



## Full wwPDB EM Validation Report ⓘ

May 20, 2025 – 03:07 AM EDT

PDB ID : 9B28 / pdb\_00009b28  
EMDB ID : EMD-44100  
Title : Cryo-EM structure of the mouse TRPM3 alpha 2 channel in complex with  
primidone  
Authors : Yin, Y.; Park, C.G.; Feng, S.; Zhang, F.; Guan, Z.; Sharma, K.; Borgnia, M.J.;  
Im, W.; Lee, S.-Y.  
Deposited on : 2024-03-14  
Resolution : 3.24 Å (reported)  
Based on initial model : 6BPQ

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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

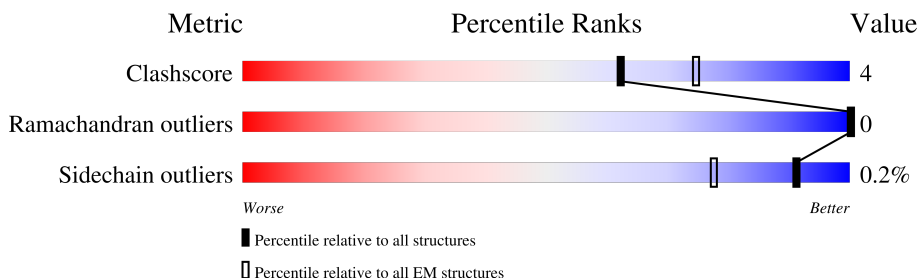
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.24 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1739	
1	B	1739	
1	C	1739	
1	D	1739	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50704 atoms, of which 23832 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel, subfamily M, member 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	925	Total	C	H	N	O	S	0	0
			12392	4264	5797	1127	1163	41		
1	C	925	Total	C	H	N	O	S	0	0
			12392	4264	5797	1127	1163	41		
1	B	925	Total	C	H	N	O	S	0	0
			12392	4264	5797	1127	1163	41		
1	D	925	Total	C	H	N	O	S	0	0
			12392	4264	5797	1127	1163	41		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1710	SER	-	expression tag	UNP Q5F4S7
A	1711	ASN	-	expression tag	UNP Q5F4S7
A	1712	SER	-	expression tag	UNP Q5F4S7
A	1713	LEU	-	expression tag	UNP Q5F4S7
A	1714	GLU	-	expression tag	UNP Q5F4S7
A	1715	VAL	-	expression tag	UNP Q5F4S7
A	1716	LEU	-	expression tag	UNP Q5F4S7
A	1717	PHE	-	expression tag	UNP Q5F4S7
A	1718	GLN	-	expression tag	UNP Q5F4S7
A	1719	GLY	-	expression tag	UNP Q5F4S7
A	1720	PRO	-	expression tag	UNP Q5F4S7
A	1721	ASP	-	expression tag	UNP Q5F4S7
A	1722	TYR	-	expression tag	UNP Q5F4S7
A	1723	LYS	-	expression tag	UNP Q5F4S7
A	1724	ASP	-	expression tag	UNP Q5F4S7
A	1725	ASP	-	expression tag	UNP Q5F4S7
A	1726	ASP	-	expression tag	UNP Q5F4S7
A	1727	ASP	-	expression tag	UNP Q5F4S7
A	1728	LYS	-	expression tag	UNP Q5F4S7
A	1729	ALA	-	expression tag	UNP Q5F4S7
A	1730	HIS	-	expression tag	UNP Q5F4S7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1731	HIS	-	expression tag	UNP Q5F4S7
A	1732	HIS	-	expression tag	UNP Q5F4S7
A	1733	HIS	-	expression tag	UNP Q5F4S7
A	1734	HIS	-	expression tag	UNP Q5F4S7
A	1735	HIS	-	expression tag	UNP Q5F4S7
A	1736	HIS	-	expression tag	UNP Q5F4S7
A	1737	HIS	-	expression tag	UNP Q5F4S7
A	1738	HIS	-	expression tag	UNP Q5F4S7
A	1739	HIS	-	expression tag	UNP Q5F4S7
C	1710	SER	-	expression tag	UNP Q5F4S7
C	1711	ASN	-	expression tag	UNP Q5F4S7
C	1712	SER	-	expression tag	UNP Q5F4S7
C	1713	LEU	-	expression tag	UNP Q5F4S7
C	1714	GLU	-	expression tag	UNP Q5F4S7
C	1715	VAL	-	expression tag	UNP Q5F4S7
C	1716	LEU	-	expression tag	UNP Q5F4S7
C	1717	PHE	-	expression tag	UNP Q5F4S7
C	1718	GLN	-	expression tag	UNP Q5F4S7
C	1719	GLY	-	expression tag	UNP Q5F4S7
C	1720	PRO	-	expression tag	UNP Q5F4S7
C	1721	ASP	-	expression tag	UNP Q5F4S7
C	1722	TYR	-	expression tag	UNP Q5F4S7
C	1723	LYS	-	expression tag	UNP Q5F4S7
C	1724	ASP	-	expression tag	UNP Q5F4S7
C	1725	ASP	-	expression tag	UNP Q5F4S7
C	1726	ASP	-	expression tag	UNP Q5F4S7
C	1727	ASP	-	expression tag	UNP Q5F4S7
C	1728	LYS	-	expression tag	UNP Q5F4S7
C	1729	ALA	-	expression tag	UNP Q5F4S7
C	1730	HIS	-	expression tag	UNP Q5F4S7
C	1731	HIS	-	expression tag	UNP Q5F4S7
C	1732	HIS	-	expression tag	UNP Q5F4S7
C	1733	HIS	-	expression tag	UNP Q5F4S7
C	1734	HIS	-	expression tag	UNP Q5F4S7
C	1735	HIS	-	expression tag	UNP Q5F4S7
C	1736	HIS	-	expression tag	UNP Q5F4S7
C	1737	HIS	-	expression tag	UNP Q5F4S7
C	1738	HIS	-	expression tag	UNP Q5F4S7
C	1739	HIS	-	expression tag	UNP Q5F4S7
B	1710	SER	-	expression tag	UNP Q5F4S7
B	1711	ASN	-	expression tag	UNP Q5F4S7
B	1712	SER	-	expression tag	UNP Q5F4S7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1713	LEU	-	expression tag	UNP Q5F4S7
B	1714	GLU	-	expression tag	UNP Q5F4S7
B	1715	VAL	-	expression tag	UNP Q5F4S7
B	1716	LEU	-	expression tag	UNP Q5F4S7
B	1717	PHE	-	expression tag	UNP Q5F4S7
B	1718	GLN	-	expression tag	UNP Q5F4S7
B	1719	GLY	-	expression tag	UNP Q5F4S7
B	1720	PRO	-	expression tag	UNP Q5F4S7
B	1721	ASP	-	expression tag	UNP Q5F4S7
B	1722	TYR	-	expression tag	UNP Q5F4S7
B	1723	LYS	-	expression tag	UNP Q5F4S7
B	1724	ASP	-	expression tag	UNP Q5F4S7
B	1725	ASP	-	expression tag	UNP Q5F4S7
B	1726	ASP	-	expression tag	UNP Q5F4S7
B	1727	ASP	-	expression tag	UNP Q5F4S7
B	1728	LYS	-	expression tag	UNP Q5F4S7
B	1729	ALA	-	expression tag	UNP Q5F4S7
B	1730	HIS	-	expression tag	UNP Q5F4S7
B	1731	HIS	-	expression tag	UNP Q5F4S7
B	1732	HIS	-	expression tag	UNP Q5F4S7
B	1733	HIS	-	expression tag	UNP Q5F4S7
B	1734	HIS	-	expression tag	UNP Q5F4S7
B	1735	HIS	-	expression tag	UNP Q5F4S7
B	1736	HIS	-	expression tag	UNP Q5F4S7
B	1737	HIS	-	expression tag	UNP Q5F4S7
B	1738	HIS	-	expression tag	UNP Q5F4S7
B	1739	HIS	-	expression tag	UNP Q5F4S7
D	1710	SER	-	expression tag	UNP Q5F4S7
D	1711	ASN	-	expression tag	UNP Q5F4S7
D	1712	SER	-	expression tag	UNP Q5F4S7
D	1713	LEU	-	expression tag	UNP Q5F4S7
D	1714	GLU	-	expression tag	UNP Q5F4S7
D	1715	VAL	-	expression tag	UNP Q5F4S7
D	1716	LEU	-	expression tag	UNP Q5F4S7
D	1717	PHE	-	expression tag	UNP Q5F4S7
D	1718	GLN	-	expression tag	UNP Q5F4S7
D	1719	GLY	-	expression tag	UNP Q5F4S7
D	1720	PRO	-	expression tag	UNP Q5F4S7
D	1721	ASP	-	expression tag	UNP Q5F4S7
D	1722	TYR	-	expression tag	UNP Q5F4S7
D	1723	LYS	-	expression tag	UNP Q5F4S7
D	1724	ASP	-	expression tag	UNP Q5F4S7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1725	ASP	-	expression tag	UNP Q5F4S7
D	1726	ASP	-	expression tag	UNP Q5F4S7
D	1727	ASP	-	expression tag	UNP Q5F4S7
D	1728	LYS	-	expression tag	UNP Q5F4S7
D	1729	ALA	-	expression tag	UNP Q5F4S7
D	1730	HIS	-	expression tag	UNP Q5F4S7
D	1731	HIS	-	expression tag	UNP Q5F4S7
D	1732	HIS	-	expression tag	UNP Q5F4S7
D	1733	HIS	-	expression tag	UNP Q5F4S7
D	1734	HIS	-	expression tag	UNP Q5F4S7
D	1735	HIS	-	expression tag	UNP Q5F4S7
D	1736	HIS	-	expression tag	UNP Q5F4S7
D	1737	HIS	-	expression tag	UNP Q5F4S7
D	1738	HIS	-	expression tag	UNP Q5F4S7
D	1739	HIS	-	expression tag	UNP Q5F4S7

- # Y01

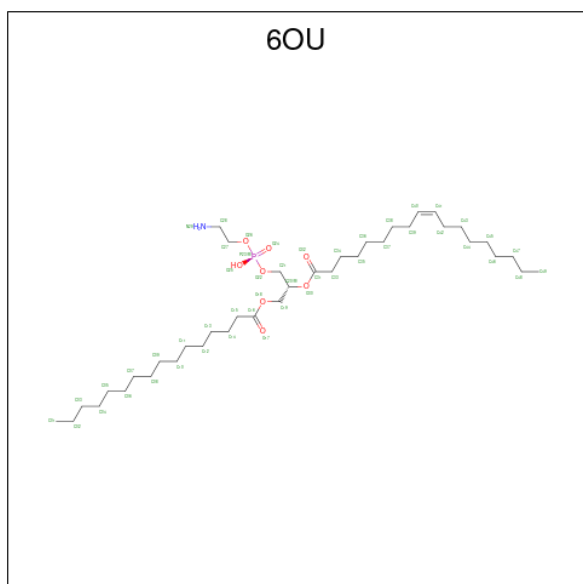
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 84	C 31	H 49	O 4	0
2	A	1	Total 84	C 31	H 49	O 4	0
2	C	1	Total 84	C 31	H 49	O 4	0
2	C	1	Total 84	C 31	H 49	O 4	0



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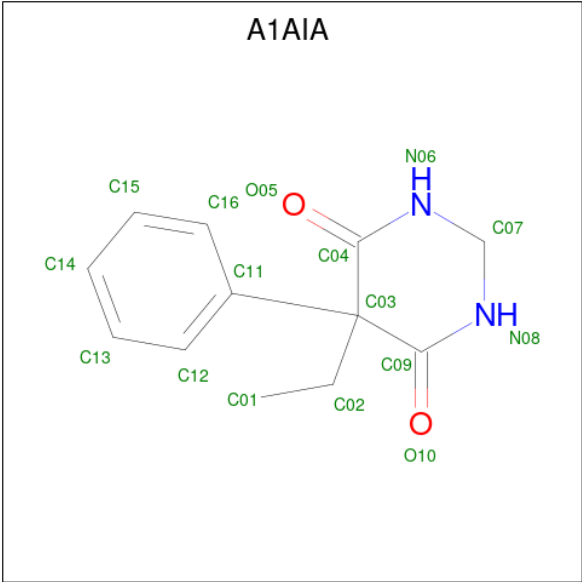
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	D	1	Total	C	H	O	0
			84	31	49	4	
2	D	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ( {Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			86	27	49	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			86	27	49	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			86	27	49	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			86	27	49	1	8	1	

- Molecule 4 is primidone (CCD ID: A1AIA) (formula: C<sub>12</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			30	12	14	2	2	
4	C	1	Total	C	H	N	O	0
			30	12	14	2	2	
4	B	1	Total	C	H	N	O	0
			30	12	14	2	2	
4	D	1	Total	C	H	N	O	0
			30	12	14	2	2	





- Molecule 1: Transient receptor potential cation channel, subfamily M, member 3



SER	ASN	CYS	K919	PRO	GLU	L647	L557	V345	TRP	PRO	MET
ASN	CYS	CYS	M925	GLU	GLU	M648	L558	V345	SER	ALA	GLY
ILE	TRP	ARG	SER	PRO	PRO	M649	D559	V349	ILE	GLN	LYS
ARG	TRP	TRP	GLU	GLU	GLU	F657	L560	SER	LYS	LYS	TRP
SER	LYS	LYS	PRO	LYS	LYS	M678	E565	G368	HIS	TRP	ARG
ARG	HIS	HIS	G929	PRO	PRO	M678	C574	S371	THR	ILE	ASP
THR	GLU	GLU	L932	THR	THR	L729	R578	T138	THR	ALA	GLY
SER	SER	ASP	SER	LYS	LYS	L729	R578	T138	THR	ALA	GLY
ASP	ASP	GLN	N944	LYS	LYS	M734	R582	D139	THR	ALA	GLY
CYS	ASP	GLU	N944	ASP	ASP	M734	R582	D139	THR	ALA	GLY
THR	THR	GLU	T951	GLU	GLU	G765	F589	GLY	THR	ALA	GLY
ASP	ASP	GLU	T951	GLU	GLU	G765	F589	GLY	THR	ALA	GLY
ASP	ASP	ASP	Q965	ASP	ASP	R768	F589	GLY	THR	ALA	GLY
ALA	ASP	ASP	P966	MET	MET	M769	R578	ILE	THR	PRO	CYS
TYR	TYR	GLU	G1180	GLU	GLU	ARG	R578	ASN	THR	ASP	ASP
ILE	ILE	LEU	R972	LEU	LEU	ASN	R582	GLU	THR	ASP	GLY
VAL	VAL	THR	R972	THR	THR	ASN	R582	GLU	THR	ASP	GLY
ARG	ARG	ILE	E1203	THR	THR	ASN	R582	S390	THR	ASP	GLY
GLN	GLN	GLN	R1206	ALA	ALA	SER	PRO	S390	THR	ASP	GLY
SER	SER	SER	I979	LEU	LEU	GLY	ALA	L399	THR	HIS	SER
SER	SER	SER	K1005	GLY	GLY	LYS	LYS	GLN	THR	ARG	ALA
PHE	PHE	PHE	R1240	ARG	ARG	VAL	LYS	THR	ARG	CYS	SER
ASN	ASN	H1241	R1241	SER	SER	ILE	LEU	PHE	THR	CYS	SER
SER	SER	S1243	M1017	ASN	ASN	GLY	GLY	THR	THR	GLY	ARG
GLN	GLN	M1244	A1030	GLY	GLY	ILE	MET	TYR	GLY	ARG	ARG
GLU	GLU	GLY	A1030	GLU	GLU	ILE	GLU	THR	THR	LEU	SER
GLY	GLY	GLN	E1037	SER	SER	LEU	ASP	ARG	GLY	ILE	ARG
ASN	ASN	THR	E1037	SER	SER	LEU	ASP	ARG	THR	ILE	ARG
THR	THR	THR	G1068	ARG	ARG	PRO	ILE	T408	ARG	GLY	SER
PHE	PHE	VAL	G1068	LYS	LYS	PRO	PRO	M432	ARG	GLN	SER
LYS	LYS	ASP	L1081	LYS	SER	SER	LEU	GLY	THR	HIS	SER
LEU	LEU	ILE	L1081	ASP	ASP	ILE	ARG	SER	THR	VAL	ARG
GLN	GLN	ARG	C1084	GLU	GLU	LEU	ARG	GLU	MET	GLY	ARG
GLU	GLU	LEU	C1084	GLU	GLU	SER	GLY	G436	ASN	LEU	ARG
SER	SER	ALA	A1102	GLU	GLU	LEU	ARG	G436	ASN	THR	PHE
ILE	ILE	GLN	A1102	VAL	VAL	GLU	ARG	ASN	PRO	ALA	ALA
ASP	ASP	LEU	L1109	GLN	GLN	PHE	THR	M453	SER	GLU	GLU
PRO	PRO	GLU	L1109	SER	SER	THR	THR	ALA	MET	ILE	SER
ALA	ALA	ASP	V1113	ARG	ARG	ASN	THR	LYS	LYS	TRP	LYS
GLY	GLY	LEU	V1113	HIS	HIS	LYS	LYS	A456	VAL	VAL	LYS
GLU	GLU	ILE	V1121	ARG	ARG	ASP	LYS	T285	LEU	LEU	ARG
GLU	GLU	GLY	V1121	ARG	ARG	ASP	ARG	L493	GLN	GLN	LEU
THR	THR	ARG	I1124	ILE	ILE	MET	GLU	L496	ASN	ASN	SER
ILE	ILE	MET	I1124	PRO	PRO	GLU	GLU	GLY	GLU	GLU	LYS
SER	SER	ALA	V1128	VAL	VAL	TYR	VAL	M514	TYR	ASN	GLN
PRO	PRO	THR	V1128	THR	THR	MET	ASP	T519	GLY	GLU	GLY
THR	THR	ALA	P1147	ALA	ALA	THR	ILE	T519	ALA	SER	SER
SER	SER	GLU	P1147	GLN	GLN	GLN	ASP	I520	ARG	THR	LYS
PRO	PRO	LEU	P1148	GLN	GLN	GLN	LEU	I520	LEU	ARG	LYS
THR	THR	ARG	P1149	GLN	GLN	GLN	ASP	E524	ASP	SER	ARG
LEU	LEU	LEU	I1150	THR	THR	ILE	ASP	E524	ASN	ARG	SER
MET	MET	THR	I1151	THR	THR	ILE	PRO	L526	THR	ASN	GLY
PRO	PRO	GLY	I1159	GLY	HIS	HIS	GLU	I527	ASP	ASN	LEU
ARG	ARG	LEU	PHE	LEU	LEU	LEU	I631	N528	THR	ASP	PRO
MET	MET	GLU	GLN	GLU	GLU	GLN	GLU	T529	ILE	ILE	PRO
ARG	ARG	ALA	HIS	GLN	GLN	GLN	L641	T529	GLY	GLN	ALA
SER	SER	CTR	CTR	LYS	LYS	CTR	V541	V541	GLY	SER	GLN
THR	THR	CTR	CTR	CTR	CTR	CTR	V541	V541	CTR	LYS	THR

