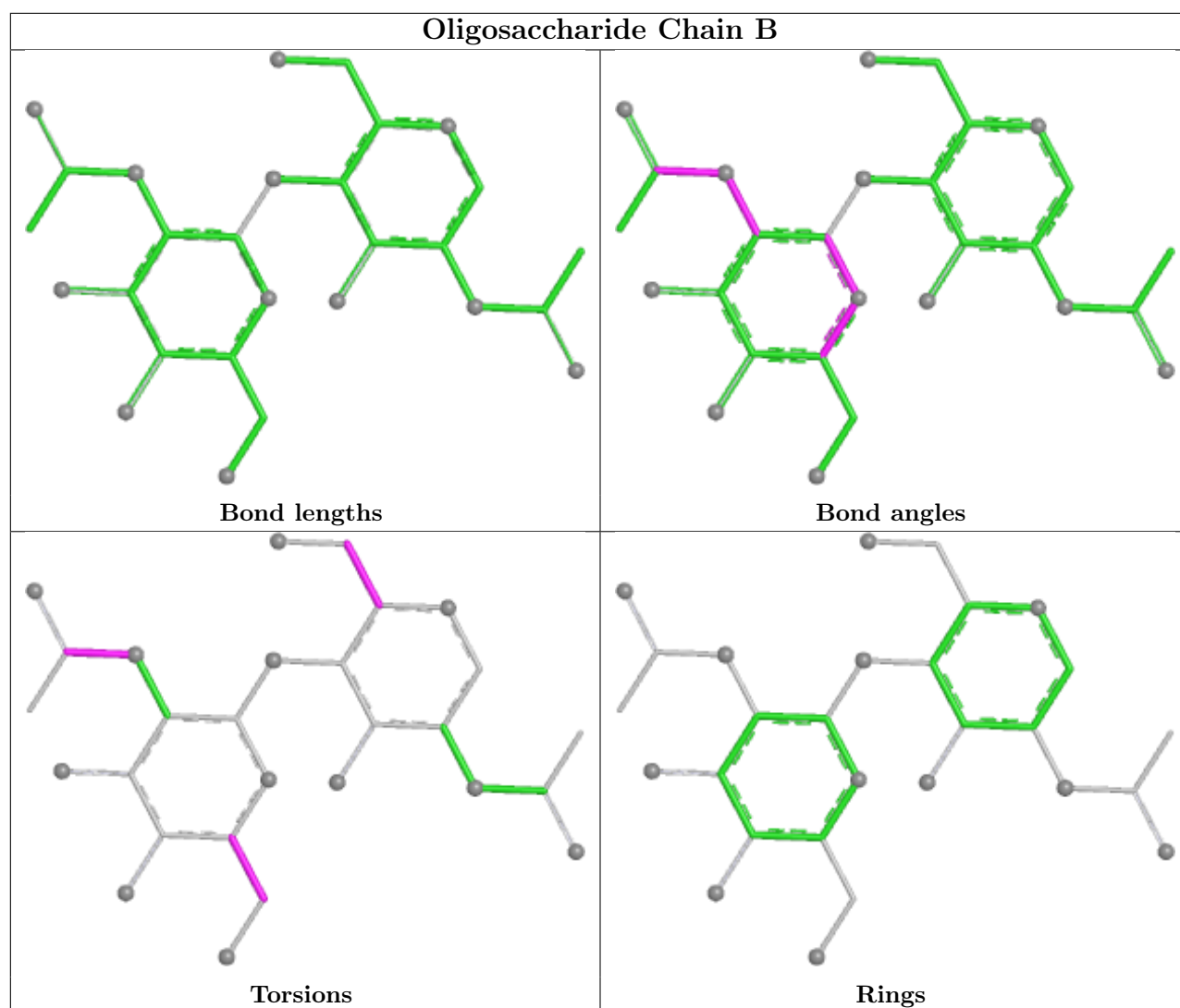
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
3	Y01	A	1502	-	38,38,38	2.09	7 (18%)	57,57,57	3.27	28 (49%)
3	Y01	A	1507	-	38,38,38	2.08	8 (21%)	57,57,57	3.26	27 (47%)
3	Y01	A	1503	-	38,38,38	2.08	9 (23%)	57,57,57	3.17	26 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	Y01	A	1505	-	38,38,38	2.09	8 (21%)	57,57,57	3.29	27 (47%)
3	Y01	A	1504	-	38,38,38	2.15	8 (21%)	57,57,57	3.30	30 (52%)
3	Y01	A	1506	-	38,38,38	2.16	11 (28%)	57,57,57	3.08	27 (47%)
3	Y01	A	1508	-	38,38,38	2.22	10 (26%)	57,57,57	3.18	25 (43%)
4	NAG	A	1510	1	14,14,15	0.18	0	17,19,21	0.53	0
3	Y01	A	1509	-	38,38,38	2.09	9 (23%)	57,57,57	3.22	29 (50%)
3	Y01	A	1501	-	38,38,38	2.47	14 (36%)	57,57,57	3.83	29 (50%)

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	A	1502	-	-	7/19/77/77	0/4/4/4
3	Y01	A	1507	-	-	10/19/77/77	0/4/4/4
3	Y01	A	1503	-	-	6/19/77/77	0/4/4/4
3	Y01	A	1505	-	-	8/19/77/77	0/4/4/4
3	Y01	A	1504	-	-	13/19/77/77	0/4/4/4
3	Y01	A	1506	-	-	10/19/77/77	0/4/4/4
3	Y01	A	1508	-	-	4/19/77/77	0/4/4/4
4	NAG	A	1510	1	-	0/6/23/26	0/1/1/1
3	Y01	A	1509	-	-	7/19/77/77	0/4/4/4
3	Y01	A	1501	-	-	7/19/77/77	0/4/4/4

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1504	Y01	CAE-CBI	6.63	1.65	1.54
3	A	1501	Y01	CAE-CBI	6.29	1.64	1.54
3	A	1506	Y01	CAE-CBI	6.15	1.64	1.54
3	A	1502	Y01	CAE-CBI	6.11	1.64	1.54
3	A	1505	Y01	CAE-CBI	6.03	1.64	1.54
3	A	1507	Y01	CAE-CBI	6.02	1.64	1.54
3	A	1508	Y01	CAE-CBI	5.85	1.64	1.54
3	A	1503	Y01	CAE-CBI	5.83	1.64	1.54
3	A	1508	Y01	CAL-CAX	5.79	1.64	1.50
3	A	1507	Y01	CAL-CAX	5.76	1.63	1.50
3	A	1509	Y01	CAL-CAX	5.70	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1506	Y01	CAL-CAX	5.63	1.63	1.50
3	A	1505	Y01	CAL-CAX	5.60	1.63	1.50
3	A	1501	Y01	CAL-CAX	5.58	1.63	1.50
3	A	1503	Y01	CAL-CAX	5.57	1.63	1.50
3	A	1504	Y01	CAL-CAX	5.54	1.63	1.50
3	A	1502	Y01	CAL-CAX	5.51	1.63	1.50
3	A	1509	Y01	CAE-CBI	5.29	1.63	1.54
3	A	1501	Y01	CAK-CBD	5.21	1.61	1.53
3	A	1506	Y01	CAD-CBH	4.73	1.62	1.54
3	A	1501	Y01	CAV-CBC	4.42	1.61	1.52
3	A	1509	Y01	CAV-CBC	4.42	1.61	1.52
3	A	1508	Y01	CAD-CBH	4.41	1.61	1.54
3	A	1508	Y01	CAV-CBC	4.28	1.61	1.52
3	A	1504	Y01	CAV-CBC	4.04	1.61	1.52
3	A	1501	Y01	CBD-CBF	4.04	1.61	1.53
3	A	1501	Y01	CAD-CBH	3.99	1.61	1.54
3	A	1505	Y01	CAV-CBC	3.94	1.60	1.52
3	A	1503	Y01	CAV-CBC	3.87	1.60	1.52
3	A	1503	Y01	CAD-CBH	3.79	1.60	1.54
3	A	1502	Y01	CAD-CBH	3.76	1.60	1.54
3	A	1501	Y01	CAV-CAZ	3.66	1.59	1.51
3	A	1507	Y01	CAD-CBH	3.63	1.60	1.54
3	A	1508	Y01	CAV-CAZ	3.57	1.58	1.51
3	A	1506	Y01	CAM-CAY	3.54	1.61	1.50
3	A	1507	Y01	CAV-CBC	3.54	1.59	1.52
3	A	1502	Y01	CAV-CBC	3.43	1.59	1.52
3	A	1502	Y01	CAM-CAY	3.35	1.60	1.50
3	A	1504	Y01	CAD-CBH	3.34	1.60	1.54
3	A	1509	Y01	CAV-CAZ	3.28	1.58	1.51
3	A	1507	Y01	CAM-CAY	3.27	1.60	1.50
3	A	1509	Y01	CAD-CBH	3.23	1.59	1.54
3	A	1505	Y01	CAM-CAY	3.17	1.59	1.50
3	A	1504	Y01	CAV-CAZ	3.12	1.57	1.51
3	A	1508	Y01	CAM-CAY	3.12	1.59	1.50
3	A	1509	Y01	CAM-CAY	3.08	1.59	1.50
3	A	1504	Y01	CAM-CAY	3.07	1.59	1.50
3	A	1503	Y01	CAM-CAY	3.01	1.59	1.50
3	A	1506	Y01	CAV-CBC	3.01	1.58	1.52
3	A	1506	Y01	CAQ-CAP	-2.97	1.45	1.54
3	A	1505	Y01	CAV-CAZ	2.97	1.57	1.51
3	A	1501	Y01	CAM-CAY	2.95	1.59	1.50
3	A	1505	Y01	CAD-CBH	2.95	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	Y01	OAW-CAY	2.82	1.42	1.34
3	A	1506	Y01	CAK-CAI	-2.80	1.44	1.50
3	A	1506	Y01	OAW-CAY	2.77	1.42	1.34
3	A	1505	Y01	OAW-CAY	2.71	1.41	1.34
3	A	1501	Y01	OAW-CAY	2.70	1.41	1.34
3	A	1507	Y01	OAW-CAY	2.67	1.41	1.34
3	A	1503	Y01	CAV-CAZ	2.67	1.57	1.51
3	A	1504	Y01	OAW-CAY	2.66	1.41	1.34
3	A	1509	Y01	OAW-CAY	2.66	1.41	1.34
3	A	1508	Y01	CAP-CBE	2.62	1.59	1.54
3	A	1501	Y01	CAK-CAI	2.61	1.55	1.50
3	A	1507	Y01	CAV-CAZ	2.54	1.56	1.51
3	A	1508	Y01	OAW-CAY	2.47	1.41	1.34
3	A	1503	Y01	OAW-CAY	2.47	1.41	1.34
3	A	1509	Y01	CAQ-CAP	-2.38	1.47	1.54
3	A	1503	Y01	CAQ-CAP	-2.38	1.47	1.54
3	A	1505	Y01	CBD-CBF	2.36	1.58	1.53
3	A	1508	Y01	CAQ-CAP	-2.21	1.48	1.54
3	A	1501	Y01	CBH-CAZ	-2.19	1.48	1.52
3	A	1507	Y01	CAQ-CAP	-2.17	1.48	1.54
3	A	1506	Y01	CAV-CAZ	2.13	1.55	1.51
3	A	1509	Y01	CBD-CBF	2.12	1.57	1.53
3	A	1508	Y01	CBD-CBF	2.09	1.57	1.53
3	A	1506	Y01	CBD-CBF	2.06	1.57	1.53
3	A	1501	Y01	CAP-CBE	2.05	1.58	1.54
3	A	1502	Y01	CAQ-CAP	-2.04	1.48	1.54
3	A	1501	Y01	CAS-CBF	-2.04	1.50	1.53
3	A	1503	Y01	CAK-CAI	-2.03	1.46	1.50
3	A	1506	Y01	CAO-CBB	2.02	1.59	1.54
3	A	1504	Y01	CBD-CBF	2.02	1.57	1.53
3	A	1501	Y01	CAO-CBB	2.00	1.59	1.54

