



## Full wwPDB EM Validation Report ⓘ

Oct 27, 2025 – 09:42 PM EDT

PDB ID : 9MFM / pdb\_00009mfm  
EMDB ID : EMD-48235  
Title : Structure of zebrafish OTOP1 in nanodisc in complex with inhibitor C2.36  
Authors : Burendei, B.; Ward, A.B.  
Deposited on : 2024-12-10  
Resolution : 3.42 Å(reported)  
Based on initial model : 6NF4

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ 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.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46



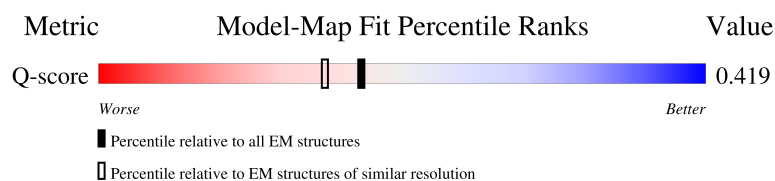
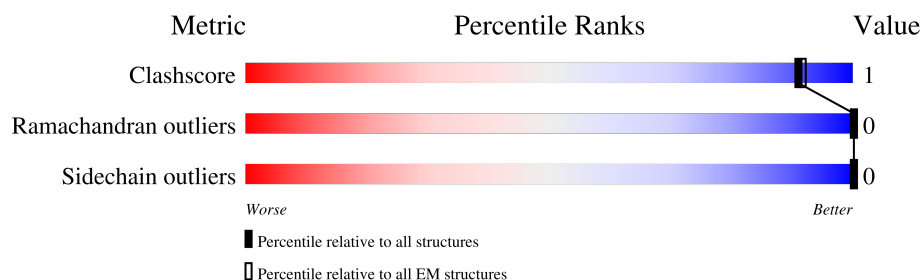
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.42 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13959 ( 2.92 - 3.92 )

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  $\geq 3$ , 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	587	
1	B	587	





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.

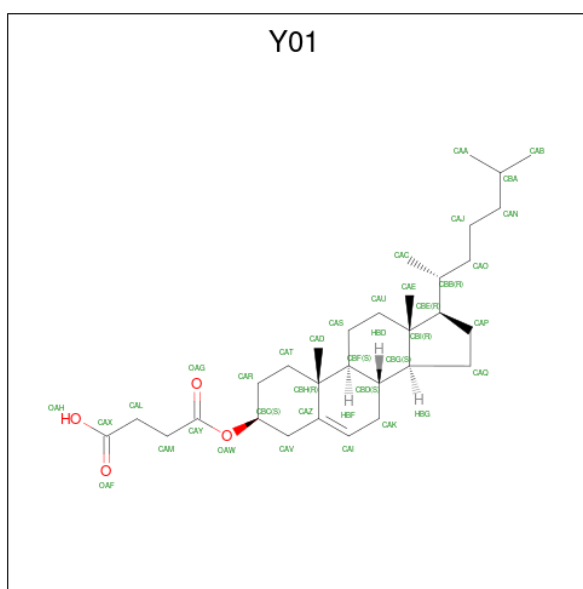
- Molecule 1 is a protein called Proton channel OTOPI.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	367	Total 2913	C 1928	N 466	O 492	S 27	0	0
1	B	367	Total 2913	C 1928	N 466	O 492	S 27	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q7ZWK8
A	1	PRO	-	expression tag	UNP Q7ZWK8
B	0	GLY	-	expression tag	UNP Q7ZWK8
B	1	PRO	-	expression tag	UNP Q7ZWK8

- 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	

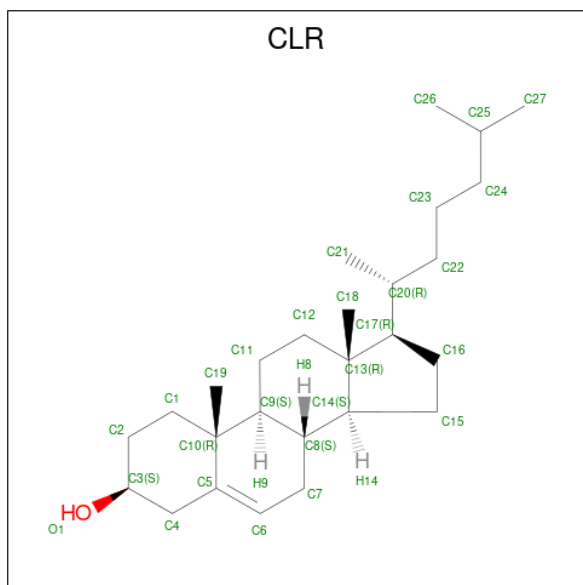
*Continued on next page...*



Continued from previous page...

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

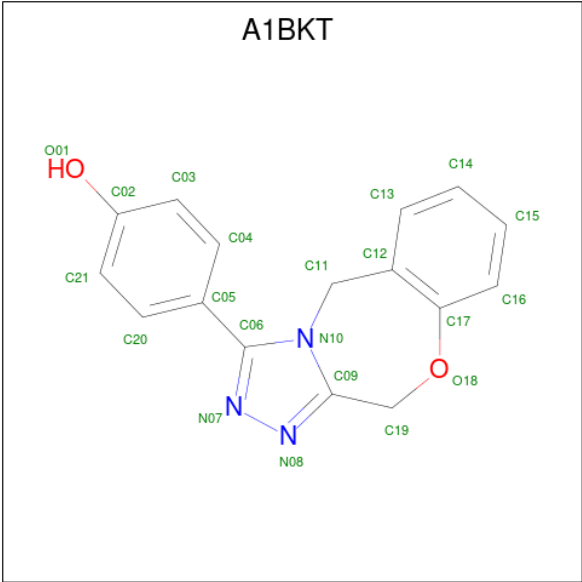
- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	

- Molecule 4 is 4-[(4R)-5H,11H-[1,2,4]triazolo[3,4-c][1,4]benzoxazepin-3-yl]phenol (CCD ID: A1BKT) (formula:  $C_{16}H_{13}N_3O_2$ ) (labeled as "Ligand of Interest" by depositor).





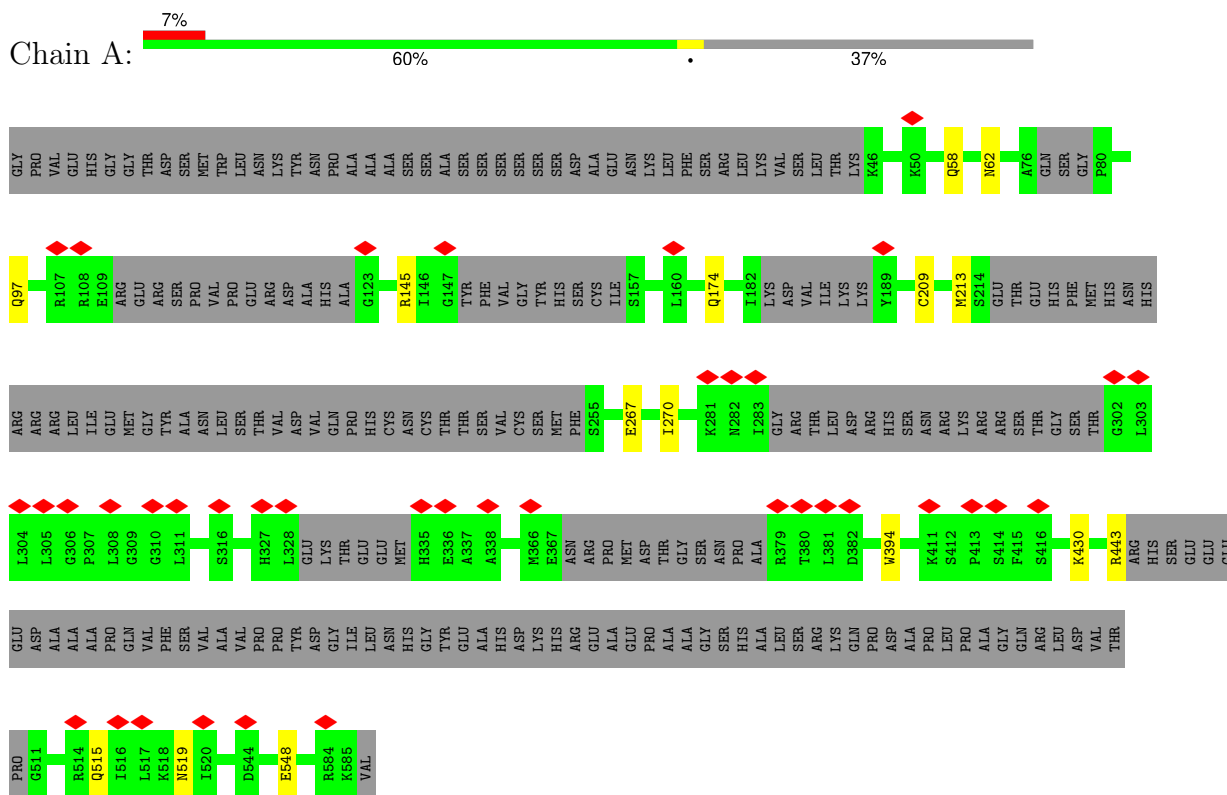
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			21	16	3	2	
4	A	1	Total	C	N	O	0
			21	16	3	2	
4	A	1	Total	C	N	O	0
			21	16	3	2	
4	B	1	Total	C	N	O	0
			21	16	3	2	
4	B	1	Total	C	N	O	0
			21	16	3	2	
4	B	1	Total	C	N	O	0
			21	16	3	2	



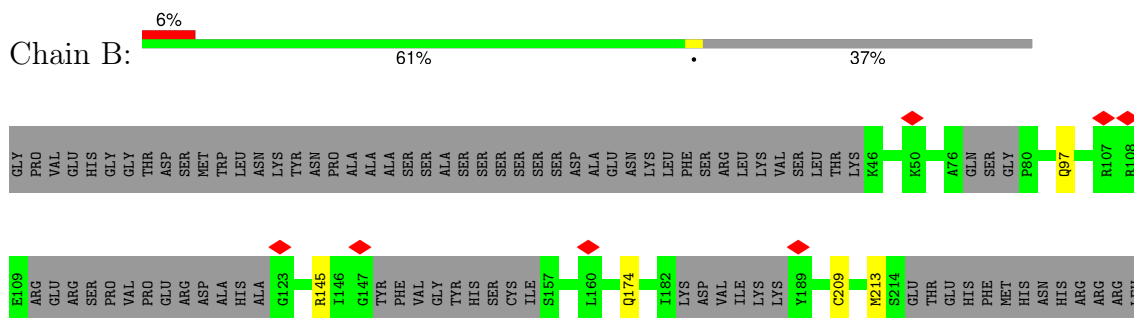
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

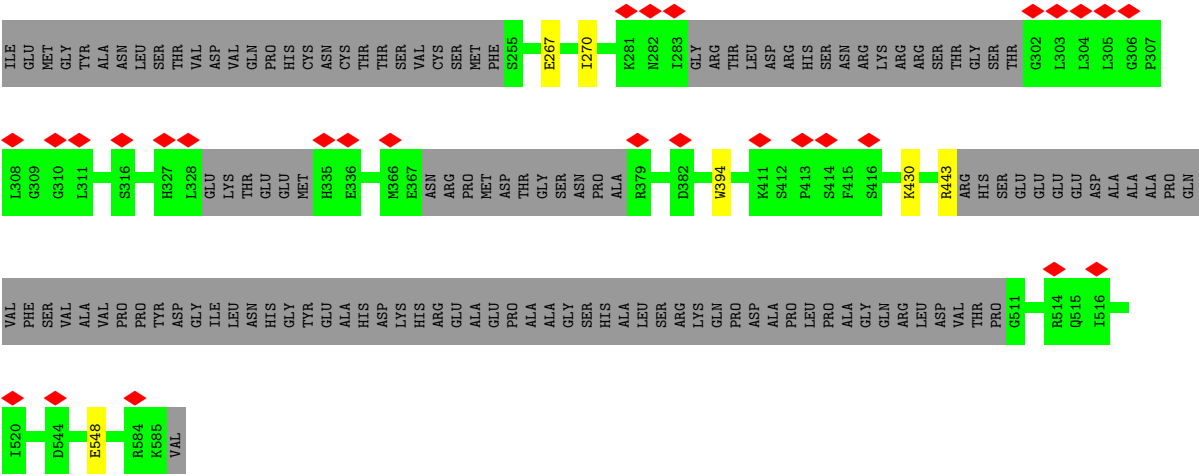
- Molecule 1: Proton channel OTOPI



- Molecule 1: Proton channel OTOPI









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	290491	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	190000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.368	Depositor
Minimum map value	-1.735	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.139	Depositor
Map size (Å)	208.8, 208.8, 208.8	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.044, 1.044, 1.044	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, CLR, A1BKT

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	0.25	0/2981	0.57	0/4039
1	B	0.25	0/2981	0.57	0/4039
All	All	0.25	0/5962	0.57	0/8078

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain
1	A	443	ARG	Sidechain
1	B	145	ARG	Sidechain
1	B	443	ARG	Sidechain



## 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	2913	0	2972	7	0
1	B	2913	0	2972	5	0
2	A	70	0	98	2	0
2	B	70	0	98	2	0
3	A	28	0	46	1	0
3	B	28	0	46	1	0
4	A	63	0	0	0	0
4	B	63	0	0	0	0
All	All	6148	0	6232	18	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 1.