[illegible]

- Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

Chain B:  49% . 47%

[illegible]





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	104425	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)	1250	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.724	Depositor
Minimum map value	-0.892	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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: 6OU, Y01, A1AIA

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	0.13	0/6731	0.25	0/9178
1	B	0.13	0/6731	0.25	0/9178
1	C	0.13	0/6731	0.25	0/9178
1	D	0.13	0/6731	0.25	0/9178
All	All	0.13	0/26924	0.25	0/36712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	6595	5797	5852	55	0
1	B	6595	5797	5852	53	0
1	C	6595	5797	5852	54	0
1	D	6595	5797	5852	53	0
2	A	70	98	98	2	0
2	B	70	98	98	2	0
2	C	70	98	98	2	0
2	D	70	98	98	3	0
3	A	37	49	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	37	49	0	0	0
3	C	37	49	0	0	0
3	D	37	49	0	0	0
4	A	16	14	0	0	0
4	B	16	14	0	0	0
4	C	16	14	0	0	0
4	D	16	14	0	0	0
All	All	26872	23832	23800	207	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 4.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:867:PHE:O	1:D:873:VAL:HG21	1.91	0.71
1:A:867:PHE:O	1:A:873:VAL:HG21	1.91	0.71
1:C:867:PHE:O	1:C:873:VAL:HG21	1.91	0.71
1:B:867:PHE:O	1:B:873:VAL:HG21	1.91	0.69
1:A:904:GLN:N	1:A:904:GLN:OE1	2.26	0.69
1:C:184:LEU:HD23	1:C:185:LEU:N	2.08	0.69
1:C:904:GLN:OE1	1:C:904:GLN:N	2.26	0.69
1:B:904:GLN:N	1:B:904:GLN:OE1	2.26	0.69
1:B:184:LEU:HD23	1:B:185:LEU:N	2.08	0.68
1:D:904:GLN:N	1:D:904:GLN:OE1	2.26	0.68
1:A:345:VAL:O	1:A:349:VAL:HG23	1.94	0.68
1:B:345:VAL:O	1:B:349:VAL:HG23	1.94	0.68
1:D:345:VAL:O	1:D:349:VAL:HG23	1.94	0.68
1:A:184:LEU:HD23	1:A:185:LEU:N	2.08	0.68
1:D:184:LEU:HD23	1:D:185:LEU:N	2.08	0.68
1:C:345:VAL:O	1:C:349:VAL:HG23	1.94	0.67
1:C:565:GLU:OE2	1:C:574:CYS:N	2.28	0.66
1:B:565:GLU:OE2	1:B:574:CYS:N	2.28	0.66
1:C:765:GLY:O	1:C:768:ARG:NE	2.29	0.66
1:D:1203:GLU:OE1	1:D:1206:ARG:NH1	2.29	0.66
1:B:765:GLY:O	1:B:768:ARG:NE	2.29	0.66
1:D:565:GLU:OE2	1:D:574:CYS:N	2.28	0.66
1:C:1203:GLU:OE1	1:C:1206:ARG:NH1	2.29	0.66
1:A:1203:GLU:OE1	1:A:1206:ARG:NH1	2.29	0.65
1:B:1203:GLU:OE1	1:B:1206:ARG:NH1	2.29	0.65
1:A:765:GLY:O	1:A:768:ARG:NE	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:GLU:OE2	1:A:574:CYS:N	2.28	0.65
1:D:765:GLY:O	1:D:768:ARG:NE	2.29	0.64
1:C:1068:GLY:N	1:C:1084:CYS:SG	2.70	0.62
1:B:1068:GLY:N	1:B:1084:CYS:SG	2.70	0.60
2:D:2002:Y01:HAC1	2:D:2002:Y01:HAU2	1.84	0.60
2:B:2002:Y01:HAU2	2:B:2002:Y01:HAC1	1.84	0.59
1:D:1068:GLY:N	1:D:1084:CYS:SG	2.70	0.59
2:A:2002:Y01:HAC1	2:A:2002:Y01:HAU2	1.84	0.59
2:C:2002:Y01:HAC1	2:C:2002:Y01:HAU2	1.84	0.58
1:A:1068:GLY:N	1:A:1084:CYS:SG	2.70	0.58
1:C:641:LEU:HD13	1:C:657:PHE:HE2	1.70	0.57
1:D:641:LEU:HD13	1:D:657:PHE:HE2	1.70	0.57
1:A:641:LEU:HD13	1:A:657:PHE:HE2	1.69	0.57
1:B:641:LEU:HD13	1:B:657:PHE:HE2	1.70	0.56
1:A:1017:MET:HE1	1:A:1102:ALA:HA	1.88	0.56
1:A:1242:HIS:HA	1:D:1240:ARG:HH22	1.70	0.56
1:D:368:GLY:O	1:D:371:SER:OG	2.21	0.55
1:B:368:GLY:O	1:B:371:SER:OG	2.21	0.55
1:D:1017:MET:HE1	1:D:1102:ALA:HA	1.88	0.55
1:A:324:ILE:N	1:A:330:GLN:O	2.39	0.55
1:D:324:ILE:N	1:D:330:GLN:O	2.39	0.55
1:D:338:ILE:CD1	1:D:349:VAL:HG22	2.37	0.55
1:A:641:LEU:HD13	1:A:657:PHE:CE2	2.42	0.55
1:D:641:LEU:HD13	1:D:657:PHE:CE2	2.42	0.55
1:C:1017:MET:HE1	1:C:1102:ALA:HA	1.88	0.54
1:C:1240:ARG:HH22	1:D:1242:HIS:HA	1.71	0.54
1:C:1242:HIS:HA	1:B:1240:ARG:HH22	1.71	0.54
1:A:338:ILE:CD1	1:A:349:VAL:HG22	2.37	0.54
1:A:1240:ARG:HH22	1:B:1242:HIS:HA	1.71	0.54
1:C:338:ILE:CD1	1:C:349:VAL:HG22	2.37	0.54
1:C:976:CYS:O	1:C:979:ILE:HG22	2.08	0.54
1:D:976:CYS:O	1:D:979:ILE:HG22	2.08	0.54
1:C:524:GLU:O	1:C:528:ASN:ND2	2.39	0.54
1:B:338:ILE:CD1	1:B:349:VAL:HG22	2.37	0.54
1:B:1017:MET:HE1	1:B:1102:ALA:HA	1.88	0.54
1:A:976:CYS:O	1:A:979:ILE:HG22	2.08	0.54
1:C:641:LEU:HD13	1:C:657:PHE:CE2	2.42	0.53
1:B:641:LEU:HD13	1:B:657:PHE:CE2	2.42	0.53
1:D:524:GLU:O	1:D:528:ASN:ND2	2.39	0.53
1:B:976:CYS:O	1:B:979:ILE:HG22	2.08	0.53
1:B:257:GLY:HA3	1:B:302:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:GLY:HA3	1:D:302:THR:HG22	1.90	0.53
1:C:257:GLY:HA3	1:C:302:THR:HG22	1.90	0.52
1:A:257:GLY:HA3	1:A:302:THR:HG22	1.91	0.52
1:C:324:ILE:N	1:C:330:GLN:O	2.39	0.52
1:D:1124:ILE:O	1:D:1128:VAL:HG23	2.10	0.52
1:A:1124:ILE:O	1:A:1128:VAL:HG23	2.10	0.51
1:C:578:ARG:O	1:C:582:ARG:HG3	2.10	0.51
1:A:578:ARG:O	1:A:582:ARG:HG3	2.11	0.51
1:B:1124:ILE:O	1:B:1128:VAL:HG23	2.10	0.51
1:B:578:ARG:O	1:B:582:ARG:HG3	2.11	0.51
1:C:368:GLY:O	1:C:371:SER:OG	2.21	0.51
1:B:524:GLU:O	1:B:528:ASN:ND2	2.39	0.51
1:A:1244:MET:HE1	1:D:1244:MET:SD	2.51	0.51
1:B:324:ILE:N	1:B:330:GLN:O	2.39	0.51
1:A:368:GLY:O	1:A:371:SER:OG	2.21	0.51
1:C:1124:ILE:O	1:C:1128:VAL:HG23	2.10	0.51
1:A:915:LEU:C	1:A:915:LEU:HD23	2.36	0.51
1:C:915:LEU:HD23	1:C:915:LEU:C	2.36	0.51
1:D:578:ARG:O	1:D:582:ARG:HG3	2.11	0.51
1:A:1244:MET:SD	1:B:1244:MET:HE1	2.52	0.50
1:B:915:LEU:C	1:B:915:LEU:HD23	2.36	0.50
1:C:1244:MET:SD	1:D:1244:MET:HE1	2.52	0.50
1:D:915:LEU:C	1:D:915:LEU:HD23	2.36	0.50
1:C:1244:MET:HE1	1:B:1244:MET:SD	2.52	0.50
1:A:524:GLU:O	1:A:528:ASN:ND2	2.39	0.49
1:C:870:ALA:O	1:C:873:VAL:HG22	2.12	0.49
1:B:647:LEU:HA	1:B:678:MET:HE1	1.95	0.49
1:B:870:ALA:O	1:B:873:VAL:HG22	2.13	0.49
1:A:647:LEU:HA	1:A:678:MET:HE1	1.95	0.49
1:D:870:ALA:O	1:D:873:VAL:HG22	2.13	0.49
1:D:915:LEU:HD22	1:D:951:ILE:HD11	1.95	0.49
1:C:647:LEU:HA	1:C:678:MET:HE1	1.95	0.48
1:D:903:THR:OG1	1:D:904:GLN:OE1	2.30	0.48
1:A:870:ALA:O	1:A:873:VAL:HG22	2.12	0.48
1:C:915:LEU:HD22	1:C:951:ILE:HD11	1.94	0.48
1:D:647:LEU:HA	1:D:678:MET:HE1	1.95	0.48
1:A:972:ARG:NH2	1:B:1030:ALA:O	2.47	0.47
1:A:915:LEU:HD22	1:A:951:ILE:HD11	1.94	0.47
1:B:915:LEU:HD22	1:B:951:ILE:HD11	1.95	0.47
1:A:184:LEU:HD23	1:A:185:LEU:H	1.79	0.47
1:C:729:LEU:O	1:C:734:ASN:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LEU:HD23	1:B:185:LEU:H	1.79	0.47
1:C:1037:GLU:OE2	1:B:896:LYS:NZ	2.39	0.46
1:D:493:LEU:C	1:D:493:LEU:HD23	2.40	0.46
1:A:493:LEU:HD23	1:A:493:LEU:C	2.40	0.46
1:C:493:LEU:C	1:C:493:LEU:HD23	2.41	0.46
1:B:903:THR:OG1	1:B:904:GLN:OE1	2.30	0.46
1:B:644:TRP:NE1	1:B:648:MET:SD	2.89	0.46
1:D:644:TRP:NE1	1:D:648:MET:SD	2.89	0.46
1:A:644:TRP:NE1	1:A:648:MET:SD	2.89	0.46
1:D:919:LYS:NZ	1:D:944:ASN:OD1	2.40	0.46
1:A:496:LEU:HD11	1:A:514:MET:HE1	1.98	0.45
1:C:496:LEU:HD11	1:C:514:MET:HE1	1.98	0.45
1:C:644:TRP:NE1	1:C:648:MET:SD	2.89	0.45
1:B:493:LEU:C	1:B:493:LEU:HD23	2.40	0.45
1:C:1030:ALA:O	1:B:972:ARG:NH2	2.47	0.45
1:D:496:LEU:HD11	1:D:514:MET:HE1	1.98	0.45
1:A:903:THR:OG1	1:A:904:GLN:OE1	2.30	0.45
1:B:496:LEU:HD11	1:B:514:MET:HE1	1.98	0.45
1:C:972:ARG:NH2	1:D:1030:ALA:O	2.47	0.44
1:A:1030:ALA:O	1:D:972:ARG:NH2	2.47	0.44
1:C:184:LEU:HD23	1:C:185:LEU:H	1.79	0.44
1:D:184:LEU:HD23	1:D:185:LEU:H	1.79	0.44
1:C:919:LYS:NZ	1:C:944:ASN:OD1	2.40	0.44
2:C:2201:Y01:HAD2	2:C:2201:Y01:HAS2	1.92	0.44
1:D:729:LEU:O	1:D:734:ASN:N	2.44	0.44
1:C:1005:LYS:HD2	1:C:1121:VAL:HG13	2.00	0.44
1:A:541:VAL:HG13	1:A:559:ASP:OD1	2.19	0.43
1:A:1005:LYS:HD2	1:A:1121:VAL:HG13	2.00	0.43
1:C:541:VAL:HG13	1:C:559:ASP:OD1	2.19	0.43
1:C:557:LEU:O	1:C:560:ILE:HG22	2.19	0.43
1:D:1005:LYS:HD2	1:D:1121:VAL:HG13	2.00	0.43
1:A:729:LEU:O	1:A:734:ASN:N	2.44	0.43
1:C:903:THR:OG1	1:C:904:GLN:OE1	2.30	0.43
1:D:526:LEU:O	1:D:529:THR:HG22	2.19	0.43
1:D:541:VAL:HG13	1:D:559:ASP:OD1	2.19	0.43
1:D:932:LEU:HD13	1:D:932:LEU:O	2.19	0.43
1:B:557:LEU:O	1:B:560:ILE:HG22	2.19	0.43
1:B:1005:LYS:HD2	1:B:1121:VAL:HG13	2.00	0.43
1:A:932:LEU:HD13	1:A:932:LEU:O	2.19	0.42
1:A:965:GLN:N	1:A:966:PRO:HD2	2.35	0.42
1:C:1081:LEU:HD12	1:C:1081:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:THR:HG22	1:B:520:ILE:N	2.34	0.42
1:B:729:LEU:O	1:B:734:ASN:N	2.44	0.42
1:D:557:LEU:O	1:D:560:ILE:HG22	2.19	0.42
1:D:1081:LEU:HD12	1:D:1081:LEU:N	2.34	0.42
1:D:257:GLY:CA	1:D:302:THR:HG22	2.49	0.42
1:D:519:THR:HG22	1:D:520:ILE:N	2.34	0.42
1:C:257:GLY:CA	1:C:302:THR:HG22	2.49	0.42
1:B:541:VAL:HG13	1:B:559:ASP:OD1	2.19	0.42
1:A:519:THR:HG22	1:A:520:ILE:N	2.34	0.42
1:A:237:LEU:C	1:A:237:LEU:HD23	2.44	0.42
1:C:237:LEU:C	1:C:237:LEU:HD23	2.44	0.42
1:C:526:LEU:O	1:C:529:THR:HG22	2.19	0.42
1:D:237:LEU:C	1:D:237:LEU:HD23	2.44	0.42
1:A:138:THR:O	1:A:139:ASP:CB	2.67	0.42
1:A:919:LYS:NZ	1:A:944:ASN:OD1	2.40	0.42
1:C:932:LEU:O	1:C:932:LEU:HD13	2.19	0.42
1:A:526:LEU:O	1:A:529:THR:HG22	2.19	0.42
1:C:1030:ALA:O	1:B:972:ARG:NH1	2.52	0.42
1:B:1081:LEU:HD12	1:B:1081:LEU:N	2.34	0.42
2:B:2201:Y01:HAE2	2:B:2201:Y01:HBB	1.96	0.42
1:D:965:GLN:N	1:D:966:PRO:HD2	2.35	0.42
1:A:1081:LEU:HD12	1:A:1081:LEU:N	2.34	0.42
1:C:519:THR:HG22	1:C:520:ILE:N	2.35	0.42
1:B:237:LEU:C	1:B:237:LEU:HD23	2.44	0.42
1:B:526:LEU:O	1:B:529:THR:HG22	2.19	0.42
1:B:932:LEU:HD13	1:B:932:LEU:O	2.19	0.42
1:B:965:GLN:N	1:B:966:PRO:HD2	2.35	0.42
1:C:972:ARG:NH1	1:D:1030:ALA:O	2.52	0.42
1:D:138:THR:O	1:D:139:ASP:CB	2.67	0.41
1:A:257:GLY:CA	1:A:302:THR:HG22	2.49	0.41
1:C:138:THR:O	1:C:139:ASP:CB	2.67	0.41
1:A:557:LEU:O	1:A:560:ILE:HG22	2.19	0.41
2:A:2201:Y01:HAE2	2:A:2201:Y01:HBB	1.96	0.41
1:D:1147:PRO:O	1:D:1151:ILE:HG23	2.21	0.41
1:C:965:GLN:N	1:C:966:PRO:HD2	2.35	0.41
1:C:1147:PRO:O	1:C:1151:ILE:HG23	2.21	0.41
1:D:1148:PRO:N	1:D:1149:PRO:CD	2.84	0.41
1:B:138:THR:O	1:B:139:ASP:CB	2.67	0.41
1:A:972:ARG:NH1	1:B:1030:ALA:O	2.52	0.41
1:A:184:LEU:O	1:A:218:ALA:HB1	2.21	0.41
1:C:184:LEU:O	1:C:218:ALA:HB1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1148:PRO:N	1:C:1149:PRO:CD	2.84	0.41
1:B:1109:LEU:O	1:B:1113:VAL:HG23	2.21	0.41
1:B:1147:PRO:O	1:B:1151:ILE:HG23	2.21	0.41
1:A:932:LEU:HD13	1:A:932:LEU:C	2.46	0.41
1:B:184:LEU:O	1:B:218:ALA:HB1	2.21	0.41
1:D:205:PHE:HE1	1:D:337:LEU:HD21	1.86	0.41
1:B:257:GLY:CA	1:B:302:THR:HG22	2.49	0.40
1:D:184:LEU:O	1:D:218:ALA:HB1	2.21	0.40
1:A:205:PHE:HE1	1:A:337:LEU:HD21	1.86	0.40
1:A:1109:LEU:O	1:A:1113:VAL:HG23	2.21	0.40
1:A:1147:PRO:O	1:A:1151:ILE:HG23	2.21	0.40
2:D:2201:Y01:HAD2	2:D:2201:Y01:HAS2	1.92	0.40
1:A:1148:PRO:N	1:A:1149:PRO:CD	2.84	0.40
1:C:1109:LEU:O	1:C:1113:VAL:HG23	2.21	0.40
1:A:1030:ALA:O	1:D:972:ARG:NH1	2.52	0.40
1:B:1017:MET:HE1	1:B:1102:ALA:CA	2.51	0.40
2:D:2201:Y01:HAE2	2:D:2201:Y01:HBB	1.96	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	895/1739 (52%)	869 (97%)	26 (3%)	0	100	100
1	B	895/1739 (52%)	869 (97%)	26 (3%)	0	100	100
1	C	895/1739 (52%)	869 (97%)	26 (3%)	0	100	100
1	D	895/1739 (52%)	869 (97%)	26 (3%)	0	100	100
All	All	3580/6956 (52%)	3476 (97%)	104 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	563/1545 (36%)	562 (100%)	1 (0%)	92	96
1	B	563/1545 (36%)	562 (100%)	1 (0%)	92	96
1	C	563/1545 (36%)	562 (100%)	1 (0%)	92	96
1	D	563/1545 (36%)	562 (100%)	1 (0%)	92	96
All	All	2252/6180 (36%)	2248 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1240	ARG
1	C	1240	ARG
1	B	1240	ARG
1	D	1240	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	633	HIS
1	A	746	HIS
1	C	633	HIS
1	B	633	HIS
1	D	633	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	Y01	B	2002	-	38,38,38	1.10	3 (7%)	57,57,57	2.31	14 (24%)
3	6OU	A	2004	-	36,36,48	1.03	4 (11%)	39,41,53	0.97	2 (5%)
3	6OU	B	2004	-	36,36,48	1.03	4 (11%)	39,41,53	0.97	2 (5%)
4	A1AIA	C	2101	-	17,17,17	5.73	9 (52%)	24,24,24	1.00	1 (4%)
3	6OU	C	2004	-	36,36,48	1.04	4 (11%)	39,41,53	0.97	2 (5%)
4	A1AIA	D	2101	-	17,17,17	5.73	9 (52%)	24,24,24	1.00	1 (4%)
4	A1AIA	B	2101	-	17,17,17	5.73	9 (52%)	24,24,24	1.00	1 (4%)
2	Y01	D	2002	-	38,38,38	1.10	3 (7%)	57,57,57	2.31	14 (24%)
3	6OU	D	2004	-	36,36,48	1.03	4 (11%)	39,41,53	0.97	2 (5%)
2	Y01	C	2201	-	38,38,38	1.14	3 (7%)	57,57,57	2.48	18 (31%)
2	Y01	B	2201	-	38,38,38	1.13	3 (7%)	57,57,57	2.48	18 (31%)
2	Y01	A	2002	-	38,38,38	1.10	3 (7%)	57,57,57	2.31	14 (24%)
2	Y01	C	2002	-	38,38,38	1.10	3 (7%)	57,57,57	2.32	13 (22%)
2	Y01	D	2201	-	38,38,38	1.13	3 (7%)	57,57,57	2.48	18 (31%)
4	A1AIA	A	2101	-	17,17,17	5.73	9 (52%)	24,24,24	0.99	0
2	Y01	A	2201	-	38,38,38	1.14	3 (7%)	57,57,57	2.48	17 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	B	2002	-	-	7/19/77/77	0/4/4/4
3	6OU	A	2004	-	-	20/40/40/52	-
3	6OU	B	2004	-	-	20/40/40/52	-
4	A1AIA	C	2101	-	-	1/9/27/27	0/2/2/2
3	6OU	C	2004	-	-	20/40/40/52	-
4	A1AIA	D	2101	-	-	1/9/27/27	0/2/2/2
4	A1AIA	B	2101	-	-	1/9/27/27	0/2/2/2
2	Y01	D	2002	-	-	7/19/77/77	0/4/4/4
3	6OU	D	2004	-	-	20/40/40/52	-
2	Y01	C	2201	-	-	15/19/77/77	0/4/4/4
2	Y01	B	2201	-	-	15/19/77/77	0/4/4/4
2	Y01	A	2002	-	-	7/19/77/77	0/4/4/4
2	Y01	C	2002	-	-	7/19/77/77	0/4/4/4
2	Y01	D	2201	-	-	15/19/77/77	0/4/4/4
4	A1AIA	A	2101	-	-	1/9/27/27	0/2/2/2
2	Y01	A	2201	-	-	15/19/77/77	0/4/4/4