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1501	Y01	CBD-CAK-CAI	-12.91	94.88	112.76
3	A	1501	Y01	CBC-CAV-CAZ	8.48	123.97	111.45
3	A	1501	Y01	CAD-CBH-CAZ	-8.32	95.67	108.38
3	A	1502	Y01	CBG-CBI-CBE	-8.29	90.58	100.10
3	A	1508	Y01	CBC-CAV-CAZ	8.09	123.40	111.45
3	A	1504	Y01	CBG-CBI-CBE	-8.08	90.83	100.10
3	A	1505	Y01	CBG-CBI-CBE	-7.95	90.98	100.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1501	Y01	CBG-CBI-CBE	-7.74	91.22	100.10
3	A	1507	Y01	CBG-CBI-CBE	-7.70	91.26	100.10
3	A	1509	Y01	CBC-CAV-CAZ	7.43	122.42	111.45
3	A	1507	Y01	OAW-CAY-CAM	7.39	127.48	111.48
3	A	1502	Y01	OAW-CAY-CAM	7.34	127.37	111.48
3	A	1509	Y01	OAW-CAY-CAM	7.31	127.30	111.48
3	A	1504	Y01	CAD-CBH-CAZ	-7.29	97.24	108.38
3	A	1501	Y01	OAW-CAY-CAM	7.29	127.25	111.48
3	A	1504	Y01	OAW-CAY-CAM	7.27	127.20	111.48
3	A	1504	Y01	CBC-CAV-CAZ	7.27	122.18	111.45
3	A	1503	Y01	CBG-CBI-CBE	-7.22	91.81	100.10
3	A	1505	Y01	CAV-CAZ-CAI	7.22	130.36	120.57
3	A	1508	Y01	CBG-CBI-CBE	-7.21	91.82	100.10
3	A	1505	Y01	OAW-CAY-CAM	7.21	127.07	111.48
3	A	1503	Y01	CBC-CAV-CAZ	7.20	122.08	111.45
3	A	1503	Y01	OAW-CAY-CAM	7.14	126.93	111.48
3	A	1508	Y01	OAW-CAY-CAM	7.11	126.86	111.48
3	A	1506	Y01	OAW-CAY-CAM	7.10	126.85	111.48
3	A	1505	Y01	CBC-CAV-CAZ	7.09	121.93	111.45
3	A	1509	Y01	CAV-CAZ-CAI	7.09	130.18	120.57
3	A	1504	Y01	CAV-CAZ-CAI	7.01	130.07	120.57
3	A	1503	Y01	CAD-CBH-CAZ	-6.99	97.70	108.38
3	A	1505	Y01	CAD-CBH-CAZ	-6.98	97.73	108.38
3	A	1507	Y01	CAV-CAZ-CAI	6.97	130.01	120.57
3	A	1509	Y01	CBG-CBI-CBE	-6.95	92.12	100.10
3	A	1502	Y01	CAD-CBH-CAZ	-6.95	97.76	108.38
3	A	1503	Y01	CAV-CAZ-CAI	6.93	129.96	120.57
3	A	1501	Y01	CAV-CAZ-CAI	6.89	129.91	120.57
3	A	1507	Y01	CAD-CBH-CAZ	-6.85	97.92	108.38
3	A	1509	Y01	CAD-CBH-CAZ	-6.84	97.93	108.38
3	A	1506	Y01	CBG-CBI-CBE	-6.82	92.27	100.10
3	A	1508	Y01	CAV-CAZ-CAI	6.77	129.74	120.57
3	A	1508	Y01	CAD-CBH-CAZ	-6.63	98.25	108.38
3	A	1502	Y01	CAV-CAZ-CAI	6.56	129.46	120.57
3	A	1507	Y01	CBC-CAV-CAZ	6.48	121.03	111.45
3	A	1506	Y01	CBD-CAK-CAI	-6.46	103.81	112.76
3	A	1506	Y01	CBC-CAV-CAZ	6.45	120.97	111.45
3	A	1501	Y01	CAK-CBD-CBF	6.39	117.10	109.72
3	A	1506	Y01	CAD-CBH-CAZ	-5.86	99.42	108.38
3	A	1502	Y01	CBC-CAV-CAZ	5.86	120.11	111.45
3	A	1507	Y01	CAV-CAZ-CBH	-5.70	109.12	116.42
3	A	1509	Y01	CBD-CAK-CAI	-5.69	104.88	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1509	Y01	CAV-CAZ-CBH	-5.64	109.21	116.42
3	A	1502	Y01	CAV-CAZ-CBH	-5.63	109.21	116.42
3	A	1505	Y01	CAV-CAZ-CBH	-5.59	109.26	116.42
3	A	1504	Y01	CAV-CAZ-CBH	-5.51	109.37	116.42
3	A	1501	Y01	CBH-CAZ-CAI	-5.48	114.93	122.93
3	A	1503	Y01	CAP-CAQ-CBG	-5.39	94.59	105.14
3	A	1508	Y01	CAP-CAQ-CBG	-5.37	94.63	105.14
3	A	1503	Y01	CAV-CAZ-CBH	-5.29	109.65	116.42
3	A	1506	Y01	CAE-CBI-CBG	5.21	121.13	111.68
3	A	1505	Y01	CBD-CAK-CAI	-5.20	105.56	112.76
3	A	1506	Y01	CAV-CAZ-CBH	-5.19	109.77	116.42
3	A	1502	Y01	CAR-CBC-CAV	-5.15	103.81	110.97
3	A	1508	Y01	CBD-CAK-CAI	-5.13	105.65	112.76
3	A	1501	Y01	CAP-CBE-CBI	-5.07	97.88	103.84
3	A	1504	Y01	CAP-CBE-CBI	-5.05	97.90	103.84
3	A	1502	Y01	CAP-CAQ-CBG	-5.02	95.33	105.14
3	A	1508	Y01	CAV-CAZ-CBH	-4.97	110.05	116.42
3	A	1507	Y01	OAW-CBC-CAV	4.95	118.24	108.04
3	A	1509	Y01	CAE-CBI-CBG	4.94	120.64	111.68
3	A	1507	Y01	CAR-CBC-CAV	-4.91	104.14	110.97
3	A	1505	Y01	CAP-CBE-CBI	-4.82	98.17	103.84
3	A	1507	Y01	CAP-CAQ-CBG	-4.82	95.71	105.14
3	A	1503	Y01	CBD-CAK-CAI	-4.82	106.09	112.76
3	A	1501	Y01	CAV-CAZ-CBH	-4.78	110.30	116.42
3	A	1507	Y01	CBD-CAK-CAI	-4.75	106.18	112.76
3	A	1504	Y01	CAP-CAQ-CBG	-4.73	95.88	105.14
3	A	1502	Y01	OAW-CBC-CAV	4.72	117.77	108.04
3	A	1506	Y01	CAR-CBC-CAV	-4.69	104.45	110.97
3	A	1502	Y01	CBD-CAK-CAI	-4.68	106.27	112.76
3	A	1504	Y01	OAW-CBC-CAV	4.68	117.67	108.04
3	A	1509	Y01	OAW-CBC-CAV	4.65	117.61	108.04
3	A	1505	Y01	CAE-CBI-CBG	4.64	120.09	111.68
3	A	1507	Y01	CAE-CBI-CBG	4.63	120.07	111.68
3	A	1501	Y01	CAP-CAQ-CBG	-4.63	96.09	105.14
3	A	1508	Y01	OAW-CBC-CAV	4.59	117.50	108.04
3	A	1506	Y01	CAE-CBI-CAU	-4.56	103.89	110.61
3	A	1505	Y01	OAW-CBC-CAV	4.53	117.38	108.04
3	A	1504	Y01	CBD-CAK-CAI	-4.53	106.49	112.76
3	A	1501	Y01	CAS-CBF-CBH	-4.45	107.59	113.08
3	A	1503	Y01	OAW-CBC-CAV	4.43	117.16	108.04
3	A	1508	Y01	CAE-CBI-CBG	4.42	119.69	111.68
3	A	1502	Y01	CAT-CBH-CAZ	4.42	116.36	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1506	Y01	CAQ-CBG-CBD	-4.40	112.07	119.10
3	A	1506	Y01	OAW-CBC-CAV	4.40	117.10	108.04
3	A	1501	Y01	OAW-CBC-CAV	4.39	117.07	108.04
3	A	1503	Y01	CAE-CBI-CBG	4.38	119.61	111.68
3	A	1502	Y01	CAS-CBF-CBH	-4.32	107.76	113.08
3	A	1505	Y01	CAR-CBC-CAV	-4.28	105.02	110.97
3	A	1505	Y01	CAP-CAQ-CBG	-4.27	96.78	105.14
3	A	1507	Y01	OAW-CAY-OAG	-4.24	113.78	123.70
3	A	1509	Y01	CAP-CAQ-CBG	-4.23	96.86	105.14
3	A	1504	Y01	CAR-CBC-CAV	-4.23	105.09	110.97
3	A	1502	Y01	OAW-CAY-OAG	-4.22	113.83	123.70
3	A	1507	Y01	CAS-CBF-CBH	-4.22	107.88	113.08
3	A	1509	Y01	OAW-CAY-OAG	-4.18	113.93	123.70
3	A	1503	Y01	OAW-CAY-OAG	-4.16	113.98	123.70
3	A	1508	Y01	OAW-CAY-OAG	-4.15	114.00	123.70
3	A	1505	Y01	OAW-CAY-OAG	-4.15	114.00	123.70
3	A	1504	Y01	OAW-CAY-OAG	-4.15	114.01	123.70
3	A	1501	Y01	OAW-CAY-OAG	-4.14	114.02	123.70
3	A	1509	Y01	CAE-CBI-CAU	-4.14	104.50	110.61
3	A	1506	Y01	OAW-CAY-OAG	-4.10	114.11	123.70
3	A	1502	Y01	CAE-CBI-CBG	4.07	119.05	111.68
3	A	1506	Y01	CAP-CAQ-CBG	-4.04	97.23	105.14
3	A	1503	Y01	CAE-CBI-CAU	-4.03	104.66	110.61
3	A	1501	Y01	CAP-CBE-CBB	4.03	118.27	112.18
3	A	1505	Y01	CAE-CBI-CAU	-4.00	104.72	110.61
3	A	1502	Y01	CAP-CBE-CBI	-3.98	99.15	103.84
3	A	1509	Y01	CAQ-CBG-CBD	-3.98	112.76	119.10
3	A	1501	Y01	CAE-CBI-CBG	3.98	118.89	111.68
3	A	1503	Y01	CAR-CBC-CAV	-3.95	105.48	110.97
3	A	1502	Y01	CAE-CBI-CAU	-3.95	104.79	110.61
3	A	1507	Y01	CAE-CBI-CAU	-3.94	104.80	110.61
3	A	1506	Y01	CAV-CAZ-CAI	3.93	125.90	120.57
3	A	1503	Y01	CAS-CBF-CBH	-3.92	108.25	113.08
3	A	1507	Y01	CAT-CBH-CAZ	3.91	115.49	108.74
3	A	1505	Y01	CAS-CBF-CBH	-3.89	108.28	113.08
3	A	1509	Y01	CAS-CBF-CBH	-3.89	108.28	113.08
3	A	1508	Y01	CAQ-CBG-CBD	-3.89	112.90	119.10
3	A	1506	Y01	CAT-CBH-CAZ	3.88	115.42	108.74
3	A	1501	Y01	CAE-CBI-CAU	-3.85	104.92	110.61
3	A	1504	Y01	CAE-CBI-CBG	3.85	118.66	111.68
3	A	1504	Y01	CAK-CAI-CAZ	3.83	131.50	125.02
3	A	1505	Y01	CAQ-CBG-CBD	-3.79	113.06	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1502	Y01	CAK-CAI-CAZ	3.78	131.41	125.02
3	A	1508	Y01	CAS-CBF-CBH	-3.78	108.43	113.08
3	A	1504	Y01	CAT-CBH-CAZ	3.77	115.25	108.74
3	A	1509	Y01	CAR-CBC-CAV	-3.75	105.77	110.97
3	A	1503	Y01	CAQ-CBG-CBD	-3.74	113.14	119.10
3	A	1504	Y01	CAQ-CBG-CBD	-3.72	113.17	119.10
3	A	1505	Y01	CAT-CBH-CAZ	3.70	115.12	108.74
3	A	1508	Y01	CAR-CBC-CAV	-3.70	105.83	110.97
3	A	1507	Y01	CAQ-CBG-CBD	-3.68	113.22	119.10
3	A	1507	Y01	CAK-CAI-CAZ	3.65	131.18	125.02
3	A	1504	Y01	CAS-CBF-CBH	-3.65	108.59	113.08
3	A	1502	Y01	CAK-CBD-CBF	3.63	113.92	109.72
3	A	1502	Y01	CAQ-CBG-CBD	-3.63	113.31	119.10
3	A	1509	Y01	CBI-CBG-CBD	-3.62	109.27	114.41
3	A	1506	Y01	CBH-CAZ-CAI	-3.61	117.66	122.93
3	A	1501	Y01	CAQ-CBG-CBD	-3.59	113.38	119.10
3	A	1503	Y01	CAT-CBH-CAZ	3.58	114.92	108.74
3	A	1505	Y01	CBI-CBG-CBD	-3.54	109.39	114.41
3	A	1507	Y01	CAP-CBE-CBI	-3.51	99.71	103.84
3	A	1507	Y01	CBI-CBG-CBD	-3.45	109.51	114.41
3	A	1509	Y01	CAT-CBH-CAZ	3.44	114.67	108.74
3	A	1504	Y01	CAK-CBD-CBF	3.38	113.63	109.72
3	A	1504	Y01	CAP-CBE-CBB	3.38	117.29	112.18
3	A	1506	Y01	CBI-CBG-CBD	-3.35	109.66	114.41
3	A	1504	Y01	CBI-CBG-CBD	-3.32	109.69	114.41
3	A	1508	Y01	CAT-CBH-CAZ	3.32	114.47	108.74
3	A	1508	Y01	CAE-CBI-CAU	-3.31	105.73	110.61
3	A	1501	Y01	CAD-CBH-CAT	3.30	114.44	109.43
3	A	1505	Y01	CAK-CAI-CAZ	3.27	130.54	125.02
3	A	1506	Y01	CBH-CBF-CBD	-3.27	107.94	112.71
3	A	1503	Y01	CBI-CBG-CBD	-3.24	109.81	114.41
3	A	1508	Y01	CAK-CAI-CAZ	3.22	130.46	125.02
3	A	1501	Y01	CAR-CBC-CAV	-3.22	106.50	110.97
3	A	1503	Y01	CAK-CAI-CAZ	3.21	130.44	125.02
3	A	1501	Y01	CAT-CBH-CAZ	3.19	114.24	108.74
3	A	1502	Y01	CBI-CBG-CBD	-3.19	109.88	114.41
3	A	1507	Y01	CAK-CBD-CBF	3.19	113.41	109.72
3	A	1501	Y01	CBI-CBG-CBD	-3.16	109.93	114.41
3	A	1505	Y01	CAP-CBE-CBB	3.15	116.95	112.18
3	A	1508	Y01	CAK-CBD-CBF	3.15	113.36	109.72
3	A	1506	Y01	CAP-CBE-CBI	-3.12	100.17	103.84
3	A	1505	Y01	CAK-CBD-CBF	3.10	113.30	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1506	Y01	CAQ-CAP-CBE	3.10	111.21	105.14
3	A	1508	Y01	CBI-CBG-CBD	-3.05	110.09	114.41
3	A	1509	Y01	CAK-CAI-CAZ	3.00	130.09	125.02
3	A	1508	Y01	CAP-CBE-CBI	-2.97	100.35	103.84
3	A	1501	Y01	CBI-CBE-CBB	-2.97	114.91	119.50
3	A	1506	Y01	CAS-CBF-CBH	-2.95	109.45	113.08
3	A	1503	Y01	CAK-CBD-CBF	2.92	113.09	109.72
3	A	1503	Y01	CBI-CBE-CBB	-2.91	115.00	119.50
3	A	1504	Y01	CBI-CBE-CBB	-2.83	115.13	119.50
3	A	1502	Y01	CAR-CAT-CBH	2.82	118.79	112.78
3	A	1501	Y01	CBH-CBF-CBD	-2.80	108.62	112.71
3	A	1508	Y01	CAQ-CAP-CBE	2.79	110.61	105.14
3	A	1506	Y01	CBI-CBE-CBB	-2.76	115.23	119.50
3	A	1507	Y01	CAQ-CAP-CBE	2.76	110.55	105.14
3	A	1503	Y01	CAQ-CAP-CBE	2.76	110.54	105.14
3	A	1506	Y01	CAQ-CBG-CBI	2.73	107.05	103.84
3	A	1502	Y01	CAP-CBE-CBB	2.72	116.30	112.18
3	A	1509	Y01	CBH-CBF-CBD	-2.72	108.74	112.71
3	A	1502	Y01	CAS-CBF-CBD	-2.71	107.99	111.78
3	A	1509	Y01	CAP-CBE-CBI	-2.71	100.65	103.84
3	A	1508	Y01	CAS-CBF-CBD	-2.69	108.02	111.78
3	A	1505	Y01	CBI-CBE-CBB	-2.68	115.36	119.50
3	A	1501	Y01	CAU-CBI-CBG	2.64	111.20	107.25
3	A	1509	Y01	CAQ-CAP-CBE	2.63	110.30	105.14
3	A	1508	Y01	CBI-CBE-CBB	-2.62	115.45	119.50
3	A	1504	Y01	CAE-CBI-CAU	-2.59	106.79	110.61
3	A	1502	Y01	CAQ-CAP-CBE	2.58	110.20	105.14
3	A	1502	Y01	CBI-CBE-CBB	-2.54	115.58	119.50
3	A	1509	Y01	CBI-CBE-CBB	-2.52	115.60	119.50
3	A	1502	Y01	CAE-CBI-CBE	2.51	116.23	111.68
3	A	1504	Y01	CAS-CBF-CBD	-2.51	108.28	111.78
3	A	1507	Y01	CAR-CAT-CBH	2.48	118.08	112.78
3	A	1509	Y01	CAU-CAS-CBF	2.44	117.28	113.14
3	A	1508	Y01	CBH-CAZ-CAI	-2.42	119.39	122.93
3	A	1507	Y01	CBI-CBE-CBB	-2.39	115.80	119.50
3	A	1505	Y01	CBH-CBF-CBD	-2.35	109.28	112.71
3	A	1506	Y01	CAU-CAS-CBF	2.34	117.11	113.14
3	A	1507	Y01	CAE-CBI-CBE	2.34	115.92	111.68
3	A	1506	Y01	CAK-CBD-CBF	2.33	112.41	109.72
3	A	1501	Y01	CAQ-CAP-CBE	2.33	109.69	105.14
3	A	1502	Y01	CAD-CBH-CAT	2.32	112.97	109.43
3	A	1504	Y01	CAQ-CAP-CBE	2.32	109.68	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1507	Y01	CAD-CBH-CAT	2.31	112.95	109.43
3	A	1502	Y01	CAU-CBI-CBG	2.31	110.70	107.25
3	A	1503	Y01	CAE-CBI-CBE	2.30	115.85	111.68
3	A	1509	Y01	CAK-CBD-CBF	2.29	112.37	109.72
3	A	1505	Y01	CAE-CBI-CBE	2.29	115.83	111.68
3	A	1501	Y01	CAE-CBI-CBE	2.27	115.80	111.68
3	A	1509	Y01	CAQ-CBG-CBI	2.27	106.51	103.84
3	A	1503	Y01	CAD-CBH-CAT	2.25	112.85	109.43
3	A	1504	Y01	CBF-CBH-CAZ	-2.25	106.36	109.65
3	A	1503	Y01	CAP-CBE-CBI	-2.25	101.20	103.84
3	A	1501	Y01	CBC-OAW-CAY	2.23	123.12	117.80
3	A	1509	Y01	CAT-CBH-CBF	2.22	111.68	108.74
3	A	1504	Y01	CAT-CBH-CBF	2.21	111.66	108.74
3	A	1505	Y01	CAQ-CBG-CBI	2.20	106.43	103.84
3	A	1504	Y01	CBH-CBF-CBD	-2.18	109.53	112.71
3	A	1506	Y01	CAK-CAI-CAZ	2.18	128.70	125.02
3	A	1503	Y01	CBH-CAZ-CAI	-2.17	119.76	122.93
3	A	1509	Y01	CBH-CAZ-CAI	-2.16	119.77	122.93
3	A	1507	Y01	CAS-CBF-CBD	-2.14	108.79	111.78
3	A	1507	Y01	CBC-OAW-CAY	2.14	122.92	117.80
3	A	1505	Y01	CAQ-CAP-CBE	2.13	109.31	105.14
3	A	1509	Y01	CAE-CBI-CBE	2.12	115.52	111.68
3	A	1509	Y01	CBC-OAW-CAY	2.12	122.86	117.80
3	A	1506	Y01	CAE-CBI-CBE	2.12	115.52	111.68
3	A	1504	Y01	CAD-CBH-CAT	2.07	112.58	109.43
3	A	1505	Y01	CBH-CAZ-CAI	-2.07	119.91	122.93
3	A	1504	Y01	CBC-OAW-CAY	2.05	122.71	117.80
3	A	1504	Y01	CAR-CAT-CBH	2.05	117.14	112.78
3	A	1501	Y01	CAT-CBH-CBF	2.03	111.43	108.74
3	A	1508	Y01	CAD-CBH-CAT	2.03	112.52	109.43
3	A	1503	Y01	CBH-CBF-CBD	-2.03	109.75	112.71

