



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2025 – 06:32 AM JST

PDB ID : 7FBS / pdb_00007fbs
EMDB ID : EMD-31519
Title : structure of a channel
Authors : Jiang, D.J.; Catterall, W.A.
Deposited on : 2021-07-12
Resolution : 3.40 Å(reported)

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 : 1.8.5 (274361), CSD as541be (2020)
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) : 2.44

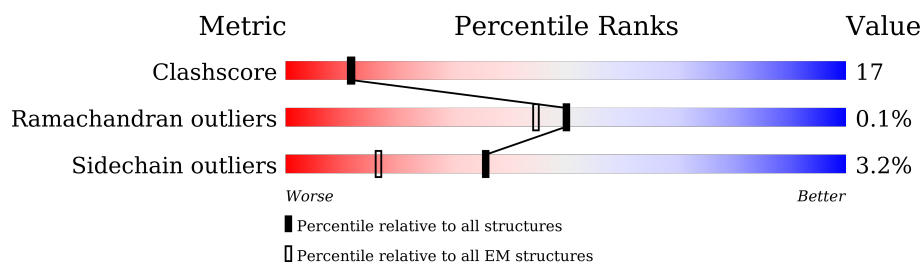
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	1838	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9274 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

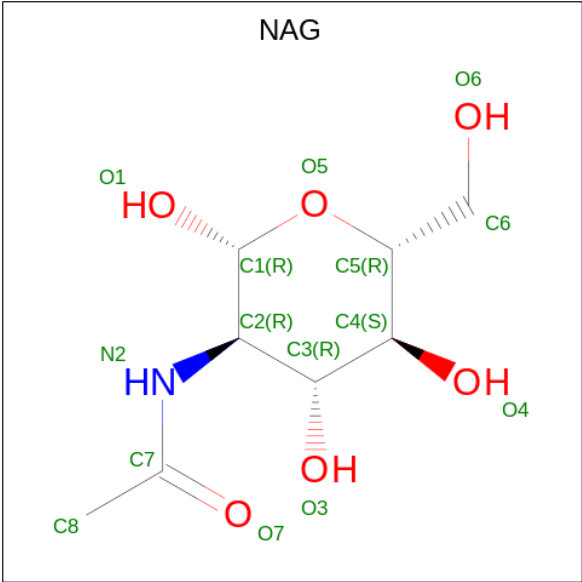
- Molecule 1 is a protein called Sodium channel protein type 5 subunit alpha,Sodium channel protein type 5 subunit alpha,Sodium channel protein type 5 subunit alpha,G protein/GFP fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1118	Total	C	N	O	S	0	0
			8849	5868	1406	1510	65		

There are 22 discrepancies between the modelled and reference sequences:

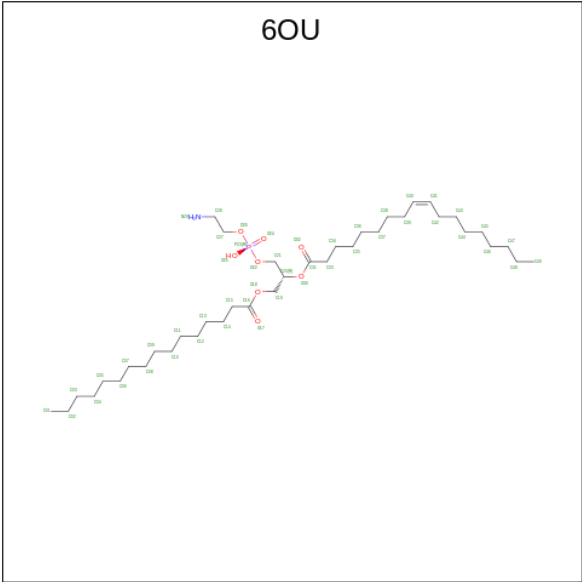
Chain	Residue	Modelled	Actual	Comment	Reference
A	1487	GLN	ILE	engineered mutation	UNP P15389
A	1488	GLN	PHE	engineered mutation	UNP P15389
A	1489	GLN	MET	engineered mutation	UNP P15389
A	1899	GLU	-	linker	UNP P15389
A	1900	VAL	-	linker	UNP P15389
A	1901	LEU	-	linker	UNP P15389
A	1902	PHE	-	linker	UNP P15389
A	1903	GLN	-	linker	UNP P15389
A	1904	GLY	-	linker	UNP P15389
A	1905	PRO	-	linker	UNP P15389
A	1906	GLY	-	linker	UNP P15389
A	1907	SER	-	linker	UNP P15389
A	2147	GLY	-	expression tag	UNP B7UCZ6
A	2148	SER	-	expression tag	UNP B7UCZ6
A	2149	ASP	-	expression tag	UNP B7UCZ6
A	2150	TYR	-	expression tag	UNP B7UCZ6
A	2151	LYS	-	expression tag	UNP B7UCZ6
A	2152	ASP	-	expression tag	UNP B7UCZ6
A	2153	ASP	-	expression tag	UNP B7UCZ6
A	2154	ASP	-	expression tag	UNP B7UCZ6
A	2155	ASP	-	expression tag	UNP B7UCZ6
A	2156	LYS	-	expression tag	UNP B7UCZ6

