



wwPDB EM Validation Summary Report ⓘ

May 20, 2025 – 03:06 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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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.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

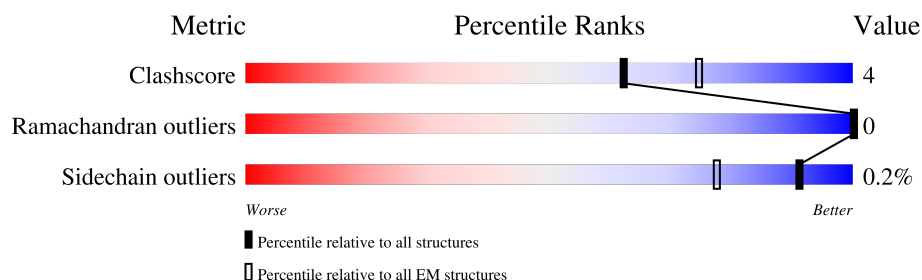
1 Overall quality at a glance

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 ≥ 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

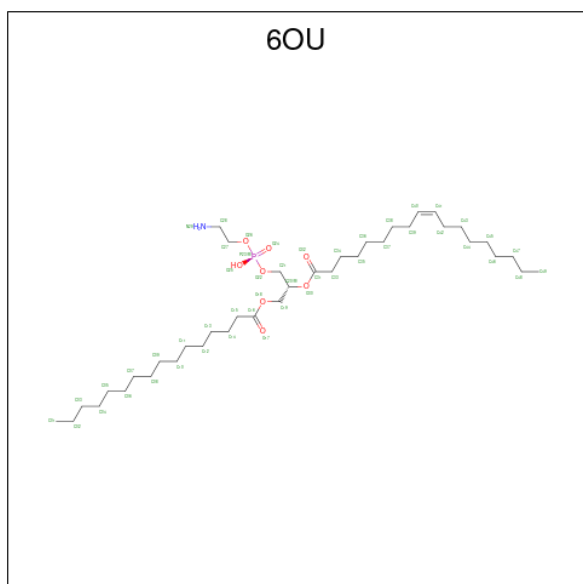
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 84	C 31	H 49	O 4	0
2	A	1	Total 84	C 31	H 49	O 4	0
2	C	1	Total 84	C 31	H 49	O 4	0
2	C	1	Total 84	C 31	H 49	O 4	0



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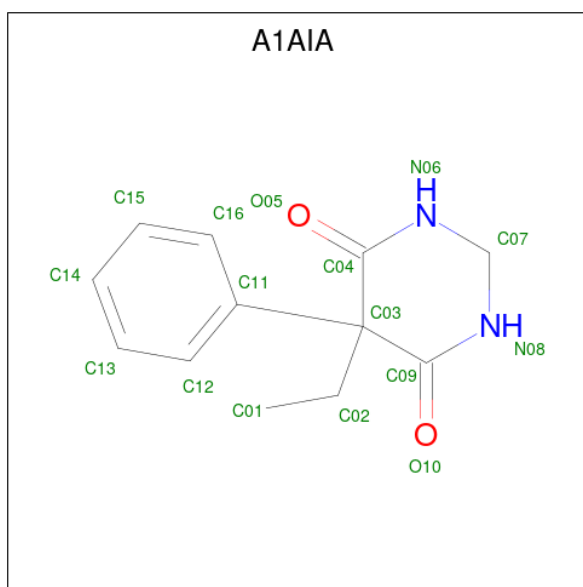
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	D	1	Total	C	H	O	0
			84	31	49	4	
2	D	1	Total	C	H	O	0
			84	31	49	4	

- 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: C₃₉H₇₆NO₈P).



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: C₁₂H₁₄N₂O₂).

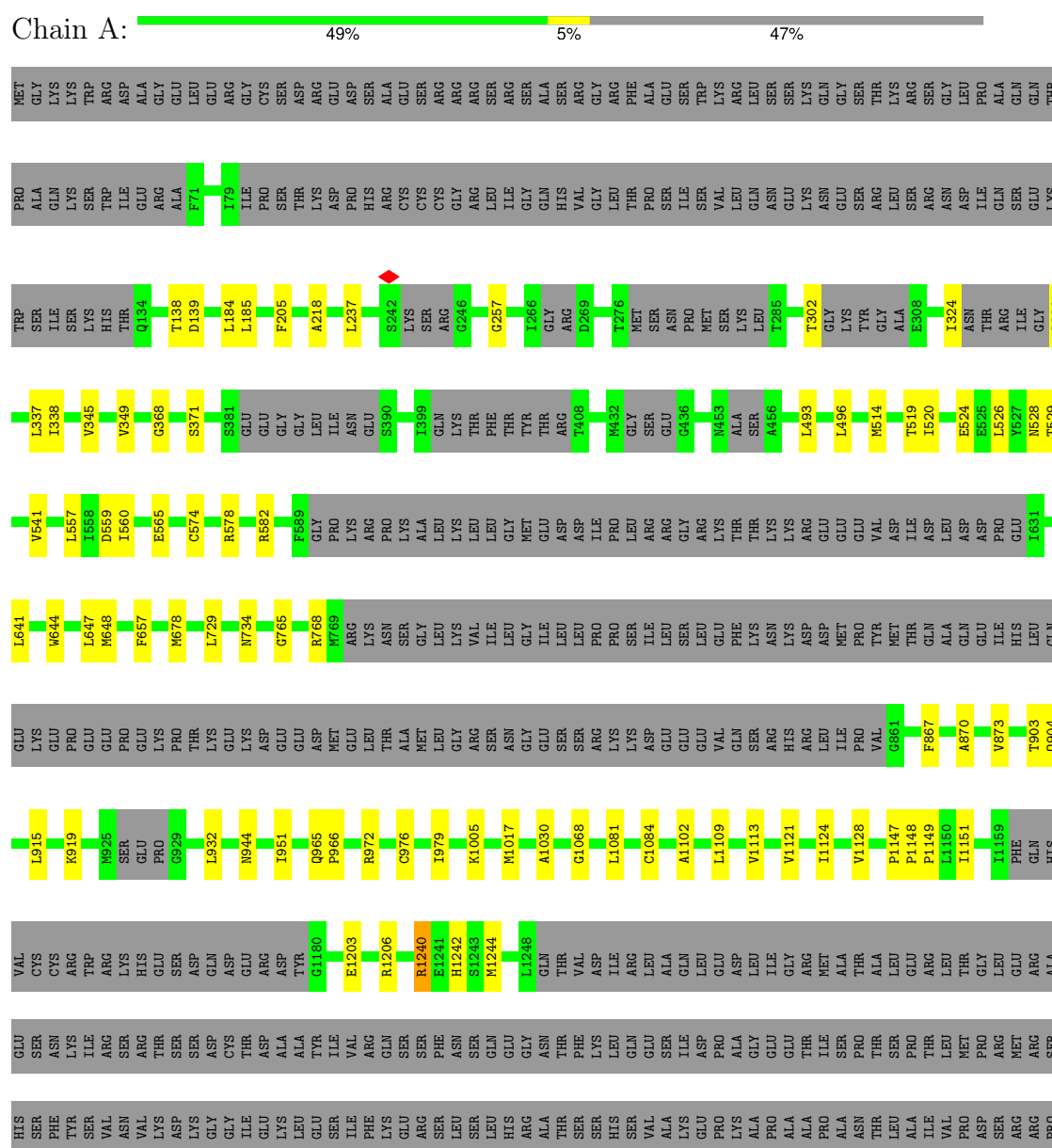


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			30	12	14	2	2	
4	C	1	Total	C	H	N	O	0
			30	12	14	2	2	
4	B	1	Total	C	H	N	O	0
			30	12	14	2	2	
4	D	1	Total	C	H	N	O	0
			30	12	14	2	2	

3 Residue-property plots

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

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



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

Chain C:



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	ARG	GLU	GLU	GLU	F657	L560	SER	LYS	LYS	TRP
SER	LYS	LYS	PRO	LYS	LYS	M678	E565	G368	HIS	TRP	ARG
ARG	HIS	GLU	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	GLU
ASP	ASP	GLN	N944	GLU	GLU	M734	R582	D139	THR	ALA	GLU
GLN	ASP	GLU	LYS	ASP	ASP	M734	R582	D139	THR	ALA	GLU
THR	THR	GLU	T951	GLU	GLU	G765	F589	GLY	THR	F71	LEU
ASP	ASP	GLU	Q965	GLU	GLU	G765	F589	GLY	THR	F71	LEU
ALA	ASP	ASP	P966	ASP	ASP	R768	R578	GLY	THR	F71	LEU
TYR	TYR	GLU	R972	GLU	GLU	M769	R578	ILE	THR	F71	LEU
ILE	ILE	LEU	R972	LEU	LEU	ARG	R582	ASN	THR	F71	LEU
VAL	VAL	THR	E1203	THR	THR	ASN	R582	GLU	THR	F71	LEU
ARG	ARG	GLN	C976	ALA	ALA	SER	R582	GLU	THR	F71	LEU
GLN	GLN	R1206	I979	MET	MET	GLY	R582	GLY	THR	F71	LEU
SER	SER	R1240	K1005	GLY	GLY	LYS	R582	GLY	THR	F71	LEU
PHE	PHE	I1241	H1242	ARG	ARG	VAL	R582	THR	THR	F71	LEU
ASN	ASN	S1243	M1017	SER	SER	ILE	R582	PHE	THR	F71	LEU
SER	SER	M1244	A1030	ASN	ASN	GLY	R582	THR	THR	F71	LEU
GLN	GLN	L1248	E1037	GLU	GLU	LEU	R582	THR	THR	F71	LEU
GLY	GLY	GLN	G1068	SER	SER	LEU	R582	ARG	THR	F71	LEU
ASN	ASN	THR	L1081	ARG	ARG	LEU	R582	ASP	THR	F71	LEU
THR	THR	VAL	C1084	GLU	GLU	LEU	R582	ASP	THR	F71	LEU
PHE	PHE	GLN	A1102	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
LYS	LYS	LEU	L1109	VAL	VAL	LEU	R582	GLY	THR	F71	LEU
ILE	ILE	GLU	V1113	SER	SER	LEU	R582	GLY	THR	F71	LEU
GLN	GLN	ASP	V1121	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
ALA	ALA	LEU	I1124	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
ASP	ASP	GLY	V1128	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
GLY	GLY	ILE	P1147	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
GLU	GLU	GLU	P1148	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
THR	THR	GLU	P1149	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
LEU	LEU	LEU	T1150	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
MET	MET	THR	T1151	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
PRO	PRO	GLY	T1159	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
ARG	ARG	LEU	PHE	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
MET	MET	GLU	GLN	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
ARG	ARG	ALA	HIS	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
SER	SER	THR	L915	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
THR	THR	GLU	HIS	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
GLN	GLN	VAL	VAL	GLU	GLU	LEU	R582	GLY	THR	F71	LEU
THR	THR	THR	THR	GLU	GLU	LEU	R582	GLY	THR	F71	LEU