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1501	Y01	OAG-CAY-OAW-CBC
3	A	1501	Y01	CAM-CAY-OAW-CBC
3	A	1502	Y01	OAG-CAY-OAW-CBC
3	A	1502	Y01	CAM-CAY-OAW-CBC
3	A	1503	Y01	OAG-CAY-OAW-CBC
3	A	1504	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	A	1504	Y01	CAM-CAY-OAW-CBC
3	A	1505	Y01	OAG-CAY-OAW-CBC
3	A	1506	Y01	OAG-CAY-OAW-CBC
3	A	1506	Y01	CAM-CAY-OAW-CBC
3	A	1507	Y01	OAG-CAY-OAW-CBC
3	A	1507	Y01	CAM-CAY-OAW-CBC
3	A	1508	Y01	OAG-CAY-OAW-CBC
3	A	1508	Y01	CAM-CAY-OAW-CBC
3	A	1509	Y01	OAG-CAY-OAW-CBC
3	A	1509	Y01	CAM-CAY-OAW-CBC
3	A	1505	Y01	CAV-CBC-OAW-CAY
3	A	1503	Y01	CAM-CAY-OAW-CBC
3	A	1505	Y01	CAM-CAY-OAW-CBC
3	A	1503	Y01	CAJ-CAO-CBB-CBE
3	A	1504	Y01	CAJ-CAO-CBB-CBE
3	A	1505	Y01	CAJ-CAO-CBB-CBE
3	A	1507	Y01	CAJ-CAO-CBB-CBE
3	A	1503	Y01	CAJ-CAO-CBB-CAC
3	A	1504	Y01	CAJ-CAO-CBB-CAC
3	A	1502	Y01	CAJ-CAO-CBB-CBE
3	A	1509	Y01	CAJ-CAO-CBB-CBE
3	A	1504	Y01	CAX-CAL-CAM-CAY
3	A	1502	Y01	CAJ-CAO-CBB-CAC
3	A	1505	Y01	CAJ-CAO-CBB-CAC
3	A	1507	Y01	CAJ-CAO-CBB-CAC
3	A	1509	Y01	CAJ-CAO-CBB-CAC
3	A	1507	Y01	CAX-CAL-CAM-CAY
3	A	1508	Y01	CAX-CAL-CAM-CAY
3	A	1504	Y01	CAN-CAJ-CAO-CBB
3	A	1505	Y01	CAO-CAJ-CAN-CBA
3	A	1501	Y01	CAN-CAJ-CAO-CBB
3	A	1506	Y01	CAX-CAL-CAM-CAY
3	A	1506	Y01	CAJ-CAN-CBA-CAB
3	A	1501	Y01	CAX-CAL-CAM-CAY
3	A	1504	Y01	CAJ-CAN-CBA-CAA
3	A	1503	Y01	CAO-CAJ-CAN-CBA
3	A	1506	Y01	CAJ-CAO-CBB-CBE
3	A	1503	Y01	CAN-CAJ-CAO-CBB
3	A	1507	Y01	CAN-CAJ-CAO-CBB
3	A	1506	Y01	CAJ-CAN-CBA-CAA
3	A	1507	Y01	CAJ-CAN-CBA-CAB
3	A	1504	Y01	CAJ-CAN-CBA-CAB