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	A1AIA	C04-N06	16.16	1.45	1.33
4	D	2101	A1AIA	C04-N06	16.16	1.45	1.33
4	A	2101	A1AIA	C04-N06	16.05	1.45	1.33
4	C	2101	A1AIA	C04-N06	16.05	1.45	1.33
4	A	2101	A1AIA	C09-N08	15.45	1.45	1.33
4	C	2101	A1AIA	C09-N08	15.45	1.45	1.33
4	B	2101	A1AIA	C09-N08	15.34	1.45	1.33
4	D	2101	A1AIA	C09-N08	15.34	1.45	1.33
4	C	2101	A1AIA	C07-N06	3.89	1.50	1.45
4	A	2101	A1AIA	C07-N06	3.83	1.50	1.45
4	B	2101	A1AIA	C07-N06	3.82	1.50	1.45
4	D	2101	A1AIA	C07-N06	3.82	1.50	1.45
4	B	2101	A1AIA	C07-N08	3.76	1.49	1.45
4	D	2101	A1AIA	C07-N08	3.76	1.49	1.45
4	C	2101	A1AIA	C07-N08	3.74	1.49	1.45
4	A	2101	A1AIA	C07-N08	3.65	1.49	1.45
2	C	2201	Y01	OAW-CAY	3.35	1.43	1.34
4	B	2101	A1AIA	C03-C04	-3.33	1.49	1.53
4	D	2101	A1AIA	C03-C04	-3.33	1.49	1.53
2	A	2201	Y01	OAW-CAY	3.32	1.43	1.34
2	B	2201	Y01	OAW-CAY	3.32	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2201	Y01	OAW-CAY	3.32	1.43	1.34
2	A	2002	Y01	OAW-CAY	3.30	1.43	1.34
2	B	2002	Y01	OAW-CAY	3.30	1.43	1.34
2	D	2002	Y01	OAW-CAY	3.30	1.43	1.34
2	C	2002	Y01	OAW-CAY	3.28	1.43	1.34
4	A	2101	A1AIA	C03-C04	-3.24	1.50	1.53
4	C	2101	A1AIA	C03-C04	-3.24	1.50	1.53
2	C	2002	Y01	OAH-CAX	-2.87	1.21	1.30
2	A	2002	Y01	OAH-CAX	-2.86	1.21	1.30
2	B	2002	Y01	OAH-CAX	-2.84	1.21	1.30
2	D	2002	Y01	OAH-CAX	-2.84	1.21	1.30
2	A	2201	Y01	OAH-CAX	-2.84	1.21	1.30
2	C	2201	Y01	OAH-CAX	-2.84	1.21	1.30
2	B	2201	Y01	OAH-CAX	-2.84	1.21	1.30
2	D	2201	Y01	OAH-CAX	-2.84	1.21	1.30
3	A	2004	6OU	O30-C20	-2.66	1.40	1.46
3	B	2004	6OU	O30-C20	-2.66	1.40	1.46
3	D	2004	6OU	O30-C20	-2.66	1.40	1.46
3	C	2004	6OU	O30-C20	-2.65	1.40	1.46
3	B	2004	6OU	O18-C16	2.44	1.40	1.33
3	D	2004	6OU	O18-C16	2.44	1.40	1.33
3	A	2004	6OU	O18-C16	2.44	1.40	1.33
3	C	2004	6OU	O18-C16	2.42	1.40	1.33
4	B	2101	A1AIA	O10-C09	-2.41	1.18	1.22
4	D	2101	A1AIA	O10-C09	-2.41	1.18	1.22
4	A	2101	A1AIA	O10-C09	-2.39	1.18	1.22
4	C	2101	A1AIA	O10-C09	-2.39	1.18	1.22
4	C	2101	A1AIA	O05-C04	-2.31	1.18	1.22
4	A	2101	A1AIA	O05-C04	-2.26	1.19	1.22
4	B	2101	A1AIA	O05-C04	-2.25	1.19	1.22
4	D	2101	A1AIA	O05-C04	-2.25	1.19	1.22
2	C	2201	Y01	CAS-CBF	2.23	1.57	1.53
2	B	2201	Y01	CAS-CBF	2.23	1.57	1.53
2	D	2201	Y01	CAS-CBF	2.23	1.57	1.53
4	B	2101	A1AIA	C03-C11	2.22	1.58	1.54
4	D	2101	A1AIA	C03-C11	2.22	1.58	1.54
4	A	2101	A1AIA	C03-C11	2.21	1.58	1.54
4	C	2101	A1AIA	C03-C11	2.21	1.58	1.54
3	C	2004	6OU	O18-C19	-2.18	1.40	1.45
3	B	2004	6OU	O18-C19	-2.18	1.40	1.45
3	D	2004	6OU	O18-C19	-2.18	1.40	1.45
2	A	2201	Y01	CAS-CBF	2.17	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2004	6OU	O18-C19	-2.16	1.40	1.45
3	C	2004	6OU	O30-C31	2.15	1.40	1.34
3	A	2004	6OU	O30-C31	2.13	1.40	1.34
3	B	2004	6OU	O30-C31	2.13	1.40	1.34
3	D	2004	6OU	O30-C31	2.13	1.40	1.34
2	A	2002	Y01	CAK-CAI	2.12	1.54	1.50
2	C	2002	Y01	CAK-CAI	2.12	1.54	1.50
2	B	2002	Y01	CAK-CAI	2.12	1.54	1.50
2	D	2002	Y01	CAK-CAI	2.12	1.54	1.50
4	A	2101	A1AIA	C03-C09	-2.01	1.51	1.53
4	C	2101	A1AIA	C03-C09	-2.01	1.51	1.53
4	B	2101	A1AIA	C03-C09	-2.01	1.51	1.53
4	D	2101	A1AIA	C03-C09	-2.01	1.51	1.53

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2002	Y01	CAT-CBH-CBF	-9.55	96.09	108.74
2	A	2002	Y01	CAT-CBH-CBF	-9.54	96.12	108.74
2	B	2002	Y01	CAT-CBH-CBF	-9.54	96.12	108.74
2	D	2002	Y01	CAT-CBH-CBF	-9.54	96.12	108.74
2	A	2201	Y01	CAT-CBH-CBF	-8.28	97.78	108.74
2	C	2201	Y01	CAT-CBH-CBF	-8.25	97.82	108.74
2	B	2201	Y01	CAT-CBH-CBF	-8.25	97.82	108.74
2	D	2201	Y01	CAT-CBH-CBF	-8.25	97.82	108.74
2	A	2201	Y01	CAV-CAZ-CAI	7.97	131.37	120.57
2	C	2201	Y01	CAV-CAZ-CAI	7.95	131.34	120.57
2	B	2201	Y01	CAV-CAZ-CAI	7.94	131.33	120.57
2	D	2201	Y01	CAV-CAZ-CAI	7.94	131.33	120.57
2	C	2002	Y01	CAV-CAZ-CAI	6.75	129.72	120.57
2	B	2002	Y01	CAV-CAZ-CAI	6.74	129.70	120.57
2	D	2002	Y01	CAV-CAZ-CAI	6.74	129.70	120.57
2	A	2002	Y01	CAV-CAZ-CAI	6.72	129.68	120.57
2	A	2201	Y01	CBH-CBF-CBD	-5.74	104.33	112.71
2	B	2201	Y01	CBH-CBF-CBD	-5.71	104.37	112.71
2	D	2201	Y01	CBH-CBF-CBD	-5.71	104.37	112.71
2	C	2201	Y01	CBH-CBF-CBD	-5.71	104.37	112.71
2	C	2002	Y01	CBH-CBF-CBD	-5.15	105.18	112.71
2	A	2002	Y01	CBH-CBF-CBD	-5.13	105.21	112.71
2	B	2002	Y01	CBH-CBF-CBD	-5.13	105.21	112.71
2	D	2002	Y01	CBH-CBF-CBD	-5.13	105.21	112.71
2	C	2201	Y01	CAV-CAZ-CBH	-4.77	110.31	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2201	Y01	CAV-CAZ-CBH	-4.76	110.33	116.42
2	B	2201	Y01	CAV-CAZ-CBH	-4.76	110.33	116.42
2	D	2201	Y01	CAV-CAZ-CBH	-4.76	110.33	116.42
2	C	2002	Y01	CBH-CAZ-CAI	-4.44	116.44	122.93
2	A	2002	Y01	CBH-CAZ-CAI	-4.42	116.47	122.93
2	B	2002	Y01	CBH-CAZ-CAI	-4.40	116.51	122.93
2	D	2002	Y01	CBH-CAZ-CAI	-4.40	116.51	122.93
2	C	2002	Y01	CAD-CBH-CBF	4.26	116.44	111.66
2	A	2002	Y01	CAD-CBH-CBF	4.24	116.42	111.66
2	B	2002	Y01	CAD-CBH-CBF	4.23	116.41	111.66
2	D	2002	Y01	CAD-CBH-CBF	4.23	116.41	111.66
2	A	2201	Y01	OAW-CAY-CAM	4.23	120.64	111.48
2	B	2201	Y01	OAW-CAY-CAM	4.23	120.64	111.48
2	D	2201	Y01	OAW-CAY-CAM	4.23	120.64	111.48
2	C	2201	Y01	OAW-CAY-CAM	4.22	120.61	111.48
2	A	2201	Y01	CAU-CBI-CBE	-3.98	110.73	116.60
2	C	2201	Y01	CAU-CBI-CBE	-3.97	110.75	116.60
2	B	2201	Y01	CAU-CBI-CBE	-3.97	110.75	116.60
2	D	2201	Y01	CAU-CBI-CBE	-3.97	110.75	116.60
3	B	2004	6OU	O30-C31-C33	3.94	120.00	111.48
3	D	2004	6OU	O30-C31-C33	3.94	120.00	111.48
3	A	2004	6OU	O30-C31-C33	3.93	119.98	111.48
3	C	2004	6OU	O30-C31-C33	3.92	119.95	111.48
2	A	2002	Y01	OAW-CAY-CAM	3.91	119.93	111.48
2	B	2002	Y01	OAW-CAY-CAM	3.91	119.93	111.48
2	D	2002	Y01	OAW-CAY-CAM	3.91	119.93	111.48
2	C	2002	Y01	OAW-CAY-CAM	3.89	119.90	111.48
2	C	2201	Y01	CBI-CBE-CBB	-3.59	113.95	119.50
2	B	2201	Y01	CBI-CBE-CBB	-3.59	113.95	119.50
2	D	2201	Y01	CBI-CBE-CBB	-3.59	113.95	119.50
2	A	2201	Y01	CBI-CBE-CBB	-3.57	113.98	119.50
2	C	2002	Y01	CAU-CBI-CBE	-3.48	111.47	116.60
2	A	2002	Y01	CAU-CBI-CBE	-3.46	111.50	116.60
2	B	2002	Y01	CAU-CBI-CBE	-3.46	111.50	116.60
2	D	2002	Y01	CAU-CBI-CBE	-3.46	111.50	116.60
2	A	2201	Y01	CBH-CAZ-CAI	-3.17	118.30	122.93
2	C	2201	Y01	CBH-CAZ-CAI	-3.15	118.34	122.93
2	B	2201	Y01	CBH-CAZ-CAI	-3.15	118.34	122.93
2	D	2201	Y01	CBH-CAZ-CAI	-3.15	118.34	122.93
2	C	2002	Y01	CAD-CBH-CAZ	3.04	113.03	108.38
2	A	2002	Y01	CAD-CBH-CAZ	3.02	112.99	108.38
2	B	2002	Y01	CAD-CBH-CAZ	2.99	112.95	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2002	Y01	CAD-CBH-CAZ	2.99	112.95	108.38
2	C	2201	Y01	CAC-CBB-CBE	-2.88	108.56	112.88
2	A	2201	Y01	CAC-CBB-CBE	-2.86	108.58	112.88
2	B	2201	Y01	CAC-CBB-CBE	-2.86	108.58	112.88
2	D	2201	Y01	CAC-CBB-CBE	-2.86	108.58	112.88
2	A	2201	Y01	CAT-CAR-CBC	2.79	114.89	110.33
2	A	2201	Y01	CAU-CAS-CBF	2.77	117.85	113.14
2	A	2002	Y01	CAU-CAS-CBF	2.77	117.84	113.14
2	B	2002	Y01	CAU-CAS-CBF	2.77	117.84	113.14
2	D	2002	Y01	CAU-CAS-CBF	2.77	117.84	113.14
2	C	2201	Y01	CAT-CAR-CBC	2.76	114.84	110.33
2	B	2201	Y01	CAT-CAR-CBC	2.76	114.84	110.33
2	D	2201	Y01	CAT-CAR-CBC	2.76	114.84	110.33
2	C	2002	Y01	CAU-CAS-CBF	2.76	117.83	113.14
2	C	2201	Y01	CAU-CAS-CBF	2.75	117.81	113.14
2	B	2201	Y01	CAU-CAS-CBF	2.75	117.81	113.14
2	D	2201	Y01	CAU-CAS-CBF	2.75	117.81	113.14
2	B	2201	Y01	CAD-CBH-CAZ	2.69	112.50	108.38
2	D	2201	Y01	CAD-CBH-CAZ	2.69	112.50	108.38
2	C	2201	Y01	CAD-CBH-CAZ	2.69	112.49	108.38
2	A	2201	Y01	CAD-CBH-CAZ	2.67	112.47	108.38
2	A	2201	Y01	CAD-CBH-CBF	2.67	114.66	111.66
2	C	2201	Y01	CAD-CBH-CBF	2.65	114.64	111.66
2	B	2201	Y01	CAD-CBH-CBF	2.63	114.61	111.66
2	D	2201	Y01	CAD-CBH-CBF	2.63	114.61	111.66
2	A	2201	Y01	CAD-CBH-CAT	2.60	113.39	109.43
2	B	2201	Y01	CAD-CBH-CAT	2.58	113.35	109.43
2	D	2201	Y01	CAD-CBH-CAT	2.58	113.35	109.43
2	C	2201	Y01	CAD-CBH-CAT	2.56	113.32	109.43
3	C	2004	6OU	O18-C16-C15	2.55	119.62	111.83
3	A	2004	6OU	O18-C16-C15	2.55	119.62	111.83
2	C	2002	Y01	CBI-CBE-CBB	-2.54	115.57	119.50
2	A	2002	Y01	CBI-CBE-CBB	-2.53	115.58	119.50
2	B	2002	Y01	CBI-CBE-CBB	-2.53	115.58	119.50
2	D	2002	Y01	CBI-CBE-CBB	-2.53	115.58	119.50
3	B	2004	6OU	O18-C16-C15	2.53	119.56	111.83
3	D	2004	6OU	O18-C16-C15	2.53	119.56	111.83
2	A	2201	Y01	CBD-CAK-CAI	-2.42	109.41	112.76
2	A	2201	Y01	CAP-CBE-CBI	-2.41	101.01	103.84
2	B	2201	Y01	CAP-CBE-CBI	-2.38	101.04	103.84
2	D	2201	Y01	CAP-CBE-CBI	-2.38	101.04	103.84
2	C	2201	Y01	CAP-CBE-CBI	-2.37	101.05	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2201	Y01	CBD-CAK-CAI	-2.36	109.49	112.76
2	B	2201	Y01	CBD-CAK-CAI	-2.35	109.51	112.76
2	D	2201	Y01	CBD-CAK-CAI	-2.35	109.51	112.76
2	C	2201	Y01	CBC-CAV-CAZ	-2.32	108.03	111.45
2	A	2201	Y01	CBC-CAV-CAZ	-2.30	108.05	111.45
2	B	2201	Y01	CBC-CAV-CAZ	-2.30	108.05	111.45
2	D	2201	Y01	CBC-CAV-CAZ	-2.30	108.05	111.45
2	C	2002	Y01	CAC-CBB-CBE	-2.24	109.52	112.88
2	A	2002	Y01	CAC-CBB-CBE	-2.22	109.56	112.88
2	B	2002	Y01	CAC-CBB-CBE	-2.22	109.56	112.88
2	D	2002	Y01	CAC-CBB-CBE	-2.22	109.56	112.88
2	C	2002	Y01	CAK-CBD-CBF	-2.13	107.26	109.72
2	A	2002	Y01	CAK-CBD-CBF	-2.08	107.31	109.72
2	B	2002	Y01	CAK-CBD-CBF	-2.08	107.31	109.72
2	D	2002	Y01	CAK-CBD-CBF	-2.08	107.31	109.72
2	B	2002	Y01	CAV-CAZ-CBH	-2.08	113.76	116.42
2	D	2002	Y01	CAV-CAZ-CBH	-2.08	113.76	116.42
2	B	2201	Y01	CAK-CBD-CBF	-2.05	107.36	109.72
2	D	2201	Y01	CAK-CBD-CBF	-2.05	107.36	109.72
2	C	2002	Y01	CAV-CAZ-CBH	-2.04	113.81	116.42
2	A	2002	Y01	CAV-CAZ-CBH	-2.03	113.82	116.42
4	C	2101	A1AIA	C01-C02-C03	-2.02	110.69	113.92
2	A	2002	Y01	CBC-CAV-CAZ	2.01	114.42	111.45
4	B	2101	A1AIA	O05-C04-N06	-2.01	119.52	122.13
4	D	2101	A1AIA	O05-C04-N06	-2.01	119.52	122.13
2	B	2002	Y01	CBC-CAV-CAZ	2.01	114.42	111.45
2	D	2002	Y01	CBC-CAV-CAZ	2.01	114.42	111.45
2	C	2201	Y01	CAK-CBD-CBF	-2.01	107.40	109.72