[illegible]

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

Chain B:  49% 1% 50%

[illegible]

SER	PHE	GLU	CYS	HIS	PHE	GLU	ASP	TRP
GLU	GLU	GLU	CYS	SER	GLU	ASP	ILE	ARG
ASN	ASN	ASN	PRO	PHE	LEU	TYR	ASN	LYS
VAL	VAL	VAL	GLU	PHE	THR	SER	THR	HIS
HIS	PRO	ARG	GLU	SER	MET	SER	SER	GLU
ASN	TYR	GLU	GLU	PRO	ASP	ASP	ASP	SER
SER	ALA	ALA	ALA	SER	ASP	GLY	GLN	ASN
ASN	HIS	GLU	LEU	ARG	THR	ILE	ASP	ASP
SER	THR	LEU	SER	TYR	SER	THR	THR	GLU
LEU	ARG	LEU	SER	TYR	PHE	GLU	ALA	ARG
GLU	LYS	HIS	PRO	TYR	ASP	LYS	ALA	ASP
VAL	SER	PRO	SER	ALA	ILE	GLU	TYR	TYR
LEU	PHE	ASN	SER	ASN	SER	ILE	GLU	ILE
LEU	ASN	SER	SER	PHE	ASP	GLU	SER	ILE
PHE	ILE	ILE	ASP	GLY	THR	PRO	VAL	ARG
GLN	GLY	GLY	SER	VAL	THR	PHE	ARG	GLN
PRO	ASP	ASP	GLU	PRO	HIS	GLU	SER	GLN
ASP	LYS	LYS	GLU	VAL	VAL	LEU	ASN	GLY
TYR	LEU	LEU	ASN	LYS	PRO	PRO	GLU	ASN
LYS	ASP	ASP	GLU	THR	THR	GLY	ARG	ASN
ALA	ALA	ALA	ARG	ILE	ASP	GLY	ALA	GLY
HIS	SER	SER	ALA	THR	THR	THR	THR	THR
HIS	LEU	ASN	ASN	ASP	ASP	PRO	SER	VAL
HIS	ARG	ASN	PRO	CYS	ILE	PRO	LYS	ASP
HIS	ASN	ILE	ILE	ASP	THR	SER	THR	ILE
HIS	PRO	SER	SER	THR	THR	THR	ALA	ARG
HIS	PHE	GLN	GLN	ARG	CYS	THR	LEU	LEU
HIS	ARG	ALA	ALA	VAL	VAL	ILE	PRO	GLU
HIS	SER	LYS	GLU	ASN	ASN	GLU	SER	GLU
HIS	SER	SER	ASN	ALA	ALA	THR	LYS	ASP
HIS	SER	LYS	ASP	PRO	GLN	THR	ALA	LEU
HIS	PRO	PRO	THR	ILE	THR	SER	GLY	ILE
HIS	GLY	LEU	THR	THR	PHE	LEU	THR	GLY
HIS	MET	MET	VAL	PRO	PRO	VAL	THR	THR
HIS	ARG	ARG	LYS	GLY	LEU	THR	LEU	LEU
HIS	ARG	LEU	ILE	LEU	LEU	ASP	PRO	MET
HIS	LEU	GLU	GLU	GLY	GLU	ASP	PRO	GLY
HIS	SER	SER	ARG	ASP	GLU	PRO	ARG	GLU
HIS	ARG	ARG	ALA	LYS	VAL	PRO	ARG	ARG
HIS	THR	THR	ASN	VAL	ALA	PRO	PRO	ALA
HIS	SER	SER	SER	GLU	ILE	SER	SER	GLU
HIS	ALA	ALA	TYR	ASP	THR	LEU	THR	SER
HIS	PHE	PHE	LEU	LEU	VAL	THR	PHE	ASN
HIS	SER	SER	ALA	SER	ILE	LYS	GLY	LYS

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

Continued on next page...

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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.

The worst 5 of 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

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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y01	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

The worst 5 of 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 172 torsion outliers are listed below:

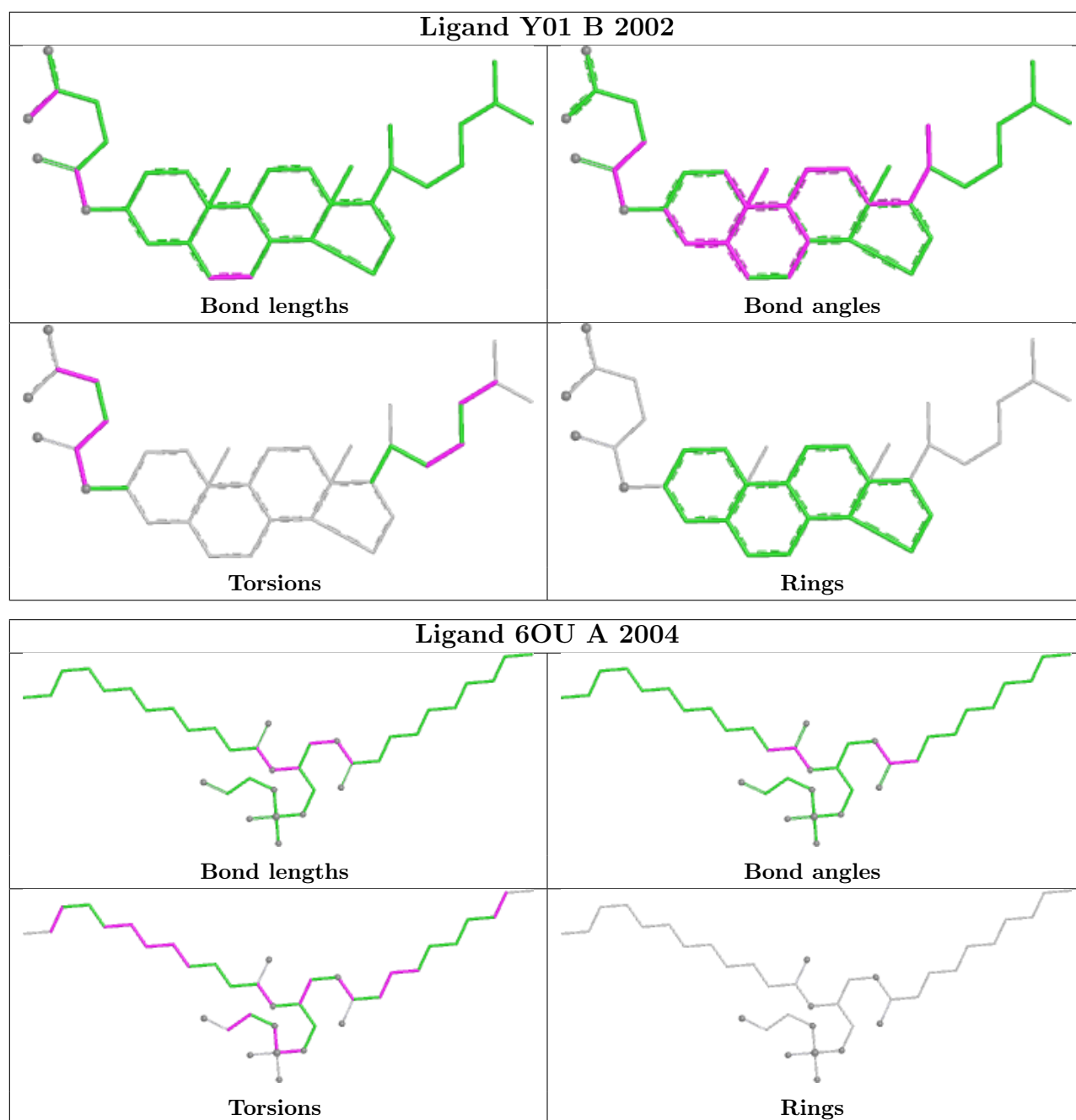
Mol	Chain	Res	Type	Atoms
3	A	2004	6OU	C21-O22-P23-O24
3	A	2004	6OU	C21-O22-P23-O26
3	A	2004	6OU	O26-C27-C28-N29
3	A	2004	6OU	O32-C31-O30-C20
3	C	2004	6OU	C21-O22-P23-O24