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Mol	Chain	Res	Type	Atoms
3	A	1506	Y01	CAR-CBC-OAW-CAY
3	A	1506	Y01	CAJ-CAO-CBB-CAC
3	A	1507	Y01	CAJ-CAN-CBA-CAA
3	A	1502	Y01	CAO-CAJ-CAN-CBA
3	A	1506	Y01	CAV-CBC-OAW-CAY
3	A	1501	Y01	CAJ-CAN-CBA-CAA
3	A	1504	Y01	CAO-CBB-CBE-CBI
3	A	1501	Y01	CAJ-CAN-CBA-CAB
3	A	1509	Y01	CAO-CAJ-CAN-CBA
3	A	1502	Y01	CAJ-CAN-CBA-CAA
3	A	1504	Y01	CAC-CBB-CBE-CBI
3	A	1506	Y01	CAO-CAJ-CAN-CBA
3	A	1502	Y01	CAJ-CAN-CBA-CAB
3	A	1504	Y01	CAL-CAM-CAY-OAW
3	A	1504	Y01	CAM-CAL-CAX-OAH
3	A	1504	Y01	CAM-CAL-CAX-OAF
3	A	1505	Y01	CAM-CAL-CAX-OAH
3	A	1509	Y01	CAM-CAL-CAX-OAF
3	A	1509	Y01	CAM-CAL-CAX-OAH
3	A	1505	Y01	CAM-CAL-CAX-OAF
3	A	1507	Y01	CAM-CAL-CAX-OAH
3	A	1501	Y01	CAL-CAM-CAY-OAW
3	A	1507	Y01	CAL-CAM-CAY-OAW
3	A	1508	Y01	CAM-CAL-CAX-OAH

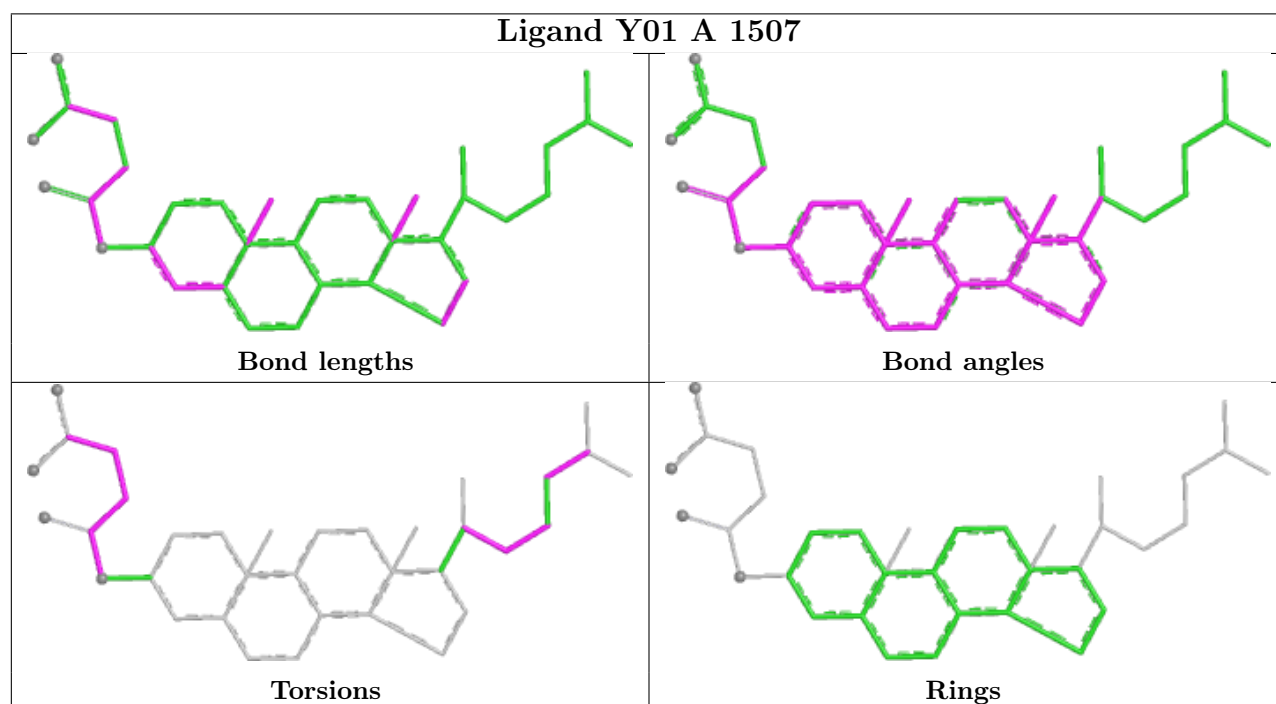
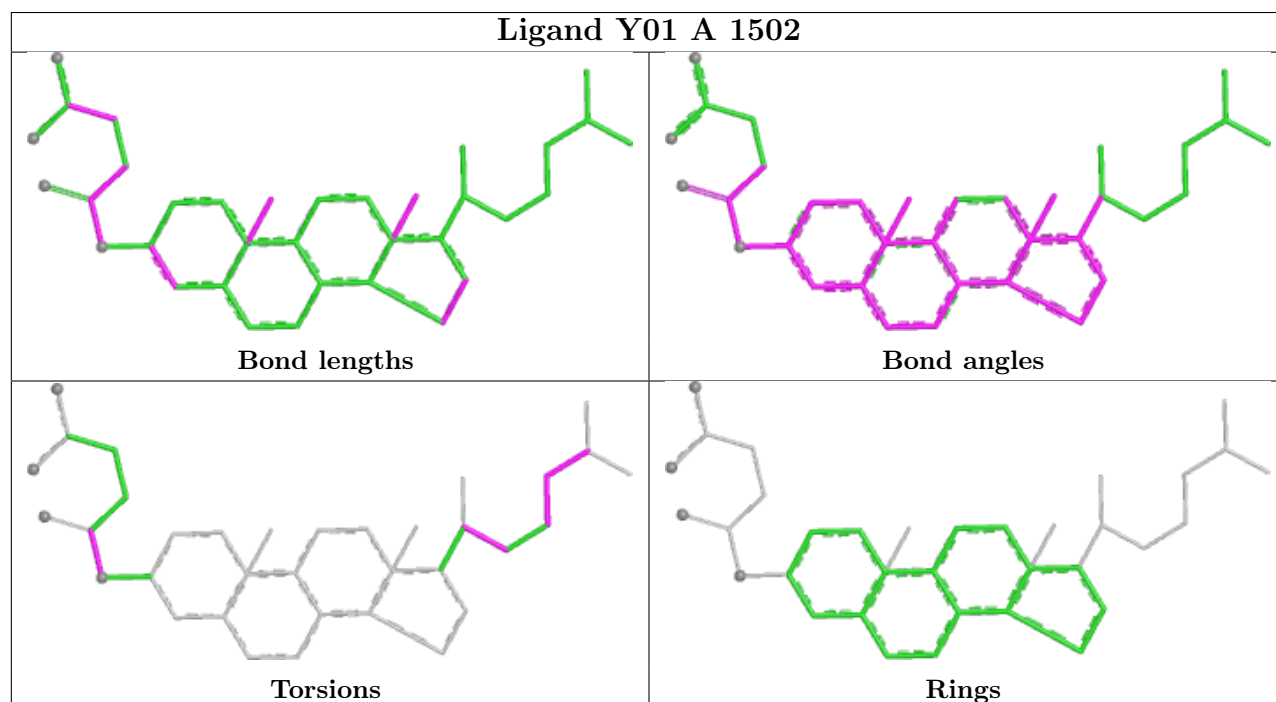
There are no ring outliers.

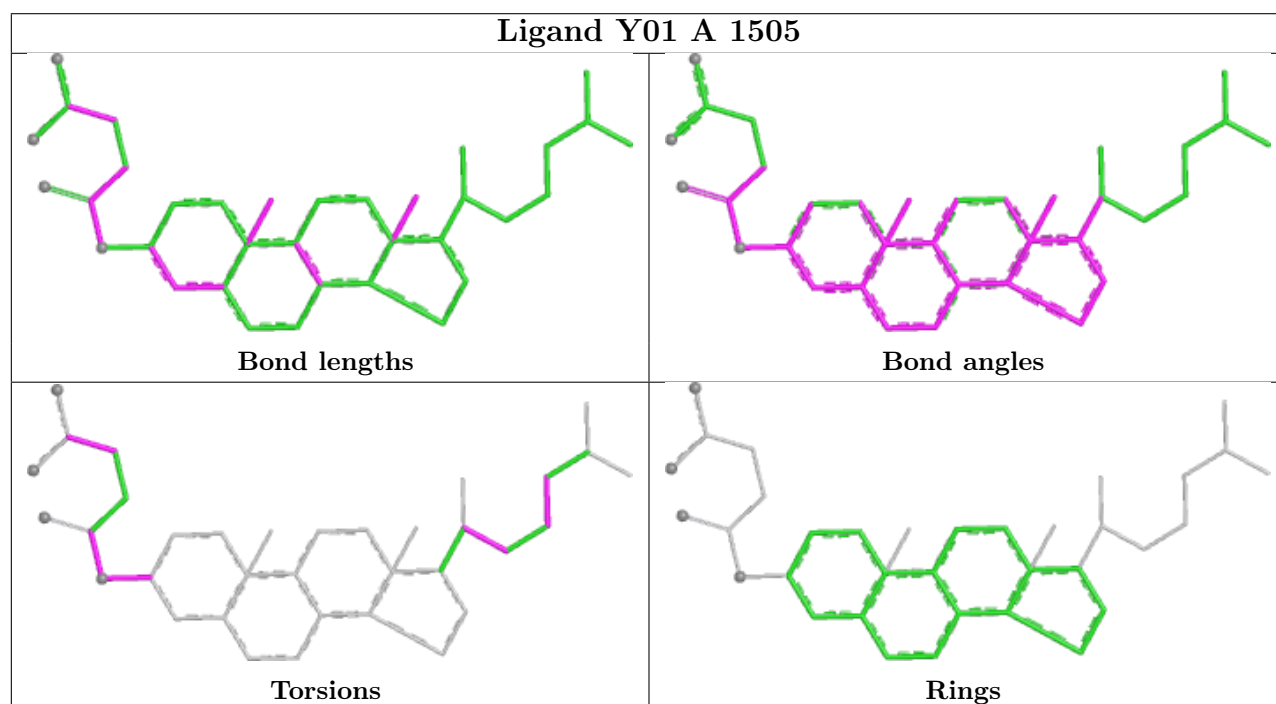
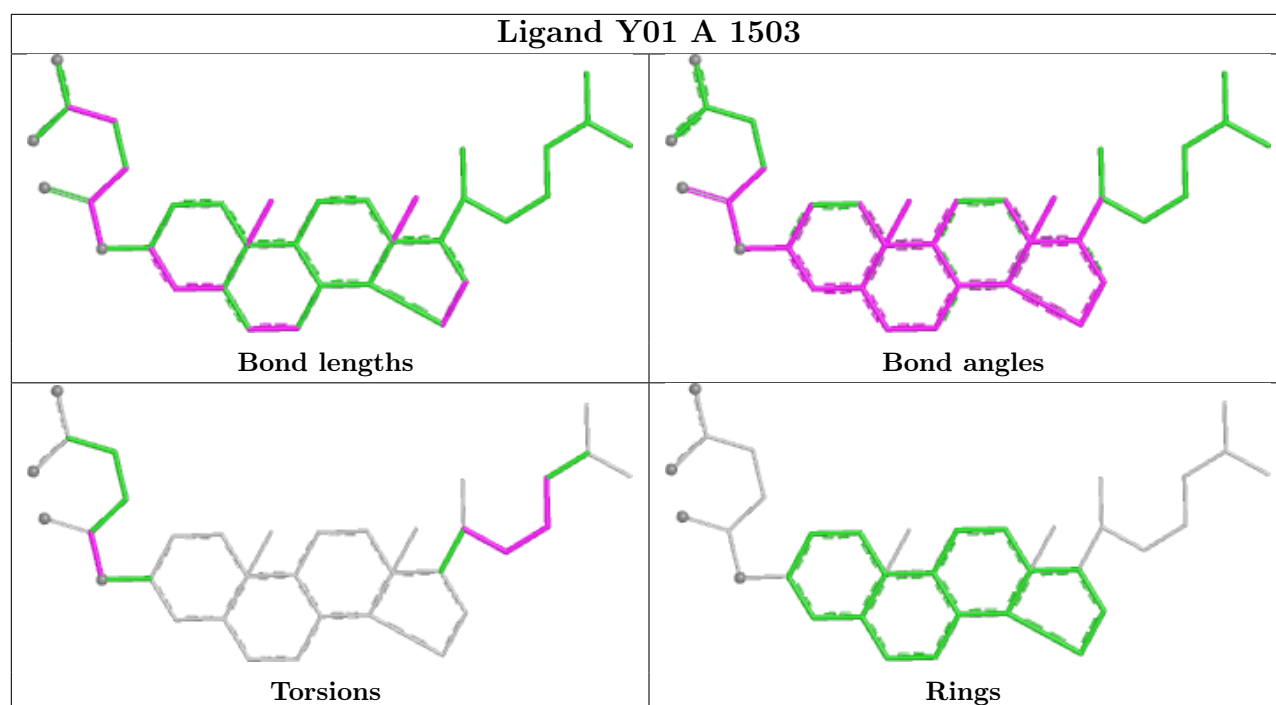
9 monomers are involved in 18 short contacts:

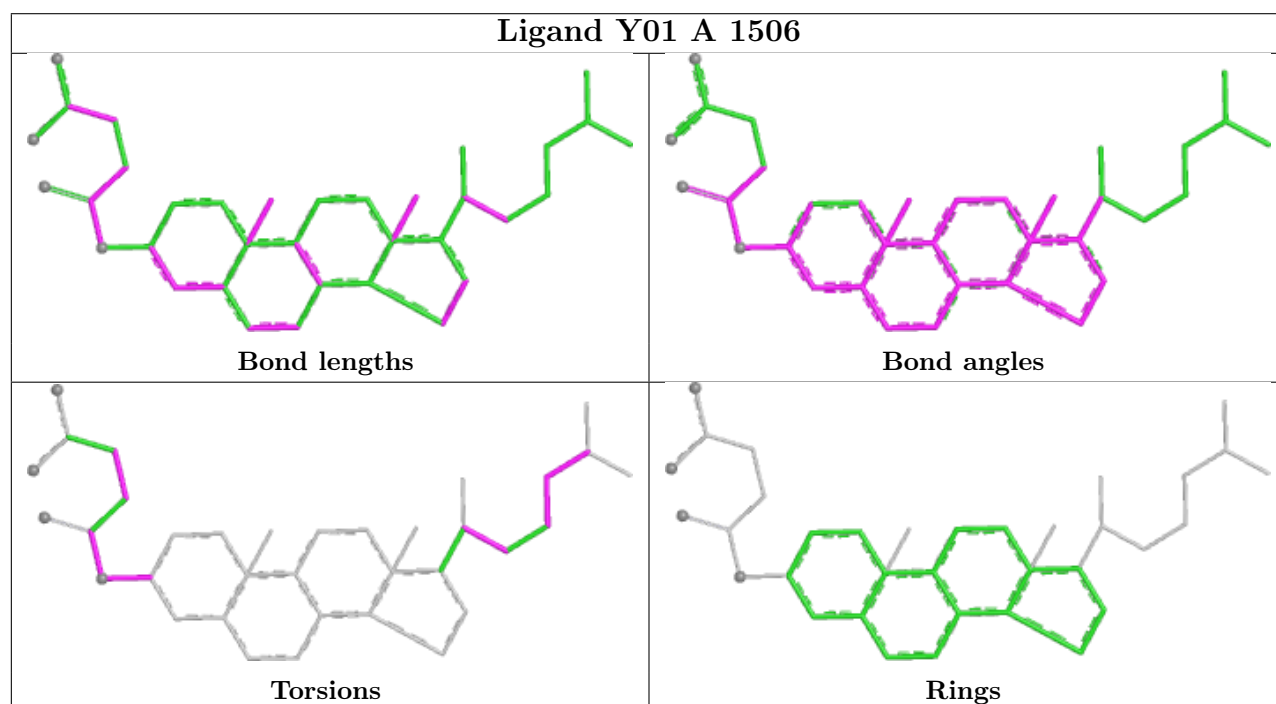
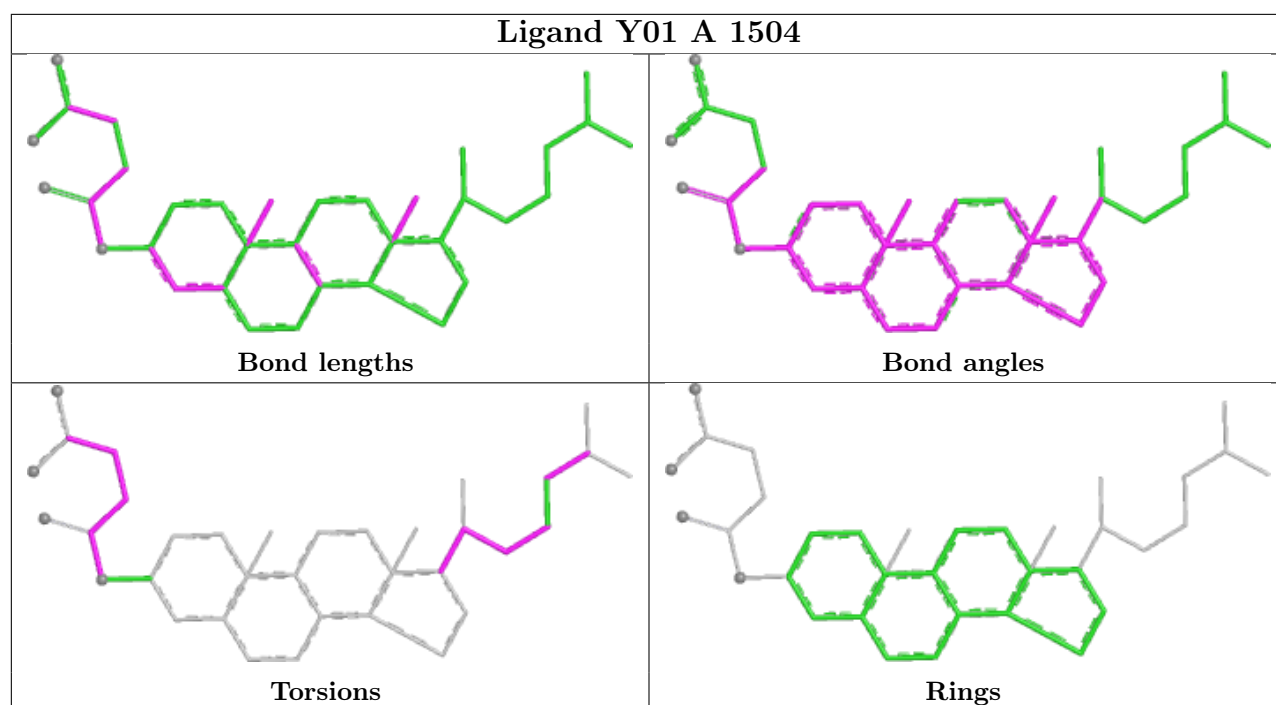
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	Y01	2	0
3	A	1507	Y01	2	0
3	A	1503	Y01	1	0
3	A	1505	Y01	3	0
3	A	1504	Y01	1	0
3	A	1506	Y01	5	0
3	A	1508	Y01	1	0
3	A	1509	Y01	1	0
3	A	1501	Y01	2	0

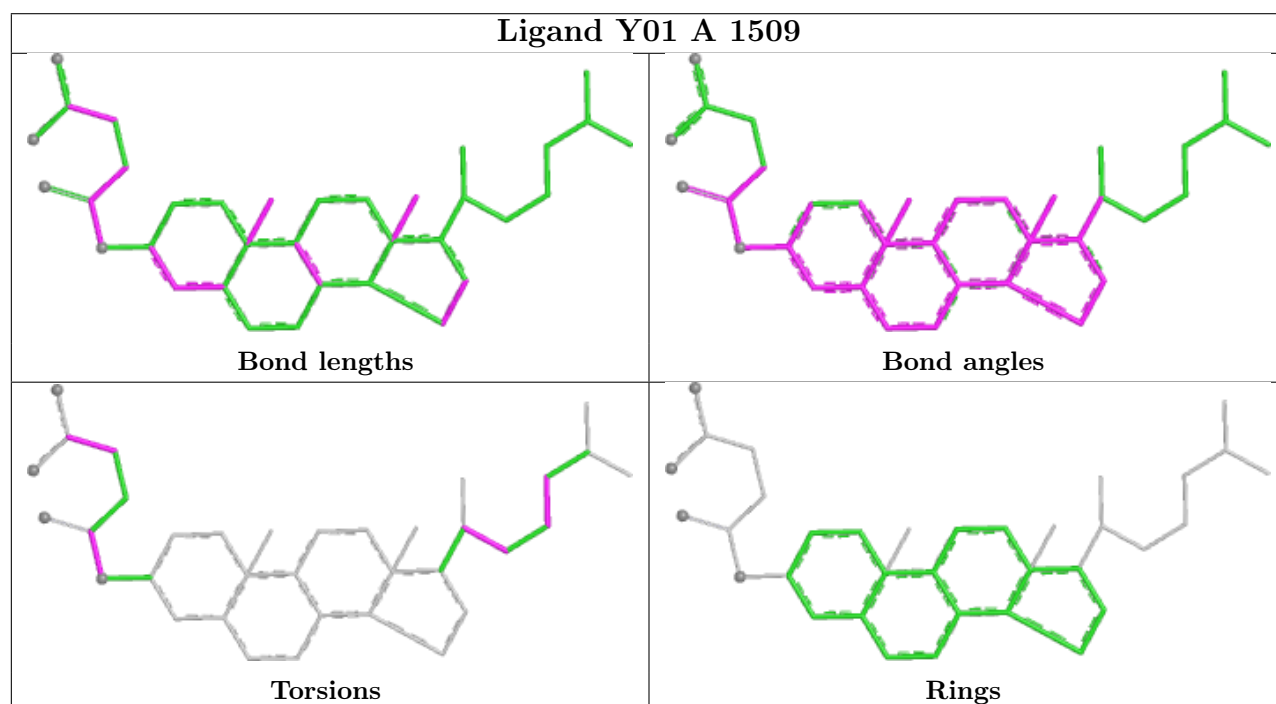
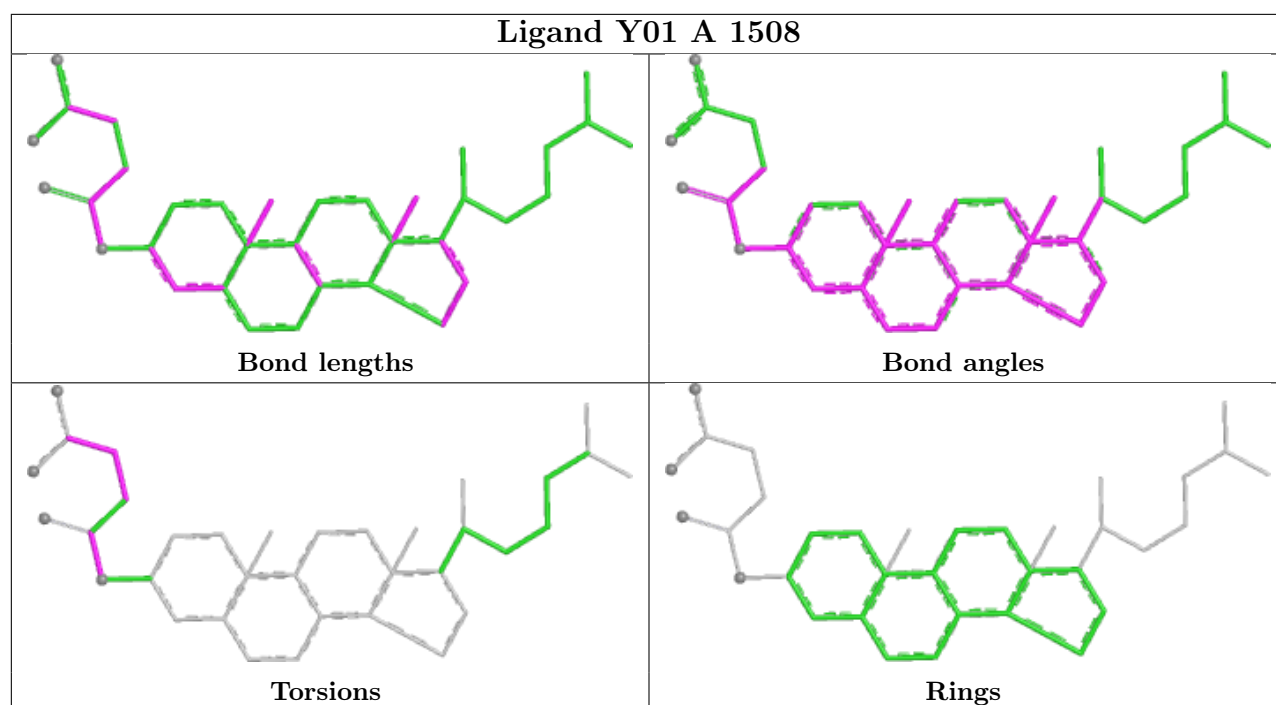
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