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



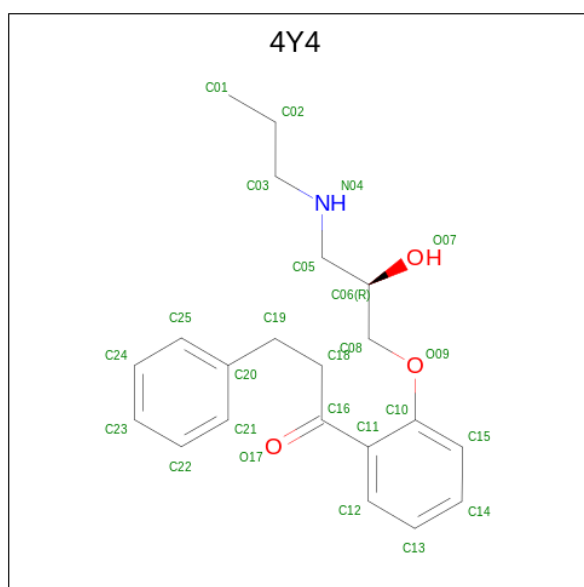
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0

- 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).



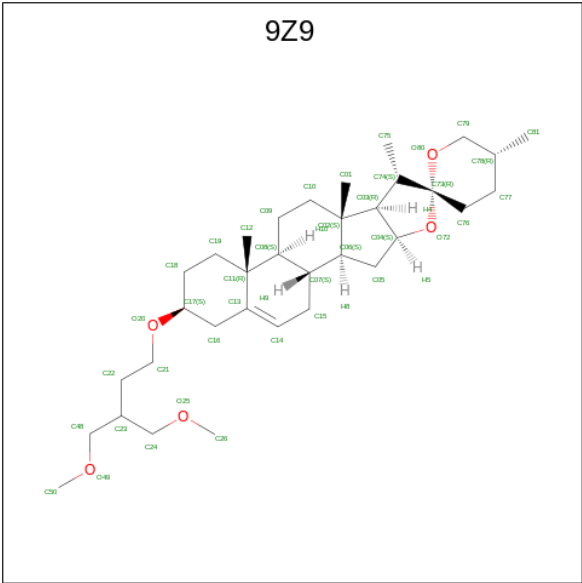
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
3	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
3	A	1	Total	C	O			0
			15	12	3			
3	A	1	Total	C	O			0
			26	21	5			
3	A	1	Total	C	O			0
			29	25	4			
3	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
3	A	1	Total	C	O			0
			27	23	4			
3	A	1	Total	C	O	P		0
			25	16	8	1		
3	A	1	Total	C	O			0
			17	15	2			
3	A	1	Total	C	O			0
			15	13	2			
3	A	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 4 is 1-[2-[(2R)-2-oxidanyl-3-(propylamino)propoxy]phenyl]-3-phenyl-propan-1-one (CCD ID: 4Y4) (formula: C₂₁H₂₇NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			25	21	1	3	

- Molecule 5 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			34	31	3	
5	A	1	Total	C	O	0
			30	27	3	

HIS	THR	GLN	ALA	ASN	GLU	F1753	L1648	V1570	K1494	K1401	K1302	W1194	PRO	THR	M859
MET	ILE	LYS	THR	PRO	PRO	F1754	L1649	A1571	K1495	K1401	K1311	R1195	ARG	ALA	Q860
VAL	GLY	ASN	TYR	SER	LEU	T1755	F1650	I1572	Y1496	G1410	R1311	R1195	SER	PRO	L861
LEU	LEU	ILE	LYS	ILE	ILE	T1756	A1651	C1577	Y1497	Y1411	R1314	K1198	ASP	GLU	F862
GLU	ASP	LYS	LEU	SER	ALA	M1768	M1653	M1581	N1498	L1414	R1314	T1199	PRO	ASP	G863
PHE	ASP	VAL	THR	TYR	LYS	Y1769	M1654	Y1587	A1499	L1414	A1345	T1199	PRO	GLY	K864
THR	ASN	ASN	LEU	GLU	PRO	S1655	S1655	Y1587	M1500	V1417	S1317	R1202	VAL	GLU	E868
ALA	TYR	ILE	PHE	GLN	ASN	A1657	L1656	L1684	M1500	V1417	S1317	R1202	GLY	MET	I873
ALA	ILE	ILE	ILE	THR	ILE	A1658	A1658	Y1587	M1501	F1420	F1319	I1203	LYS	ASN	S874
ILE	THR	THR	THR	THR	SER	L1659	L1659	Y1587	K1502	F1420	E1320	V1204	VAL	ASN	D875
THR	THR	THR	THR	THR	SER	F1777	F1777	Y1587	L1503	W1423	V1326	E1205	PRO	GLN	S876
THR	ILE	ILE	THR	LEU	ILE	SER	SER	W1593	G1504	M1424	V1326	E1205	LEU	GLN	H206
LEU	GLY	GLY	GLY	GLU	ASN	VAL	VAL	M1594	G1504	M1424	V1326	E1205	ALA	LEU	G877
LEU	GLY	GLY	GLY	GLU	VAL	ALA	ALA	I1595	S1505	M1424	V1326	E1205	ARG	LEU	L878
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	F1596	K1506	V1431	I1333	P1334	LYS	ALA	L879
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	D1597	K1507	V1431	I1333	P1334	ARG	ALA	P880
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	F1598	P1508	R1434	N1338	T1211	THR	ILE	R881
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	F1599	Q1509	G1435	V1339	I1214	ARG	GLN	W882
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	G1600	Q1509	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	V1601	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1602	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	L1603	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	S1604	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1605	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	V1606	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	G1607	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	V1609	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	L1610	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	S1611	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	D1612	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1613	P1511	G1435	V1339	I1214	ARG	GLN	D886
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LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	Q1615	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	K1616	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	Y1617	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	F1619	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	S1620	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	F1624	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1627	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	R1628	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	R1631	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1632	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	G1633	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1635	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	R1631	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	G1633	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1635	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	R1631	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	G1633	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1635	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	R1631	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	G1633	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1635	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	R1631	P1511	G1435	V1339	I1214	ARG	GLN	A890
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LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1635	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	R1631	P1511	G1435	V1339	I1214	ARG	GLN	F887
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	G1633	P1511	G1435	V1339	I1214	ARG	GLN	F888
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	I1635	P1511	G1435	V1339	I1214	ARG	GLN	A890
LEU	GLY	GLY	GLY	GLU	VAL	THR	THR	R1631	P1511	G1435	V1339	I1214	ARG	GLN	D886
LEU	GLY	GLY	GLY	GLU</											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287306	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.486	Depositor
Minimum map value	-3.763	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.65	Depositor
Map size (\AA)	337.91998, 337.91998, 337.91998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.056, 1.056, 1.056	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: 9Z9, NAG, 6OU, 4Y4