All (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLN:NE2	1:B:174:GLN:OE1	2.38	0.56
1:A:97:GLN:NE2	1:A:174:GLN:OE1	2.39	0.55
1:B:548:GLU:OE1	1:B:548:GLU:N	2.43	0.51
1:A:267:GLU:HA	1:A:270:ILE:HG22	1.95	0.48
1:A:548:GLU:OE1	1:A:548:GLU:N	2.43	0.48
1:A:394:TRP:HE1	1:A:430:LYS:HB2	1.79	0.48
1:B:267:GLU:HA	1:B:270:ILE:HG22	1.95	0.48
2:B:602:Y01:HAE2	2:B:602:Y01:HAC2	1.96	0.47
2:A:602:Y01:HAE2	2:A:602:Y01:HAC2	1.96	0.47
1:B:394:TRP:HE1	1:B:430:LYS:HB2	1.79	0.46
1:A:58:GLN:O	1:A:62:ASN:ND2	2.50	0.44
3:A:603:CLR:H222	3:A:603:CLR:H272	2.00	0.43
3:B:603:CLR:H222	3:B:603:CLR:H272	2.00	0.42
1:A:515:GLN:O	1:A:519:ASN:ND2	2.49	0.41
2:B:602:Y01:HAC2	2:B:602:Y01:CAE	2.51	0.41
1:B:209:CYS:O	1:B:213:MET:HG2	2.21	0.41
2:A:602:Y01:HAC2	2:A:602:Y01:CAE	2.51	0.41
1:A:209:CYS:O	1:A:213:MET:HG2	2.21	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	347/587 (59%)	345 (99%)	2 (1%)	0	100	100
1	B	347/587 (59%)	345 (99%)	2 (1%)	0	100	100
All	All	694/1174 (59%)	690 (99%)	4 (1%)	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	319/506 (63%)	319 (100%)	0	100	100
1	B	319/506 (63%)	319 (100%)	0	100	100
All	All	638/1012 (63%)	638 (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	210	ASN
1	A	265	ASN
1	A	269	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	210	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 ⓘ

12 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	CLR	A	603	-	31,31,31	3.44	16 (51%)	48,48,48	2.72	20 (41%)
4	A1BKT	B	605	-	21,24,24	2.23	4 (19%)	25,34,34	1.47	2 (8%)
4	A1BKT	A	605	-	21,24,24	2.21	4 (19%)	25,34,34	1.47	2 (8%)
2	Y01	B	601	-	38,38,38	1.71	7 (18%)	57,57,57	2.22	17 (29%)
4	A1BKT	A	604	-	21,24,24	2.07	5 (23%)	25,34,34	1.52	2 (8%)
4	A1BKT	B	606	-	21,24,24	1.73	4 (19%)	25,34,34	0.87	2 (8%)
4	A1BKT	B	604	-	21,24,24	2.08	5 (23%)	25,34,34	1.52	2 (8%)
2	Y01	A	601	-	38,38,38	1.70	7 (18%)	57,57,57	2.21	17 (29%)
3	CLR	B	603	-	31,31,31	3.44	15 (48%)	48,48,48	2.72	20 (41%)
2	Y01	A	602	-	38,38,38	1.49	6 (15%)	57,57,57	2.49	15 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	A1BKT	A	606	-	21,24,24	1.74	4 (19%)	25,34,34	0.86	2 (8%)
2	Y01	B	602	-	38,38,38	1.48	6 (15%)	57,57,57	2.50	15 (26%)

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	CLR	A	603	-	-	4/10/68/68	0/4/4/4
4	A1BKT	B	605	-	-	4/4/13/13	0/3/4/4
4	A1BKT	A	605	-	-	4/4/13/13	0/3/4/4
2	Y01	B	601	-	-	7/19/77/77	0/4/4/4
4	A1BKT	A	604	-	-	0/4/13/13	0/3/4/4
4	A1BKT	B	606	-	-	0/4/13/13	0/3/4/4
4	A1BKT	B	604	-	-	0/4/13/13	0/3/4/4
2	Y01	A	601	-	-	7/19/77/77	0/4/4/4
3	CLR	B	603	-	-	4/10/68/68	0/4/4/4
2	Y01	A	602	-	-	11/19/77/77	0/4/4/4
4	A1BKT	A	606	-	-	0/4/13/13	0/3/4/4
2	Y01	B	602	-	-	11/19/77/77	0/4/4/4

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	CLR	C10-C9	7.54	1.68	1.56
3	A	603	CLR	C10-C9	7.53	1.68	1.56
3	A	603	CLR	C13-C17	6.49	1.66	1.55
3	B	603	CLR	C13-C17	6.47	1.66	1.55
3	B	603	CLR	C4-C5	6.41	1.64	1.51
4	B	605	A1BKT	C19-C09	-6.41	1.44	1.50
3	A	603	CLR	C4-C5	6.40	1.64	1.51
4	A	605	A1BKT	C19-C09	-6.34	1.45	1.50
3	B	603	CLR	C8-C14	5.98	1.64	1.53
3	A	603	CLR	C8-C14	5.95	1.64	1.53
3	A	603	CLR	C4-C3	5.55	1.61	1.52
3	B	603	CLR	C4-C3	5.53	1.61	1.52
4	A	604	A1BKT	C19-C09	-4.92	1.46	1.50
3	B	603	CLR	C7-C6	4.91	1.60	1.50
3	A	603	CLR	C7-C6	4.89	1.60	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	A1BKT	C19-C09	-4.89	1.46	1.50
2	B	601	Y01	CAK-CAI	-4.83	1.40	1.50
2	A	601	Y01	CAK-CAI	-4.83	1.40	1.50
4	B	605	A1BKT	C11-C12	4.55	1.59	1.51
3	A	603	CLR	C11-C9	4.53	1.61	1.53
3	B	603	CLR	C11-C9	4.50	1.61	1.53
2	A	602	Y01	CAK-CAI	-4.50	1.41	1.50
2	B	602	Y01	CAK-CAI	-4.48	1.41	1.50
4	A	605	A1BKT	C11-C12	4.46	1.59	1.51
2	B	601	Y01	CBH-CBF	4.27	1.62	1.56
2	A	601	Y01	CBH-CBF	4.26	1.62	1.56
3	B	603	CLR	C12-C11	4.24	1.61	1.53
3	A	603	CLR	C12-C11	4.22	1.61	1.53
4	A	604	A1BKT	C11-C12	4.13	1.58	1.51
4	B	604	A1BKT	C11-C12	4.12	1.58	1.51
3	B	603	CLR	C7-C8	3.88	1.59	1.53
3	A	603	CLR	C7-C8	3.87	1.59	1.53
3	A	603	CLR	C8-C9	3.85	1.60	1.53
3	B	603	CLR	C8-C9	3.85	1.60	1.53
3	B	603	CLR	C1-C10	3.77	1.61	1.54
3	A	603	CLR	C1-C10	3.76	1.61	1.54
4	B	606	A1BKT	C09-N08	3.37	1.39	1.33
4	A	606	A1BKT	C09-N08	3.35	1.39	1.33
2	B	602	Y01	CBI-CBE	3.34	1.61	1.55
3	A	603	CLR	C20-C17	3.32	1.60	1.54
3	B	603	CLR	C20-C17	3.32	1.60	1.54
2	A	602	Y01	CBI-CBE	3.32	1.61	1.55
2	A	602	Y01	CBH-CAZ	-3.26	1.46	1.52
2	B	602	Y01	CBH-CAZ	-3.19	1.46	1.52
4	B	605	A1BKT	C09-N08	3.15	1.38	1.33
4	A	606	A1BKT	O18-C19	3.15	1.47	1.44
4	B	606	A1BKT	O18-C19	3.15	1.47	1.44
4	A	604	A1BKT	C09-N08	3.15	1.38	1.33
4	A	605	A1BKT	C09-N08	3.14	1.38	1.33
4	B	604	A1BKT	C09-N08	3.11	1.38	1.33
2	B	601	Y01	CAS-CBF	3.05	1.58	1.53
2	A	601	Y01	CAS-CBF	3.05	1.58	1.53
3	A	603	CLR	C15-C14	2.94	1.60	1.54
3	B	603	CLR	C15-C14	2.90	1.60	1.54
2	B	601	Y01	CBH-CAZ	-2.86	1.47	1.52
2	A	601	Y01	CBH-CAZ	-2.82	1.47	1.52
4	B	605	A1BKT	C06-N07	2.79	1.40	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	A1BKT	C06-N07	2.77	1.40	1.33
4	B	604	A1BKT	C06-N07	2.75	1.40	1.33
4	A	604	A1BKT	C06-N07	2.74	1.40	1.33
4	A	606	A1BKT	C06-N07	2.70	1.40	1.33
4	B	606	A1BKT	C06-N07	2.69	1.40	1.33
2	B	602	Y01	CAI-CAZ	2.68	1.38	1.33
2	A	602	Y01	CAI-CAZ	2.66	1.38	1.33
2	B	601	Y01	CAI-CAZ	2.64	1.38	1.33
4	B	604	A1BKT	O18-C19	-2.63	1.42	1.44
2	A	601	Y01	CAI-CAZ	2.61	1.38	1.33
4	A	604	A1BKT	O18-C19	-2.51	1.42	1.44
2	B	602	Y01	CAL-CAX	2.31	1.55	1.50
2	A	602	Y01	CAL-CAX	2.29	1.55	1.50
4	A	606	A1BKT	C19-C09	2.29	1.52	1.50
2	A	601	Y01	CAK-CBD	-2.22	1.49	1.53
2	B	601	Y01	CAK-CBD	-2.18	1.49	1.53
4	B	606	A1BKT	C19-C09	2.15	1.52	1.50
3	B	603	CLR	C22-C20	2.15	1.59	1.54
3	B	603	CLR	C13-C14	2.12	1.58	1.55
3	A	603	CLR	C22-C20	2.11	1.59	1.54
3	A	603	CLR	C13-C14	2.09	1.58	1.55
2	A	601	Y01	CAU-CAS	2.05	1.57	1.53
2	B	601	Y01	CAU-CAS	2.04	1.57	1.53
3	A	603	CLR	C10-C5	2.02	1.56	1.52
2	A	602	Y01	CAP-CBE	2.00	1.58	1.54
2	B	602	Y01	CAP-CBE	2.00	1.58	1.54

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	Y01	CAV-CAZ-CBH	10.28	129.59	116.42
2	A	602	Y01	CAV-CAZ-CBH	10.24	129.53	116.42
2	B	601	Y01	CAV-CAZ-CBH	7.24	125.69	116.42
2	A	601	Y01	CAV-CAZ-CBH	7.17	125.61	116.42
3	A	603	CLR	C4-C5-C6	6.84	129.84	120.57
3	B	603	CLR	C4-C5-C6	6.80	129.78	120.57
3	A	603	CLR	C18-C13-C12	-6.45	101.10	110.61
3	B	603	CLR	C18-C13-C12	-6.44	101.11	110.61
2	B	602	Y01	CAV-CAZ-CAI	-6.28	112.06	120.57
2	A	602	Y01	CAV-CAZ-CAI	-6.25	112.09	120.57
3	A	603	CLR	C3-C4-C5	6.20	121.93	112.05
3	B	603	CLR	C3-C4-C5	6.19	121.91	112.05

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	CLR	C4-C5-C10	-5.85	108.93	116.42
3	B	603	CLR	C4-C5-C10	-5.83	108.96	116.42
2	B	602	Y01	OAW-CAY-CAM	5.59	123.58	111.48
2	A	602	Y01	OAW-CAY-CAM	5.56	123.51	111.48
4	A	604	A1BKT	C12-C11-N10	5.21	126.12	112.27
4	B	604	A1BKT	C12-C11-N10	5.20	126.09	112.27
3	B	603	CLR	C7-C8-C14	5.11	118.17	110.93
3	A	603	CLR	C7-C8-C14	5.10	118.16	110.93
2	A	601	Y01	OAW-CAY-CAM	5.02	122.35	111.48
2	B	601	Y01	OAW-CAY-CAM	5.02	122.34	111.48
4	A	605	A1BKT	C12-C11-N10	4.91	125.33	112.27
4	B	605	A1BKT	C12-C11-N10	4.89	125.28	112.27
2	A	601	Y01	OAW-CAY-OAG	-4.84	112.39	123.70
2	B	602	Y01	OAW-CAY-OAG	-4.83	112.41	123.70
2	B	601	Y01	OAW-CAY-OAG	-4.82	112.43	123.70
2	A	602	Y01	OAW-CAY-OAG	-4.78	112.54	123.70
2	B	601	Y01	CAT-CBH-CAZ	-4.71	100.63	108.74
2	A	601	Y01	CAT-CBH-CAZ	-4.70	100.63	108.74
2	B	601	Y01	CAV-CAZ-CAI	-4.52	114.44	120.57
2	A	601	Y01	CAV-CAZ-CAI	-4.49	114.48	120.57
2	B	602	Y01	CAS-CBF-CBD	-4.41	105.63	111.78
3	A	603	CLR	C1-C10-C5	4.39	116.31	108.74
3	B	603	CLR	C1-C10-C5	4.37	116.27	108.74
2	A	602	Y01	CAS-CBF-CBD	-4.36	105.70	111.78
3	B	603	CLR	C12-C13-C17	4.21	122.81	116.60
3	A	603	CLR	C12-C13-C17	4.21	122.80	116.60
3	B	603	CLR	C17-C13-C14	4.18	104.89	100.10
3	B	603	CLR	C19-C10-C5	-4.17	102.02	108.38
3	A	603	CLR	C19-C10-C5	-4.15	102.05	108.38
2	B	601	Y01	CAS-CBF-CBH	4.13	118.18	113.08
2	A	601	Y01	CAS-CBF-CBH	4.12	118.17	113.08
3	A	603	CLR	C17-C13-C14	4.11	104.81	100.10
4	A	605	A1BKT	C11-C12-C17	3.83	126.38	119.62
4	B	605	A1BKT	C11-C12-C17	3.81	126.33	119.62
4	B	604	A1BKT	C11-C12-C17	3.81	126.33	119.62
4	A	604	A1BKT	C11-C12-C17	3.80	126.31	119.62
2	B	602	Y01	CAT-CBH-CAZ	-3.55	102.61	108.74
2	A	602	Y01	CAT-CBH-CAZ	-3.53	102.65	108.74
2	A	602	Y01	CBD-CAK-CAI	3.47	117.57	112.76
2	B	602	Y01	CBD-CAK-CAI	3.45	117.54	112.76
2	B	601	Y01	CBF-CBH-CAZ	3.41	114.64	109.65
2	A	602	Y01	CBI-CBE-CBB	3.40	124.74	119.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	Y01	CBI-CBE-CBB	3.39	124.73	119.50
2	A	601	Y01	CBF-CBH-CAZ	3.37	114.59	109.65
2	A	601	Y01	OAW-CBC-CAV	-3.36	101.11	108.04
2	B	601	Y01	OAW-CBC-CAV	-3.35	101.14	108.04
2	A	602	Y01	CAP-CAQ-CBG	-3.32	98.64	105.14
2	B	602	Y01	CAP-CAQ-CBG	-3.31	98.67	105.14
2	B	601	Y01	CAS-CBF-CBD	-3.26	107.23	111.78
2	A	601	Y01	CAS-CBF-CBD	-3.24	107.25	111.78
3	B	603	CLR	C15-C14-C8	3.20	124.21	119.10
2	B	601	Y01	CAR-CBC-CAV	3.18	115.40	110.97
2	A	601	Y01	CAR-CBC-CAV	3.18	115.39	110.97
3	A	603	CLR	C15-C14-C8	3.15	124.13	119.10
2	B	602	Y01	CBH-CAZ-CAI	-3.15	118.34	122.93
2	A	602	Y01	CBH-CAZ-CAI	-3.12	118.37	122.93
2	A	601	Y01	CAT-CAR-CBC	3.12	115.43	110.33
3	B	603	CLR	C18-C13-C17	-3.12	106.01	111.68
2	B	601	Y01	CAT-CAR-CBC	3.11	115.40	110.33
3	A	603	CLR	C18-C13-C17	-3.09	106.07	111.68
2	A	601	Y01	CAU-CAS-CBF	3.03	118.29	113.14
2	B	601	Y01	CAU-CAS-CBF	3.03	118.29	113.14
3	B	603	CLR	C12-C11-C9	3.00	118.23	113.14
3	A	603	CLR	C12-C11-C9	2.98	118.20	113.14
2	A	602	Y01	CBC-CAV-CAZ	2.92	115.76	111.45
3	A	603	CLR	C19-C10-C1	-2.91	105.00	109.43
2	B	602	Y01	CBC-CAV-CAZ	2.90	115.73	111.45
3	B	603	CLR	C19-C10-C1	-2.88	105.05	109.43
3	A	603	CLR	C1-C10-C9	2.73	112.35	108.74
3	B	603	CLR	C1-C10-C9	2.71	112.32	108.74
2	A	602	Y01	CAS-CBF-CBH	2.58	116.27	113.08
2	B	602	Y01	CAE-CBI-CBE	2.58	116.35	111.68
3	B	603	CLR	C16-C17-C13	-2.56	100.83	103.84
2	A	602	Y01	CAE-CBI-CBE	2.55	116.29	111.68
2	B	602	Y01	CAS-CBF-CBH	2.54	116.22	113.08
3	A	603	CLR	C16-C17-C13	-2.54	100.85	103.84
2	B	602	Y01	CAE-CBI-CAU	-2.46	106.98	110.61
2	A	602	Y01	CBG-CBI-CBE	-2.45	97.28	100.10
2	A	602	Y01	CAE-CBI-CAU	-2.45	106.99	110.61
2	B	602	Y01	CBG-CBI-CBE	-2.44	97.29	100.10
3	A	603	CLR	C10-C5-C6	-2.35	119.50	122.93
2	B	601	Y01	CAP-CBE-CBI	-2.33	101.09	103.84
3	B	603	CLR	C10-C5-C6	-2.33	119.52	122.93
3	A	603	CLR	C21-C20-C17	-2.32	109.39	112.88