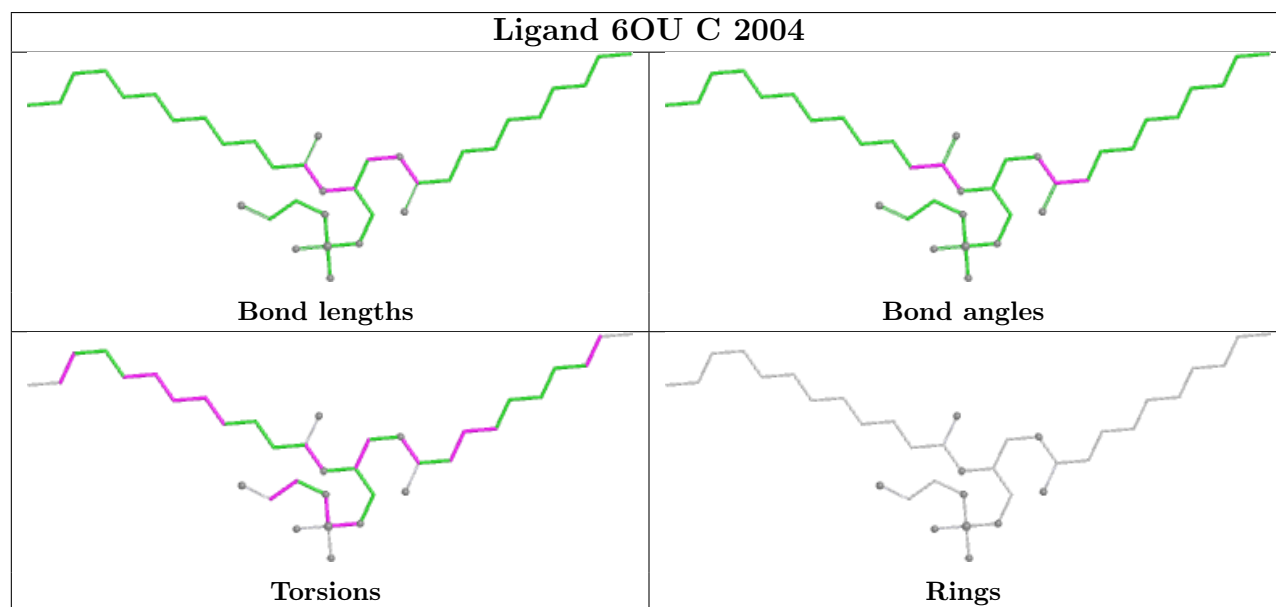
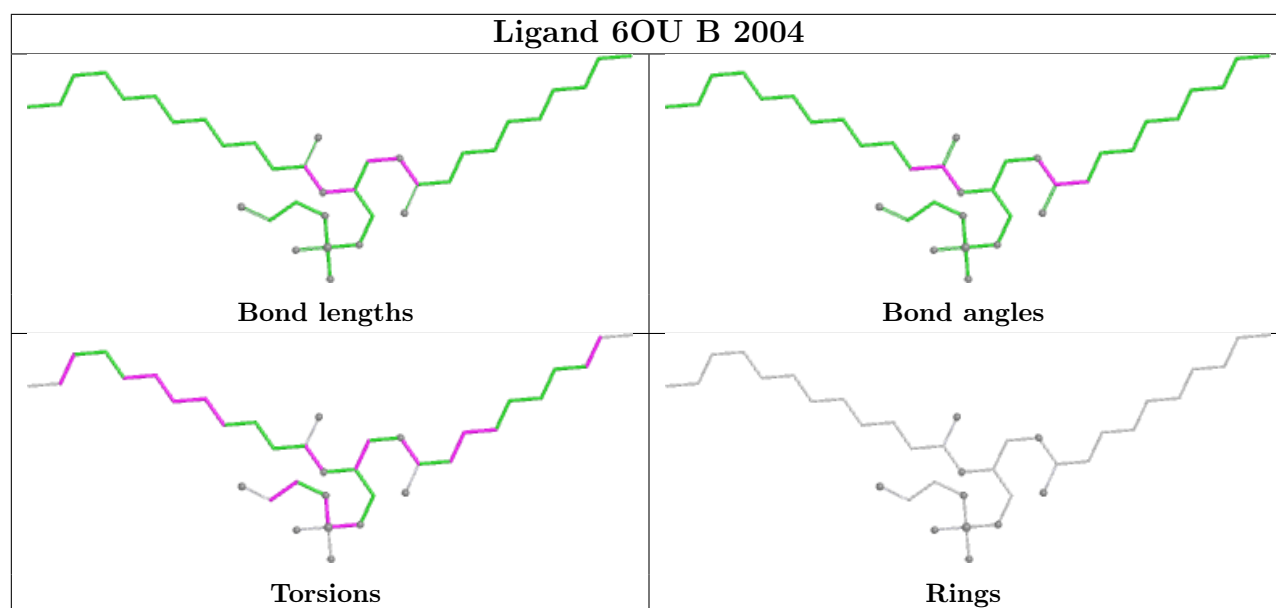
There are no ring outliers.

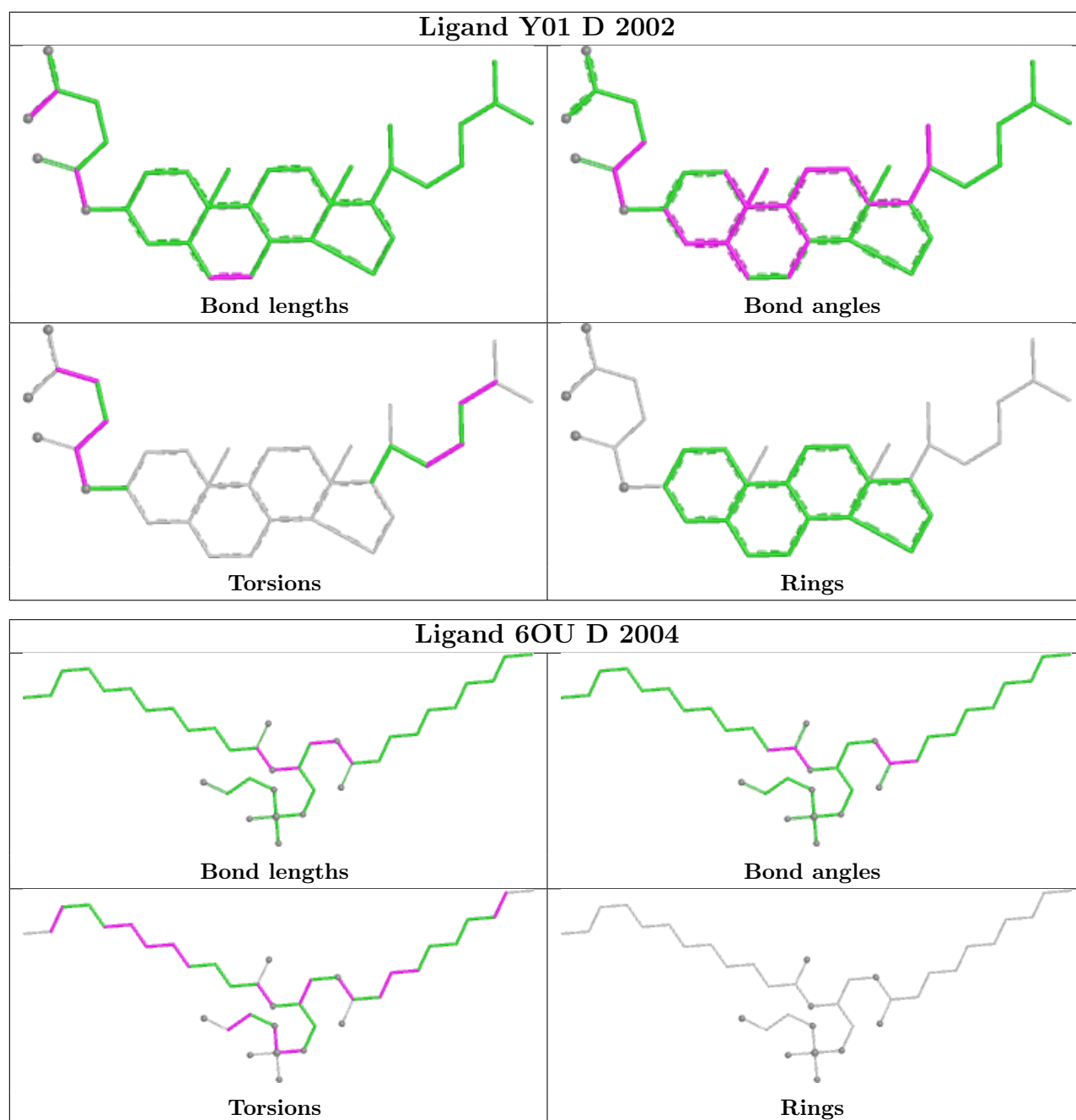
8 monomers are involved in 9 short contacts:

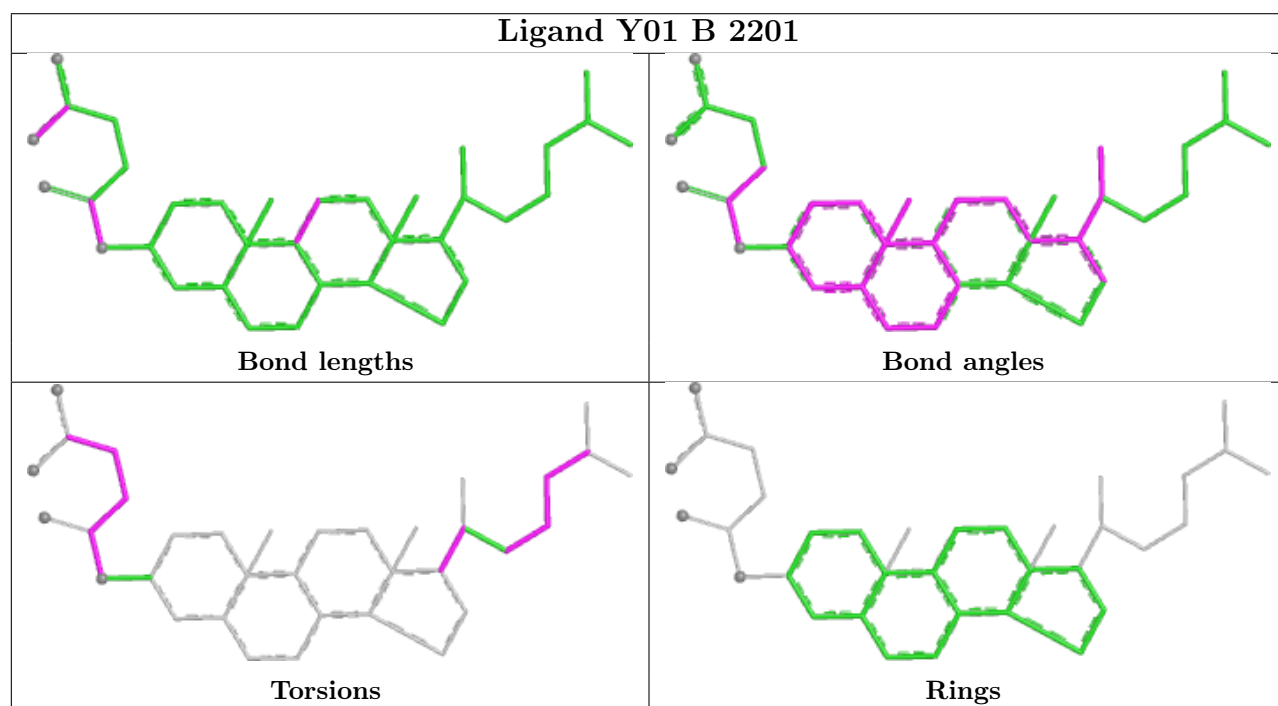
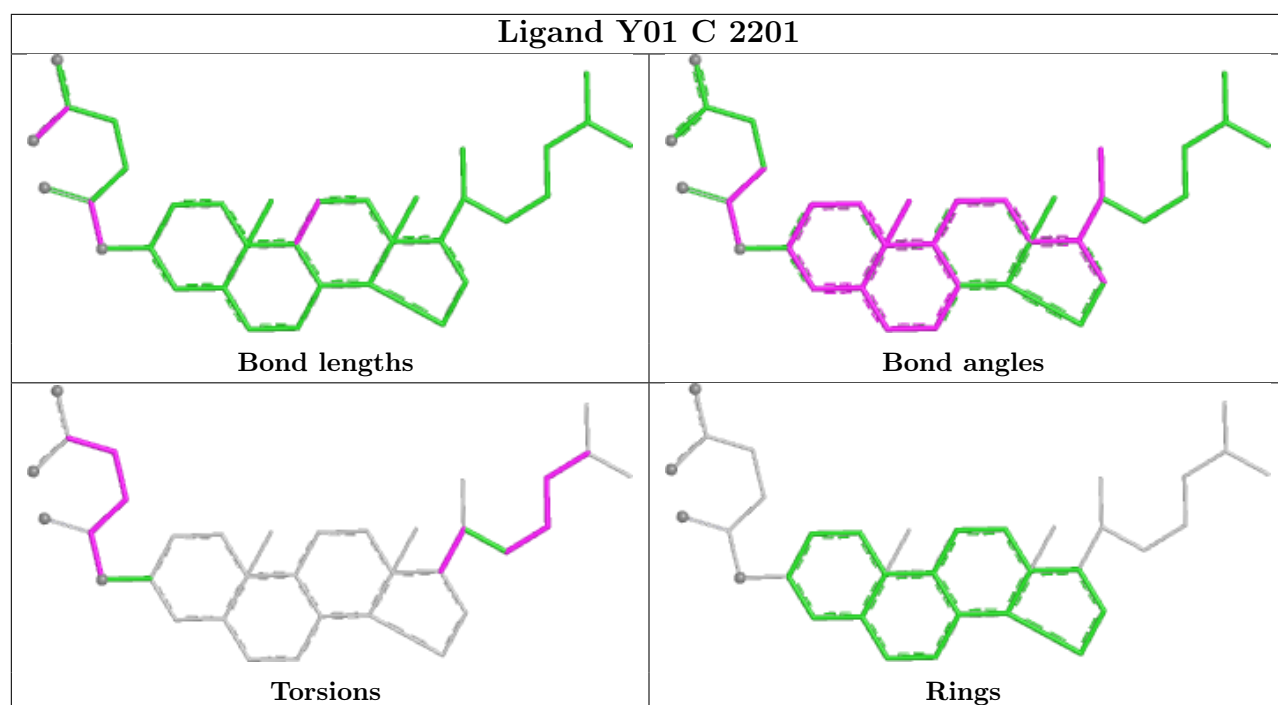
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	Y01	1	0
2	D	2002	Y01	1	0
2	C	2201	Y01	1	0
2	B	2201	Y01	1	0
2	A	2002	Y01	1	0
2	C	2002	Y01	1	0
2	D	2201	Y01	2	0
2	A	2201	Y01	1	0