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	0.37	0/9063	0.50	3/12315 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1373	LEU	CA-C-N	6.95	128.53	119.84
1	A	1373	LEU	C-N-CA	6.95	128.53	119.84
1	A	1368	GLN	N-CA-C	5.60	117.38	111.28

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	8849	0	8919	311	0
2	A	42	0	39	8	0
3	A	294	0	0	0	0
4	A	25	0	0	0	0
5	A	64	0	0	13	0
All	All	9274	0	8958	317	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 17.

The worst 5 of 317 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)
5:A:2216:9Z9:C04	5:A:2216:9Z9:C05	1.77	1.43
5:A:2217:9Z9:C04	5:A:2217:9Z9:C05	1.77	1.40
1:A:403:PHE:HB3	5:A:2217:9Z9:C81	1.61	1.29
1:A:257:LEU:HD12	1:A:1645:ILE:HA	1.33	1.09
1:A:418:GLU:HG2	5:A:2216:9Z9:C22	1.90	1.01

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	1104/1838 (60%)	1021 (92%)	82 (7%)	1 (0%)	48 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1374	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	947/1612 (59%)	917 (97%)	30 (3%)	34 59

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1199	THR
1	A	1656	LEU
1	A	1351	SER
1	A	1774	LEU
1	A	1512	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1439	GLN
1	A	1560	ASN
1	A	1701	ASN
1	A	1566	ASN
1	A	835	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6OU	A	2204	-	31,31,48	1.08	4 (12%)	34,36,53	1.29	2 (5%)
3	6OU	A	2205	-	34,34,48	1.04	2 (5%)	37,39,53	1.17	2 (5%)
2	NAG	A	2201	-	14,14,15	0.38	0	17,19,21	0.42	0
3	6OU	A	2206	-	14,14,48	0.94	1 (7%)	14,14,53	1.32	1 (7%)
3	6OU	A	2212	-	16,16,48	1.26	3 (18%)	16,16,53	1.12	1 (6%)
3	6OU	A	2215	-	33,33,48	1.04	3 (9%)	35,38,53	1.22	2 (5%)
3	6OU	A	2207	-	25,25,48	1.07	3 (12%)	27,27,53	1.33	2 (7%)
4	4Y4	A	2214	-	26,26,26	1.61	5 (19%)	30,32,32	1.01	1 (3%)
3	6OU	A	2211	-	24,24,48	1.26	4 (16%)	28,29,53	1.28	2 (7%)
2	NAG	A	2203	-	14,14,15	0.43	0	17,19,21	0.39	0
3	6OU	A	2208	-	28,28,48	1.16	3 (10%)	30,30,53	1.40	3 (10%)
3	6OU	A	2209	-	38,38,48	0.97	3 (7%)	41,43,53	1.17	3 (7%)
3	6OU	A	2213	-	14,14,48	1.34	3 (21%)	14,14,53	0.99	0
5	9Z9	A	2216	-	38,38,44	8.22	23 (60%)	60,61,68	2.28	25 (41%)
3	6OU	A	2210	-	26,26,48	0.95	2 (7%)	27,27,53	1.27	2 (7%)
5	9Z9	A	2217	-	35,35,44	8.14	23 (65%)	58,58,68	2.15	23 (39%)
2	NAG	A	2202	-	14,14,15	0.25	0	17,19,21	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6OU	A	2204	-	-	17/35/35/52	-
3	6OU	A	2205	-	-	23/38/38/52	-
2	NAG	A	2201	-	-	2/6/23/26	0/1/1/1
3	6OU	A	2206	-	-	5/13/13/52	-
3	6OU	A	2212	-	-	4/15/15/52	-
3	6OU	A	2215	-	-	17/37/37/52	-
3	6OU	A	2207	-	-	12/27/27/52	-
4	4Y4	A	2214	-	-	11/19/19/19	0/2/2/2
3	6OU	A	2211	-	-	13/26/26/52	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2203	-	-	4/6/23/26	0/1/1/1
3	6OU	A	2208	-	-	15/29/29/52	-
3	6OU	A	2209	-	-	24/42/42/52	-
3	6OU	A	2213	-	-	5/13/13/52	-
5	9Z9	A	2216	-	-	2/4/92/100	0/6/6/6
3	6OU	A	2210	-	-	18/26/26/52	-
5	9Z9	A	2217	-	-	-	0/6/6/6
2	NAG	A	2202	-	-	2/6/23/26	0/1/1/1