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	Y01	CAP-CBE-CBI	-2.32	101.11	103.84
3	B	603	CLR	C21-C20-C17	-2.28	109.45	112.88
2	B	601	Y01	CBI-CBE-CBB	2.28	123.02	119.50
2	A	601	Y01	CBI-CBE-CBB	2.28	123.02	119.50
2	A	601	Y01	OAW-CBC-CAR	2.23	113.65	108.37
4	B	606	A1BKT	O18-C17-C12	-2.22	117.09	121.20
2	B	601	Y01	OAW-CBC-CAR	2.21	113.59	108.37
4	A	606	A1BKT	O18-C17-C12	-2.21	117.11	121.20
3	B	603	CLR	C16-C15-C14	2.18	109.41	105.14
3	A	603	CLR	C16-C15-C14	2.17	109.40	105.14
2	B	601	Y01	OAF-CAX-CAL	-2.16	116.24	123.09
2	B	601	Y01	CBH-CAZ-CAI	-2.15	119.78	122.93
2	A	601	Y01	OAF-CAX-CAL	-2.15	116.28	123.09
3	A	603	CLR	C22-C20-C17	2.12	114.73	110.33
2	A	601	Y01	CBH-CAZ-CAI	-2.12	119.83	122.93
3	B	603	CLR	C22-C20-C17	2.12	114.72	110.33
3	B	603	CLR	C2-C1-C10	2.09	117.23	112.78
3	A	603	CLR	C2-C1-C10	2.07	117.20	112.78
4	A	606	A1BKT	C11-C12-C13	2.06	123.00	119.77
4	B	606	A1BKT	C11-C12-C13	2.05	122.99	119.77

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	A1BKT	C04-C05-C06-N07
4	A	605	A1BKT	C04-C05-C06-N10
4	A	605	A1BKT	C20-C05-C06-N10
4	B	605	A1BKT	C04-C05-C06-N07
4	B	605	A1BKT	C04-C05-C06-N10
4	B	605	A1BKT	C20-C05-C06-N10
2	A	602	Y01	CAM-CAY-OAW-CBC
2	B	602	Y01	CAM-CAY-OAW-CBC
2	A	602	Y01	OAG-CAY-OAW-CBC
2	B	602	Y01	OAG-CAY-OAW-CBC
2	A	601	Y01	CAO-CAJ-CAN-CBA
2	A	602	Y01	CAO-CAJ-CAN-CBA
2	B	601	Y01	CAO-CAJ-CAN-CBA
2	B	602	Y01	CAO-CAJ-CAN-CBA
4	A	605	A1BKT	C20-C05-C06-N07
4	B	605	A1BKT	C20-C05-C06-N07
2	B	602	Y01	CAJ-CAN-CBA-CAB

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	602	Y01	CAJ-CAN-CBA-CAB
2	A	602	Y01	CAO-CBB-CBE-CAP
2	B	602	Y01	CAO-CBB-CBE-CAP
2	A	602	Y01	CAJ-CAN-CBA-CAA
2	B	602	Y01	CAJ-CAN-CBA-CAA
2	B	602	Y01	CAO-CBB-CBE-CBI
2	A	602	Y01	CAO-CBB-CBE-CBI
2	A	601	Y01	CAM-CAY-OAW-CBC
2	B	601	Y01	CAM-CAY-OAW-CBC
2	A	602	Y01	CAC-CBB-CBE-CAP
2	B	602	Y01	CAC-CBB-CBE-CAP
2	A	601	Y01	CAO-CBB-CBE-CAP
2	B	601	Y01	CAO-CBB-CBE-CAP
2	A	601	Y01	OAG-CAY-OAW-CBC
2	B	601	Y01	OAG-CAY-OAW-CBC
2	A	602	Y01	CAX-CAL-CAM-CAY
2	B	602	Y01	CAX-CAL-CAM-CAY
3	A	603	CLR	C22-C23-C24-C25
3	B	603	CLR	C22-C23-C24-C25
3	A	603	CLR	C20-C22-C23-C24
3	B	603	CLR	C20-C22-C23-C24
3	A	603	CLR	C23-C24-C25-C27
3	B	603	CLR	C23-C24-C25-C27
2	A	602	Y01	CAM-CAL-CAX-OAF
2	B	602	Y01	CAM-CAL-CAX-OAF
2	A	602	Y01	CAM-CAL-CAX-OAH
2	B	602	Y01	CAM-CAL-CAX-OAH
2	A	601	Y01	CAM-CAL-CAX-OAF
2	B	601	Y01	CAM-CAL-CAX-OAF
2	B	601	Y01	CAC-CBB-CBE-CAP
2	A	601	Y01	CAC-CBB-CBE-CAP
2	A	601	Y01	CAM-CAL-CAX-OAH
3	A	603	CLR	C23-C24-C25-C26
3	B	603	CLR	C23-C24-C25-C26
2	B	601	Y01	CAM-CAL-CAX-OAH

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	CLR	1	0
3	B	603	CLR	1	0

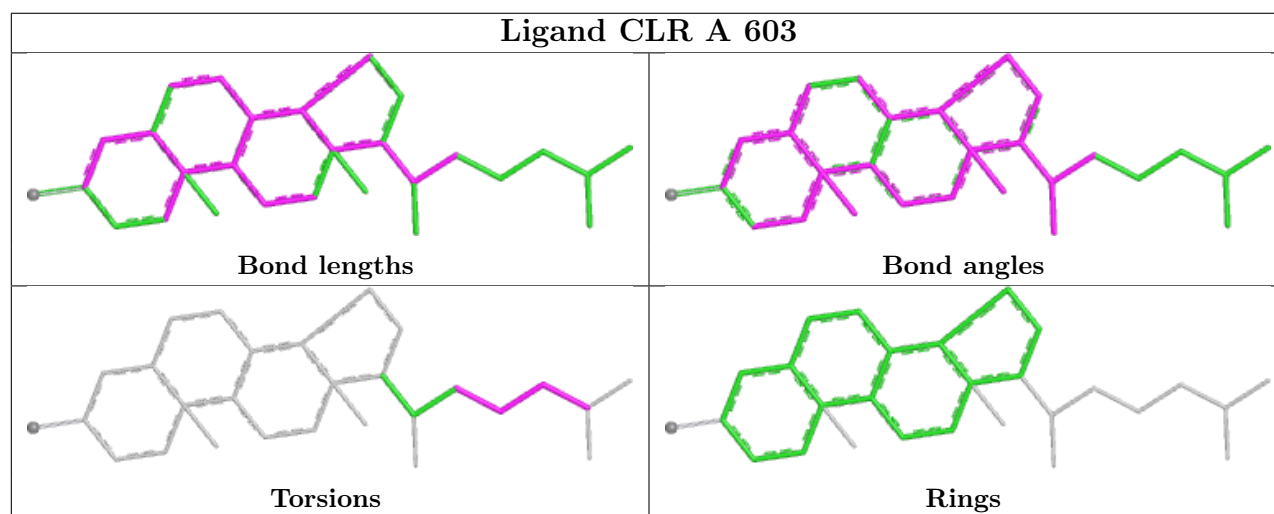
*Continued on next page...*



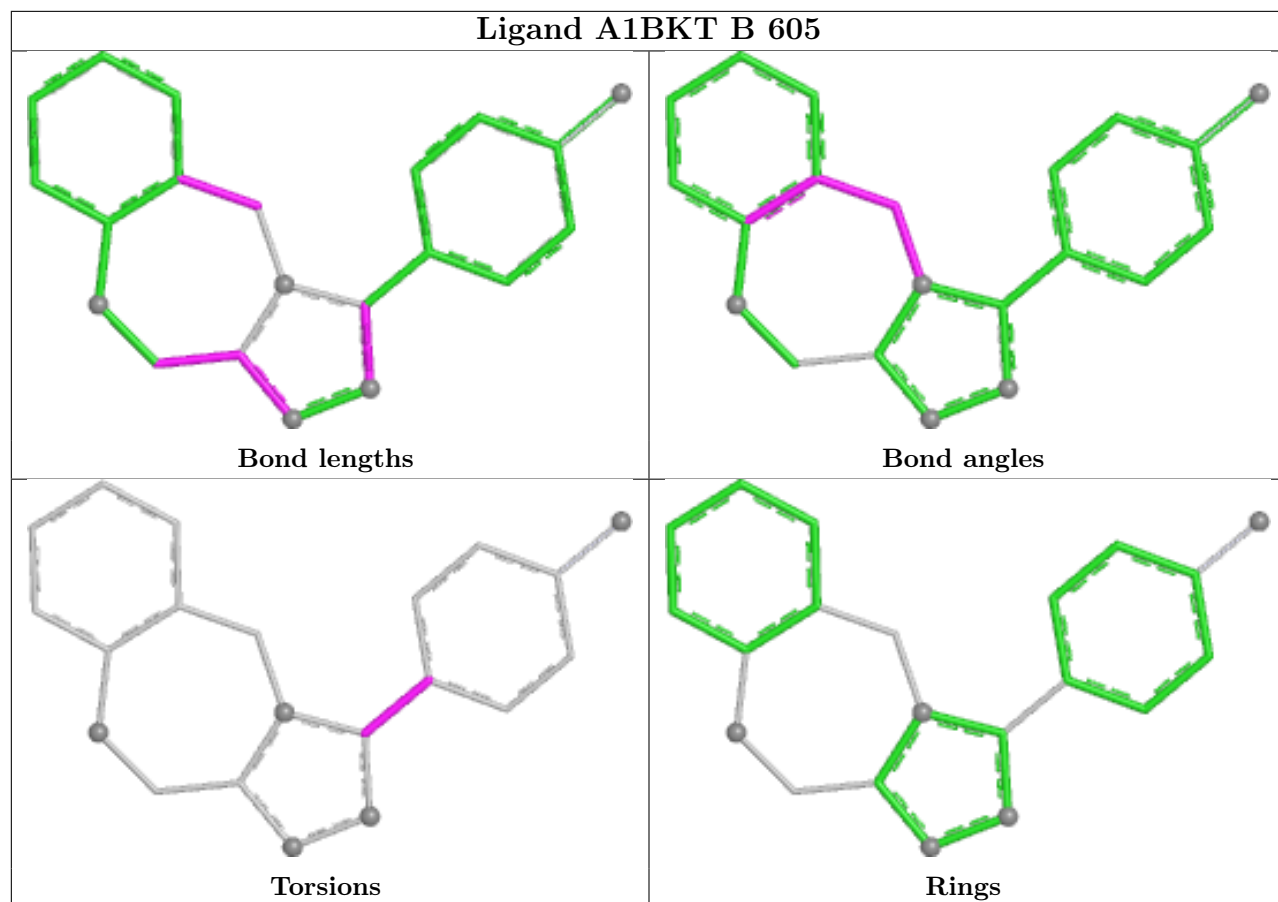
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	Y01	2	0
2	B	602	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.