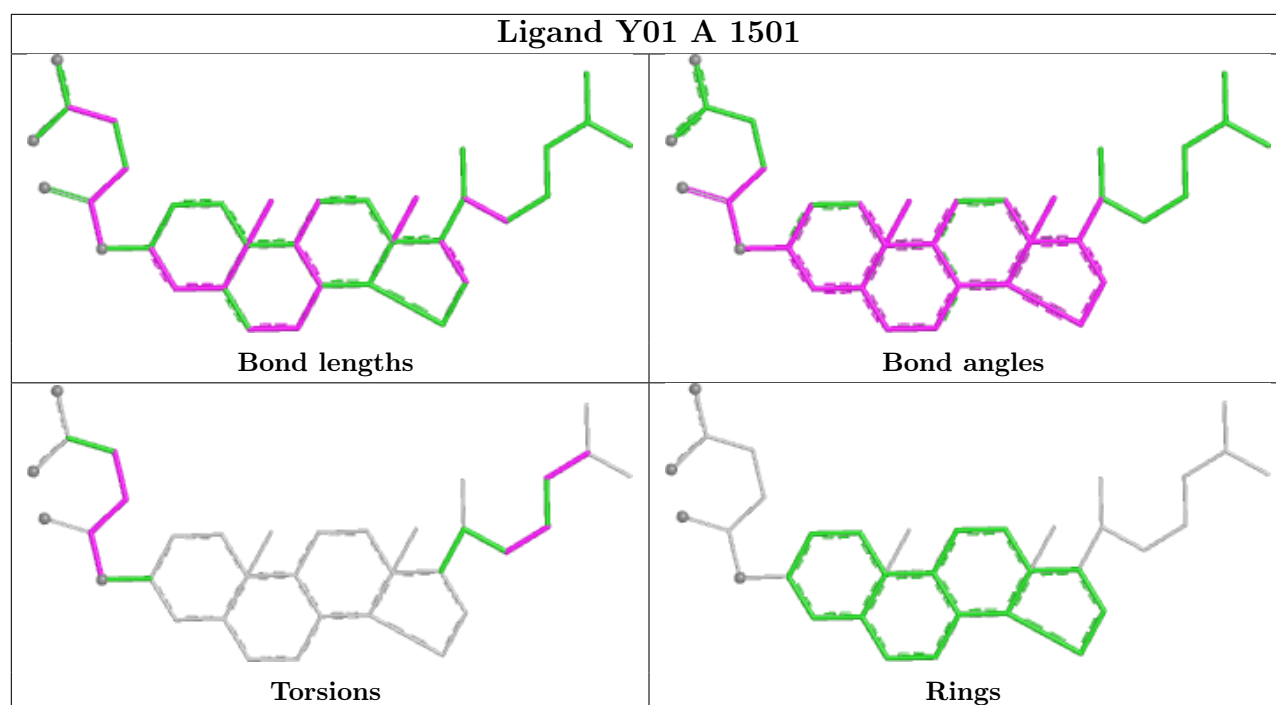
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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](#)

There are no chain breaks in this entry.

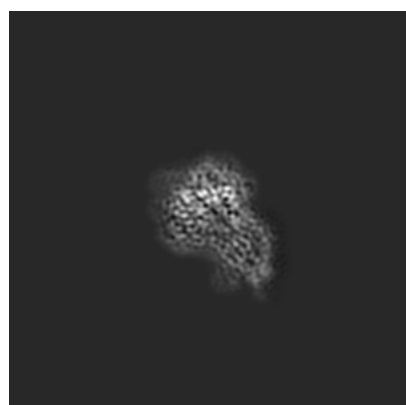
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10452. These allow visual inspection of the internal detail of the map and identification of artifacts.

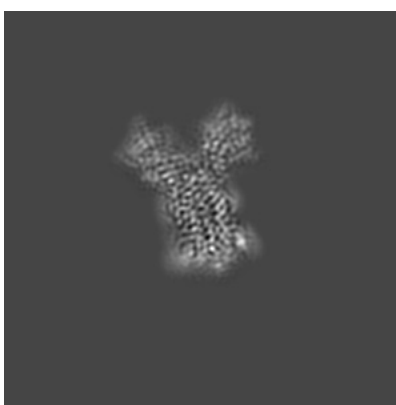
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

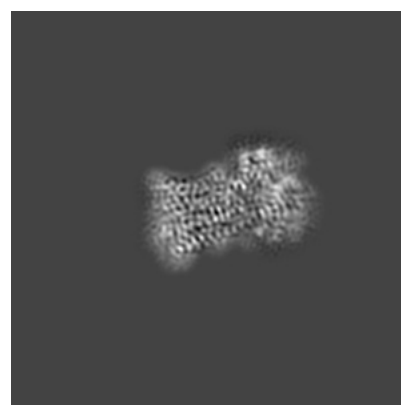
6.1.1 Primary map



X



Y



Z

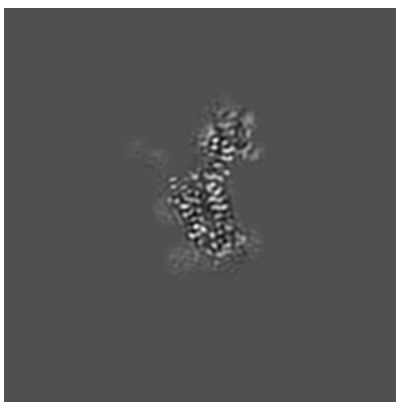
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

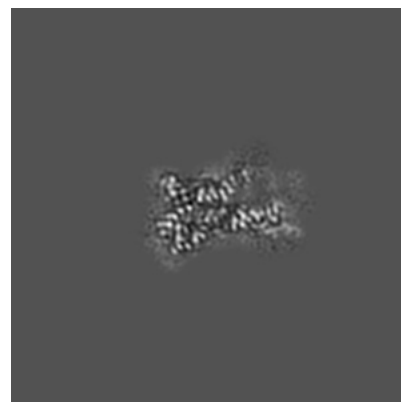
6.2.1 Primary map



X Index: 152



Y Index: 152

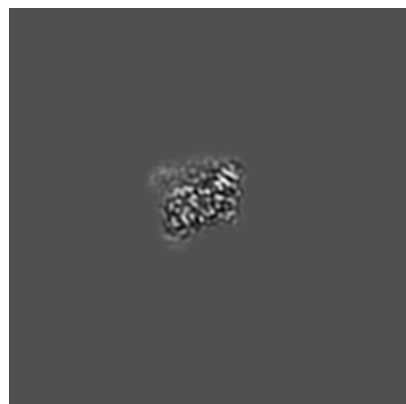


Z Index: 152

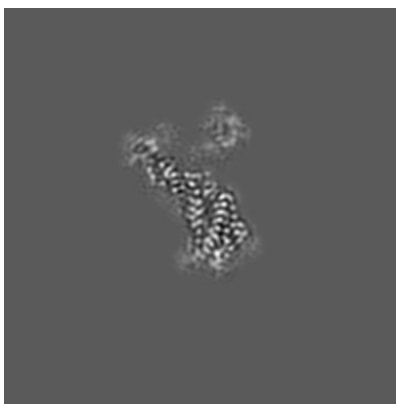
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