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2216	9Z9	C15-C07	-20.91	1.17	1.53
5	A	2217	9Z9	C15-C07	-20.88	1.17	1.53
5	A	2216	9Z9	C07-C06	-20.45	1.14	1.53
5	A	2217	9Z9	C07-C06	-20.20	1.15	1.53
5	A	2217	9Z9	C11-C13	-18.40	1.16	1.52

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2216	9Z9	C15-C14-C13	-4.91	116.00	125.06
5	A	2217	9Z9	C16-C13-C11	-4.84	109.99	116.42
5	A	2217	9Z9	C11-C13-C14	-4.62	115.83	122.90
3	A	2204	6OU	O30-C31-C33	4.49	121.17	111.50
5	A	2216	9Z9	C11-C13-C14	-4.46	116.08	122.90

There are no chirality outliers.

5 of 174 torsion outliers are listed below:

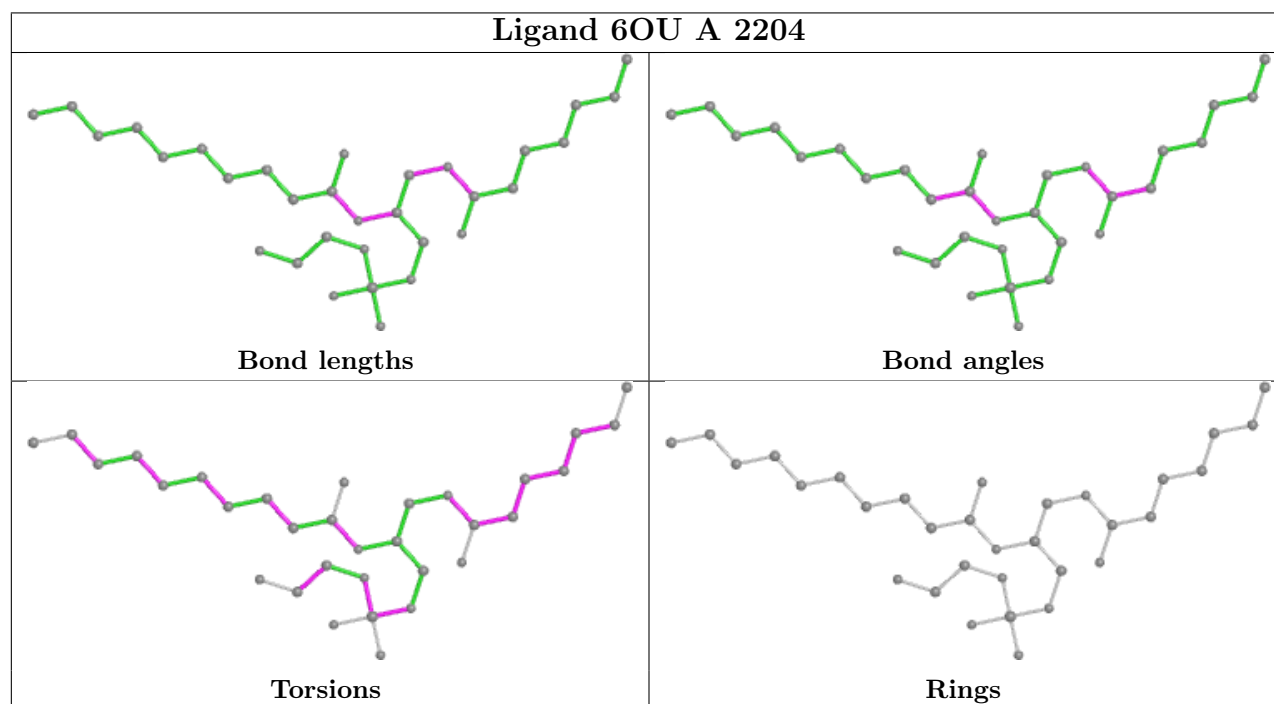
Mol	Chain	Res	Type	Atoms
3	A	2204	6OU	O26-C27-C28-N29
3	A	2205	6OU	C27-O26-P23-O22
3	A	2205	6OU	C27-O26-P23-O24
3	A	2205	6OU	C27-O26-P23-O25
3	A	2209	6OU	C27-O26-P23-O24