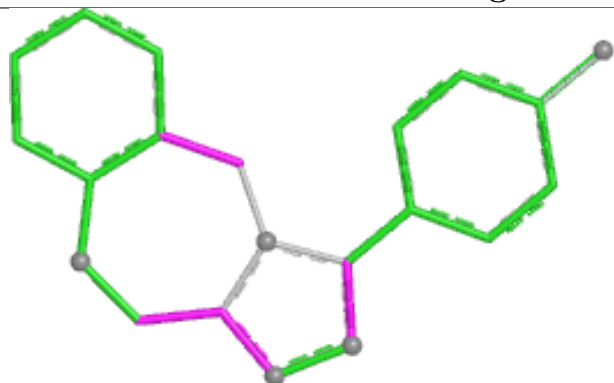




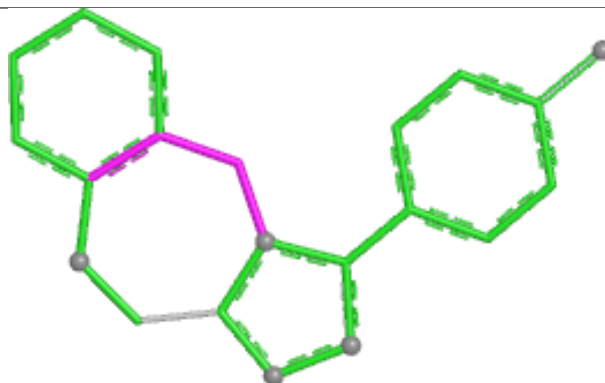




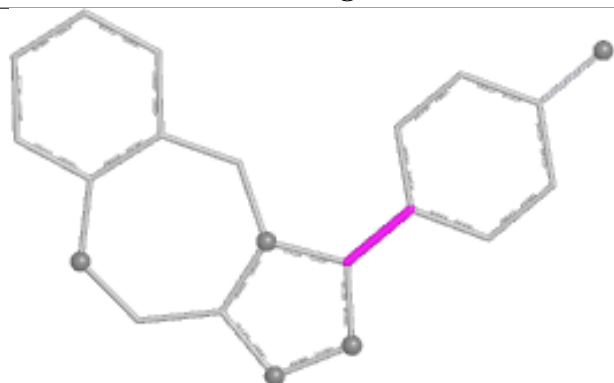
## Ligand A1BKT A 605



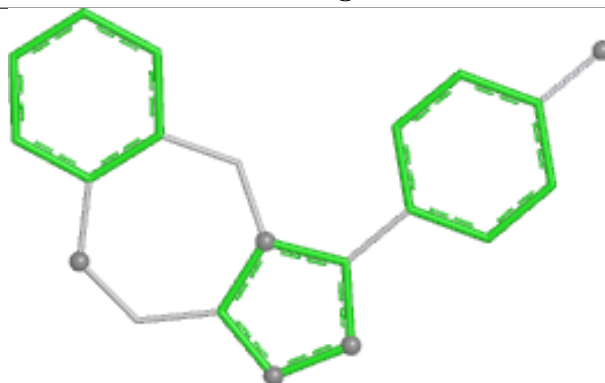
Bond lengths



Bond angles

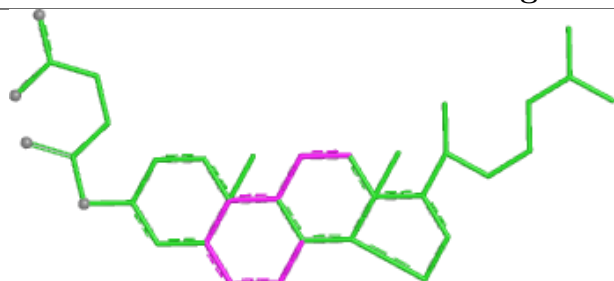


Torsions

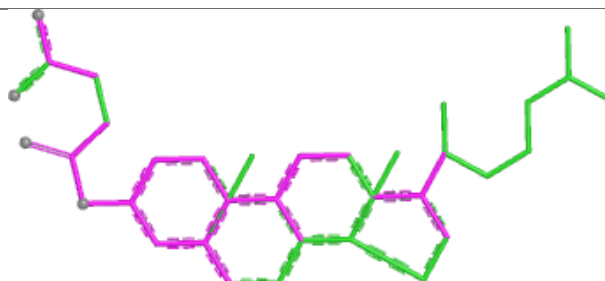


Rings

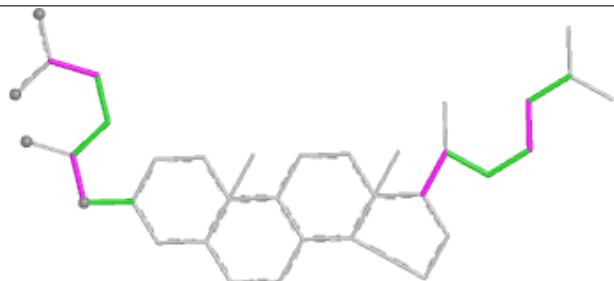
## Ligand Y01 B 601



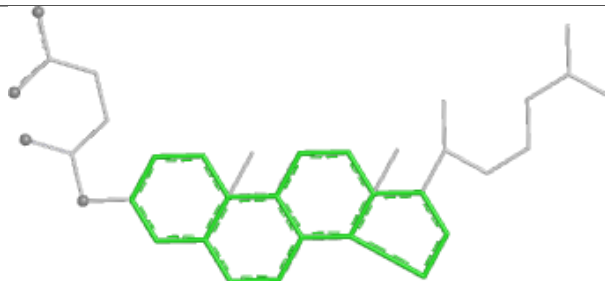
Bond lengths



Bond angles

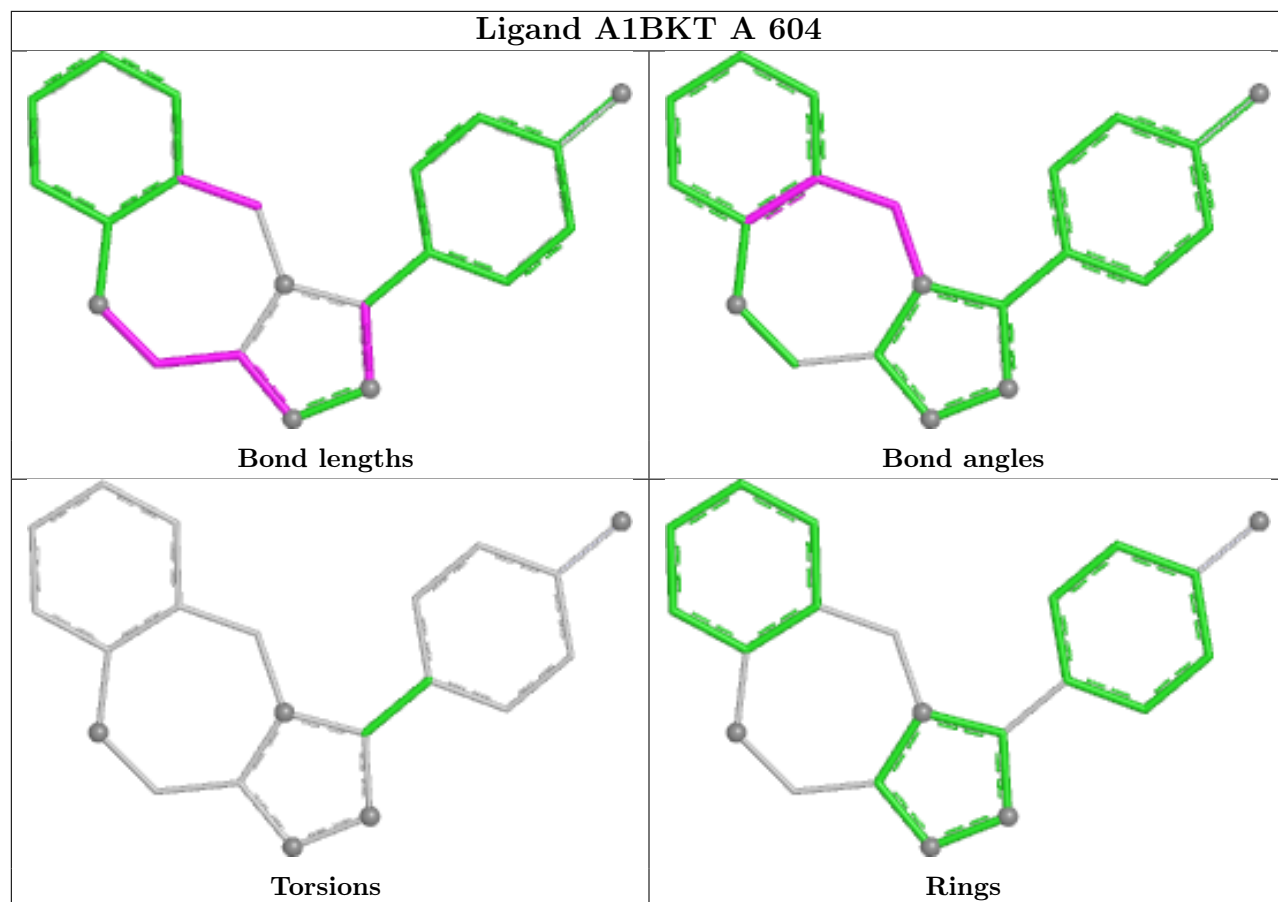


Torsions

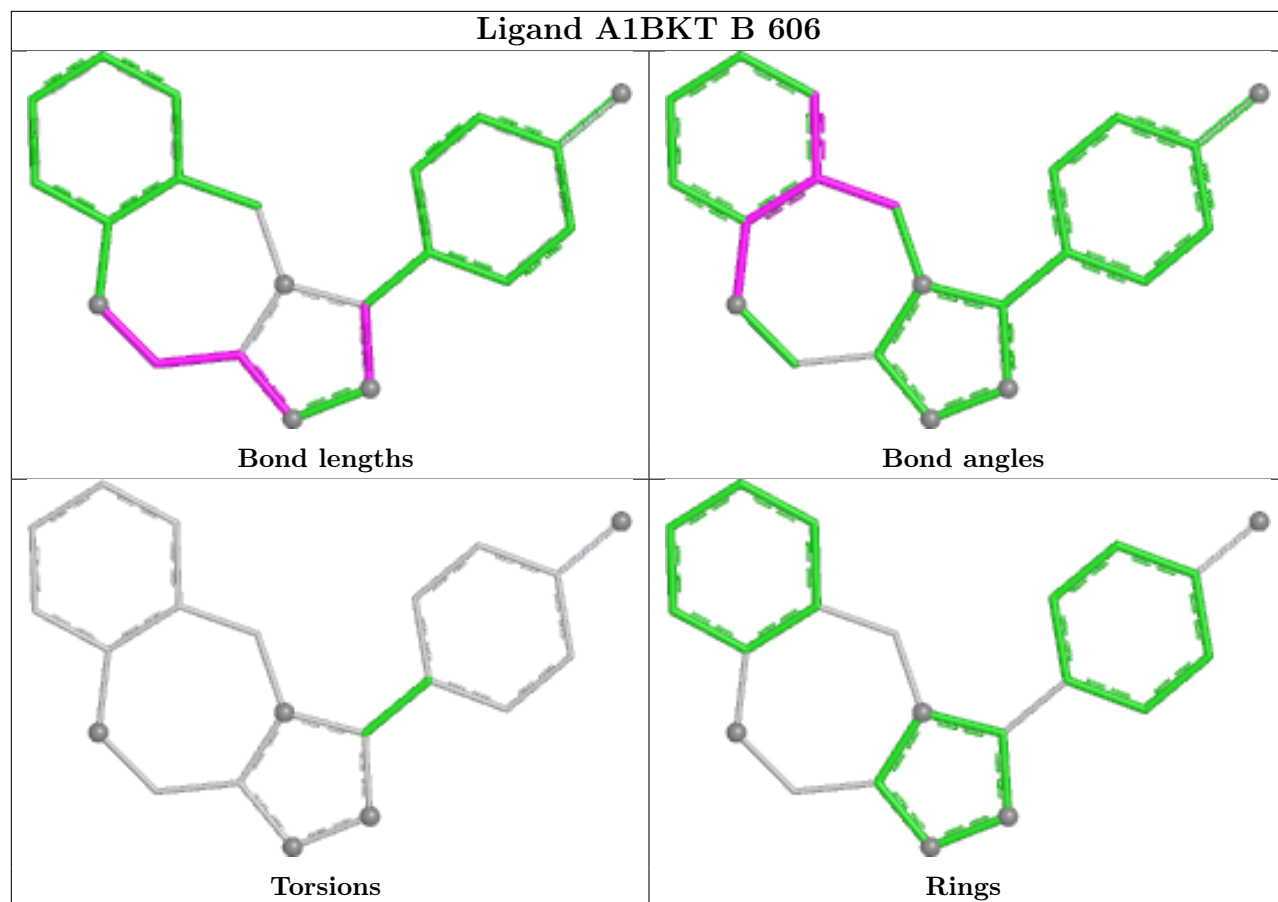


Rings



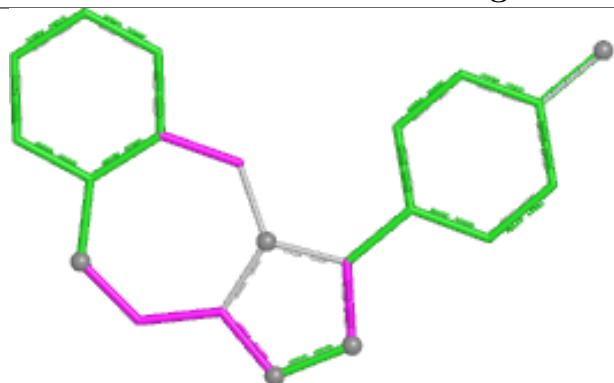




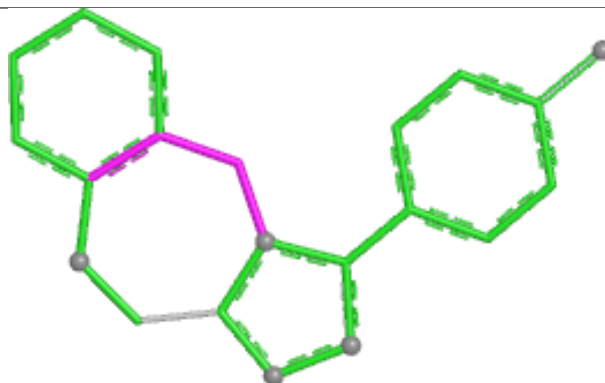




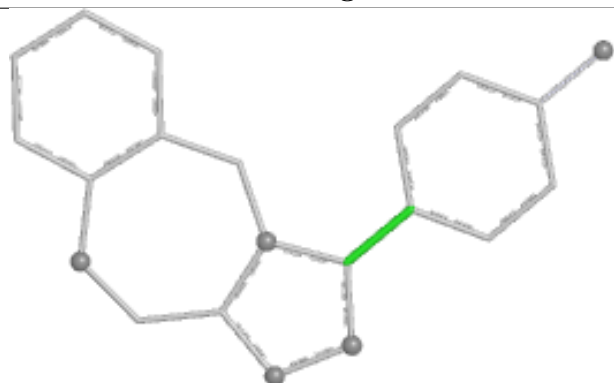