There are no chirality outliers.

All (172) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2004	6OU	C21-O22-P23-O24
3	A	2004	6OU	C21-O22-P23-O26
3	A	2004	6OU	O26-C27-C28-N29
3	A	2004	6OU	O32-C31-O30-C20
3	C	2004	6OU	C21-O22-P23-O24
3	C	2004	6OU	C21-O22-P23-O26
3	C	2004	6OU	O26-C27-C28-N29
3	C	2004	6OU	O32-C31-O30-C20
3	B	2004	6OU	C21-O22-P23-O24

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Mol	Chain	Res	Type	Atoms
3	B	2004	6OU	C21-O22-P23-O26
3	B	2004	6OU	O26-C27-C28-N29
3	B	2004	6OU	O32-C31-O30-C20
3	D	2004	6OU	C21-O22-P23-O24
3	D	2004	6OU	C21-O22-P23-O26
3	D	2004	6OU	O26-C27-C28-N29
3	D	2004	6OU	O32-C31-O30-C20
2	A	2201	Y01	CAC-CBB-CBE-CBI
2	C	2201	Y01	CAC-CBB-CBE-CBI
2	B	2201	Y01	CAC-CBB-CBE-CBI
2	D	2201	Y01	CAC-CBB-CBE-CBI
3	A	2004	6OU	C33-C31-O30-C20
3	C	2004	6OU	C33-C31-O30-C20
3	B	2004	6OU	C33-C31-O30-C20
3	D	2004	6OU	C33-C31-O30-C20
2	A	2201	Y01	CAO-CBB-CBE-CBI
2	C	2201	Y01	CAO-CBB-CBE-CBI
2	B	2201	Y01	CAO-CBB-CBE-CBI
2	D	2201	Y01	CAO-CBB-CBE-CBI
2	A	2201	Y01	CAC-CBB-CBE-CAP
2	C	2201	Y01	CAC-CBB-CBE-CAP
2	B	2201	Y01	CAC-CBB-CBE-CAP
2	D	2201	Y01	CAC-CBB-CBE-CAP
3	A	2004	6OU	C13-C14-C15-C16
3	C	2004	6OU	C13-C14-C15-C16
3	B	2004	6OU	C13-C14-C15-C16
3	D	2004	6OU	C13-C14-C15-C16
2	A	2002	Y01	CAN-CAJ-CAO-CBB
2	C	2002	Y01	CAN-CAJ-CAO-CBB
2	B	2002	Y01	CAN-CAJ-CAO-CBB
2	D	2002	Y01	CAN-CAJ-CAO-CBB
3	A	2004	6OU	C15-C16-O18-C19
3	C	2004	6OU	C15-C16-O18-C19
3	B	2004	6OU	C15-C16-O18-C19
3	D	2004	6OU	C15-C16-O18-C19
2	B	2201	Y01	CAN-CAJ-CAO-CBB
2	D	2201	Y01	CAN-CAJ-CAO-CBB
2	A	2201	Y01	CAN-CAJ-CAO-CBB
2	C	2201	Y01	CAN-CAJ-CAO-CBB
3	C	2004	6OU	O17-C16-O18-C19
3	B	2004	6OU	O17-C16-O18-C19
3	D	2004	6OU	O17-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
3	A	2004	6OU	O17-C16-O18-C19
3	A	2004	6OU	C37-C38-C39-C40
3	C	2004	6OU	C37-C38-C39-C40
3	B	2004	6OU	C37-C38-C39-C40
3	D	2004	6OU	C37-C38-C39-C40
2	A	2002	Y01	CAM-CAY-OAW-CBC
2	C	2002	Y01	CAM-CAY-OAW-CBC
2	B	2002	Y01	CAM-CAY-OAW-CBC
2	D	2002	Y01	CAM-CAY-OAW-CBC
2	A	2201	Y01	CAX-CAL-CAM-CAY
2	C	2201	Y01	CAX-CAL-CAM-CAY
2	B	2201	Y01	CAX-CAL-CAM-CAY
2	D	2201	Y01	CAX-CAL-CAM-CAY
3	A	2004	6OU	O18-C19-C20-C21
3	C	2004	6OU	O18-C19-C20-C21
3	B	2004	6OU	O18-C19-C20-C21
3	D	2004	6OU	O18-C19-C20-C21
2	A	2201	Y01	CAJ-CAN-CBA-CAB
2	C	2201	Y01	CAJ-CAN-CBA-CAB
2	B	2201	Y01	CAJ-CAN-CBA-CAB
2	D	2201	Y01	CAJ-CAN-CBA-CAB
2	A	2201	Y01	CAO-CBB-CBE-CAP
2	C	2201	Y01	CAO-CBB-CBE-CAP
2	B	2201	Y01	CAO-CBB-CBE-CAP
2	D	2201	Y01	CAO-CBB-CBE-CAP
3	A	2004	6OU	C07-C08-C09-C10
3	C	2004	6OU	C07-C08-C09-C10
3	B	2004	6OU	C07-C08-C09-C10
3	D	2004	6OU	C07-C08-C09-C10
3	A	2004	6OU	C34-C35-C36-C37
3	C	2004	6OU	C34-C35-C36-C37
3	B	2004	6OU	C34-C35-C36-C37
3	D	2004	6OU	C34-C35-C36-C37
2	A	2002	Y01	OAG-CAY-OAW-CBC
2	C	2002	Y01	OAG-CAY-OAW-CBC
2	B	2002	Y01	OAG-CAY-OAW-CBC
2	D	2002	Y01	OAG-CAY-OAW-CBC
2	A	2201	Y01	CAM-CAY-OAW-CBC
2	C	2201	Y01	CAM-CAY-OAW-CBC
2	B	2201	Y01	CAM-CAY-OAW-CBC
2	D	2201	Y01	CAM-CAY-OAW-CBC
2	A	2201	Y01	CAJ-CAN-CBA-CAA

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Mol	Chain	Res	Type	Atoms
2	C	2201	Y01	CAJ-CAN-CBA-CAA
2	B	2201	Y01	CAJ-CAN-CBA-CAA
2	D	2201	Y01	CAJ-CAN-CBA-CAA
3	A	2004	6OU	O18-C19-C20-O30
3	C	2004	6OU	O18-C19-C20-O30
3	B	2004	6OU	O18-C19-C20-O30
3	D	2004	6OU	O18-C19-C20-O30
2	A	2002	Y01	CAJ-CAN-CBA-CAA
2	C	2002	Y01	CAJ-CAN-CBA-CAA
2	B	2002	Y01	CAJ-CAN-CBA-CAA
2	D	2002	Y01	CAJ-CAN-CBA-CAA
3	B	2004	6OU	C35-C36-C37-C38
3	D	2004	6OU	C35-C36-C37-C38
3	A	2004	6OU	C35-C36-C37-C38
3	C	2004	6OU	C35-C36-C37-C38
2	A	2201	Y01	OAG-CAY-OAW-CBC
2	C	2201	Y01	OAG-CAY-OAW-CBC
2	B	2201	Y01	OAG-CAY-OAW-CBC
2	D	2201	Y01	OAG-CAY-OAW-CBC
3	A	2004	6OU	C27-O26-P23-O22
3	A	2004	6OU	C27-O26-P23-O24
3	A	2004	6OU	C27-O26-P23-O25
3	C	2004	6OU	C27-O26-P23-O22
3	C	2004	6OU	C27-O26-P23-O24
3	C	2004	6OU	C27-O26-P23-O25
3	B	2004	6OU	C27-O26-P23-O22
3	B	2004	6OU	C27-O26-P23-O24
3	B	2004	6OU	C27-O26-P23-O25
3	D	2004	6OU	C27-O26-P23-O22
3	D	2004	6OU	C27-O26-P23-O24
3	D	2004	6OU	C27-O26-P23-O25
3	A	2004	6OU	C36-C37-C38-C39
3	C	2004	6OU	C36-C37-C38-C39
3	B	2004	6OU	C36-C37-C38-C39
3	D	2004	6OU	C36-C37-C38-C39
3	A	2004	6OU	C40-C41-C42-C43
3	C	2004	6OU	C40-C41-C42-C43
3	B	2004	6OU	C40-C41-C42-C43
3	D	2004	6OU	C40-C41-C42-C43
3	A	2004	6OU	C12-C13-C14-C15
3	C	2004	6OU	C12-C13-C14-C15
3	B	2004	6OU	C12-C13-C14-C15

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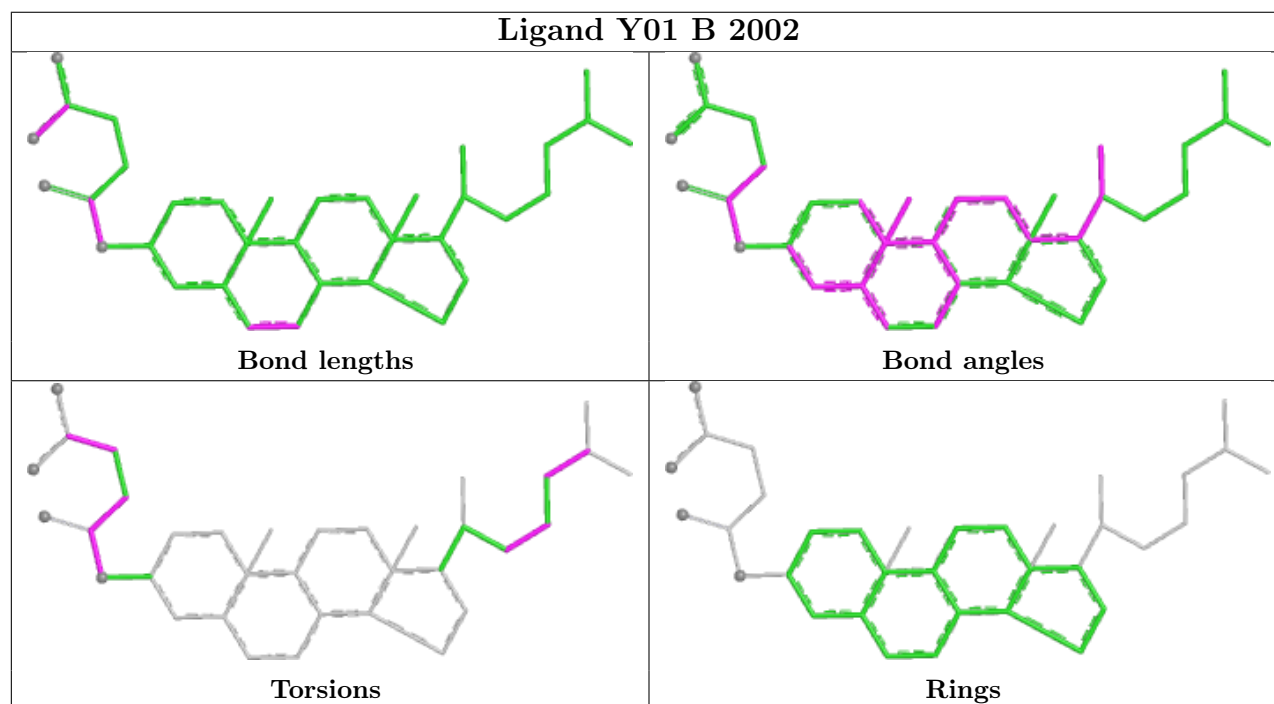
Mol	Chain	Res	Type	Atoms
3	D	2004	6OU	C12-C13-C14-C15
2	A	2002	Y01	CAM-CAL-CAX-OAH
2	C	2002	Y01	CAM-CAL-CAX-OAH
2	B	2002	Y01	CAM-CAL-CAX-OAH
2	D	2002	Y01	CAM-CAL-CAX-OAH
2	C	2002	Y01	CAM-CAL-CAX-OAF
2	A	2201	Y01	CAL-CAM-CAY-OAW
2	B	2201	Y01	CAL-CAM-CAY-OAW
2	D	2201	Y01	CAL-CAM-CAY-OAW
2	A	2002	Y01	CAM-CAL-CAX-OAF
2	B	2002	Y01	CAM-CAL-CAX-OAF
2	D	2002	Y01	CAM-CAL-CAX-OAF
2	C	2201	Y01	CAL-CAM-CAY-OAW
2	A	2201	Y01	CAM-CAL-CAX-OAF
2	B	2201	Y01	CAM-CAL-CAX-OAF
2	D	2201	Y01	CAM-CAL-CAX-OAF
2	C	2201	Y01	CAM-CAL-CAX-OAF
2	B	2201	Y01	CAM-CAL-CAX-OAH
2	D	2201	Y01	CAM-CAL-CAX-OAH
2	A	2201	Y01	CAM-CAL-CAX-OAH
2	C	2201	Y01	CAM-CAL-CAX-OAH
2	A	2201	Y01	CAO-CAJ-CAN-CBA
2	C	2201	Y01	CAO-CAJ-CAN-CBA
2	B	2201	Y01	CAO-CAJ-CAN-CBA
2	D	2201	Y01	CAO-CAJ-CAN-CBA
4	A	2101	A1AIA	C02-C03-C11-C16
4	C	2101	A1AIA	C02-C03-C11-C16
4	B	2101	A1AIA	C02-C03-C11-C16
4	D	2101	A1AIA	C02-C03-C11-C16
2	A	2201	Y01	CAL-CAM-CAY-OAG
2	B	2201	Y01	CAL-CAM-CAY-OAG
2	D	2201	Y01	CAL-CAM-CAY-OAG
2	C	2201	Y01	CAL-CAM-CAY-OAG
2	A	2002	Y01	CAL-CAM-CAY-OAW
2	C	2002	Y01	CAL-CAM-CAY-OAW
2	B	2002	Y01	CAL-CAM-CAY-OAW
2	D	2002	Y01	CAL-CAM-CAY-OAW