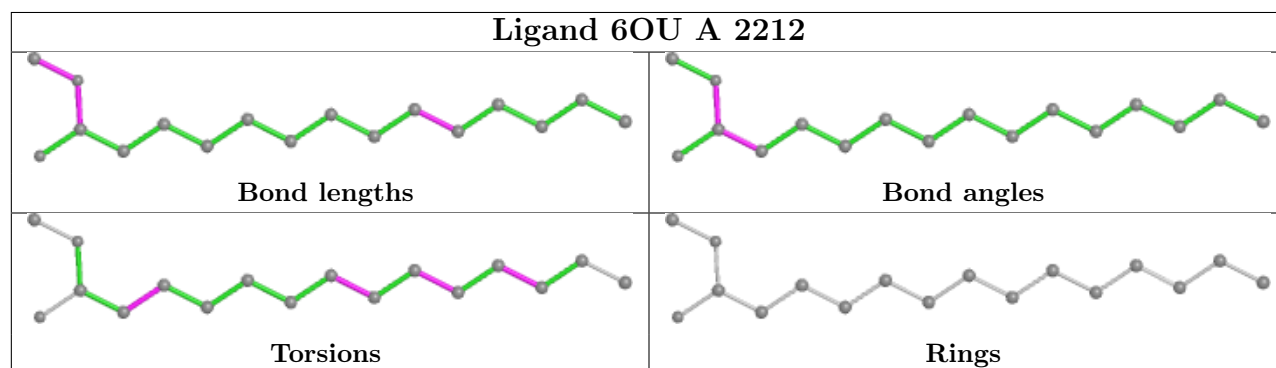
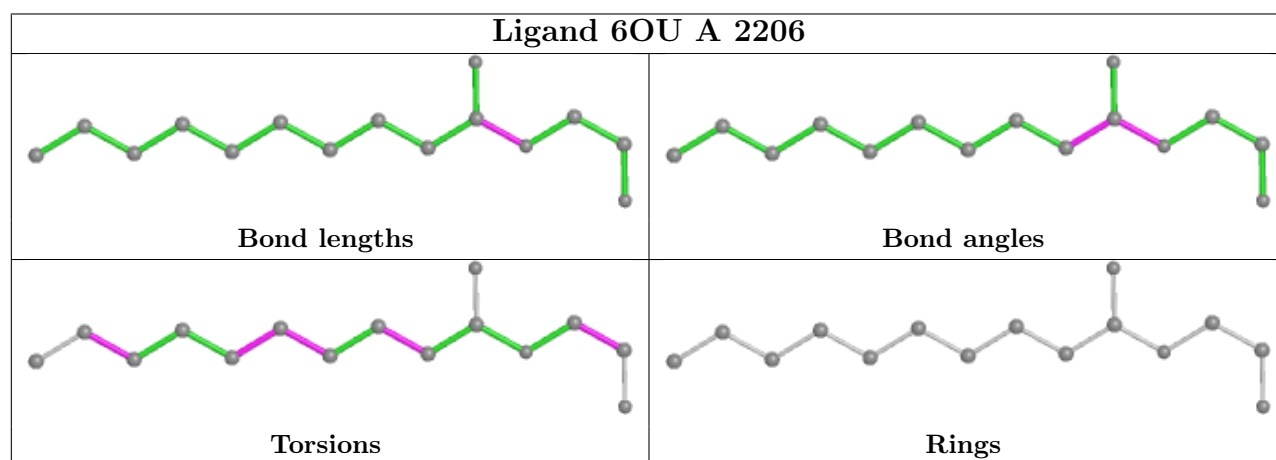
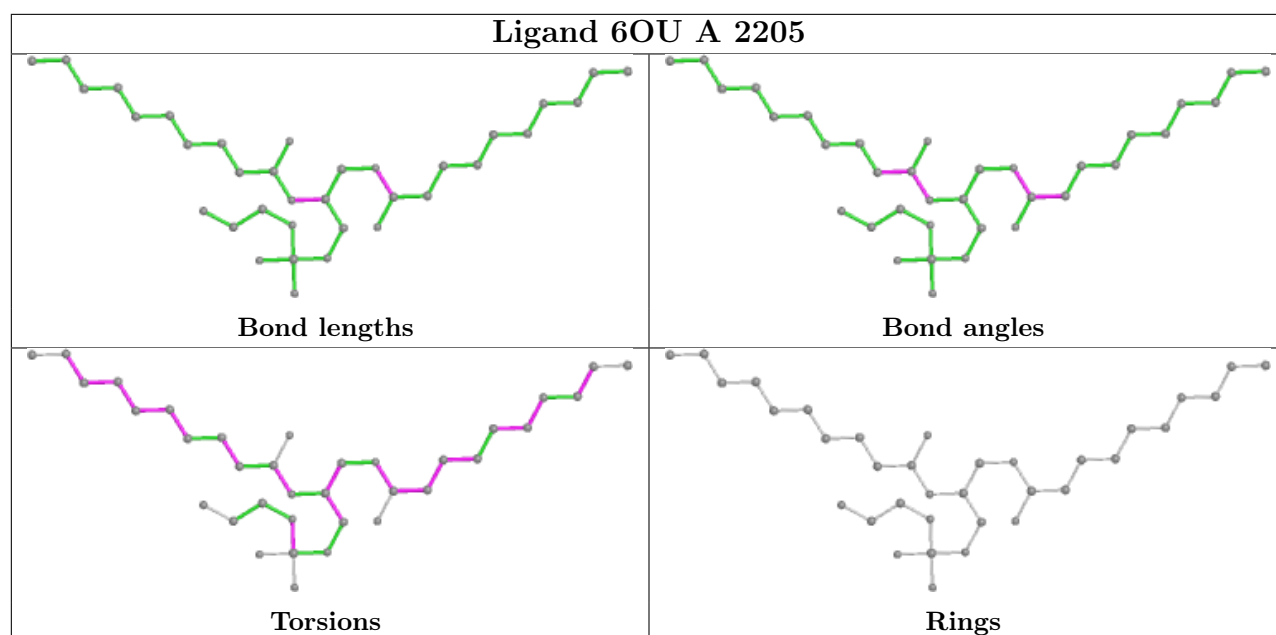
There are no ring outliers.