## Ligand A1BKT B 604



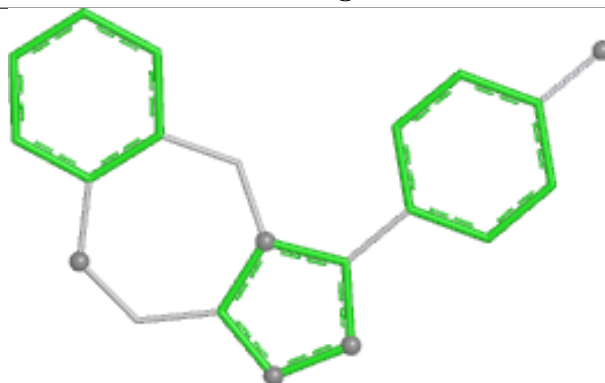
Bond lengths



Bond angles

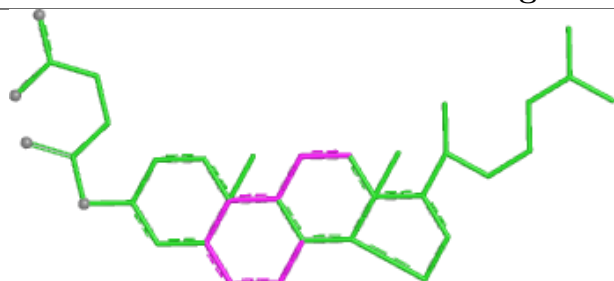


Torsions

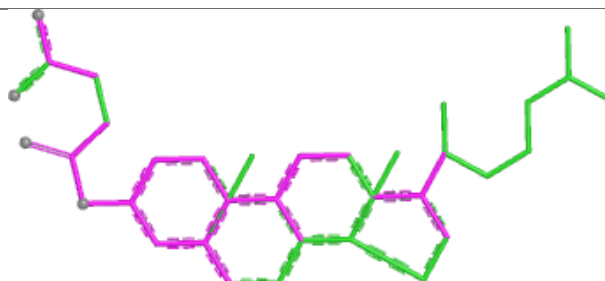


Rings

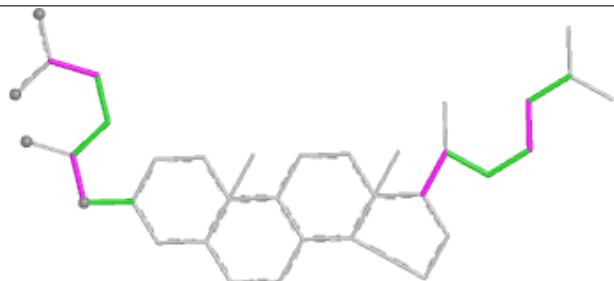
## Ligand Y01 A 601



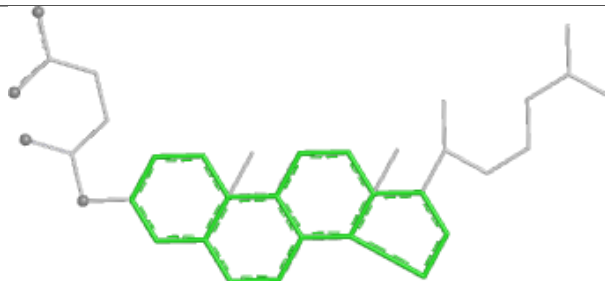
Bond lengths



Bond angles

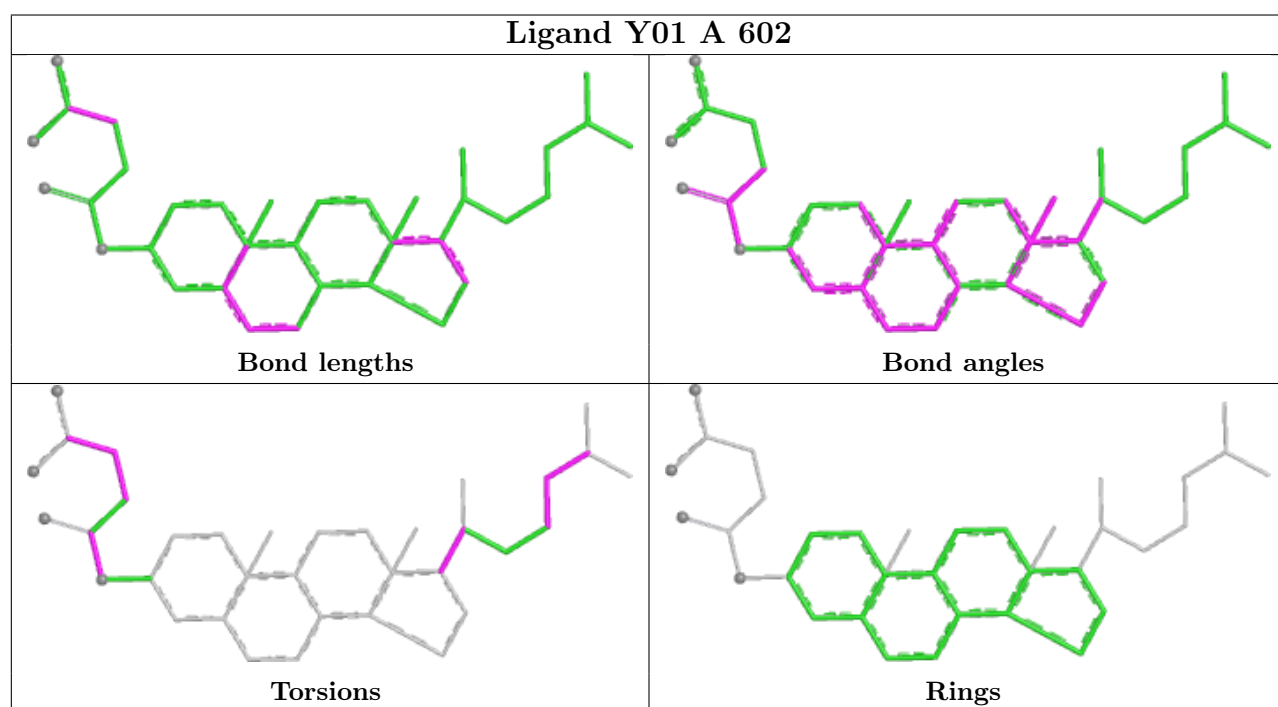
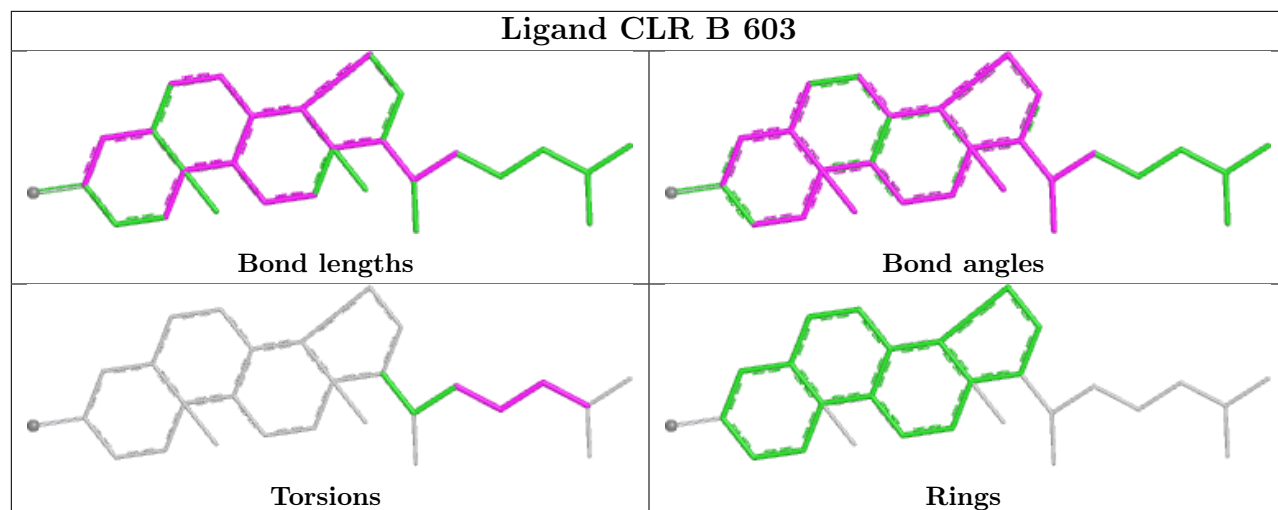


Torsions

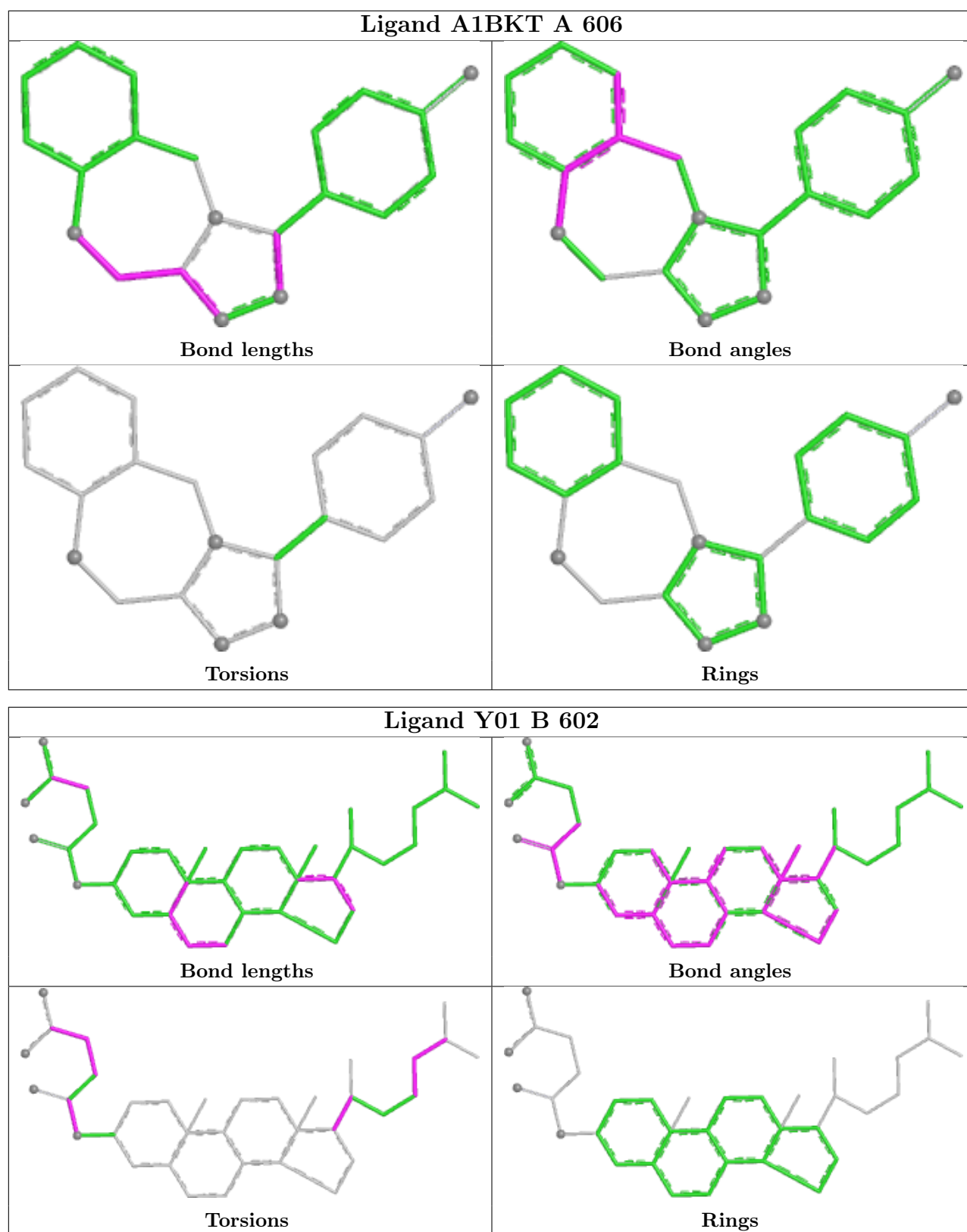


Rings









## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



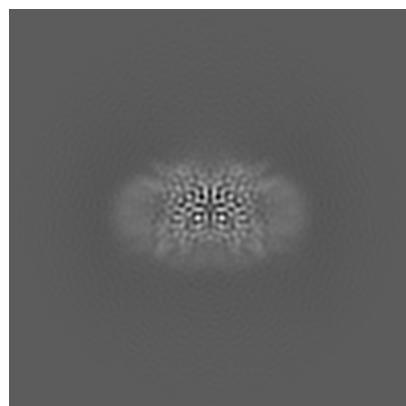
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48235. These allow visual inspection of the internal detail of the map and identification of artifacts.