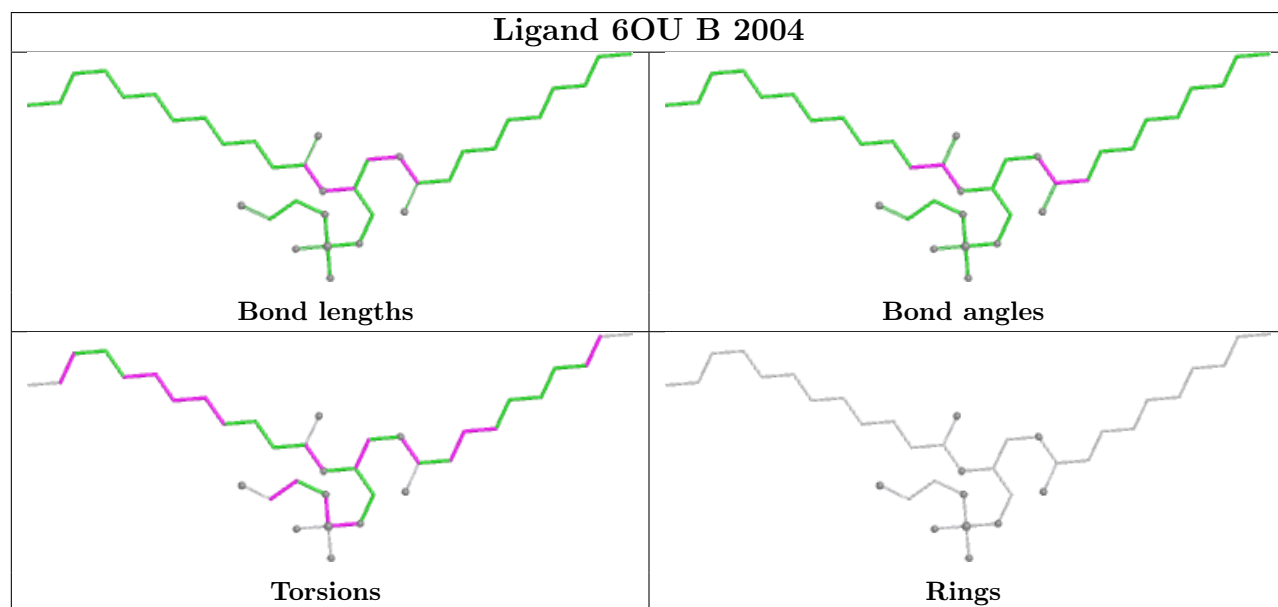
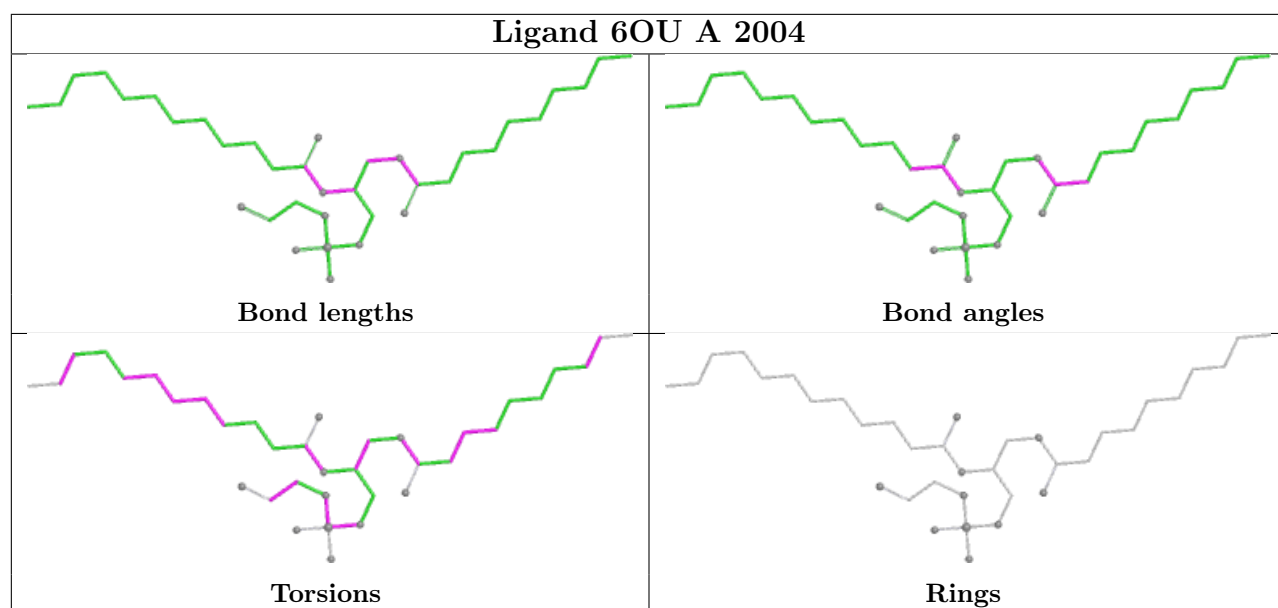
There are no ring outliers.

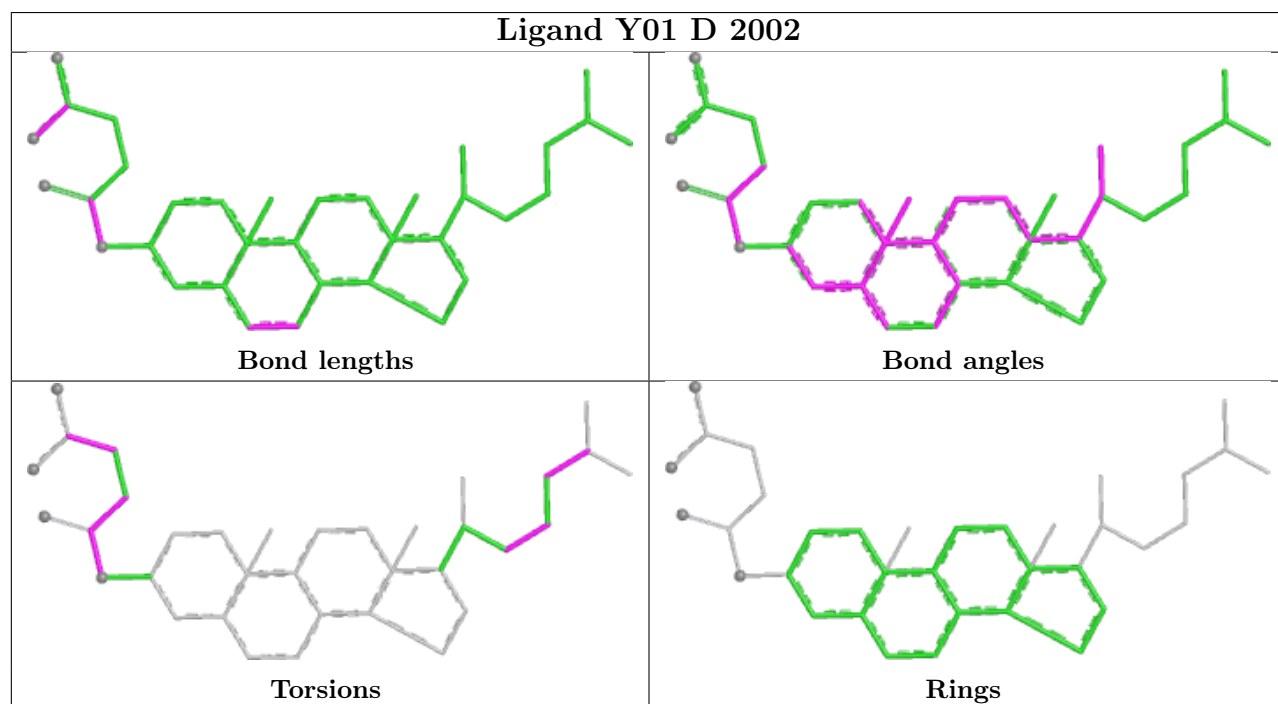
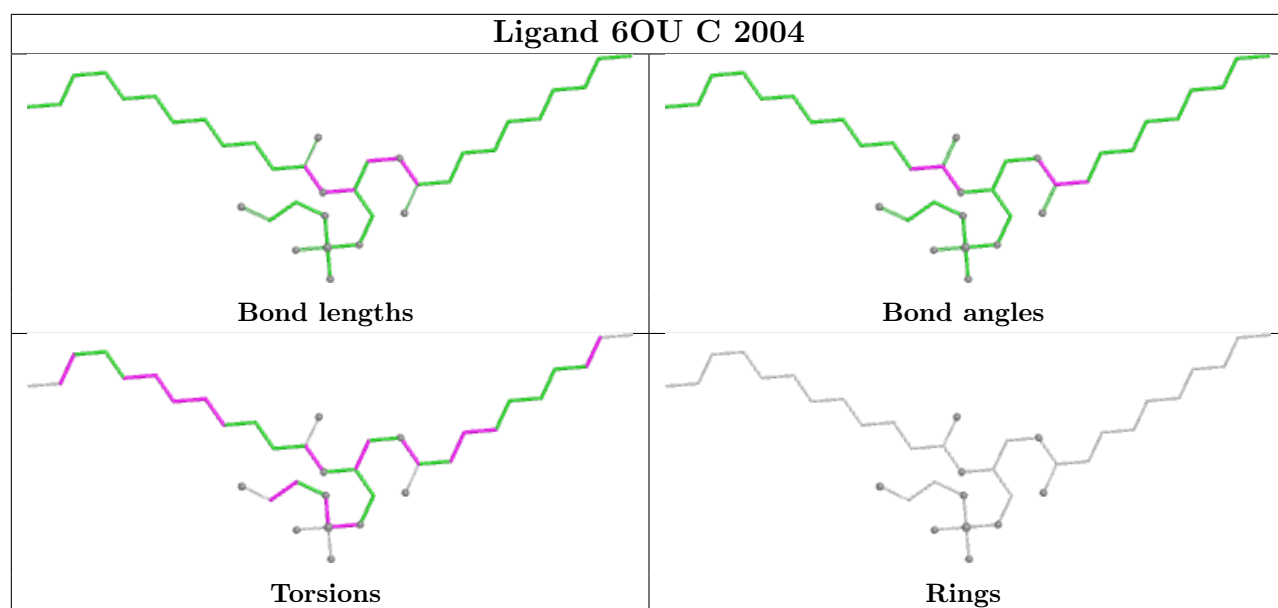
8 monomers are involved in 9 short contacts:

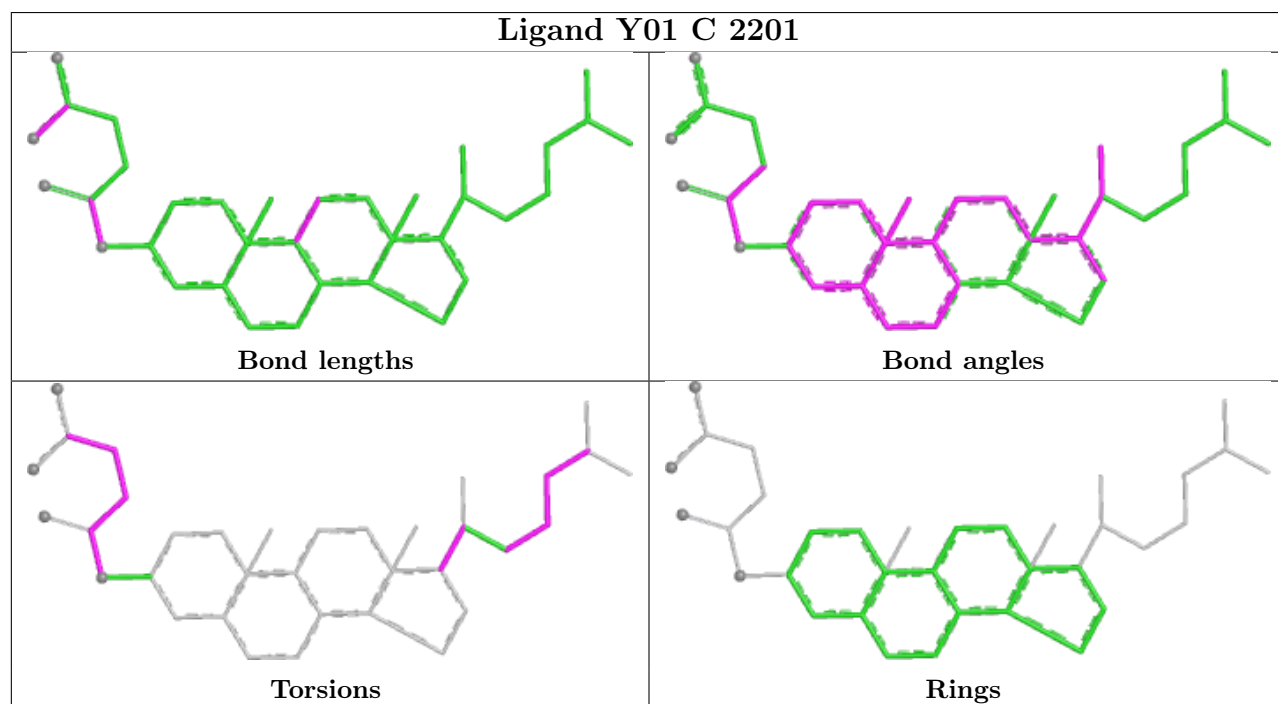
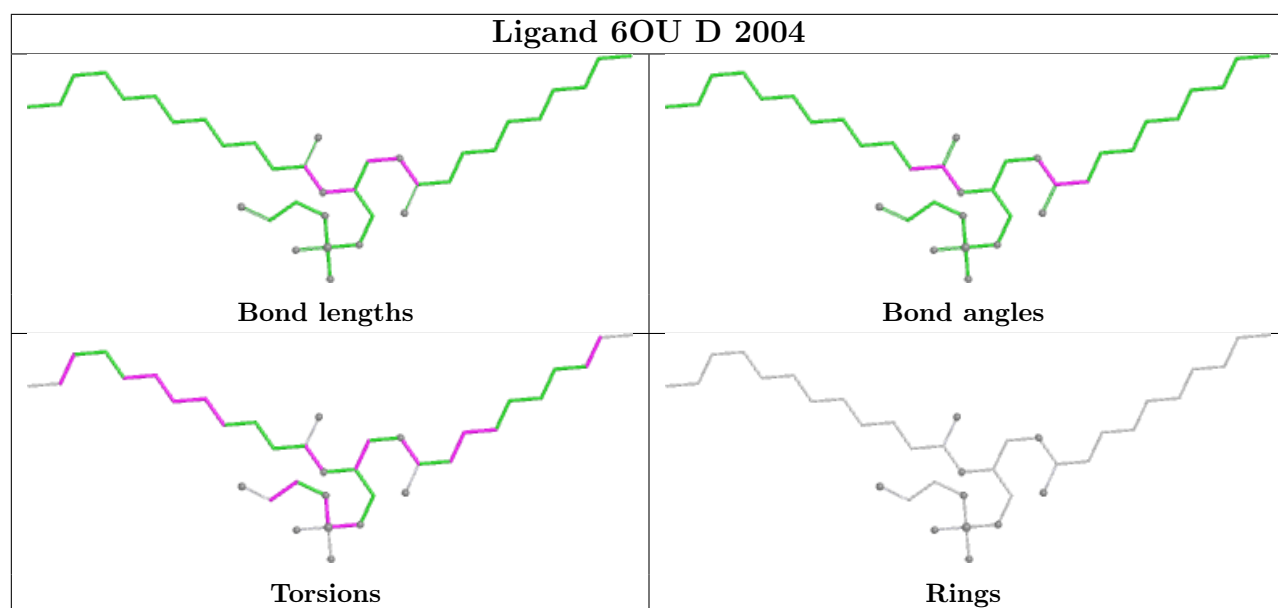
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	Y01	1	0
2	D	2002	Y01	1	0
2	C	2201	Y01	1	0
2	B	2201	Y01	1	0
2	A	2002	Y01	1	0
2	C	2002	Y01	1	0
2	D	2201	Y01	2	0
2	A	2201	Y01	1	0