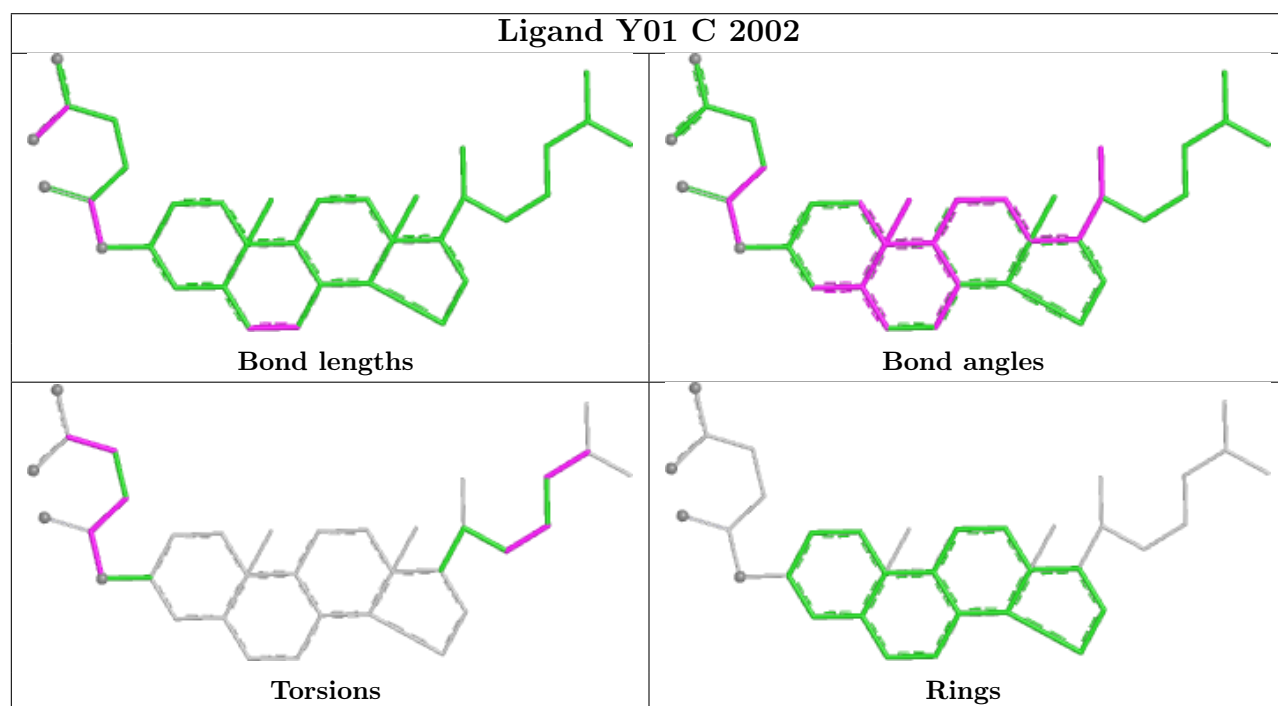
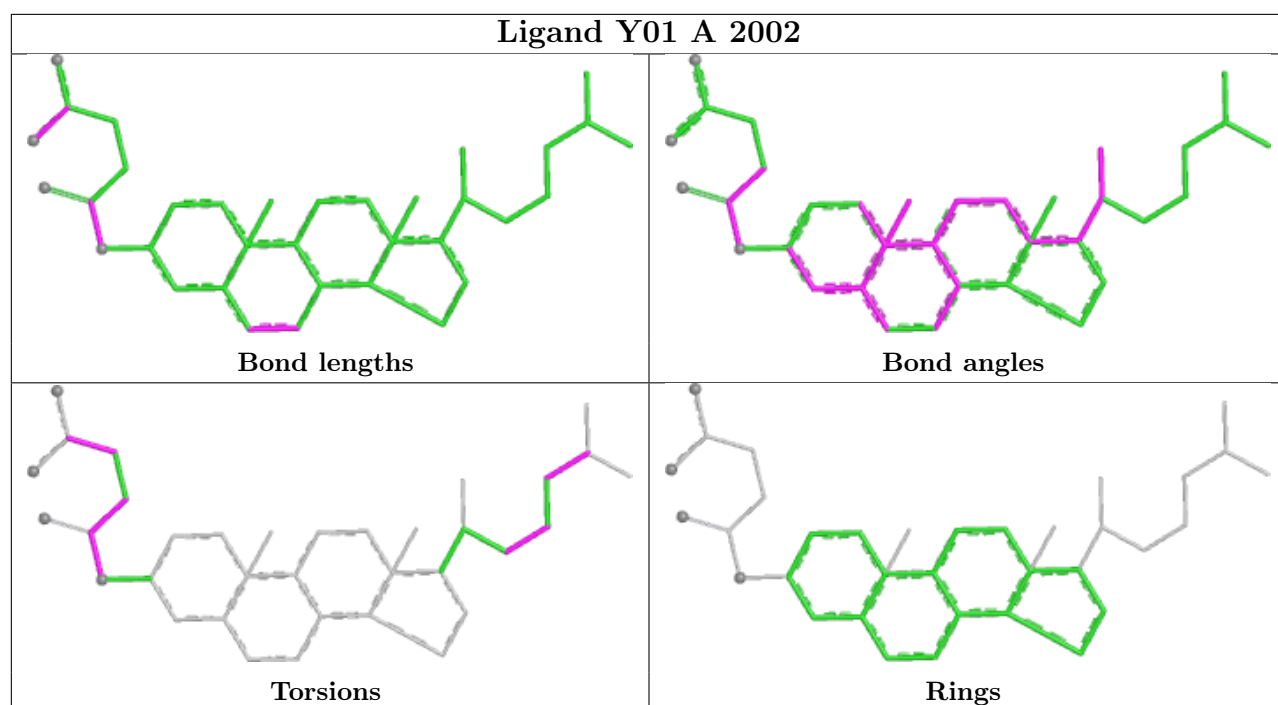
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

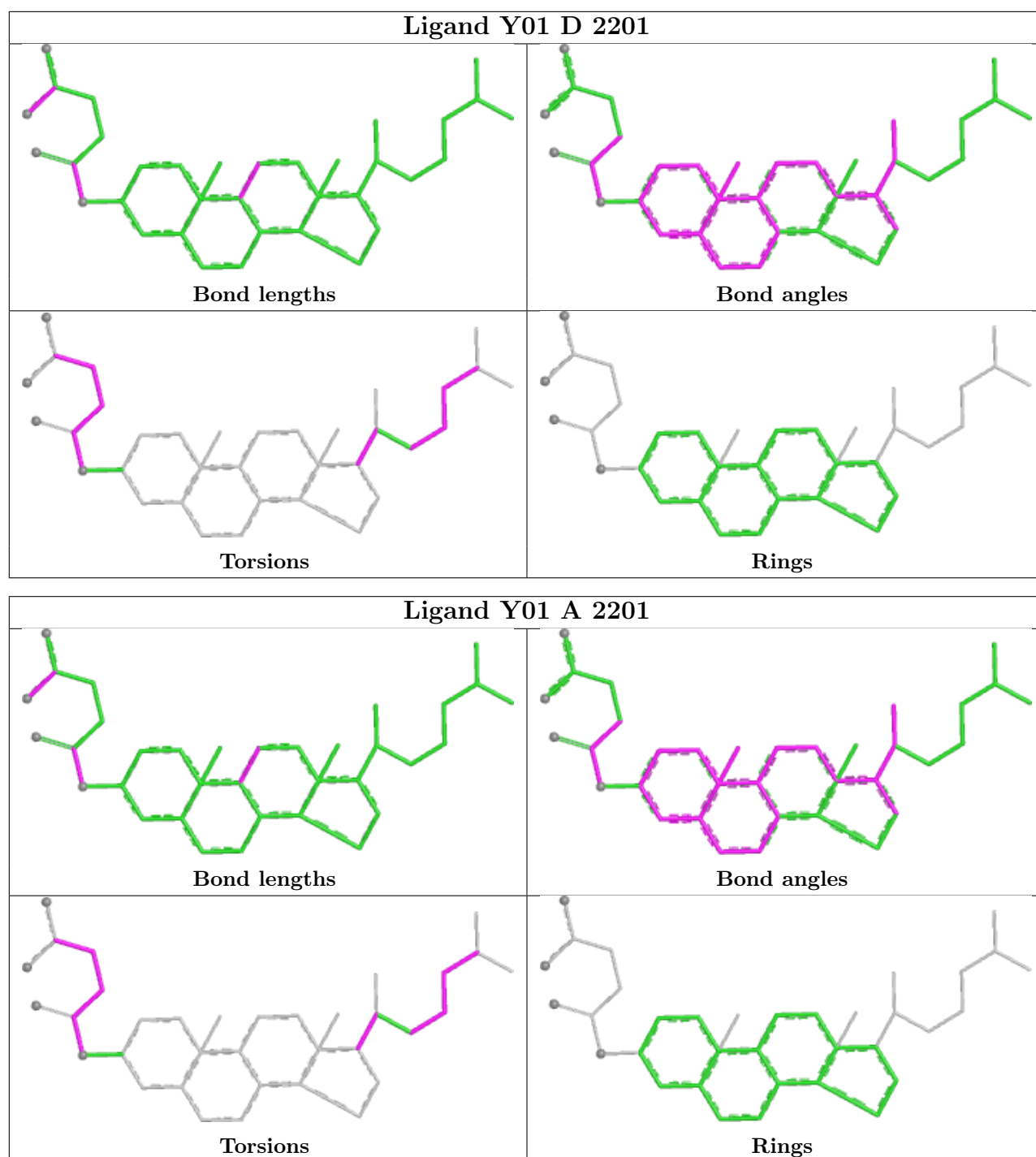












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

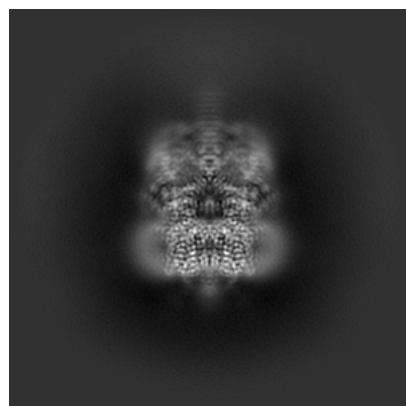
6 Map visualisation [i](#)