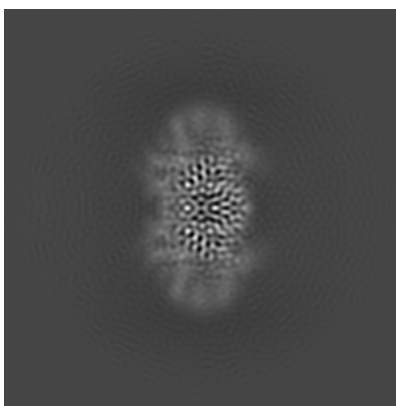
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

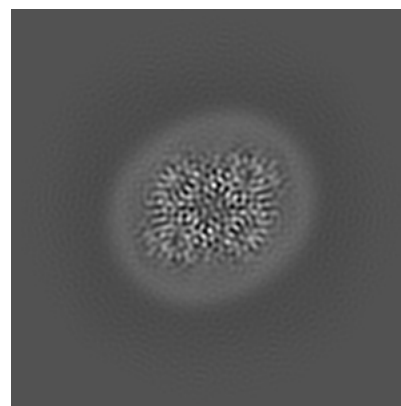
#### 6.1.1 Primary map



X

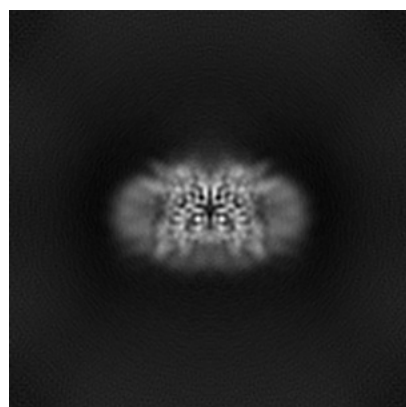


Y

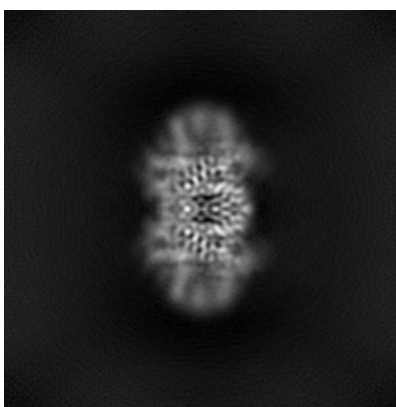


Z

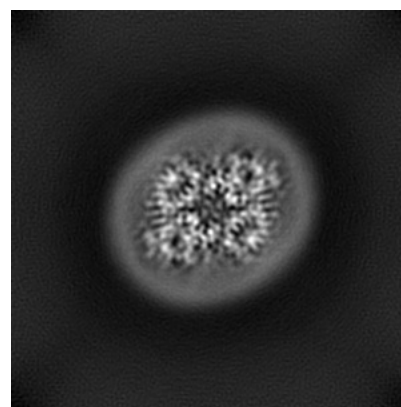
#### 6.1.2 Raw map



X



Y



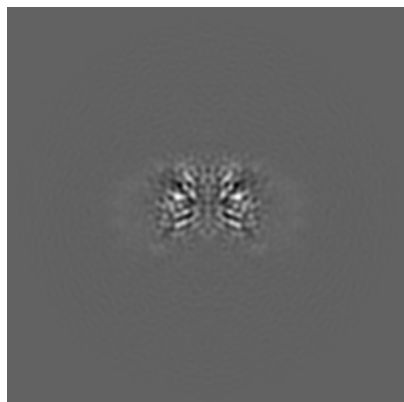
Z

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

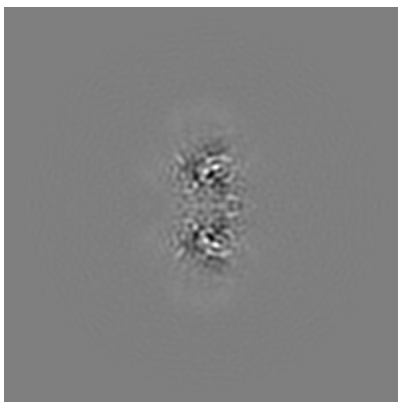


## 6.2 Central slices [i](#)

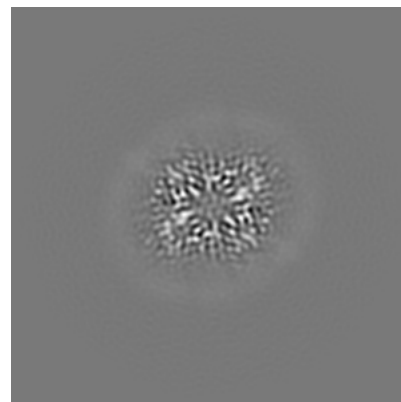
### 6.2.1 Primary map



X Index: 100

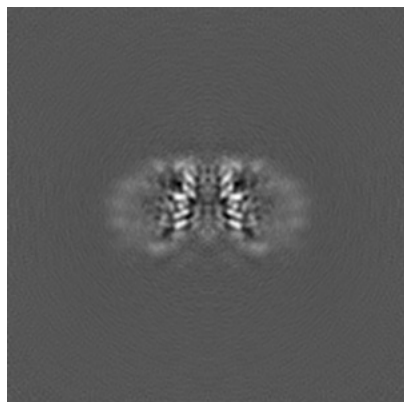


Y Index: 100

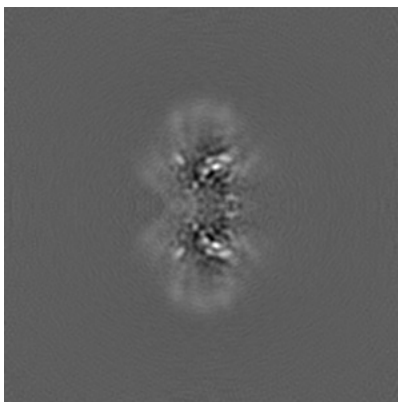


Z Index: 100

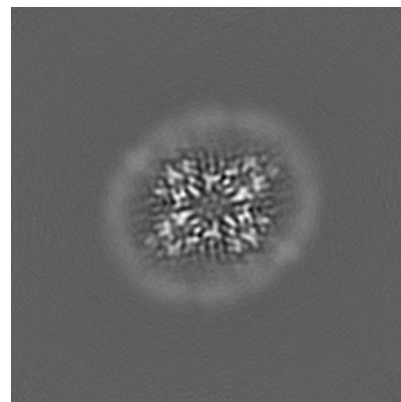
### 6.2.2 Raw map



X Index: 100



Y Index: 100



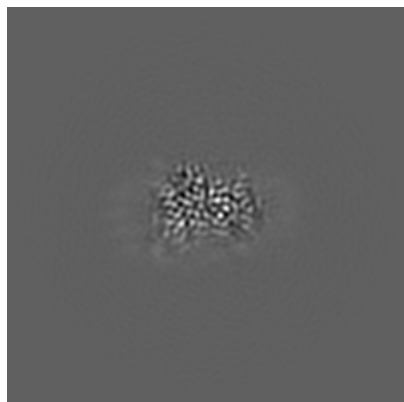
Z Index: 100

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

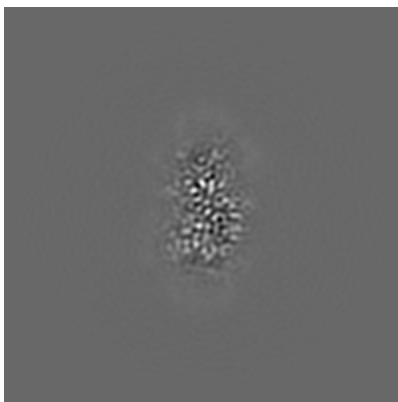


## 6.3 Largest variance slices [i](#)

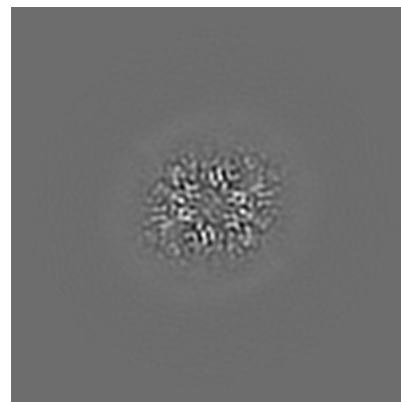
### 6.3.1 Primary map



X Index: 89

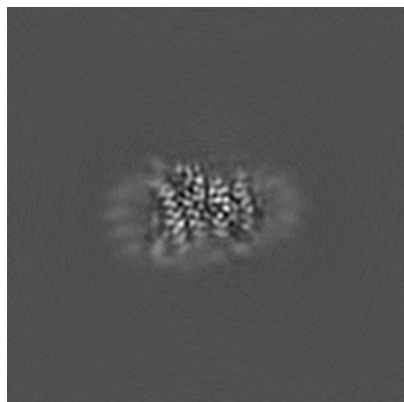


Y Index: 91

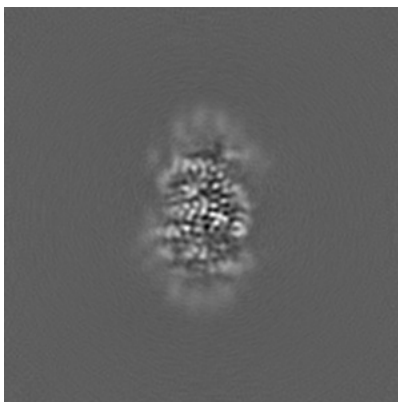


Z Index: 104

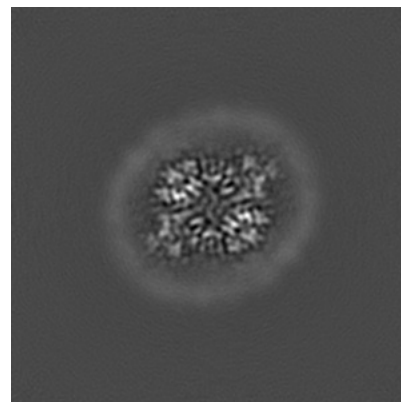
### 6.3.2 Raw map



X Index: 89



Y Index: 86



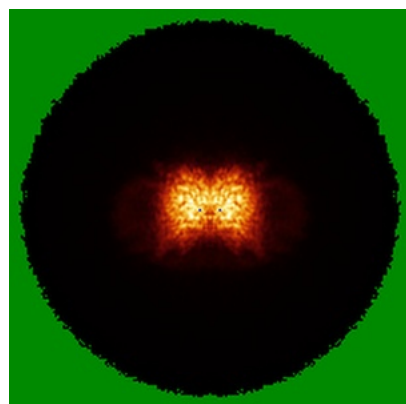
Z Index: 99

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

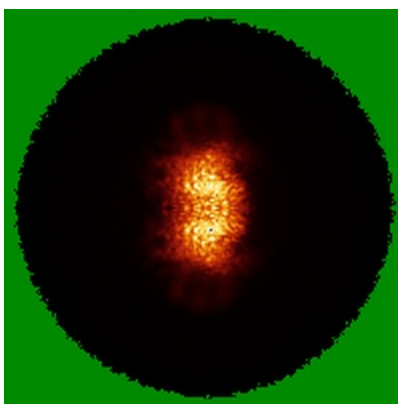


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

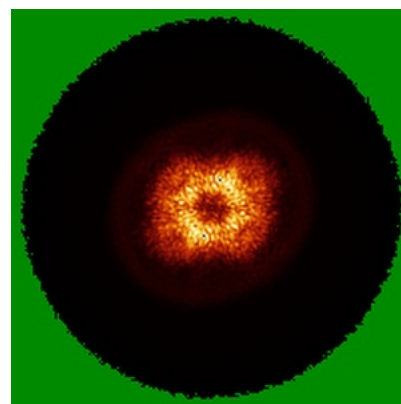
### 6.4.1 Primary map



X

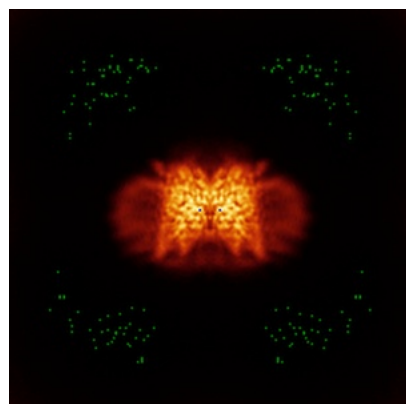


Y

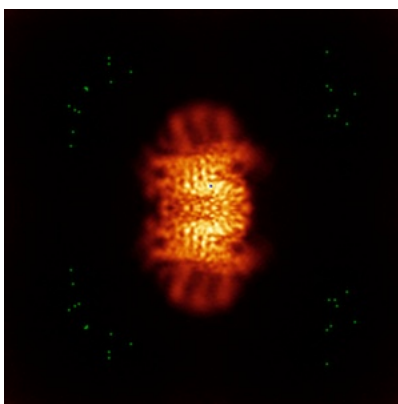


Z

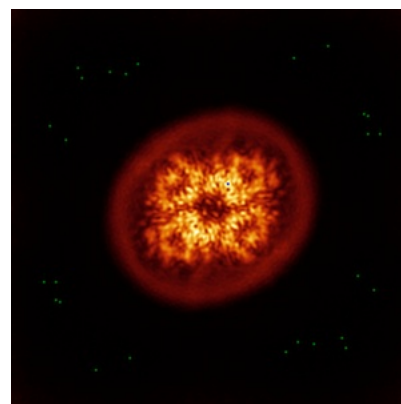
### 6.4.2 Raw map



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.