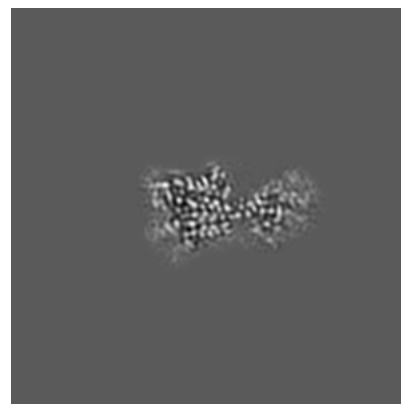
6.3.1 Primary map



X Index: 133



Y Index: 169

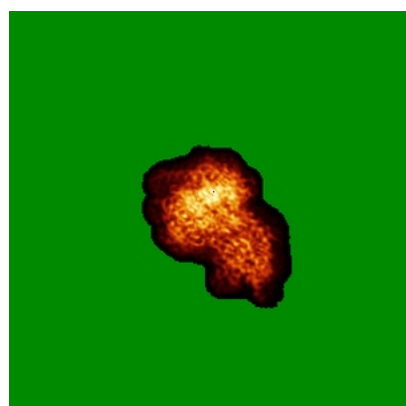


Z Index: 162

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

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

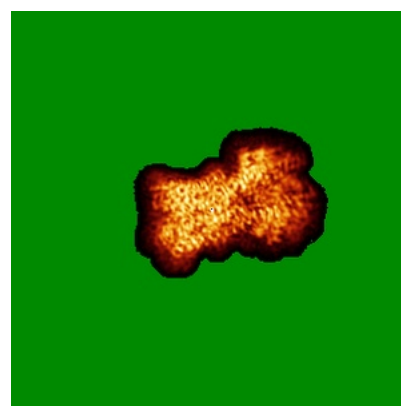
6.4.1 Primary map



X



Y

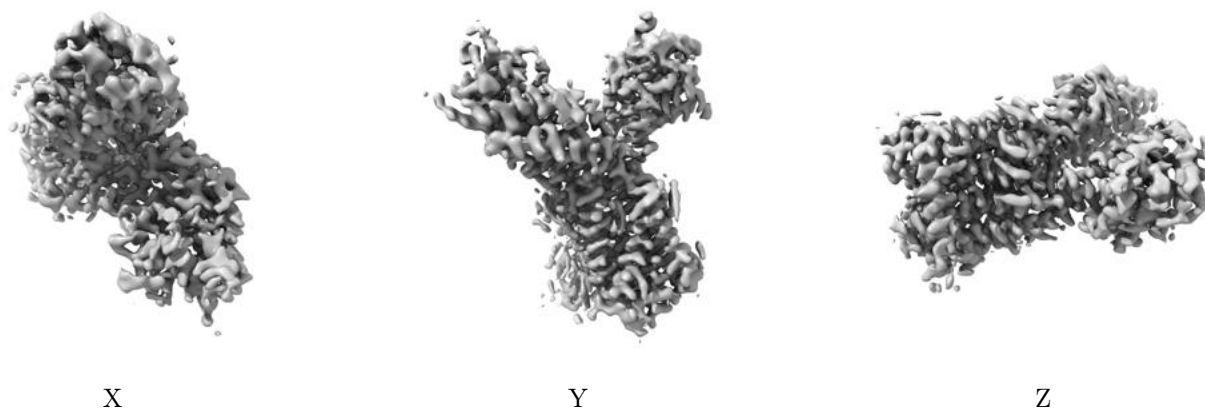


Z

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

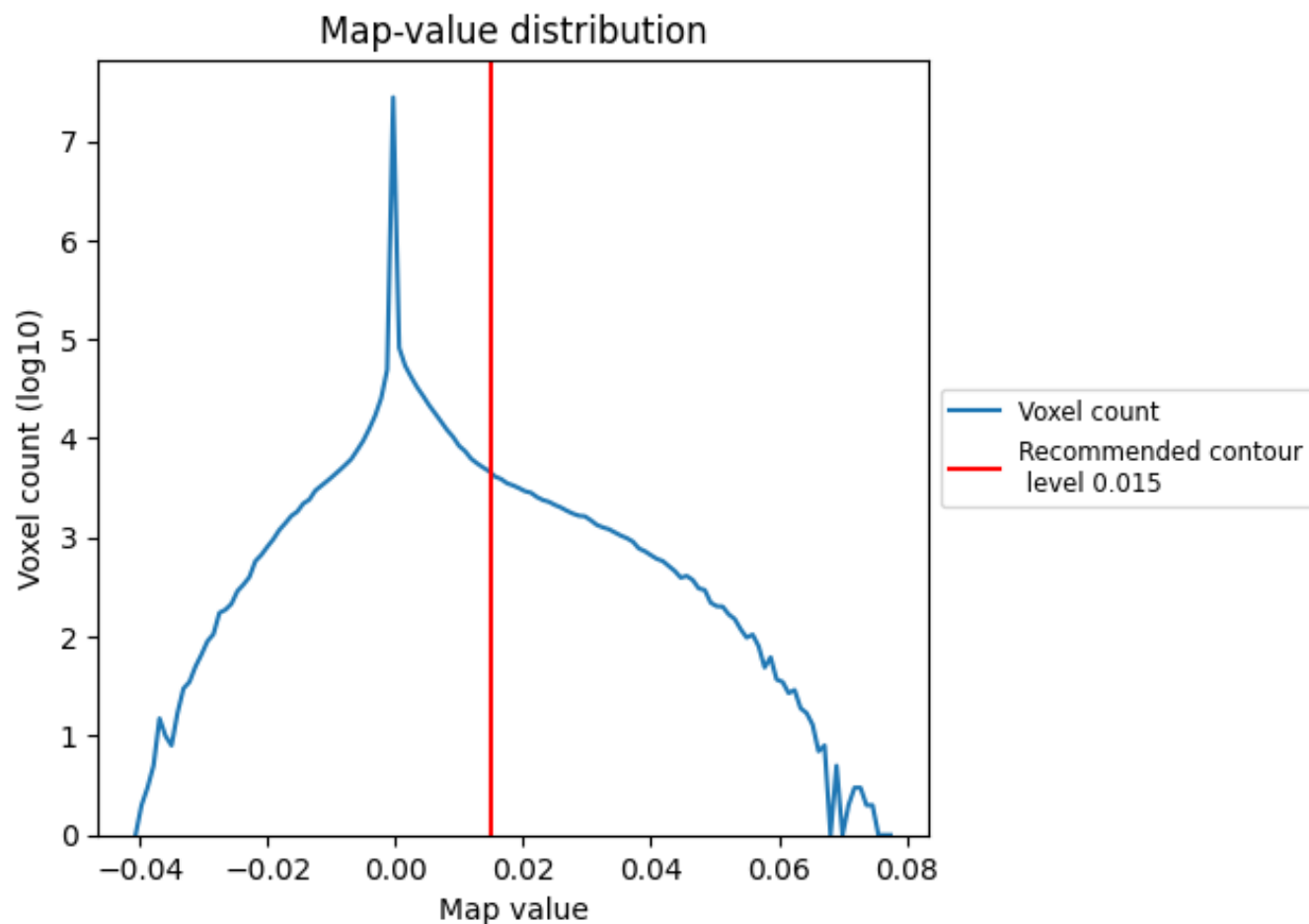
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

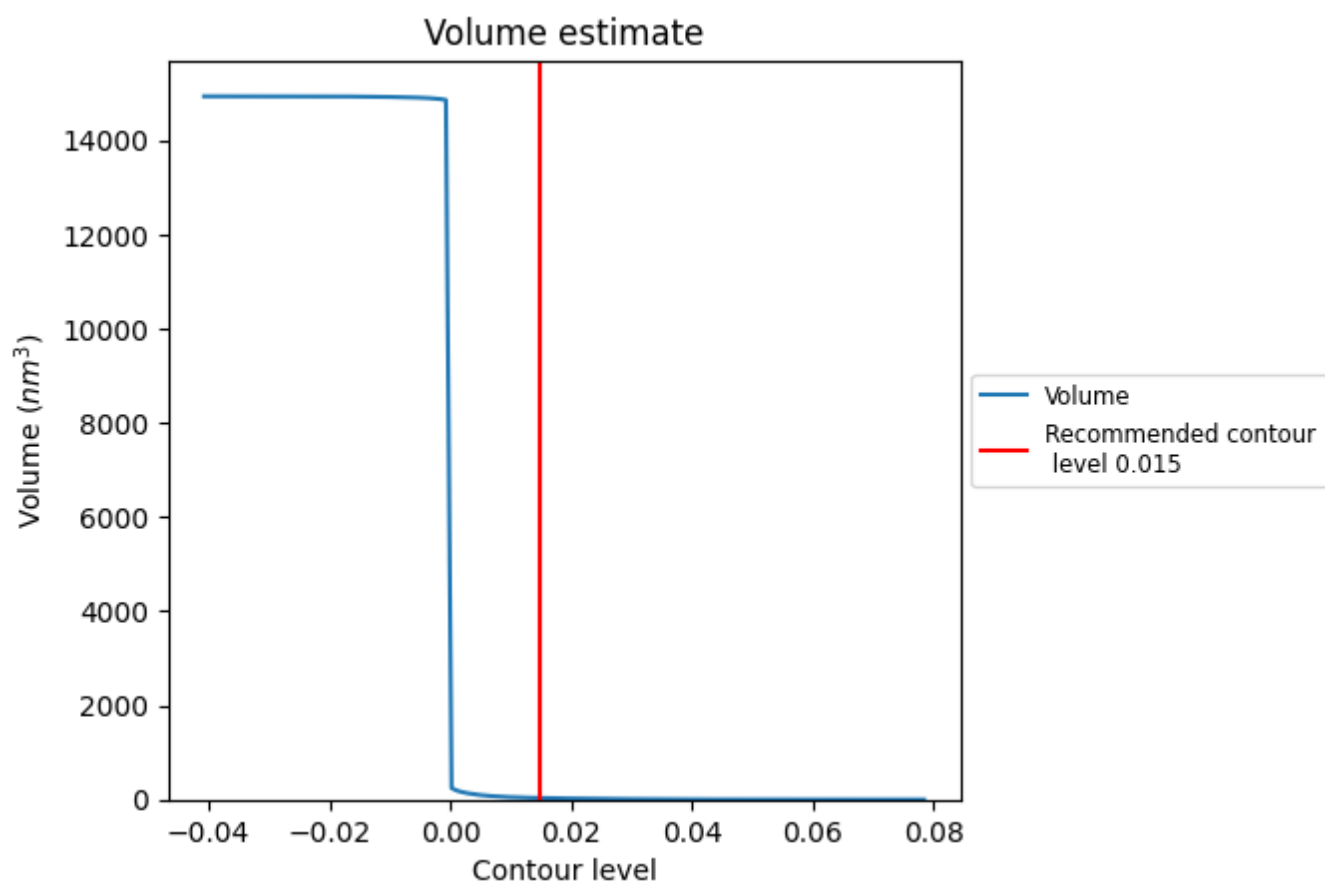
This section contains the results of statistical analysis of the map.

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.

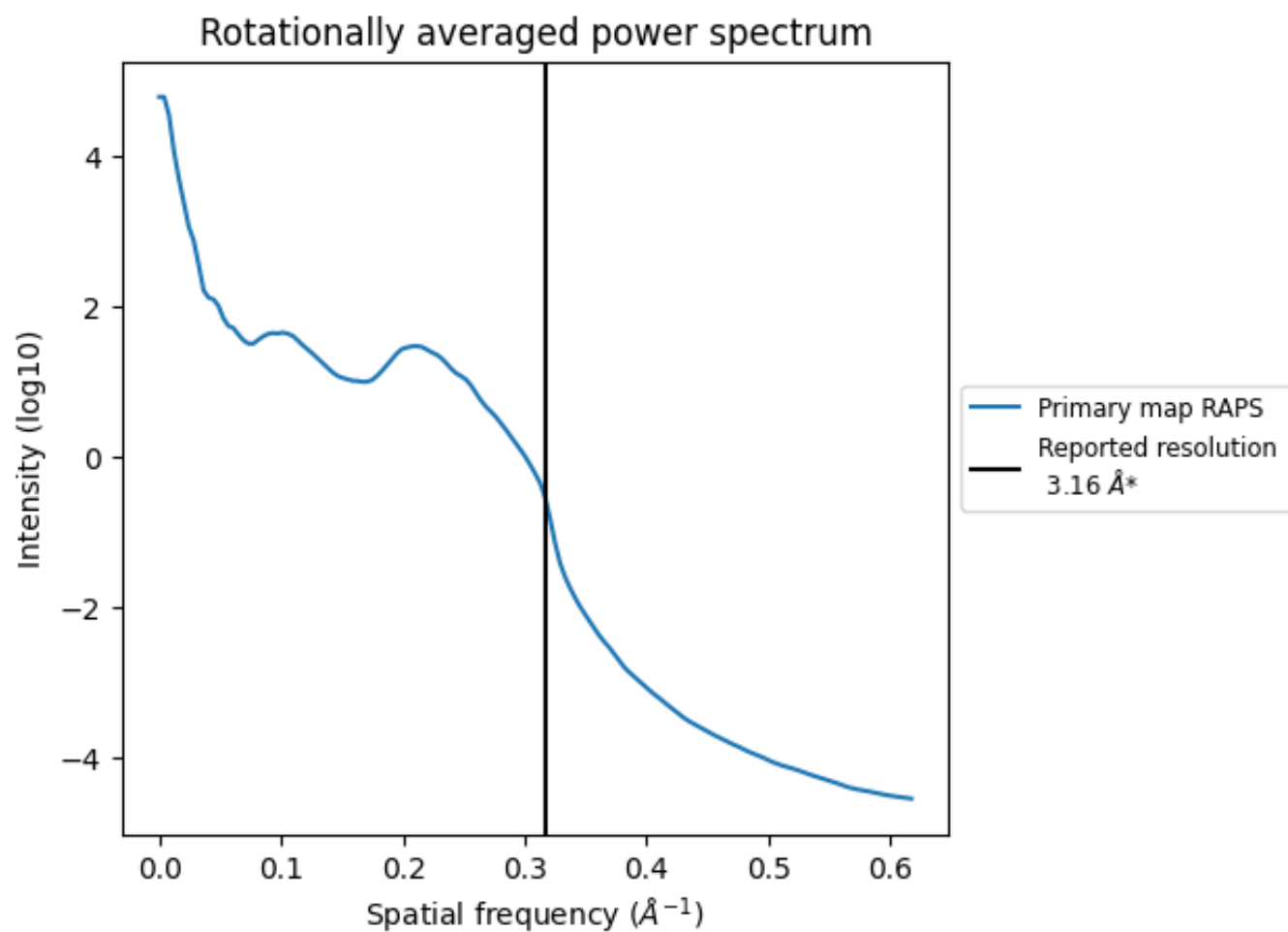
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm³; this corresponds to an approximate mass of 30 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 ⓘ