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.

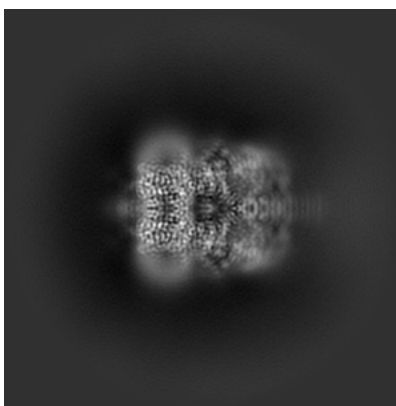
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

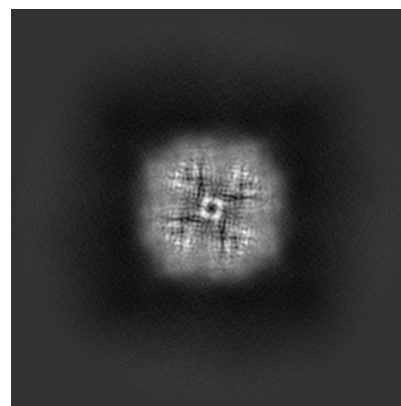
6.1.1 Primary map



X

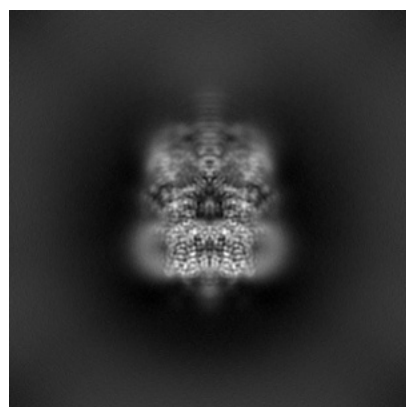


Y

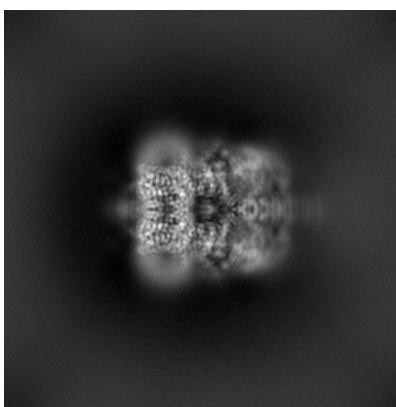


Z

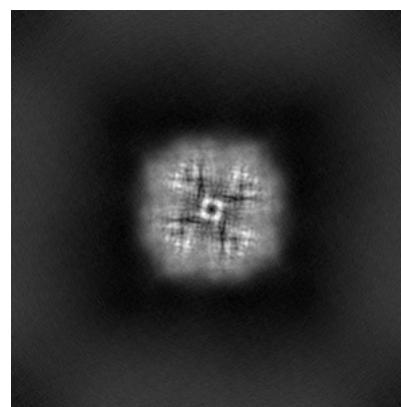
6.1.2 Raw map



X



Y

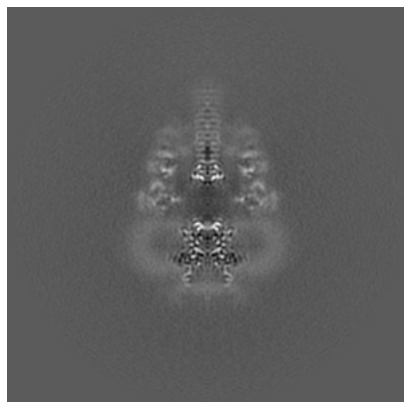


Z

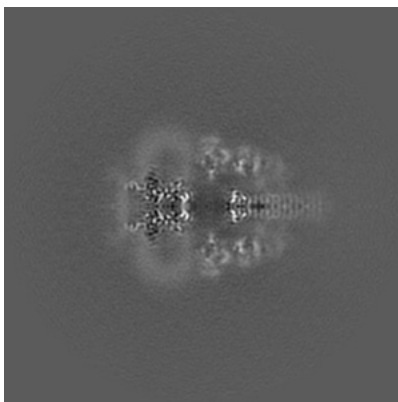
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

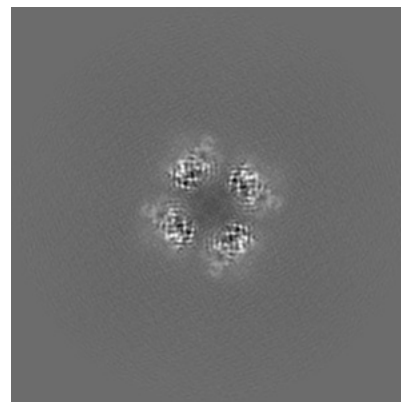
6.2.1 Primary map



X Index: 160

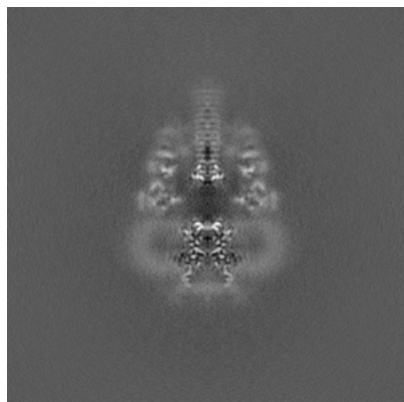


Y Index: 160

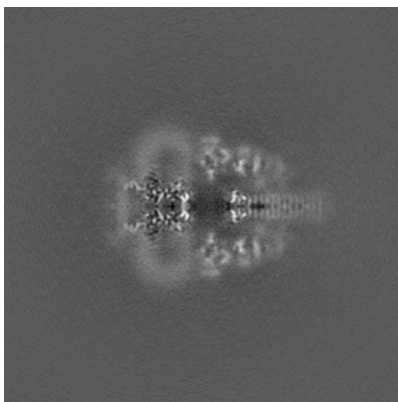


Z Index: 160

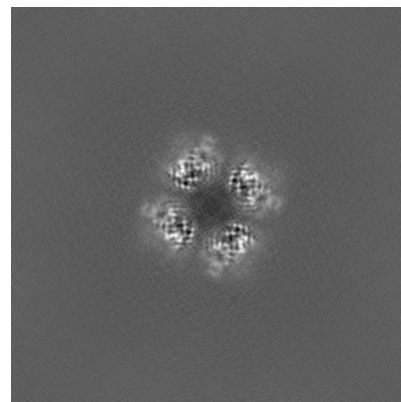
6.2.2 Raw map



X Index: 160



Y Index: 160

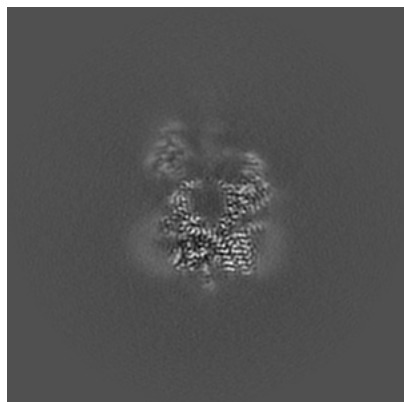


Z Index: 160

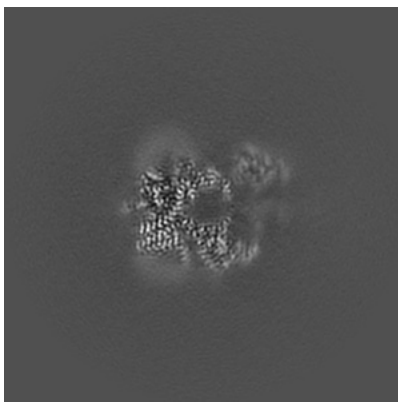
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