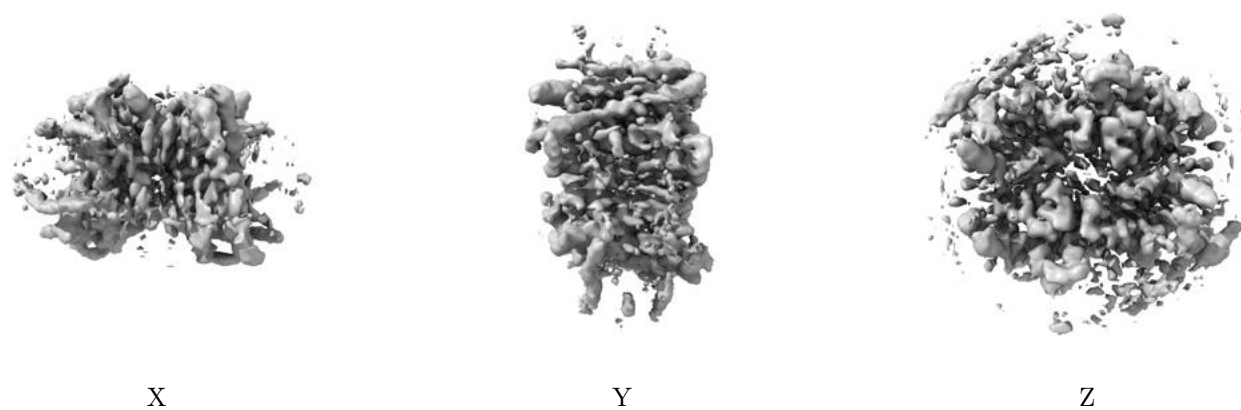
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.139. 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.



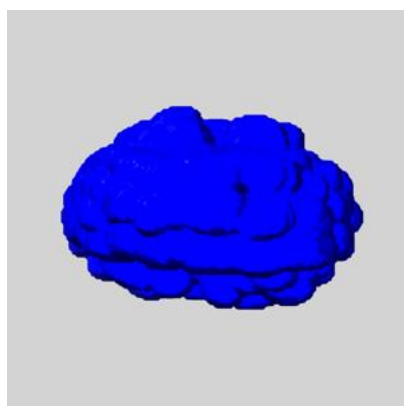
## 6.6 Mask visualisation [i](#)

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

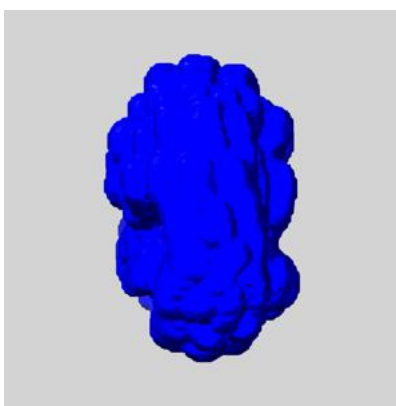
A mask typically either:

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

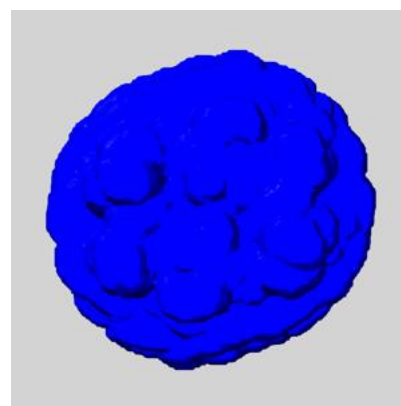
### 6.6.1 emd\_48235\_msk\_1.map [i](#)



X



Y



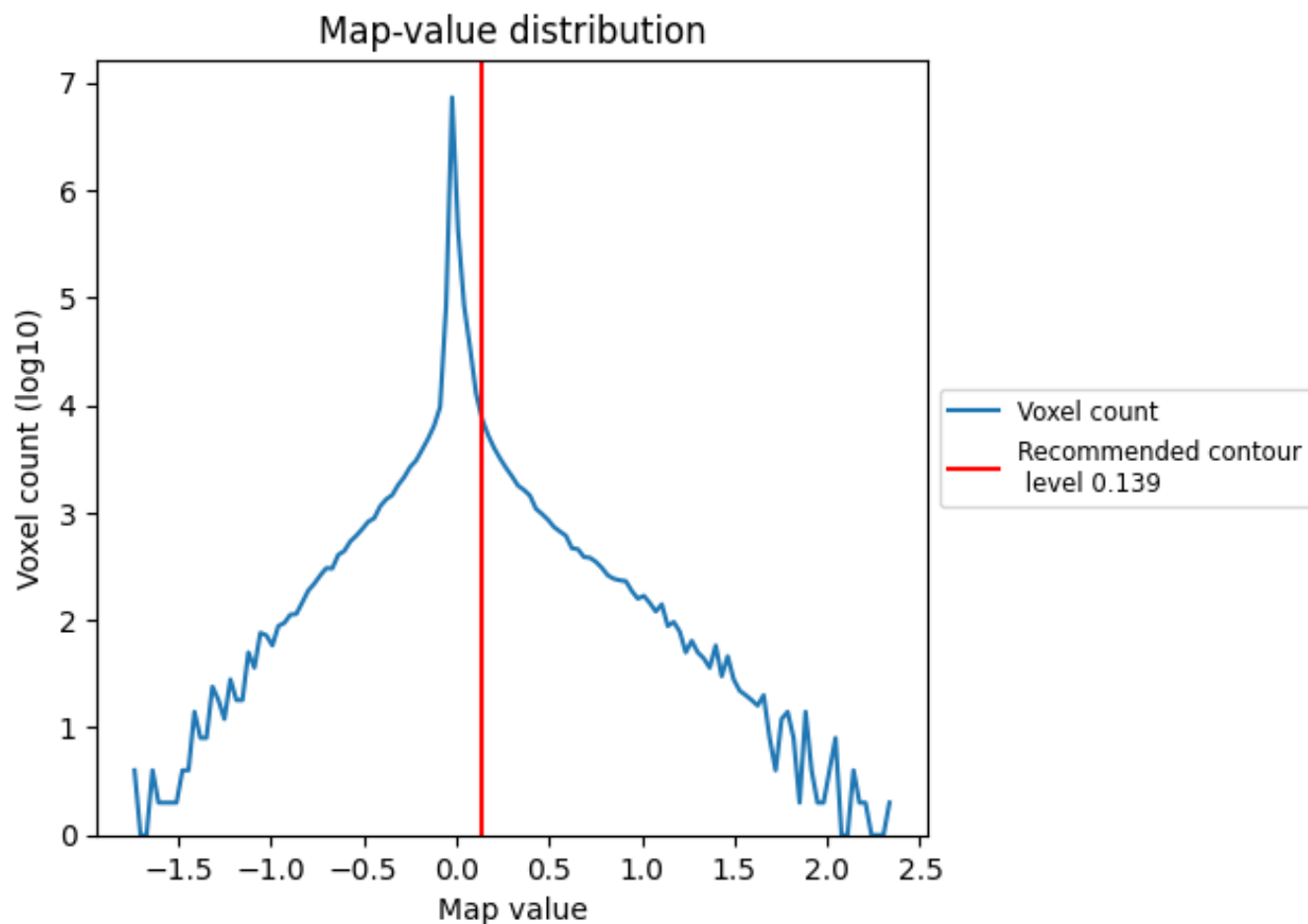
Z



## 7 Map analysis [i](#)

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

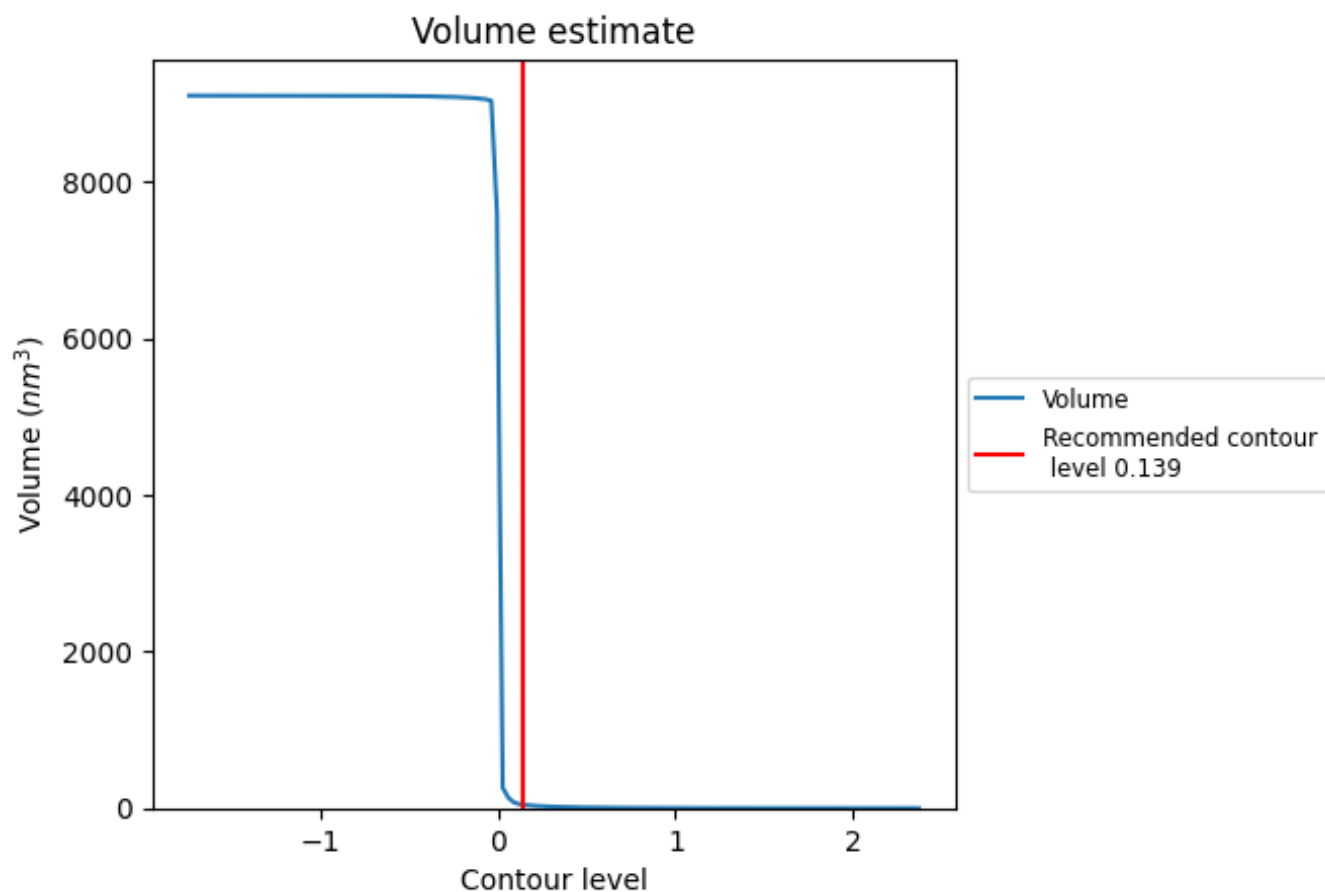
### 7.1 Map-value distribution [i](#)



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](#)

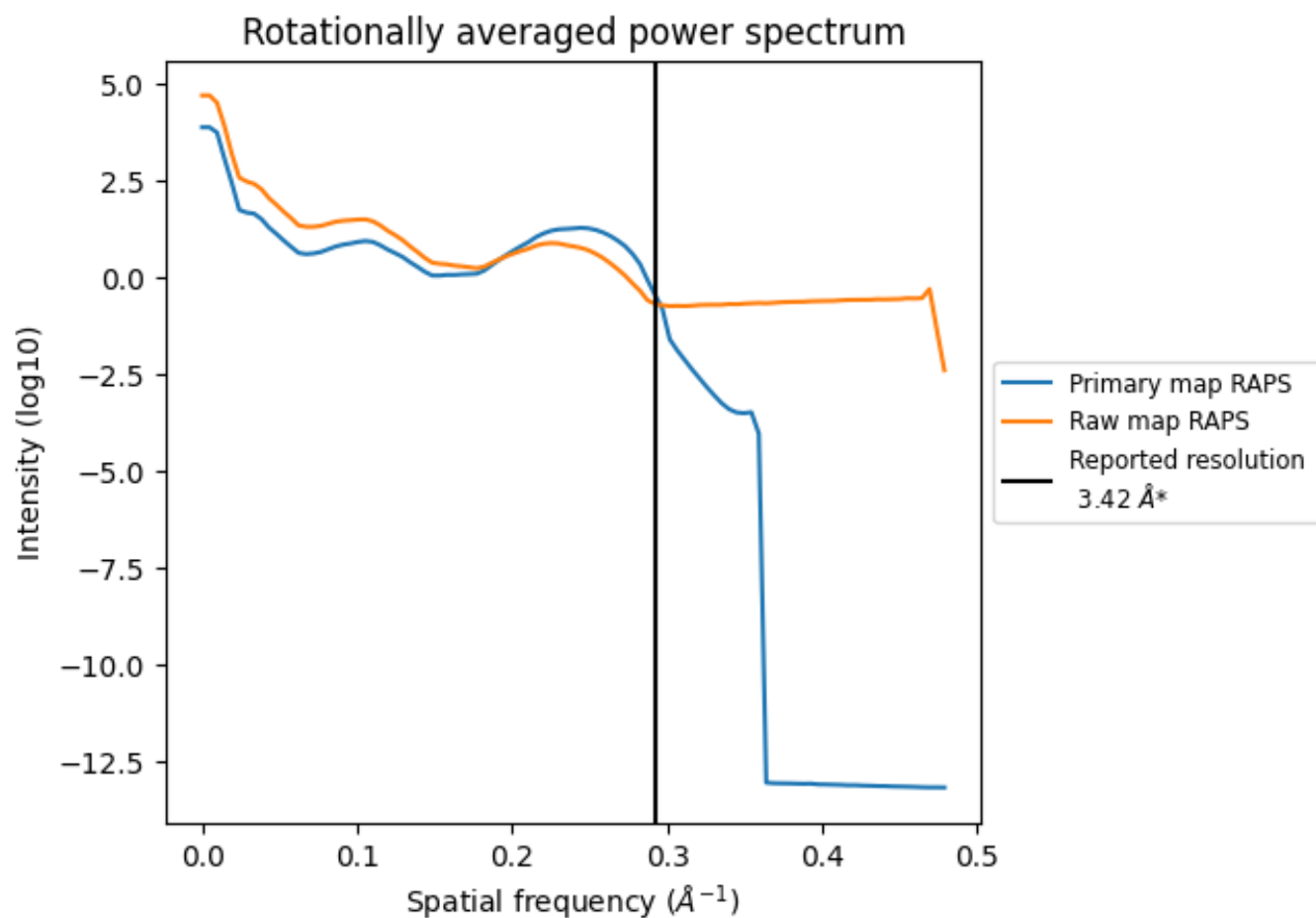


The volume at the recommended contour level is 45 nm<sup>3</sup>; this corresponds to an approximate mass of 41 kDa.