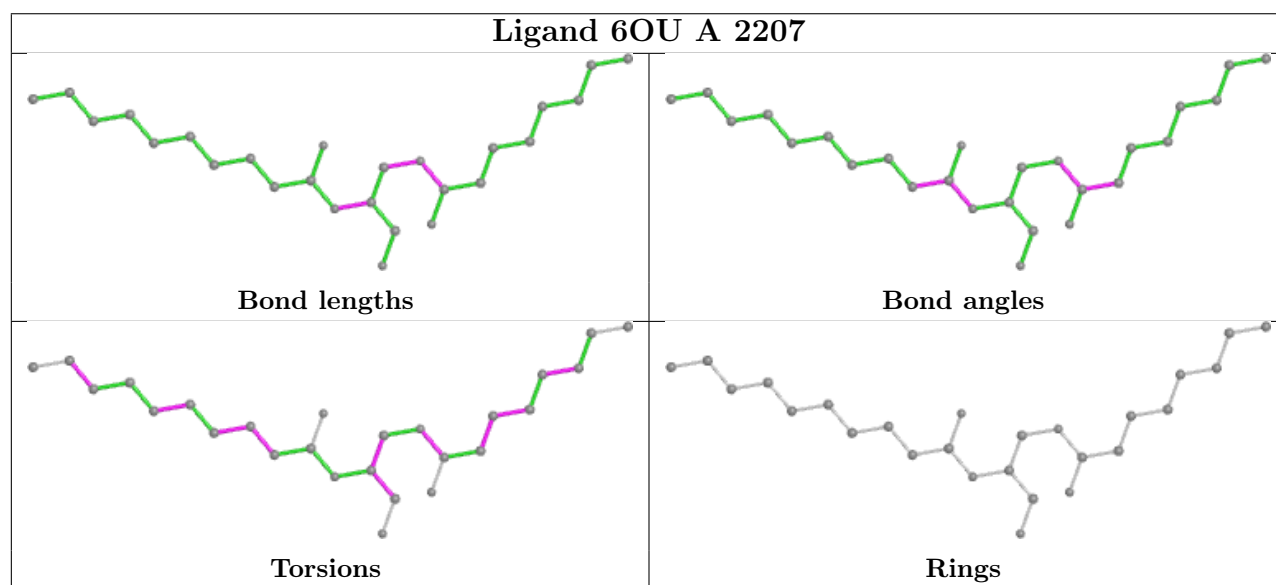
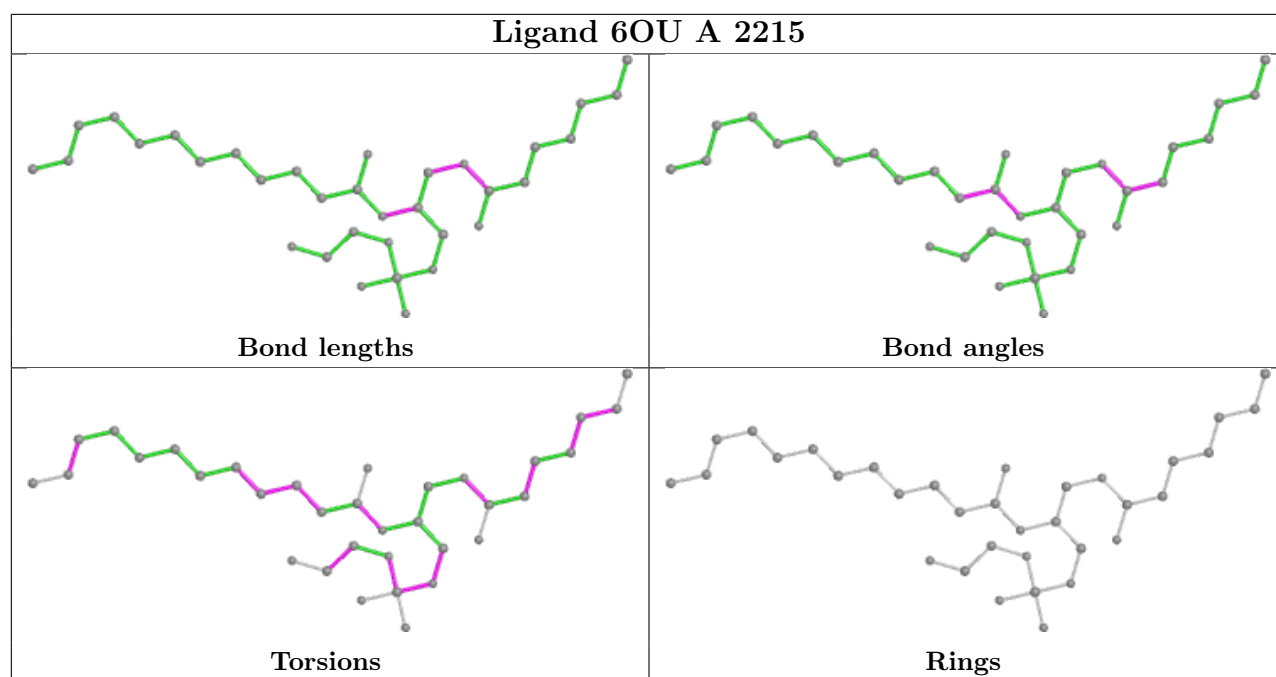
4 monomers are involved in 21 short contacts:

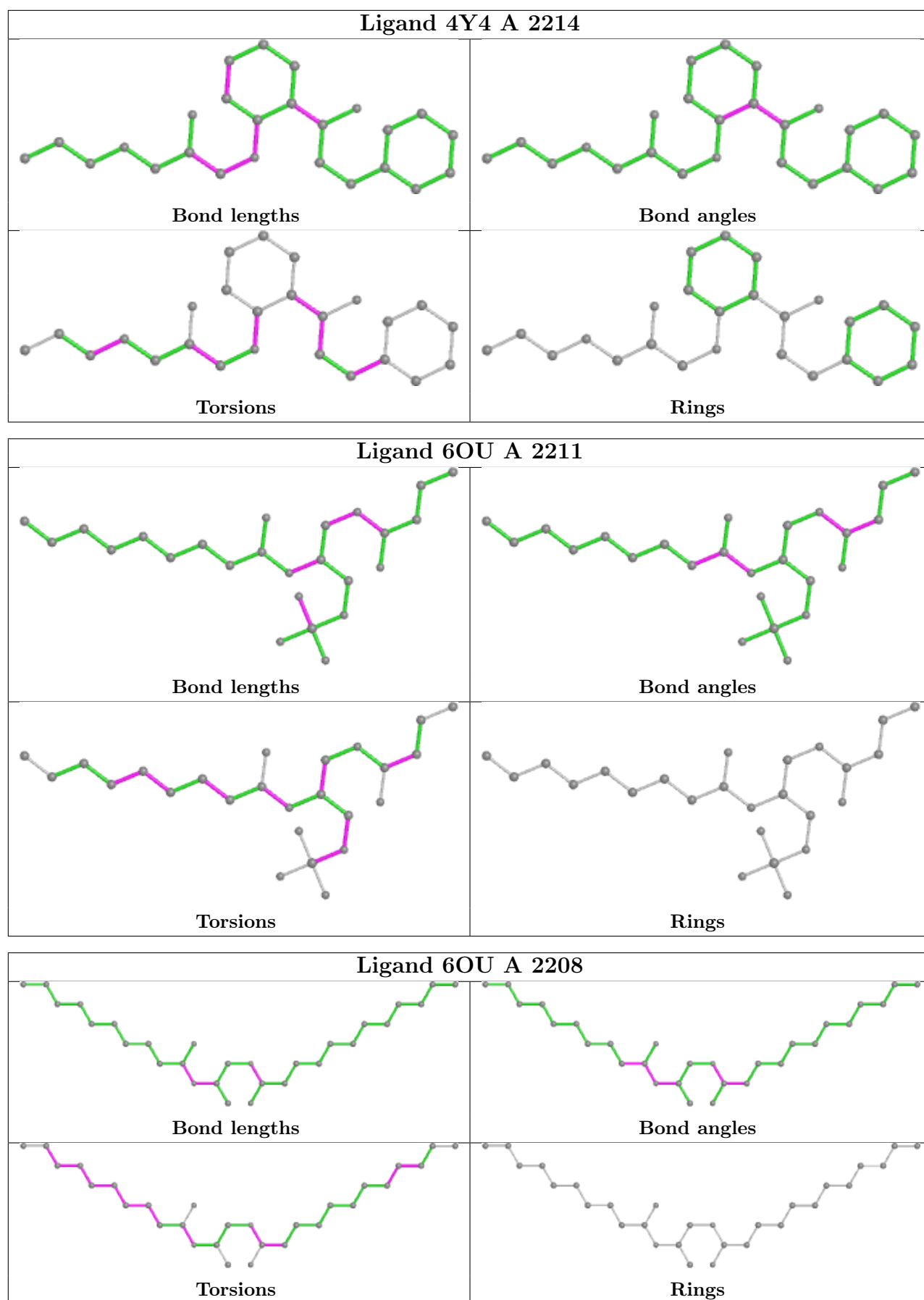
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2201	NAG	5	0
5	A	2216	9Z9	8	0
5	A	2217	9Z9	5	0
2	A	2202	NAG	4	0