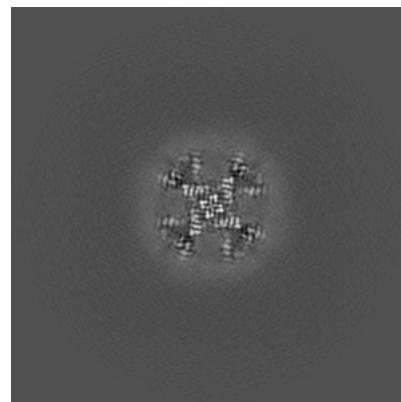
6.3.1 Primary map



X Index: 146

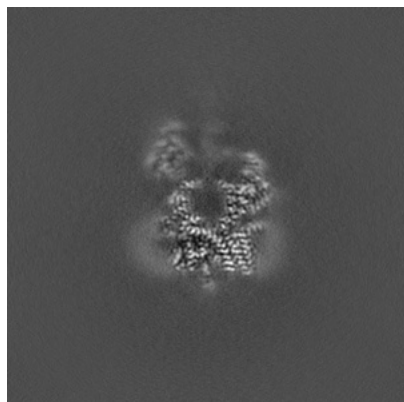


Y Index: 146

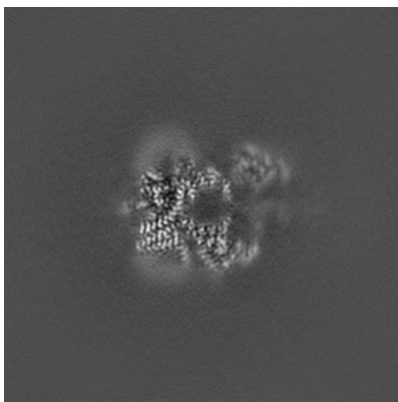


Z Index: 142

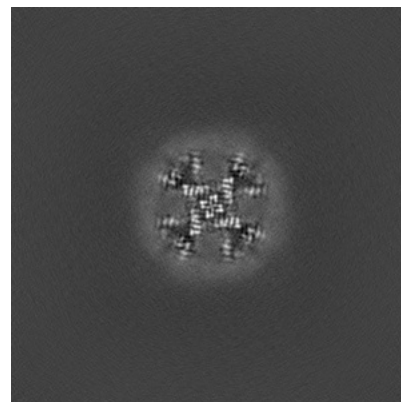
6.3.2 Raw map



X Index: 146



Y Index: 146

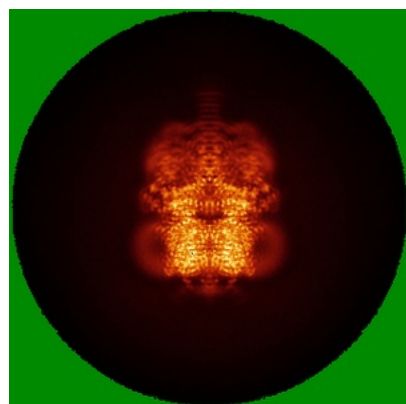


Z Index: 142

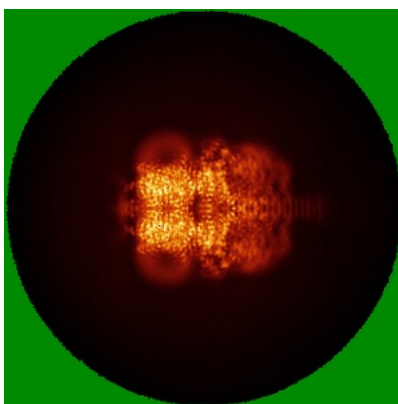
The images above show the largest variance slices of the map in three orthogonal directions.

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

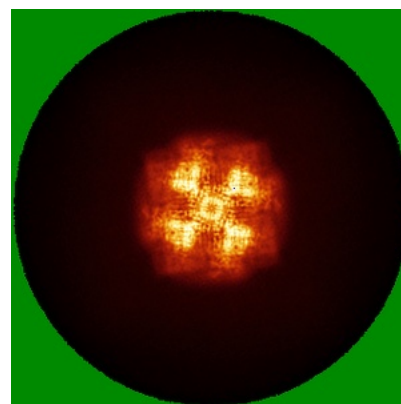
6.4.1 Primary map



X

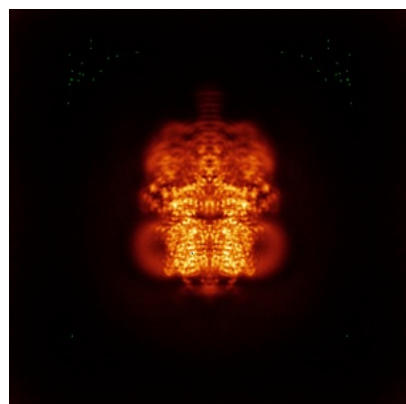


Y

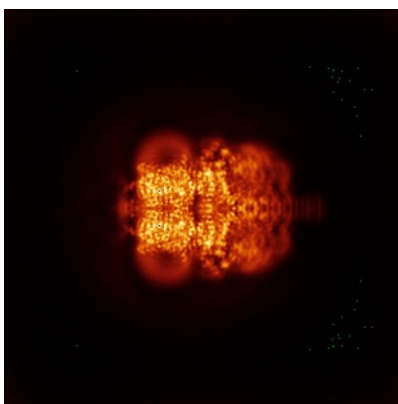


Z

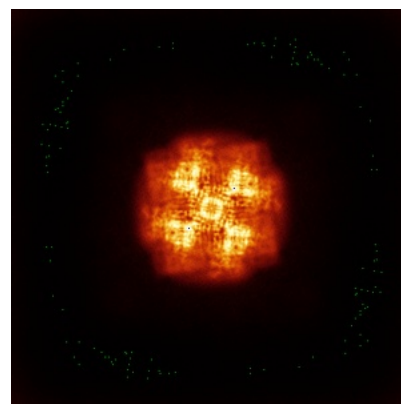
6.4.2 Raw map



X



Y

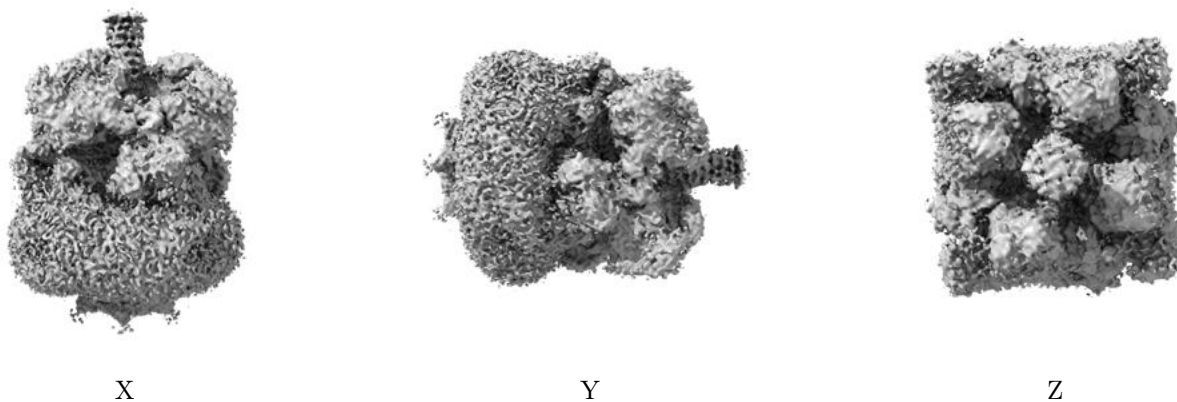


Z

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.

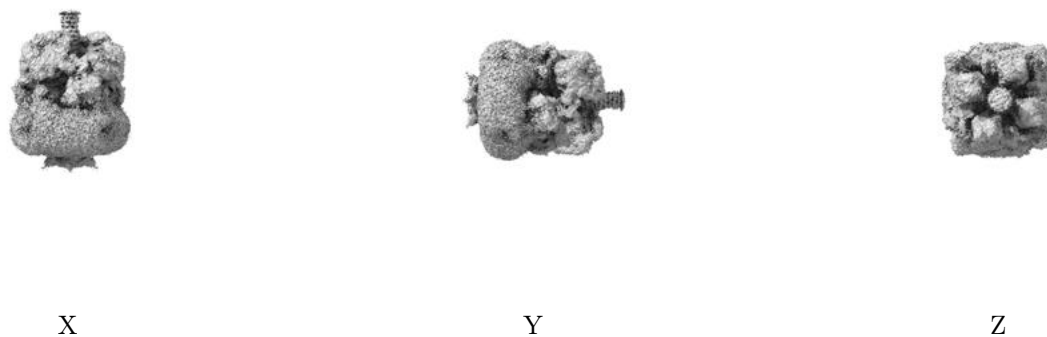
6.5 Orthogonal surface views [i](#)

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.

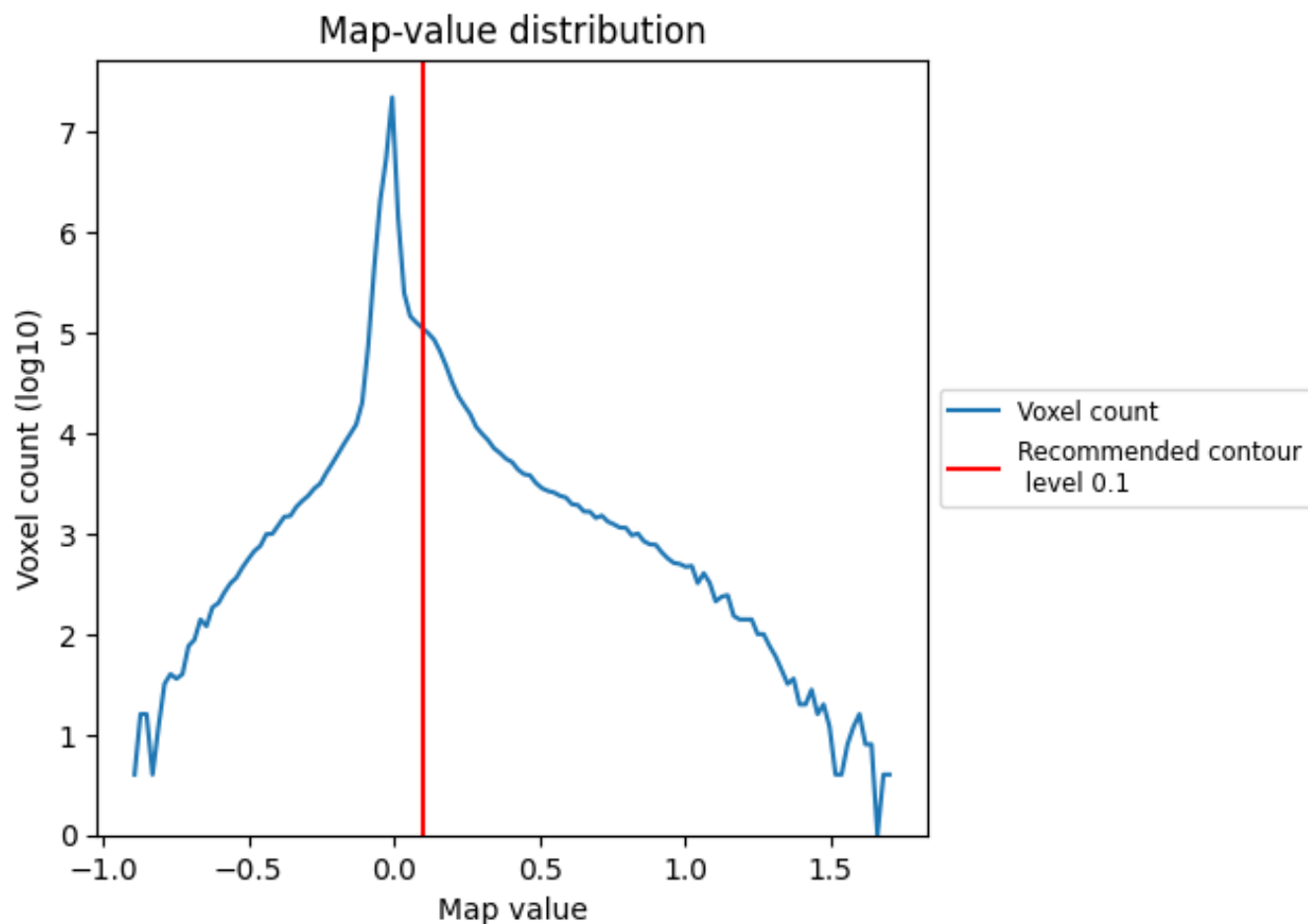
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