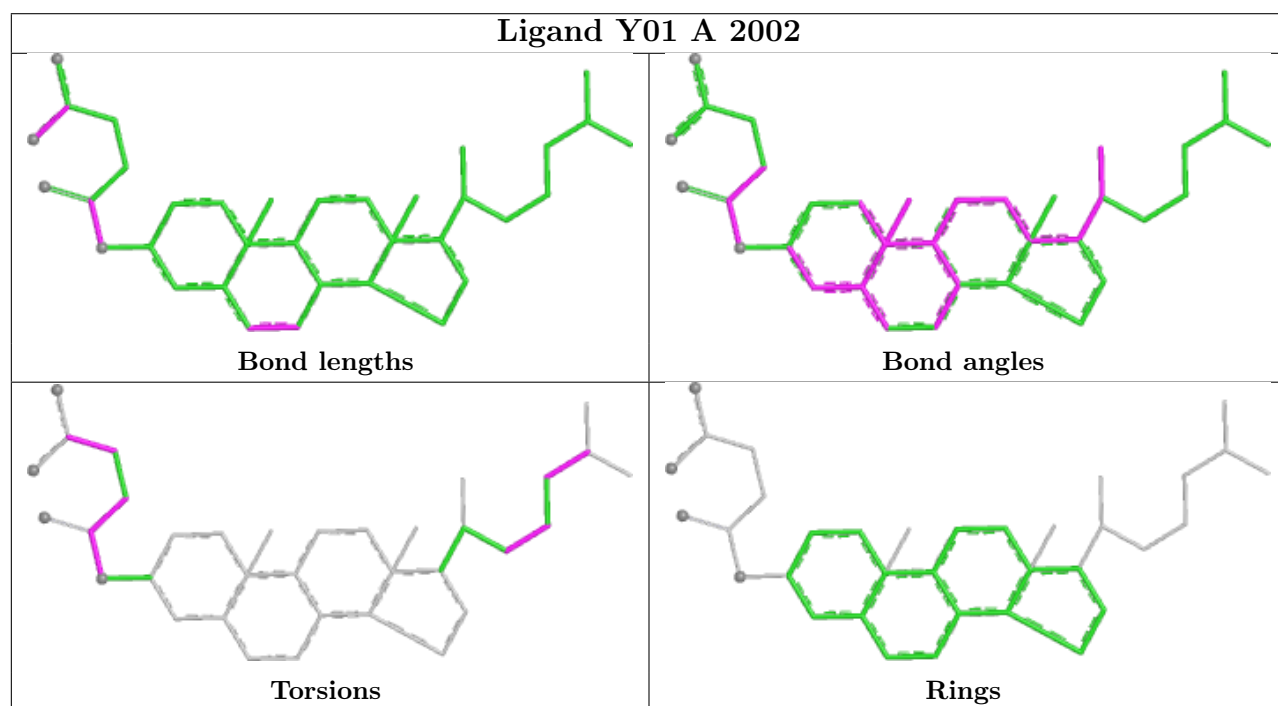
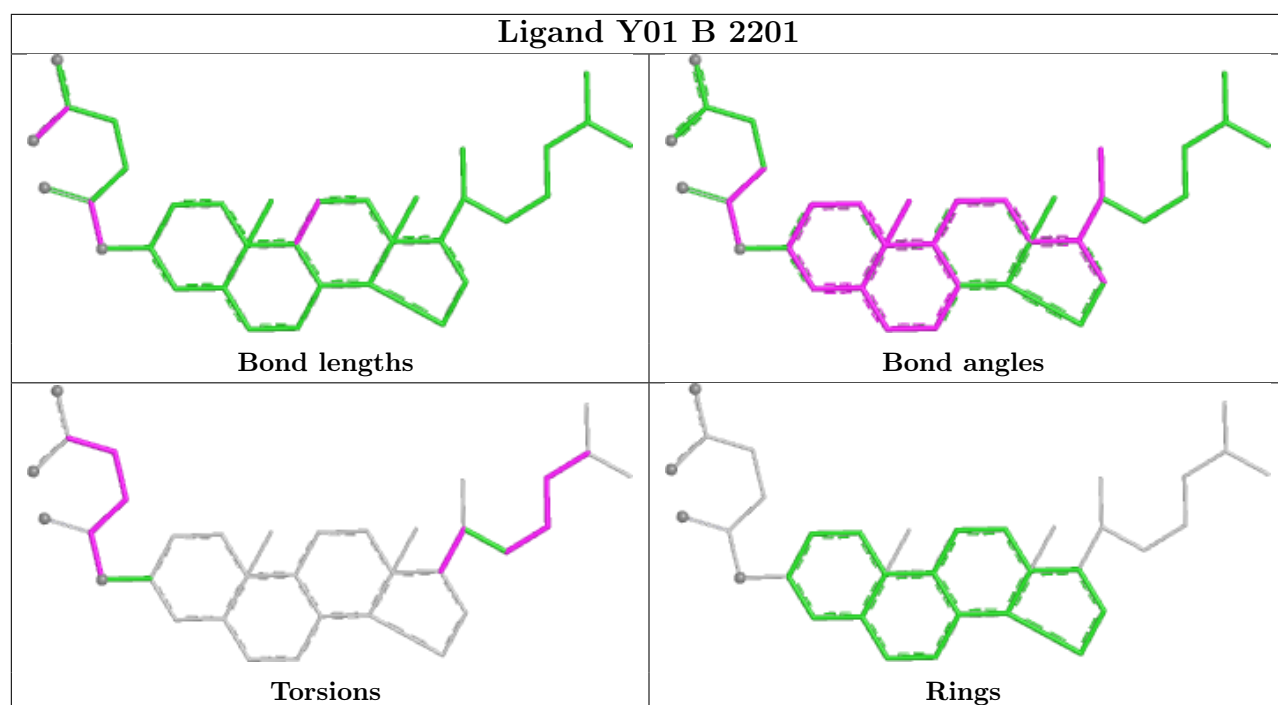
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

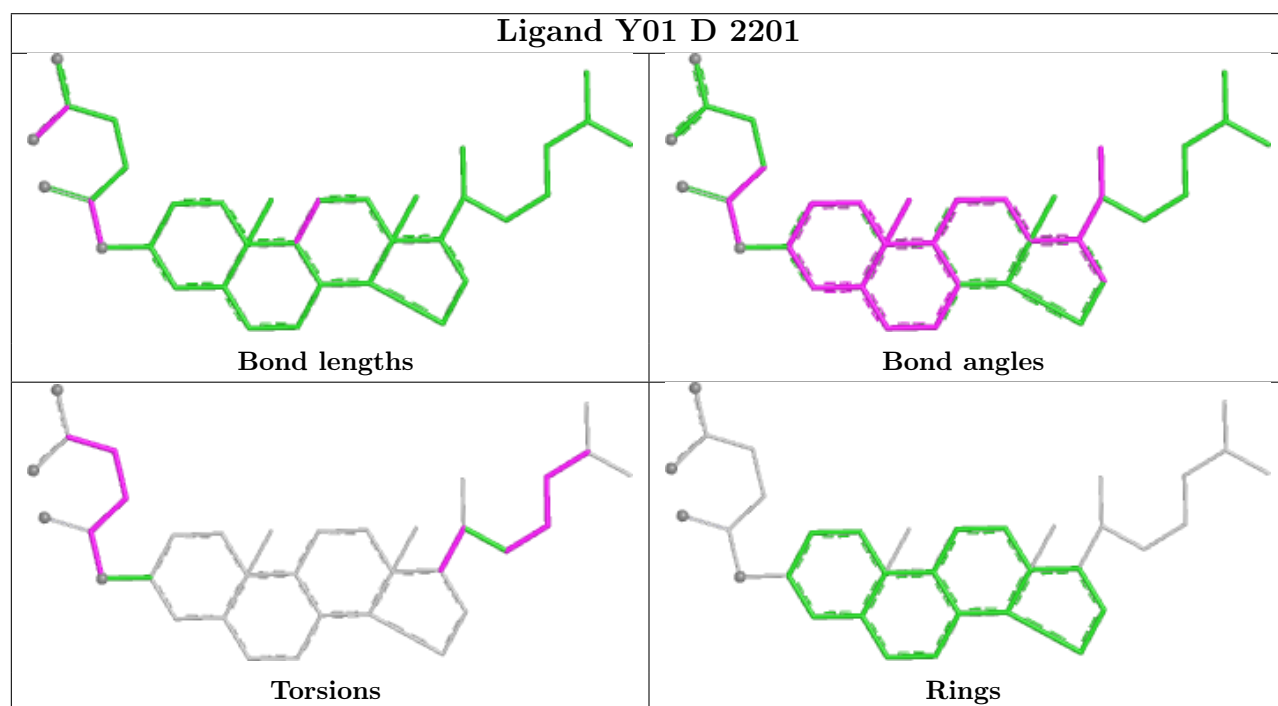
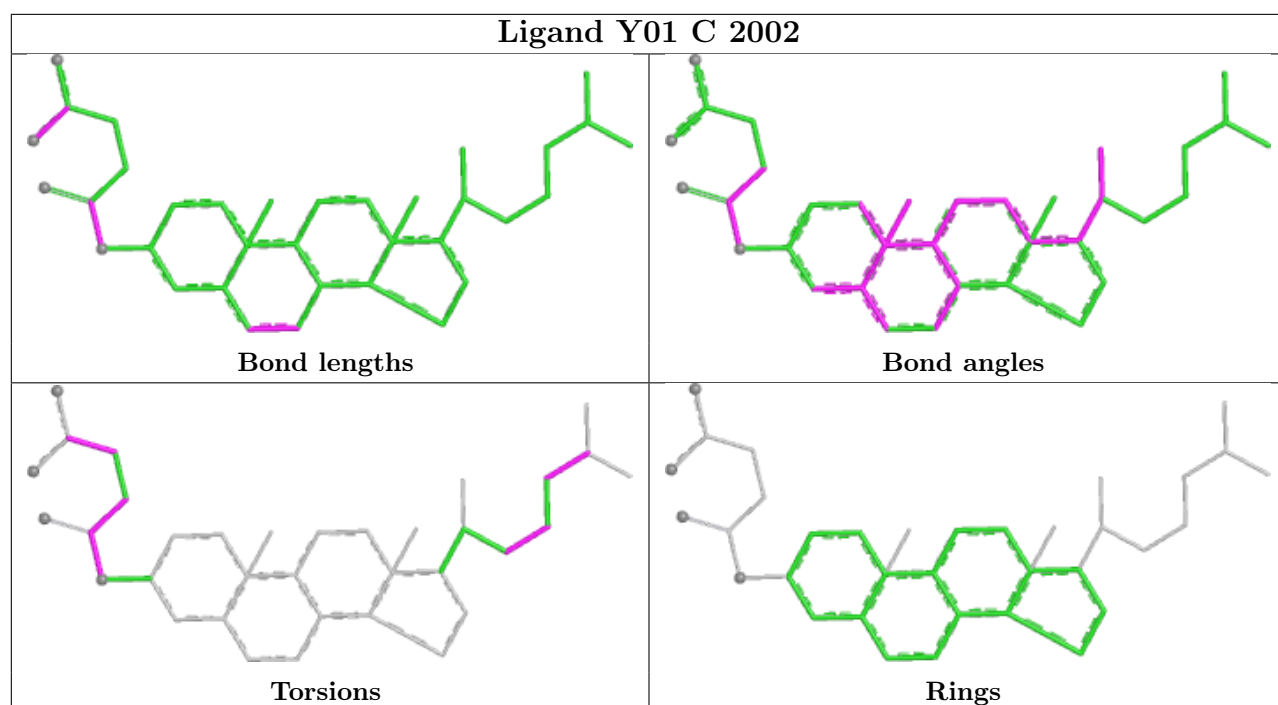


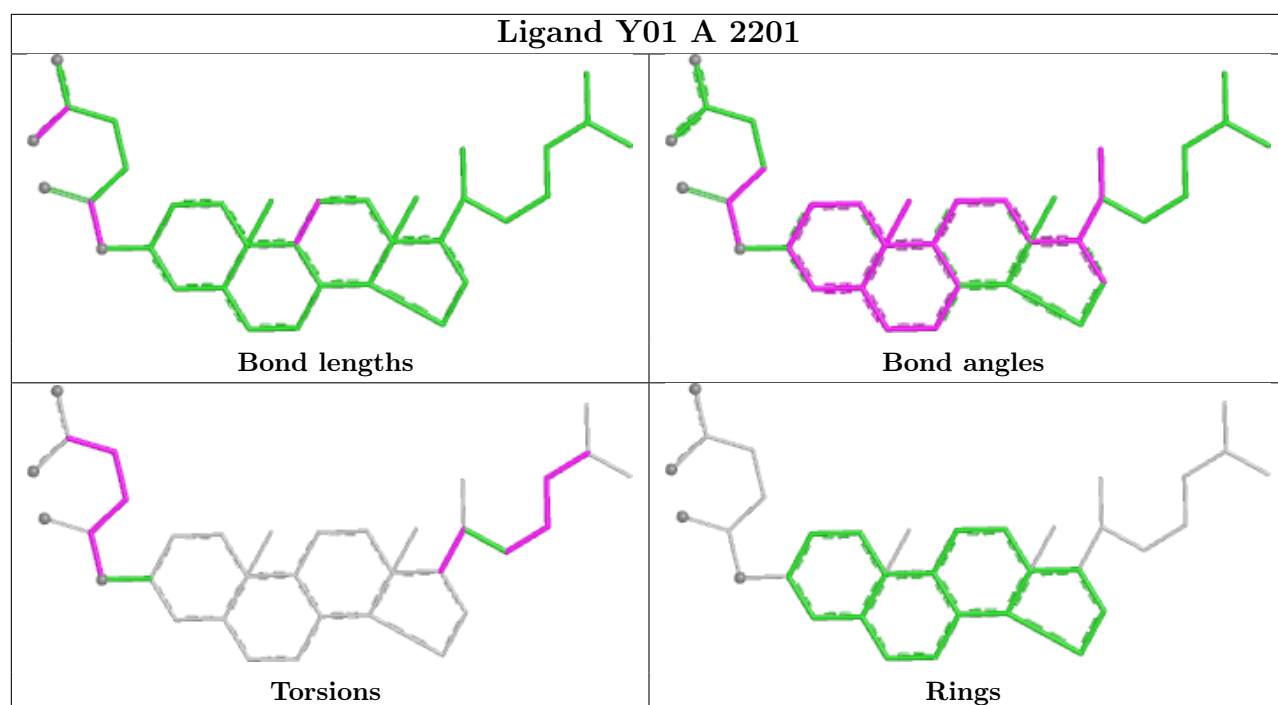












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



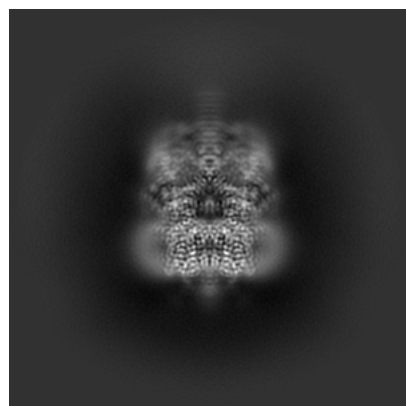
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44100. These allow visual inspection of the internal detail of the map and identification of artifacts.

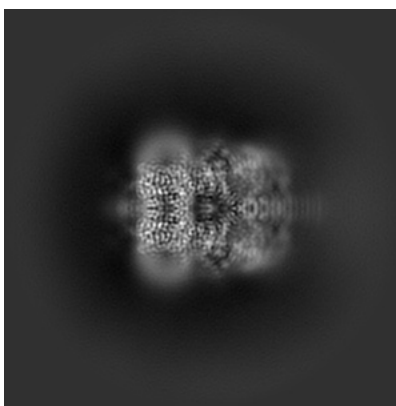
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

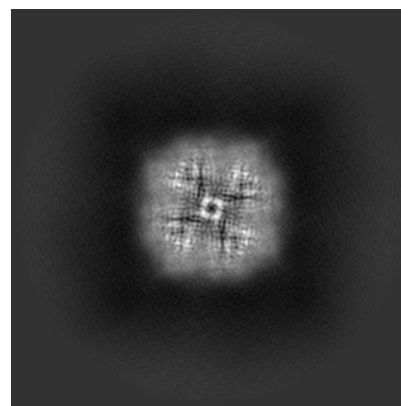
#### 6.1.1 Primary map



X

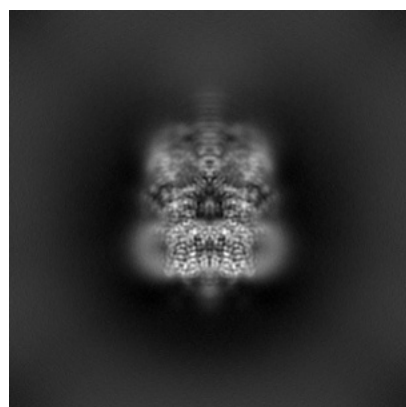


Y

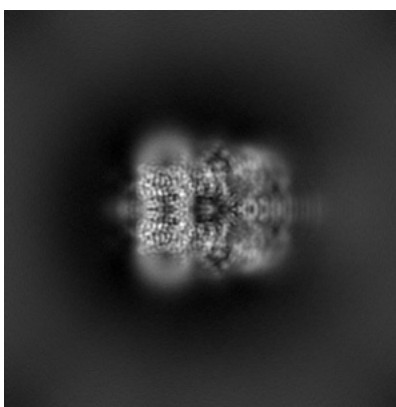


Z

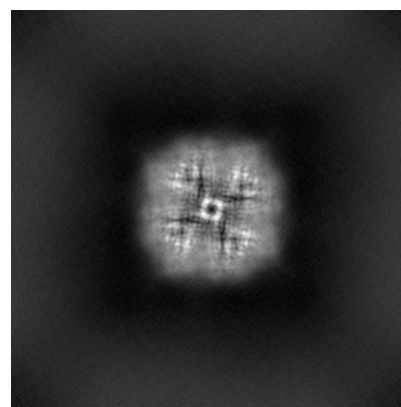
#### 6.1.2 Raw map



X



Y

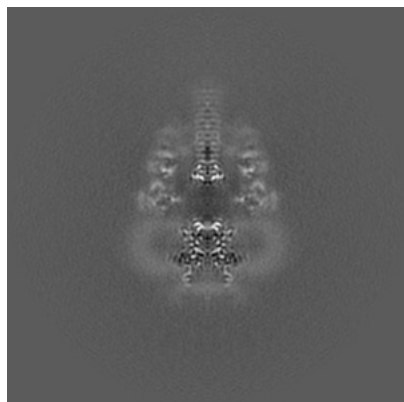


Z

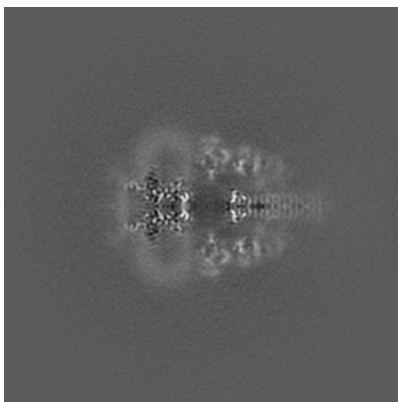
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

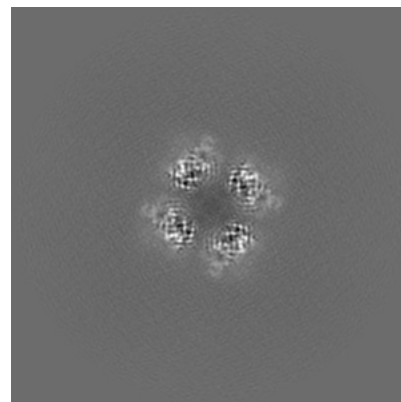
### 6.2.1 Primary map



X Index: 160

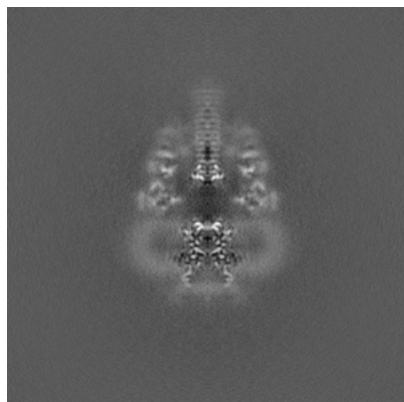


Y Index: 160

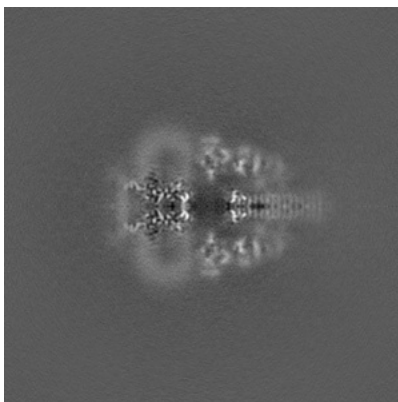


Z Index: 160

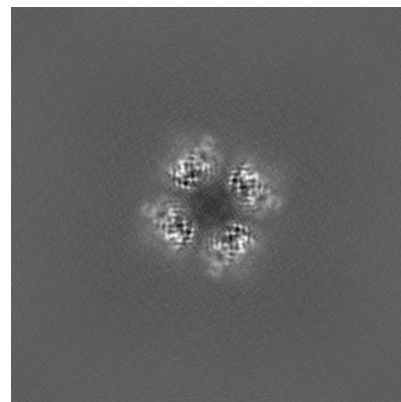
### 6.2.2 Raw map



X Index: 160



Y Index: 160

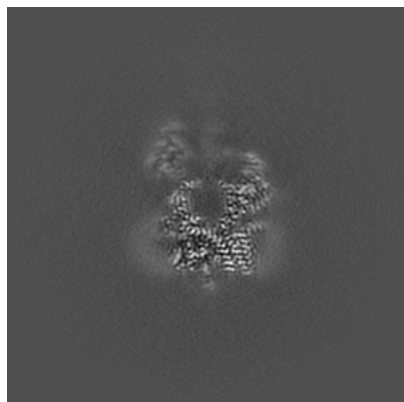


Z Index: 160

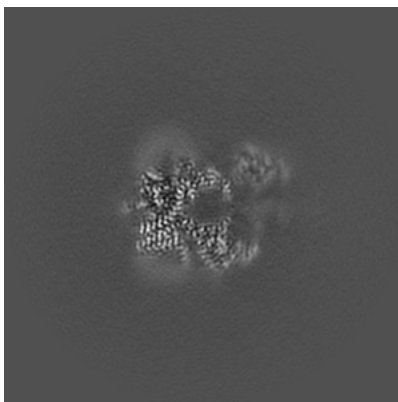
The images above show central slices of the map in three orthogonal directions.