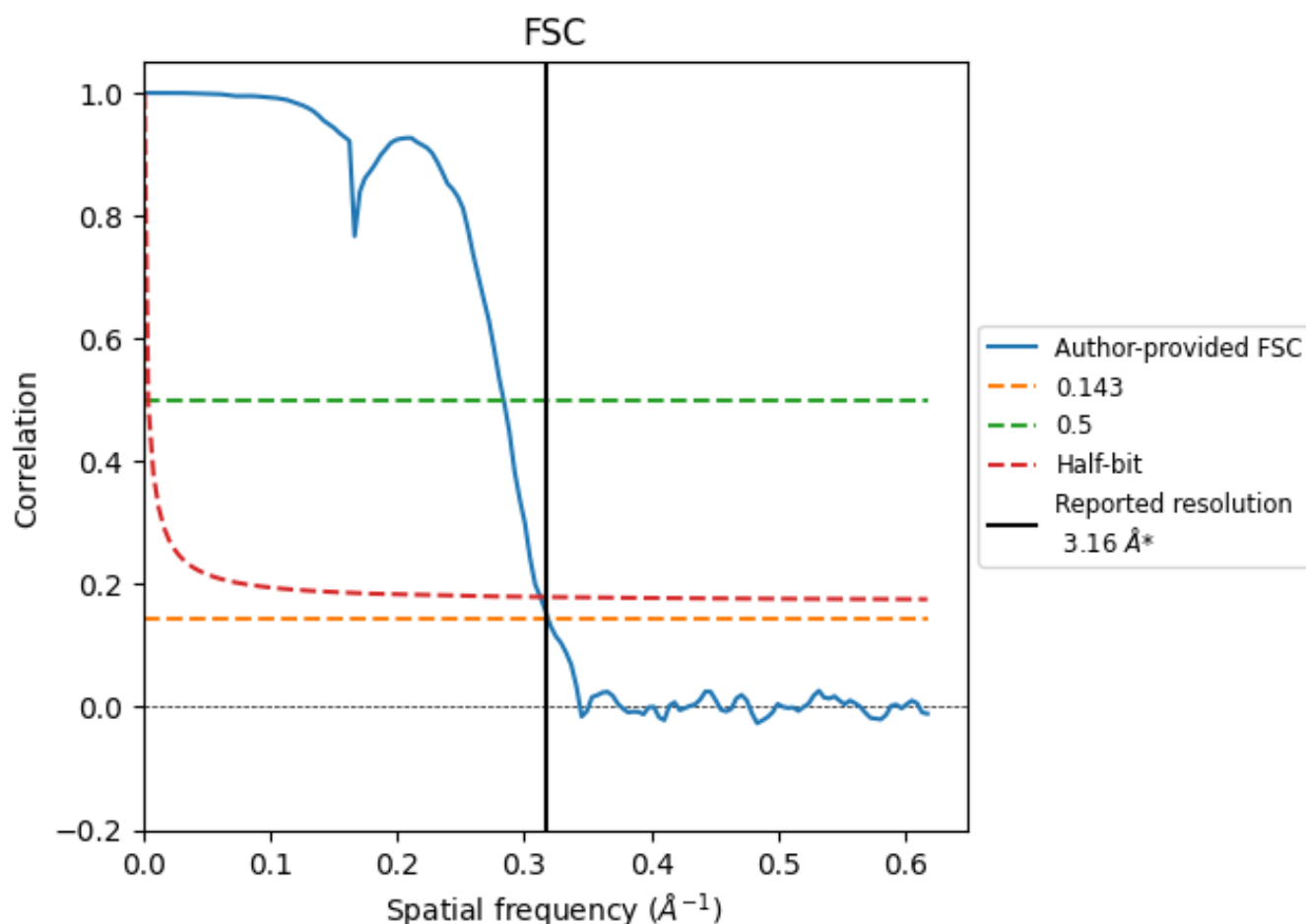


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

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 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

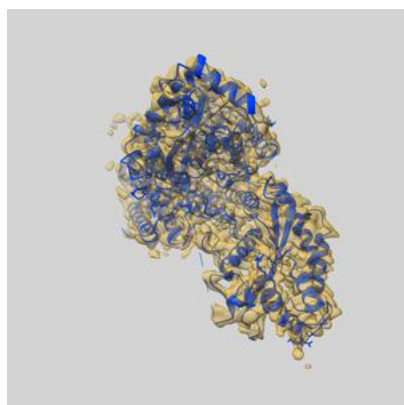
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.14	3.52	3.20
Unmasked-calculated*	-	-	-

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

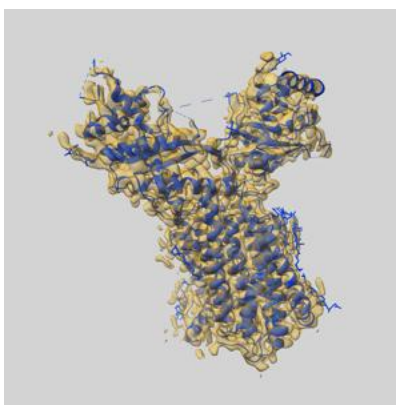
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10452 and PDB model 6TBU. Per-residue inclusion information can be found in section 3 on page 7.

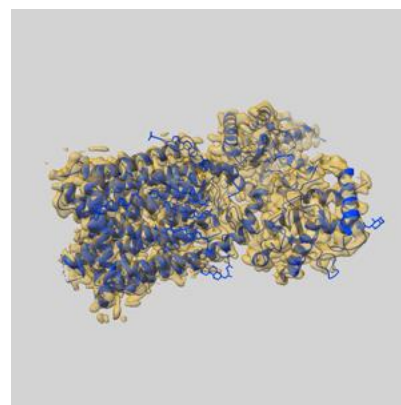
9.1 Map-model overlay [i](#)



X



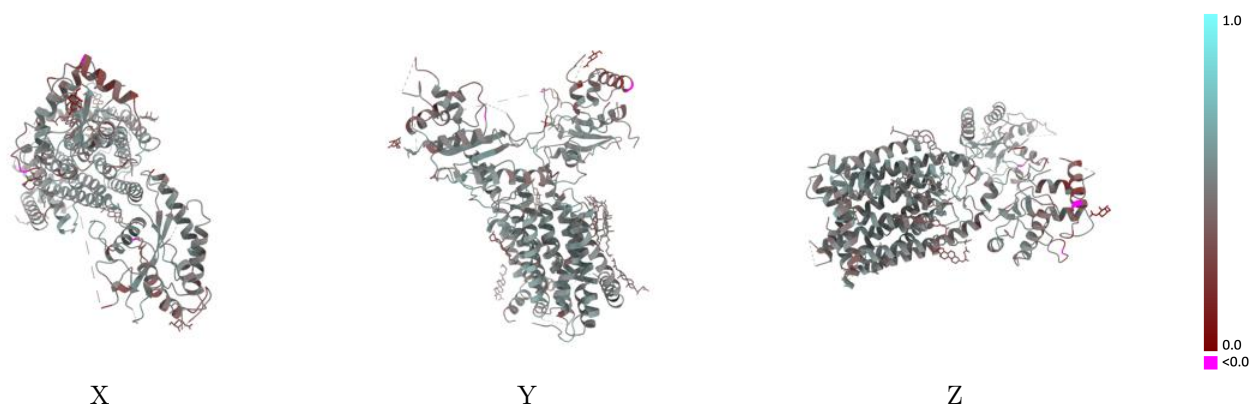
Y



Z

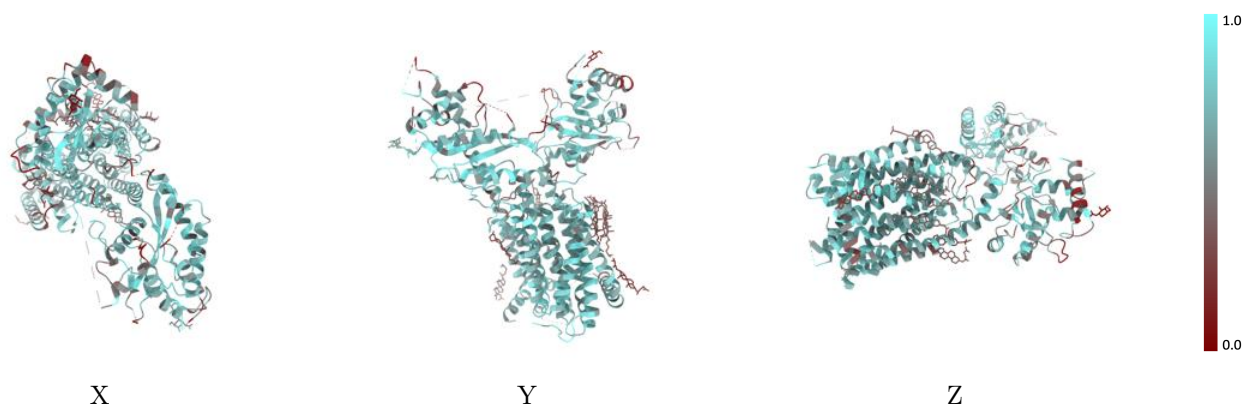
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



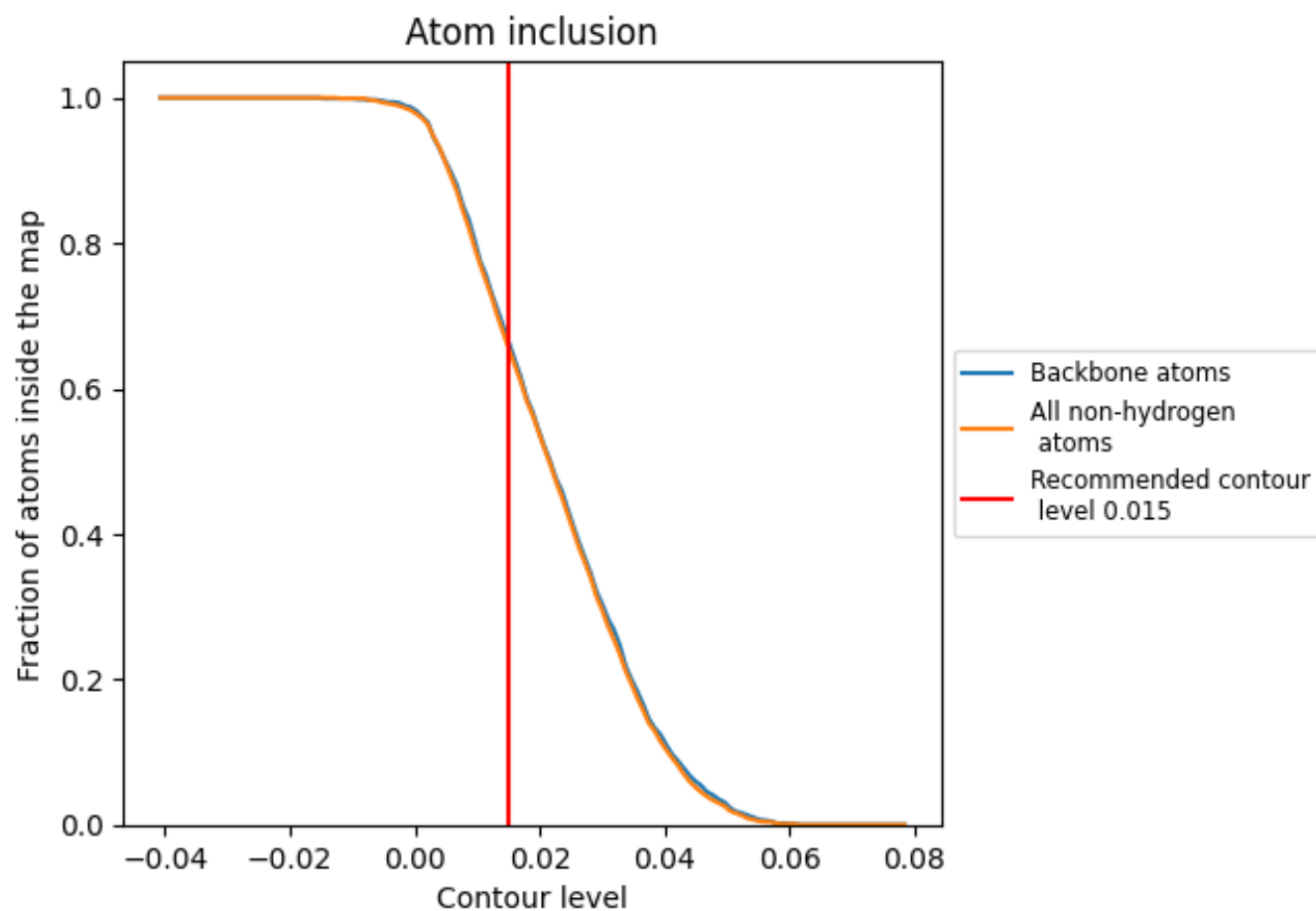
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.4800
A	0.6630	0.4800
B	0.6430	0.4030