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 ⓘ



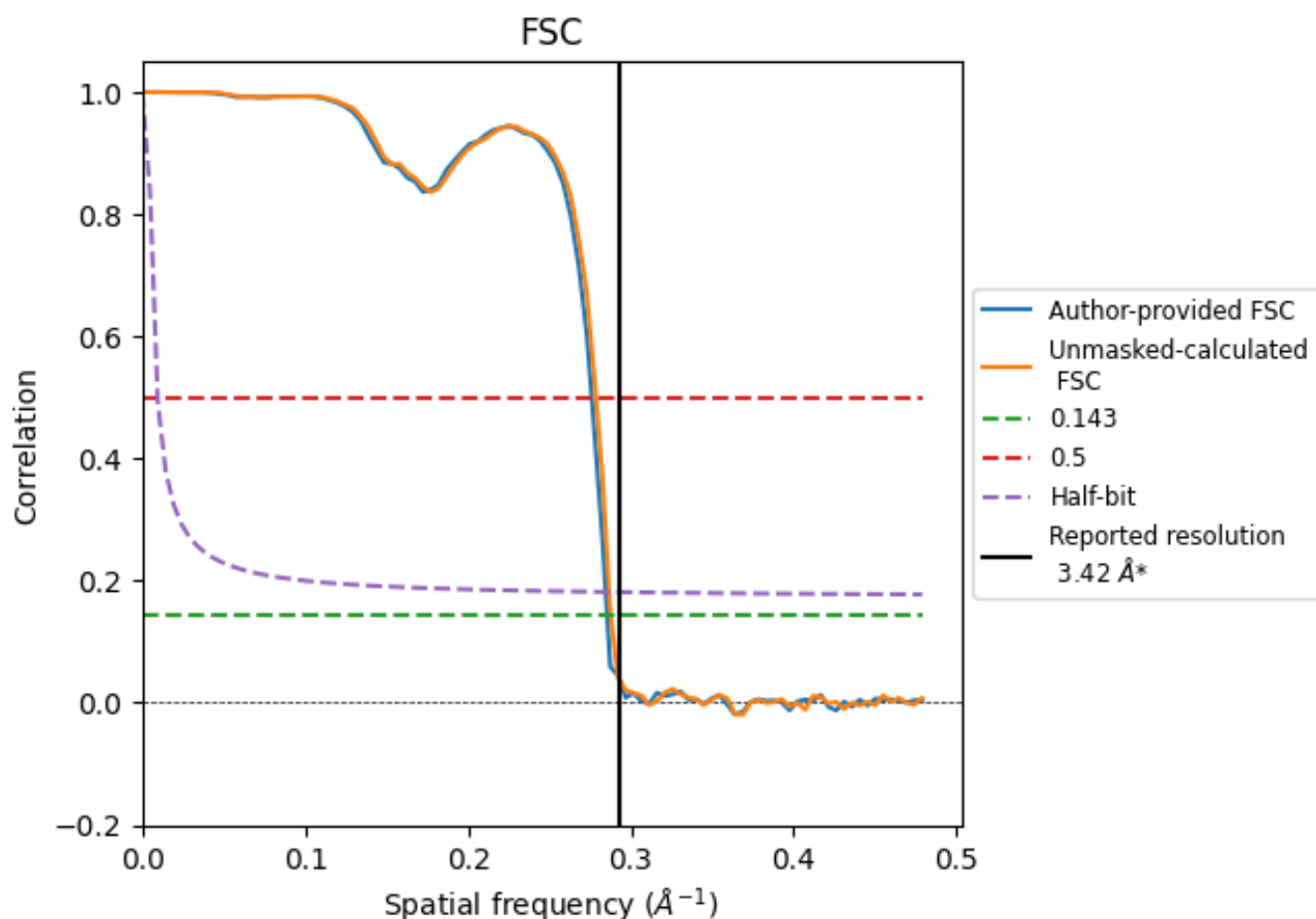
\*Reported resolution corresponds to spatial frequency of 0.292 Å<sup>-1</sup>



## 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 0.292  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.50	3.62	3.51
Unmasked-calculated*	3.48	3.59	3.49

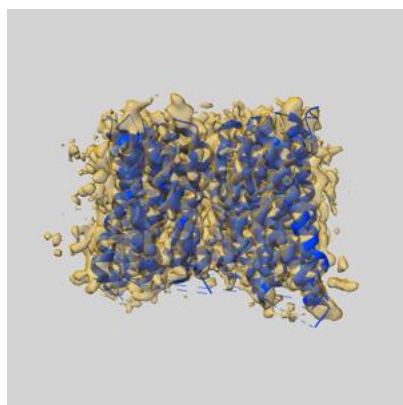
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



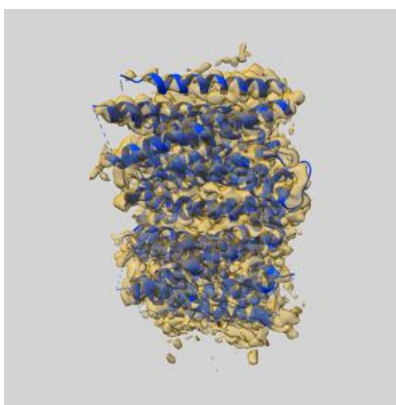
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48235 and PDB model 9MFM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

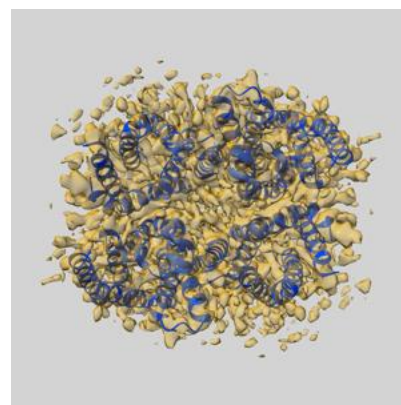
### 9.1 Map-model overlay [i](#)



X



Y

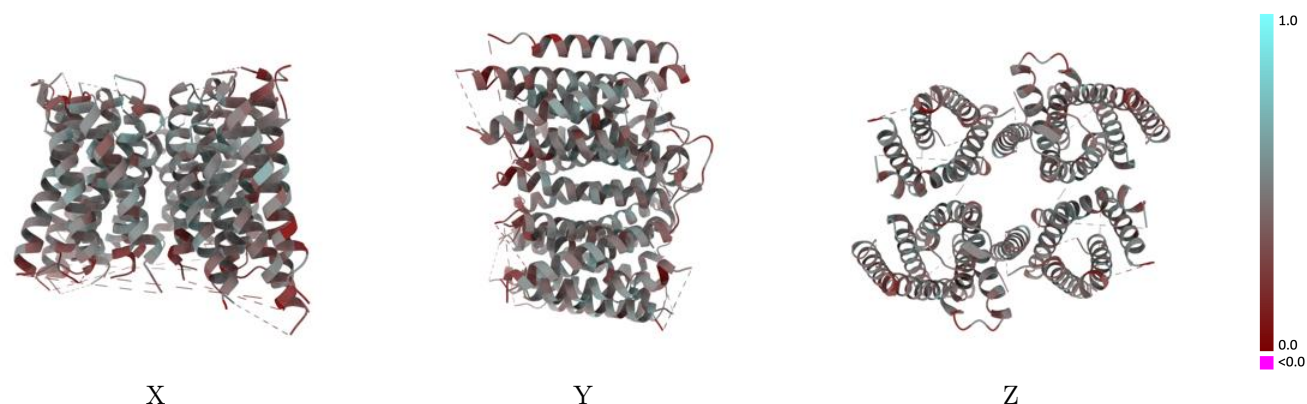


Z

The images above show the 3D surface view of the map at the recommended contour level 0.139 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.

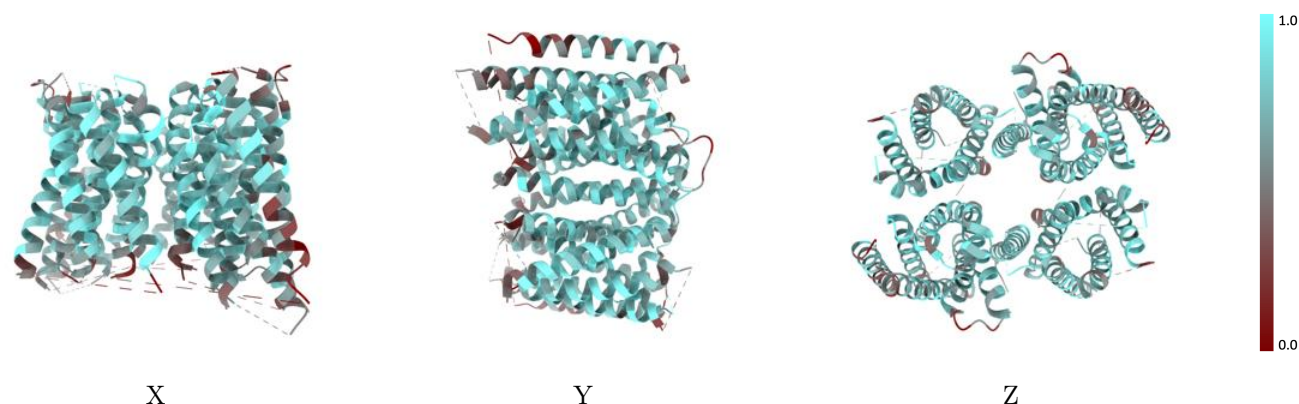


## 9.2 Q-score mapped to coordinate model [i](#)



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.

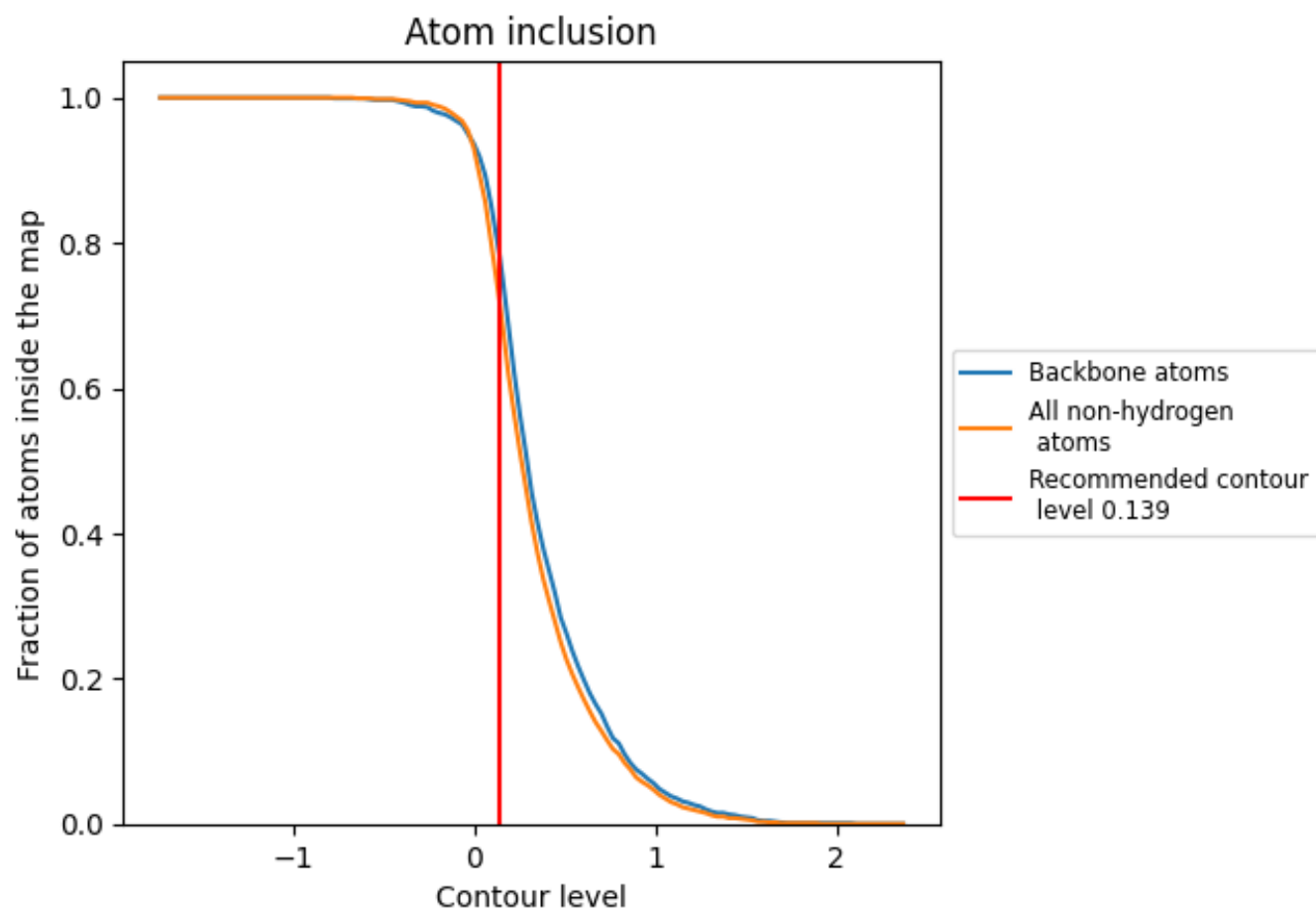
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.139).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.139) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7190	<div></div> 0.4190
A	<div></div> 0.7190	<div></div> 0.4200
B	<div></div> 0.7190	<div></div> 0.4190