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

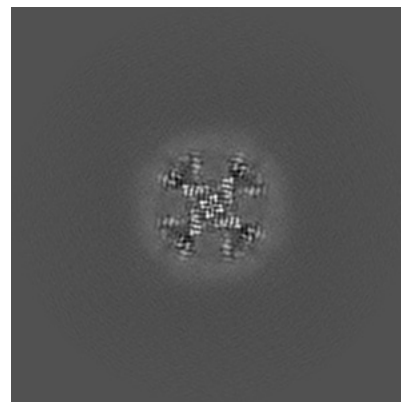
### 6.3.1 Primary map



X Index: 146

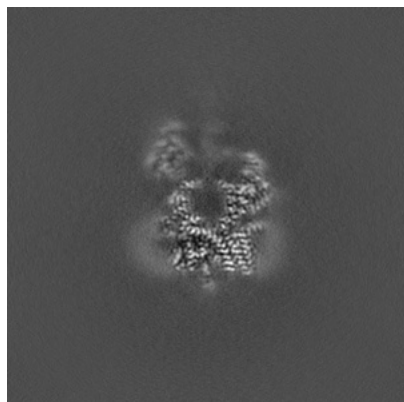


Y Index: 146

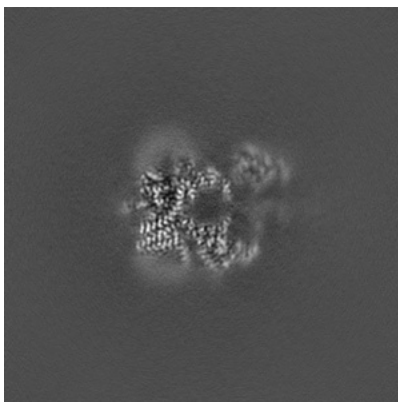


Z Index: 142

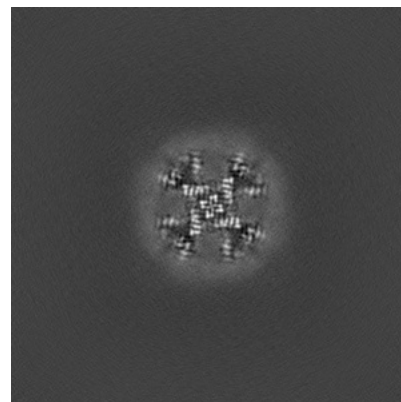
### 6.3.2 Raw map



X Index: 146



Y Index: 146

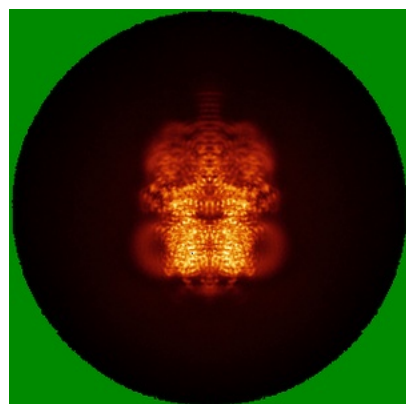


Z Index: 142

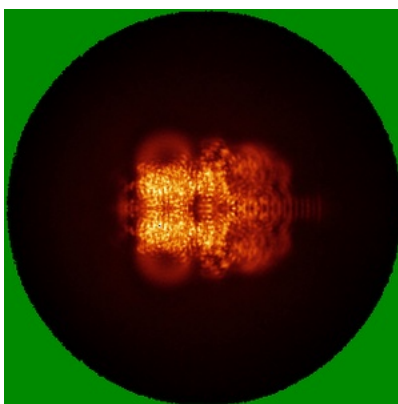
The images above show the largest variance slices of the map in three orthogonal directions.

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

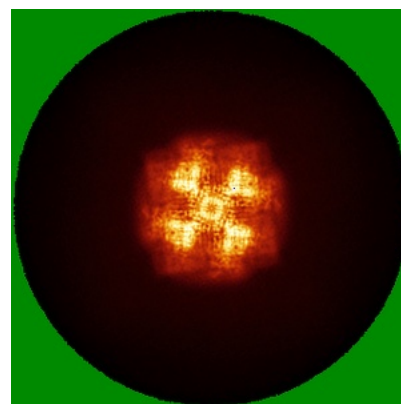
### 6.4.1 Primary map



X

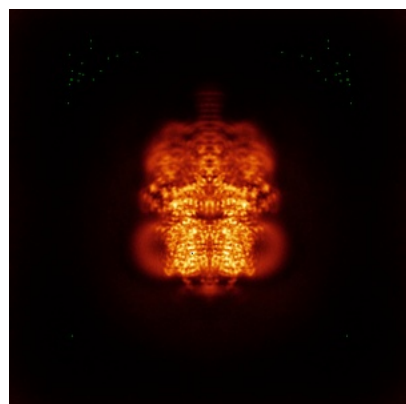


Y

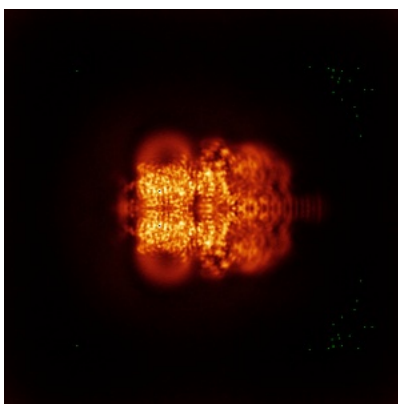


Z

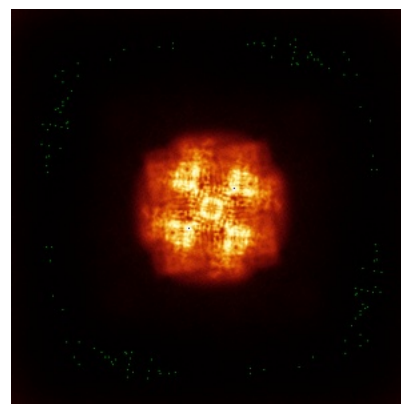
### 6.4.2 Raw map



X



Y

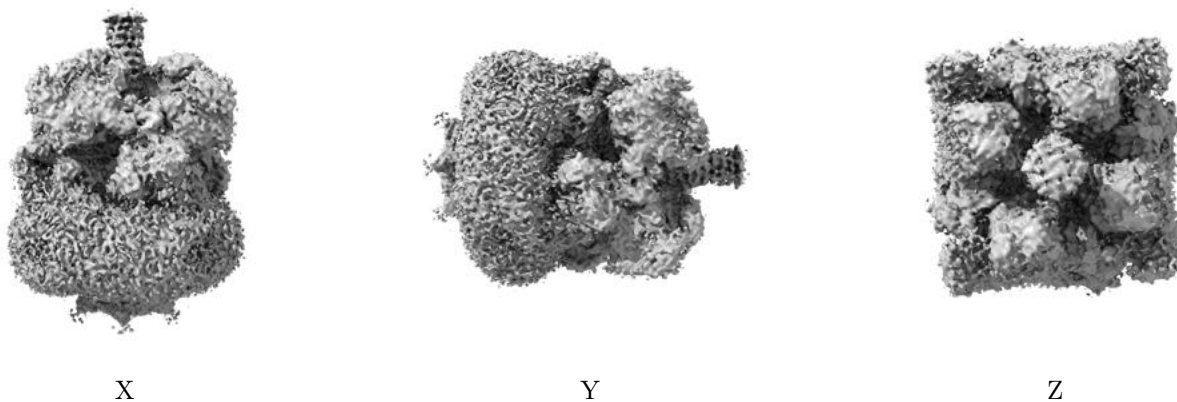


Z

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.

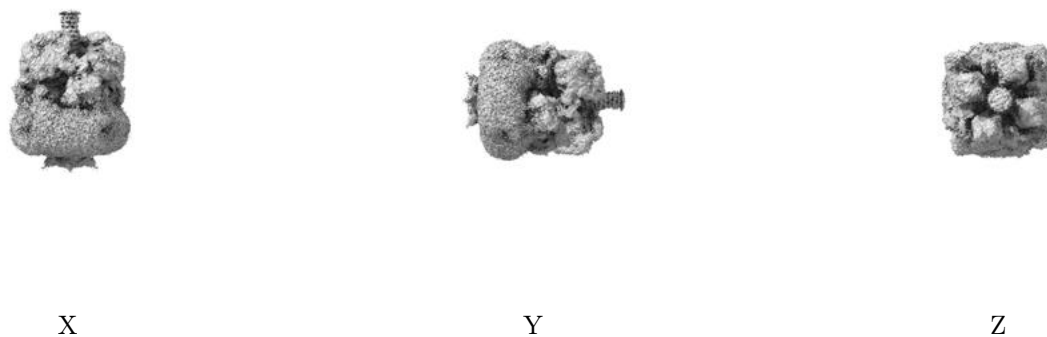
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

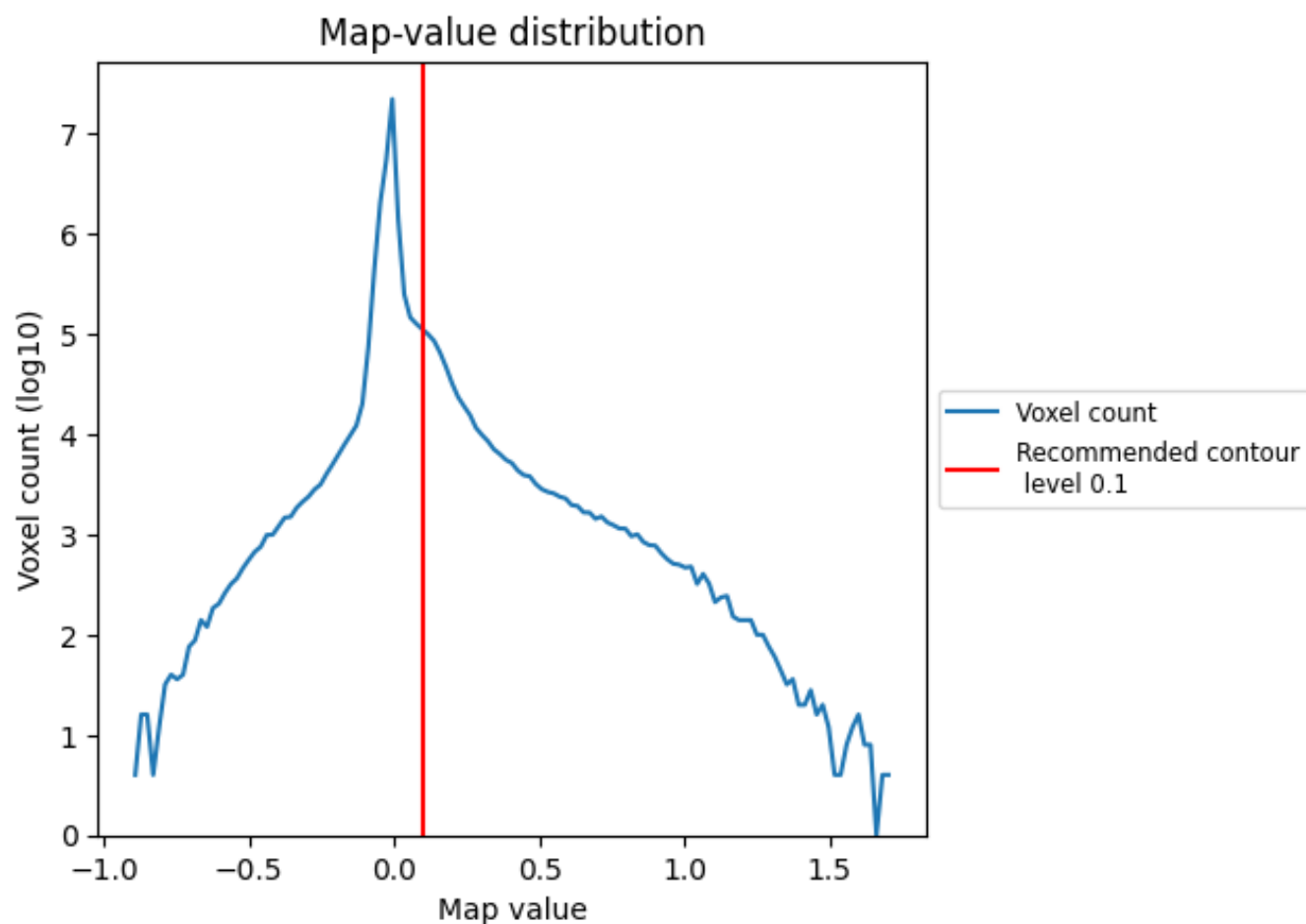
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

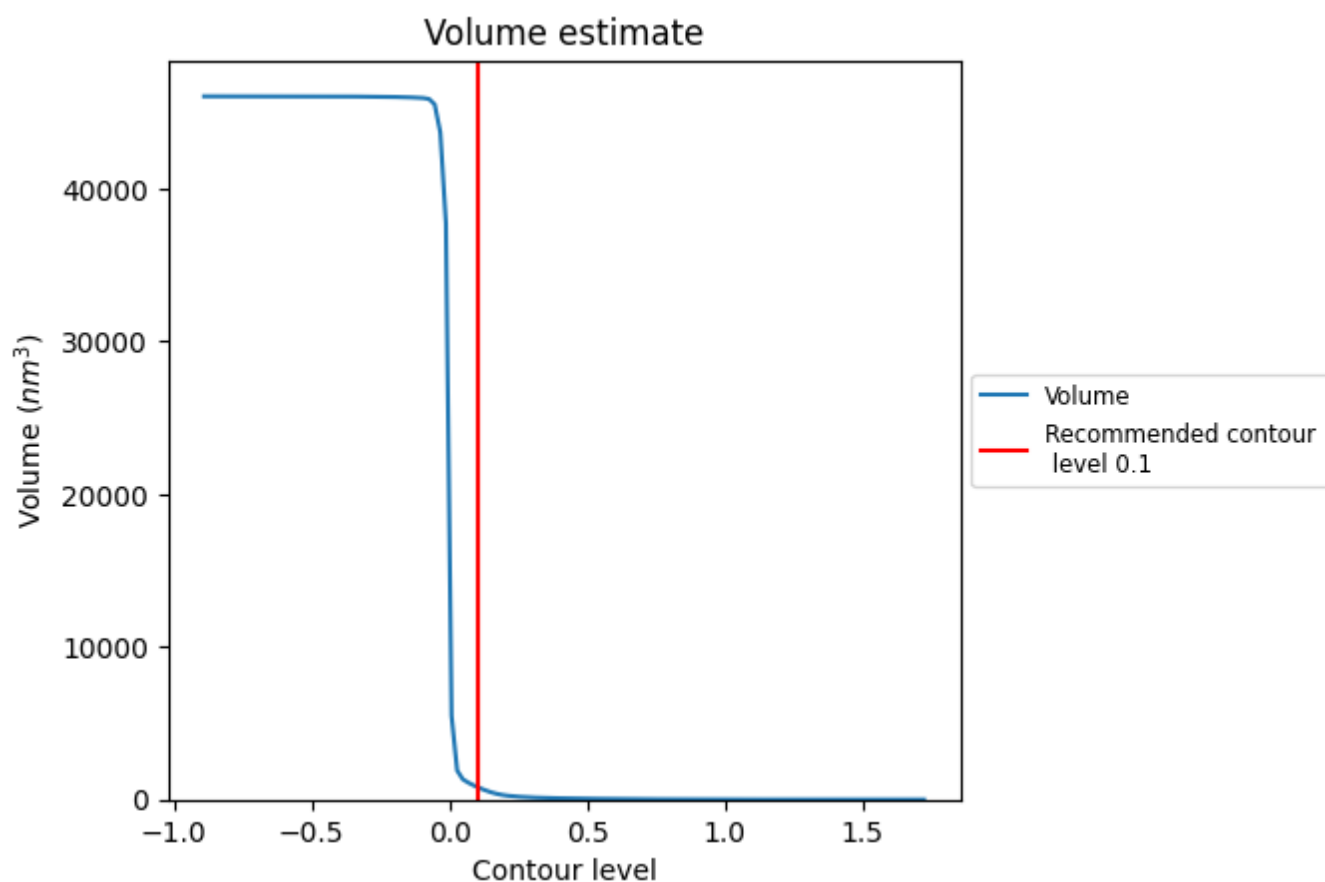
This section contains the results of statistical analysis of the map.