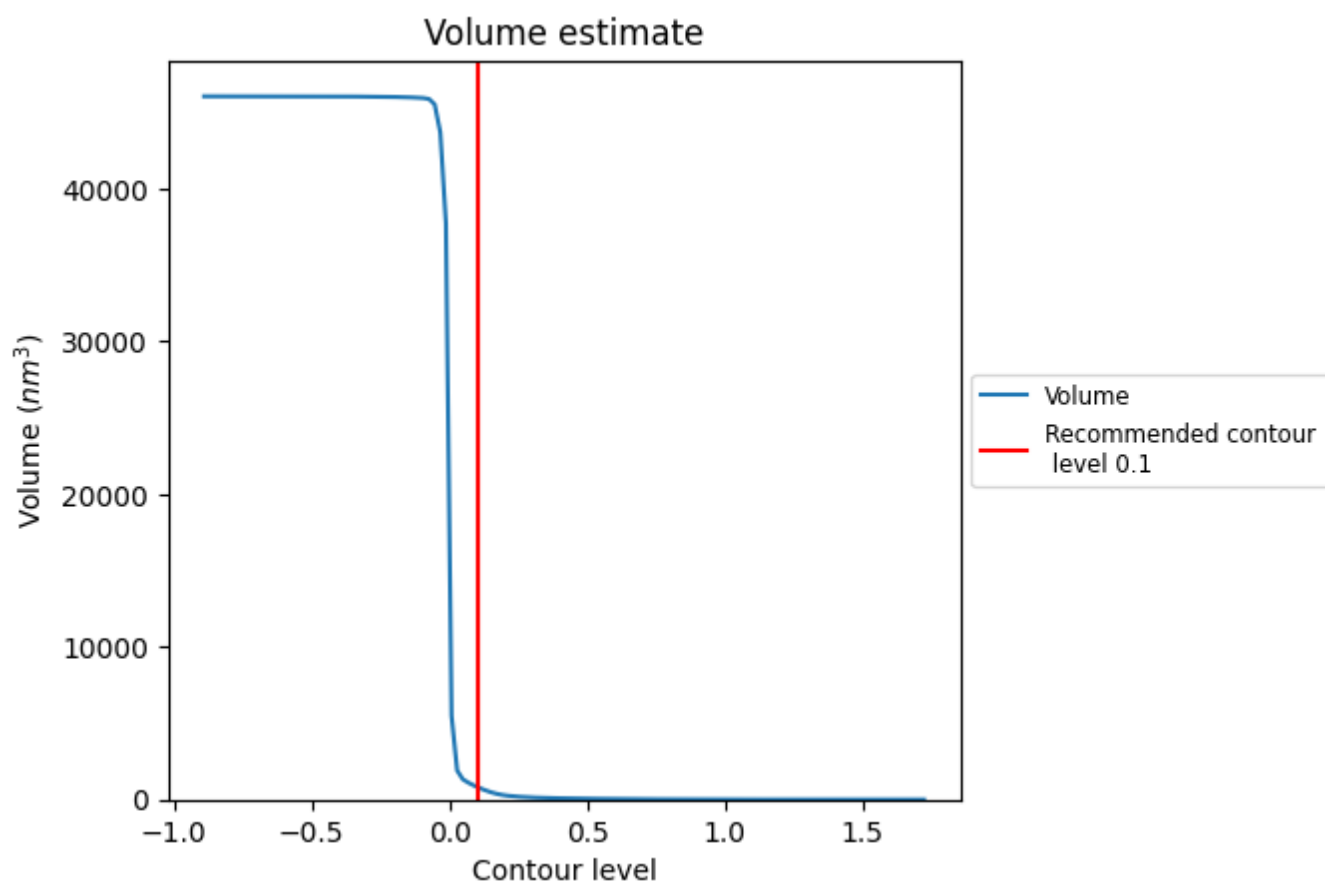
This section contains the results of statistical analysis of the map.

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.

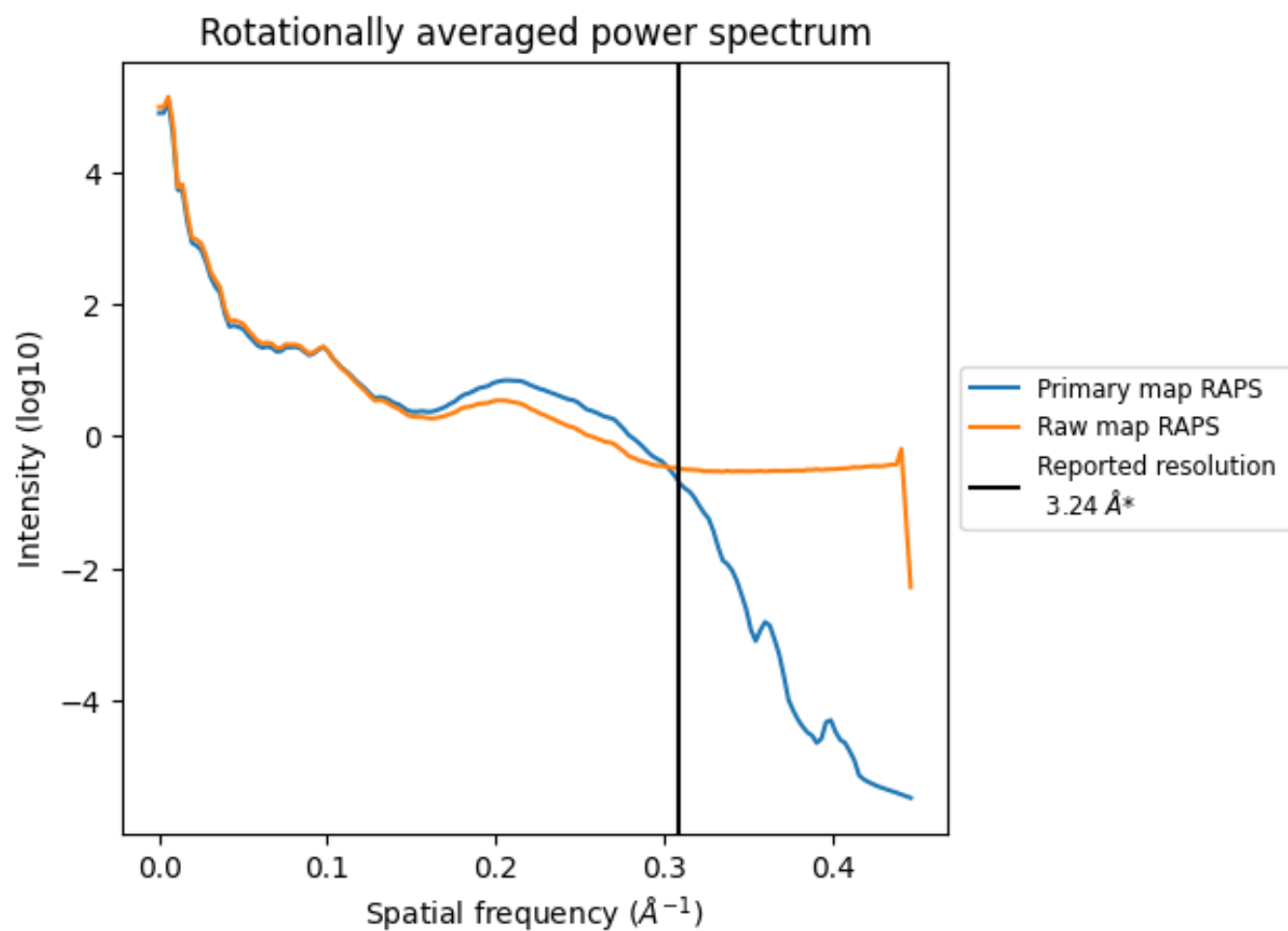
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 834 nm^3 ; 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 ⓘ

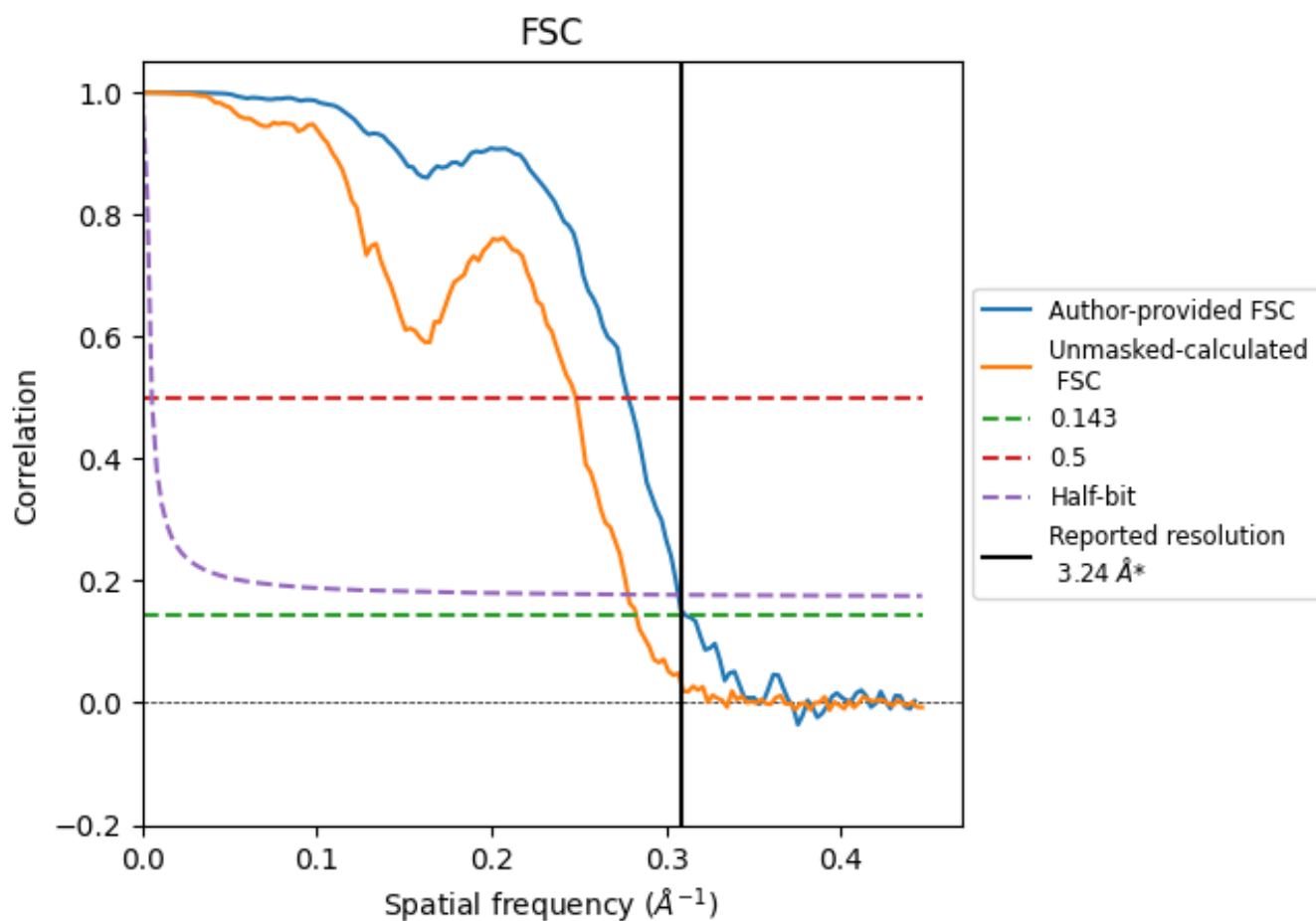


*Reported resolution corresponds to spatial frequency of 0.309 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.309 \AA^{-1}