### 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.

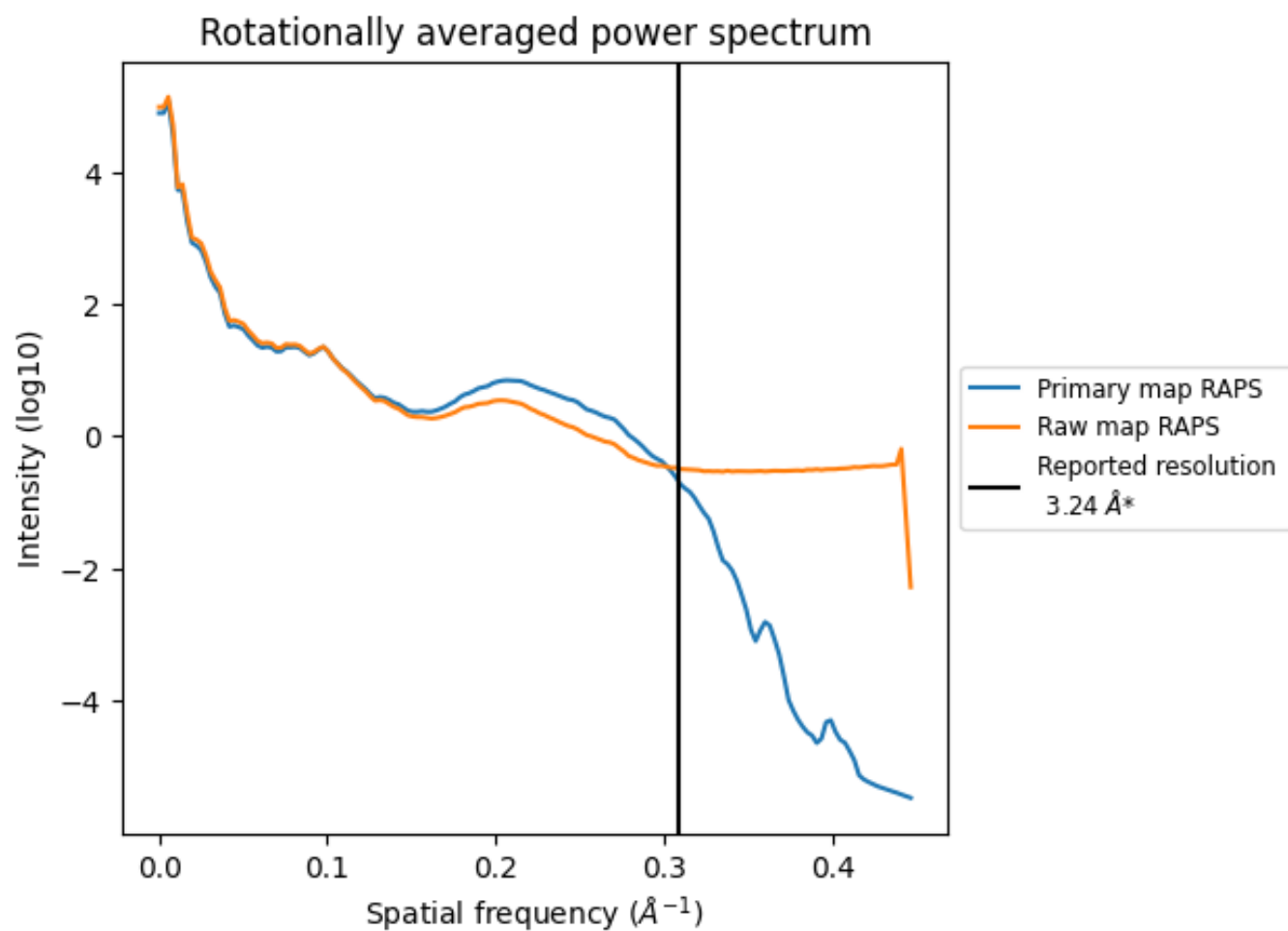
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 834 nm<sup>3</sup>; this corresponds to an approximate mass of 753 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 ⓘ



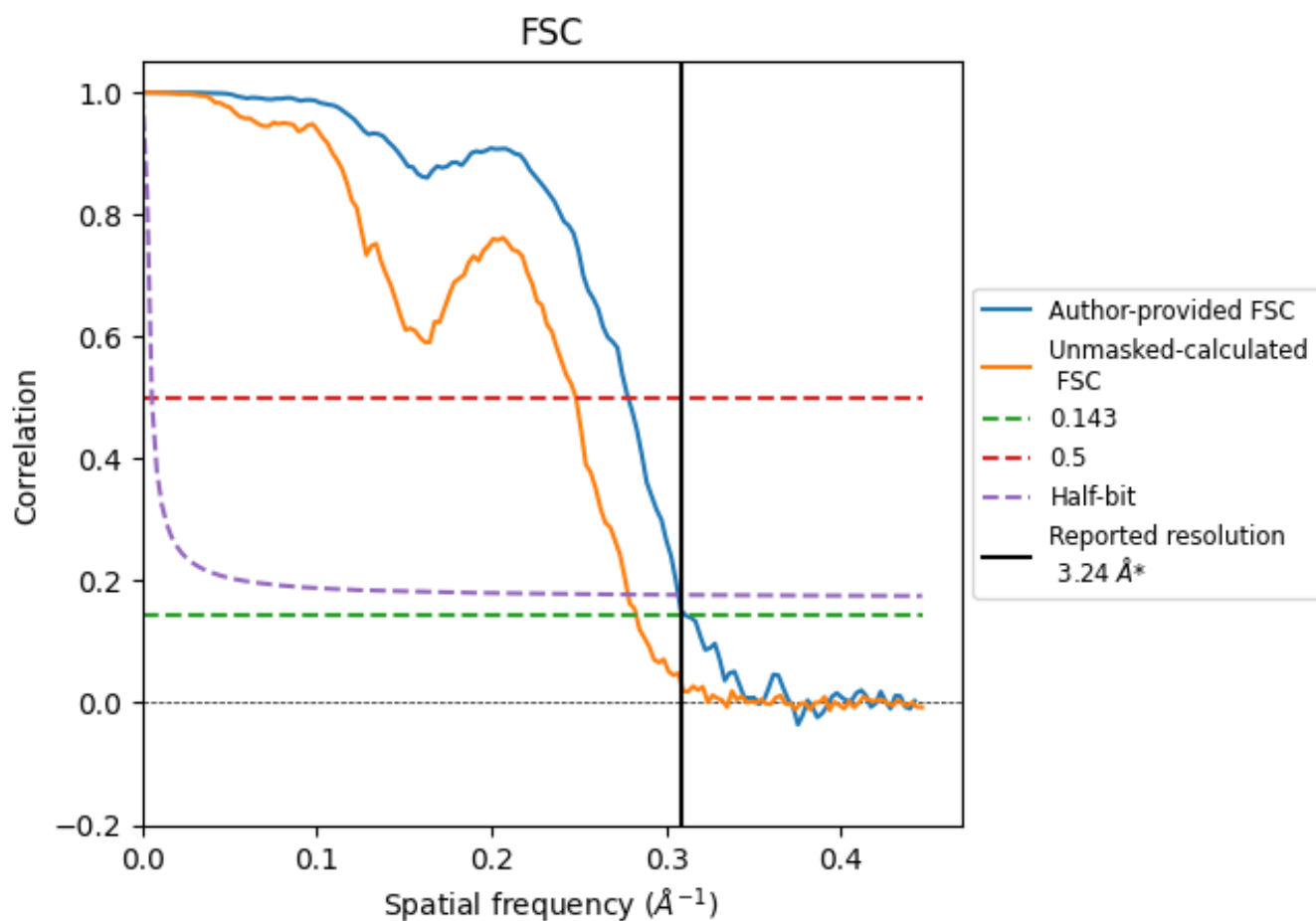
\*Reported resolution corresponds to spatial frequency of 0.309 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

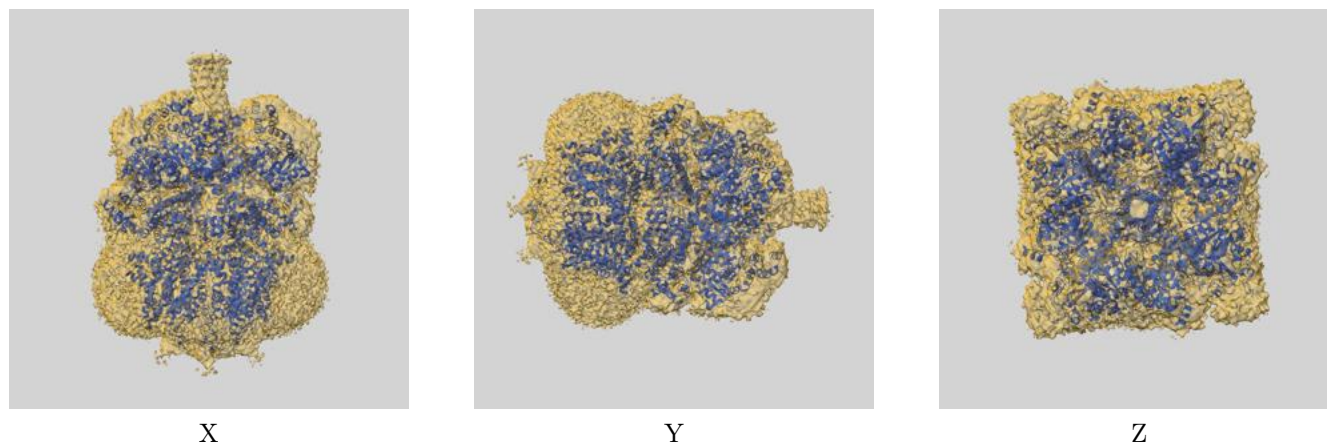
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.21	3.60	3.26
Unmasked-calculated*	3.54	4.03	3.60

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

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

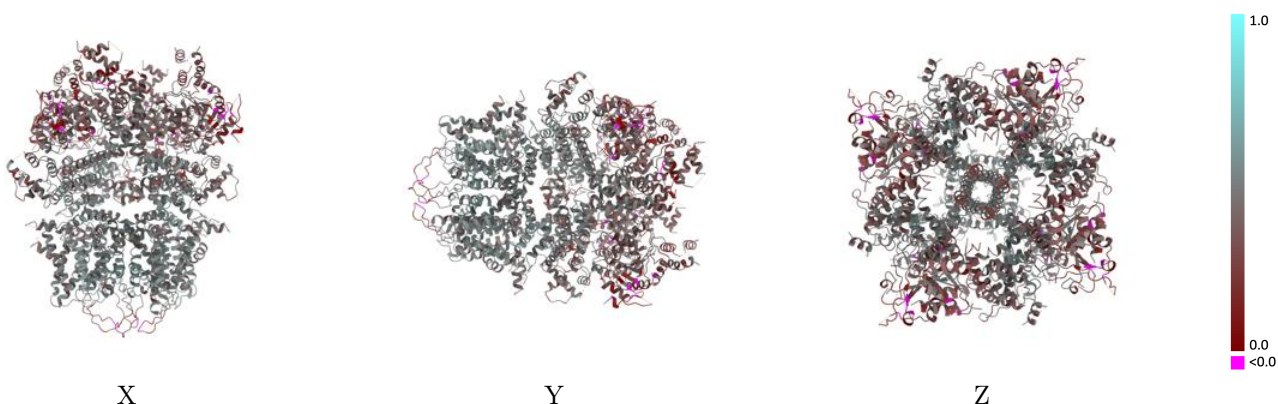
This section contains information regarding the fit between EMDB map EMD-44100 and PDB model 9B28. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



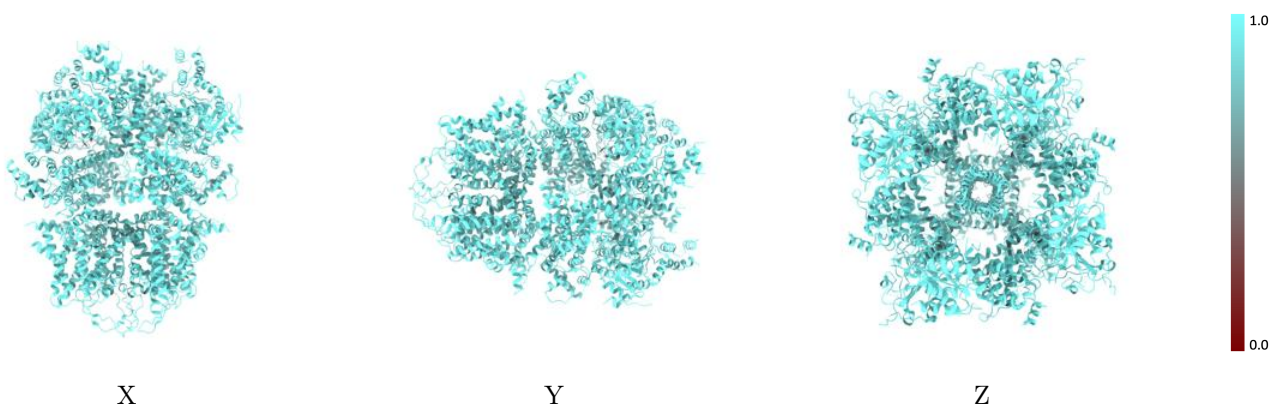
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



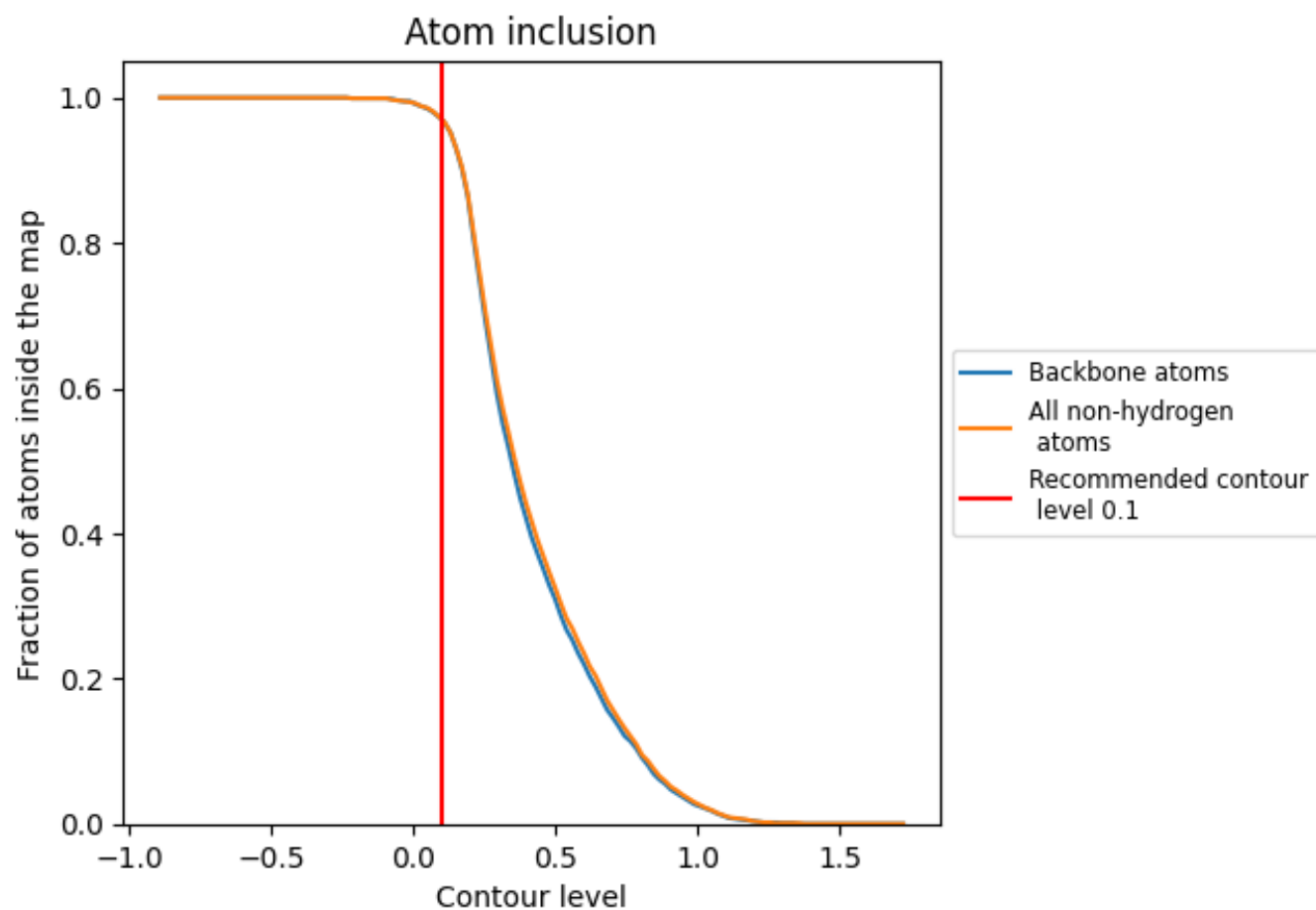
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9700	<div></div> 0.4380
A	<div></div> 0.9710	<div></div> 0.4380
B	<div></div> 0.9700	<div></div> 0.4380
C	<div></div> 0.9700	<div></div> 0.4380
D	<div></div> 0.9700	<div></div> 0.4370