8.2 Resolution estimates [i](#)

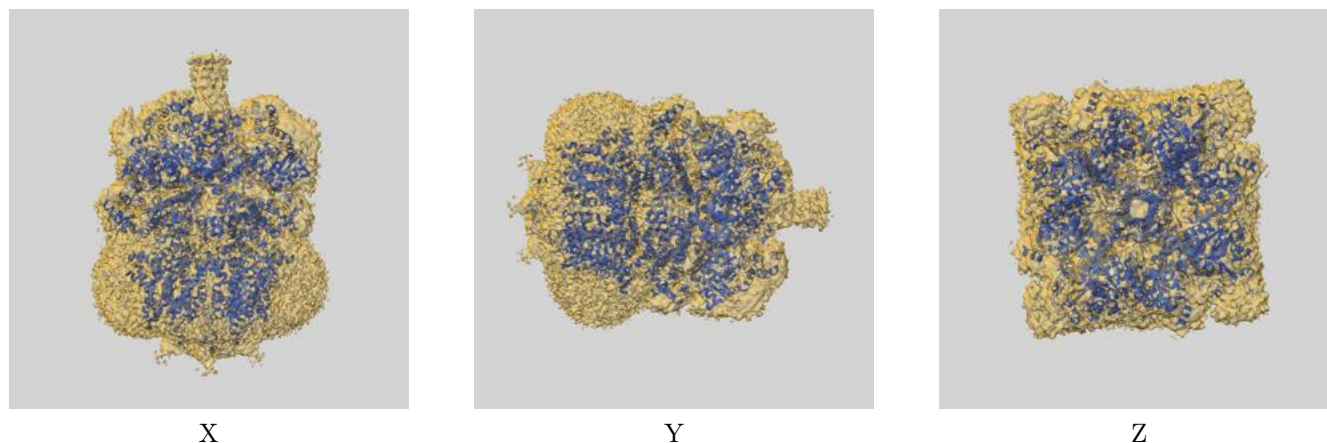
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.21	3.60	3.26
Unmasked-calculated*	3.54	4.03	3.60

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

9 Map-model fit [i](#)

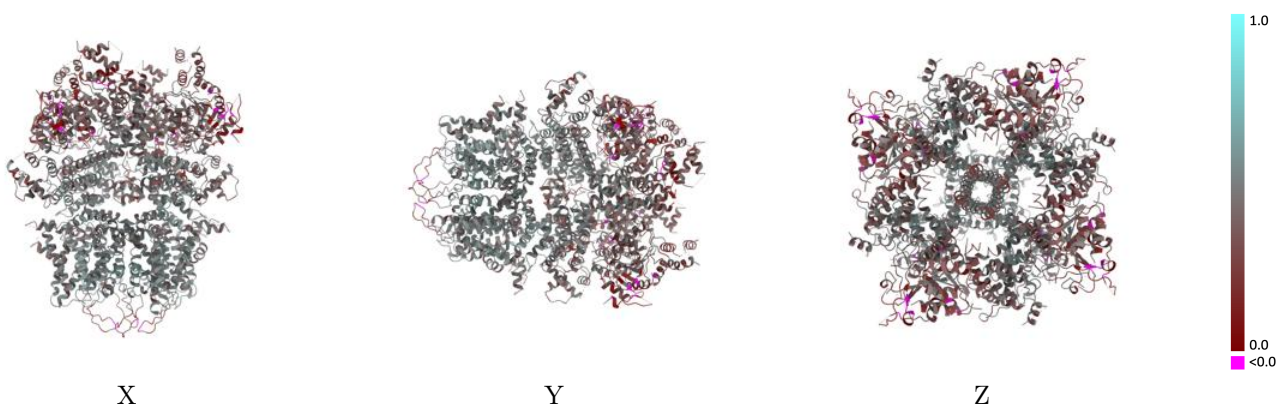
This section contains information regarding the fit between EMDB map EMD-44100 and PDB model 9B28. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



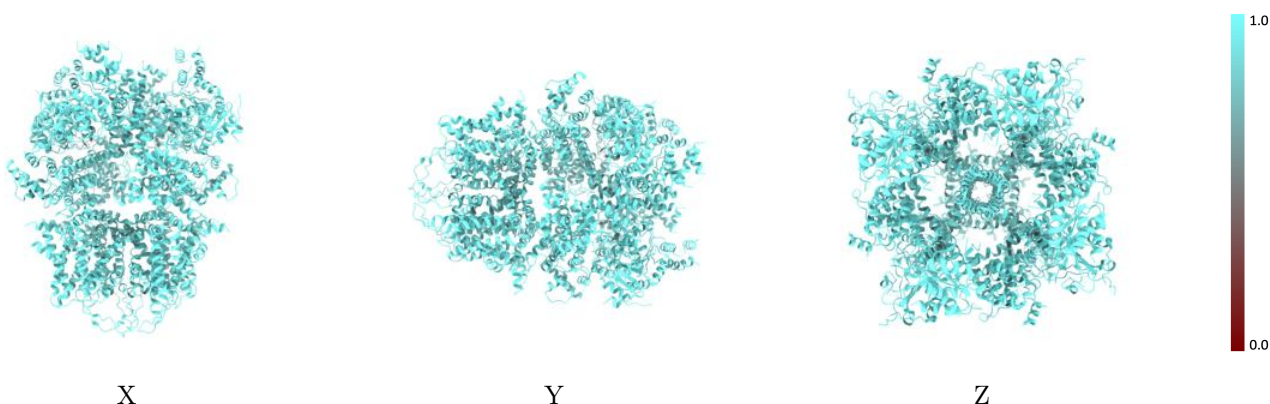
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



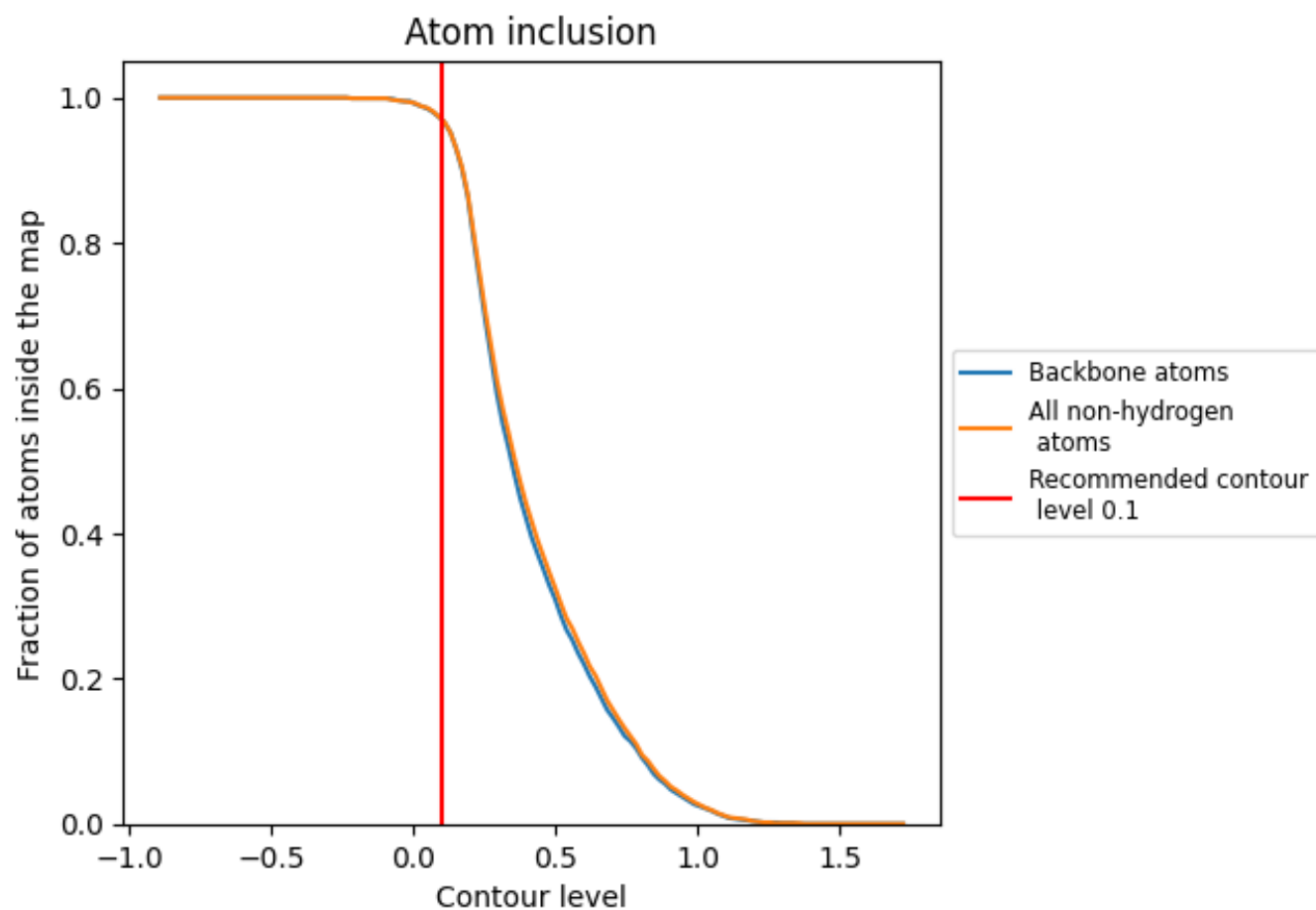
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