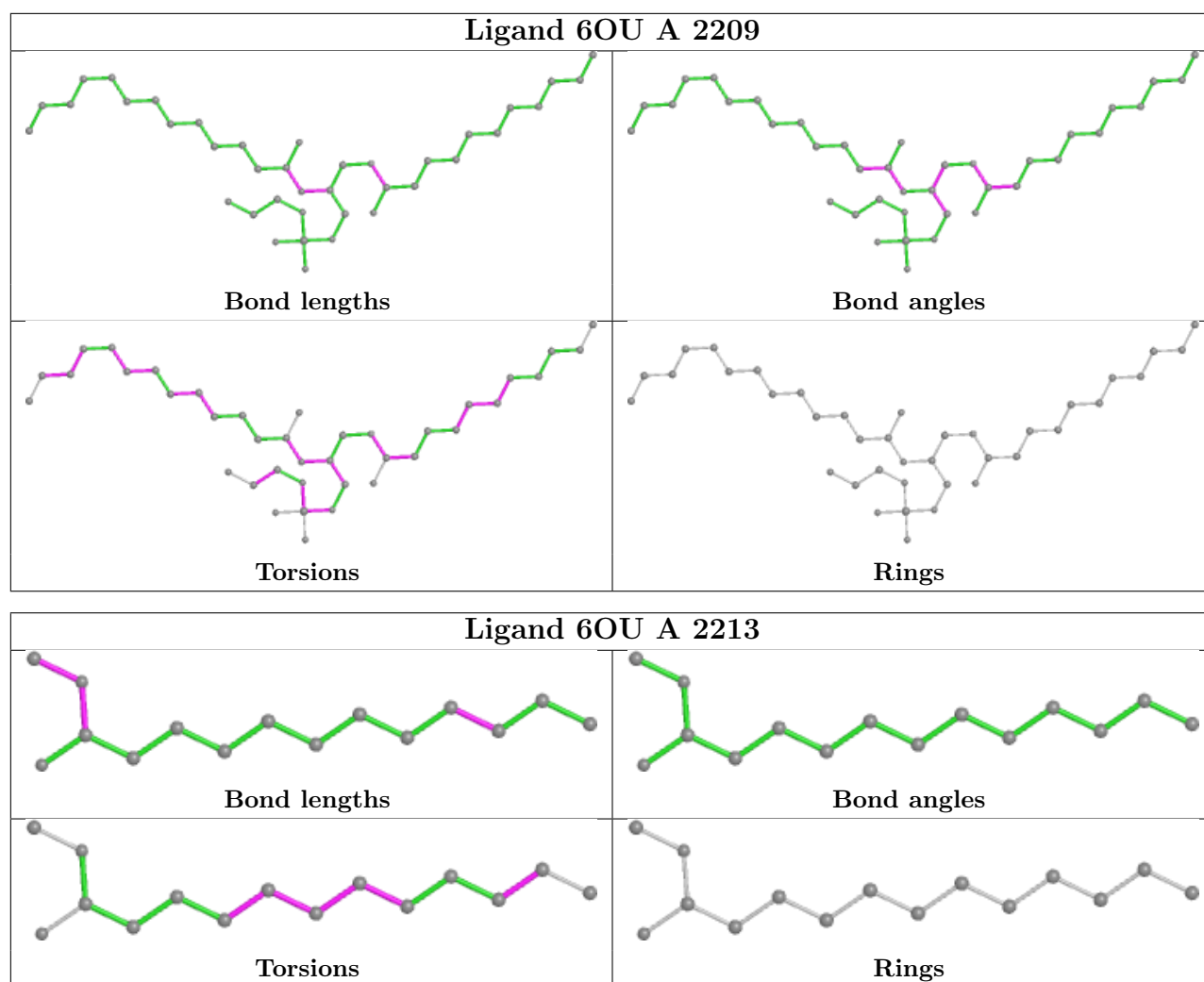
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

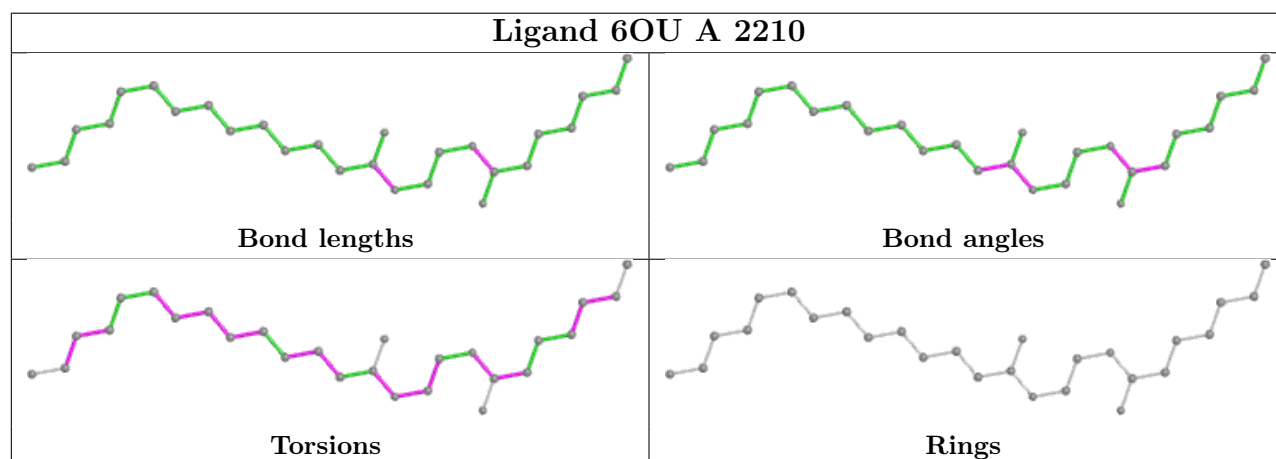
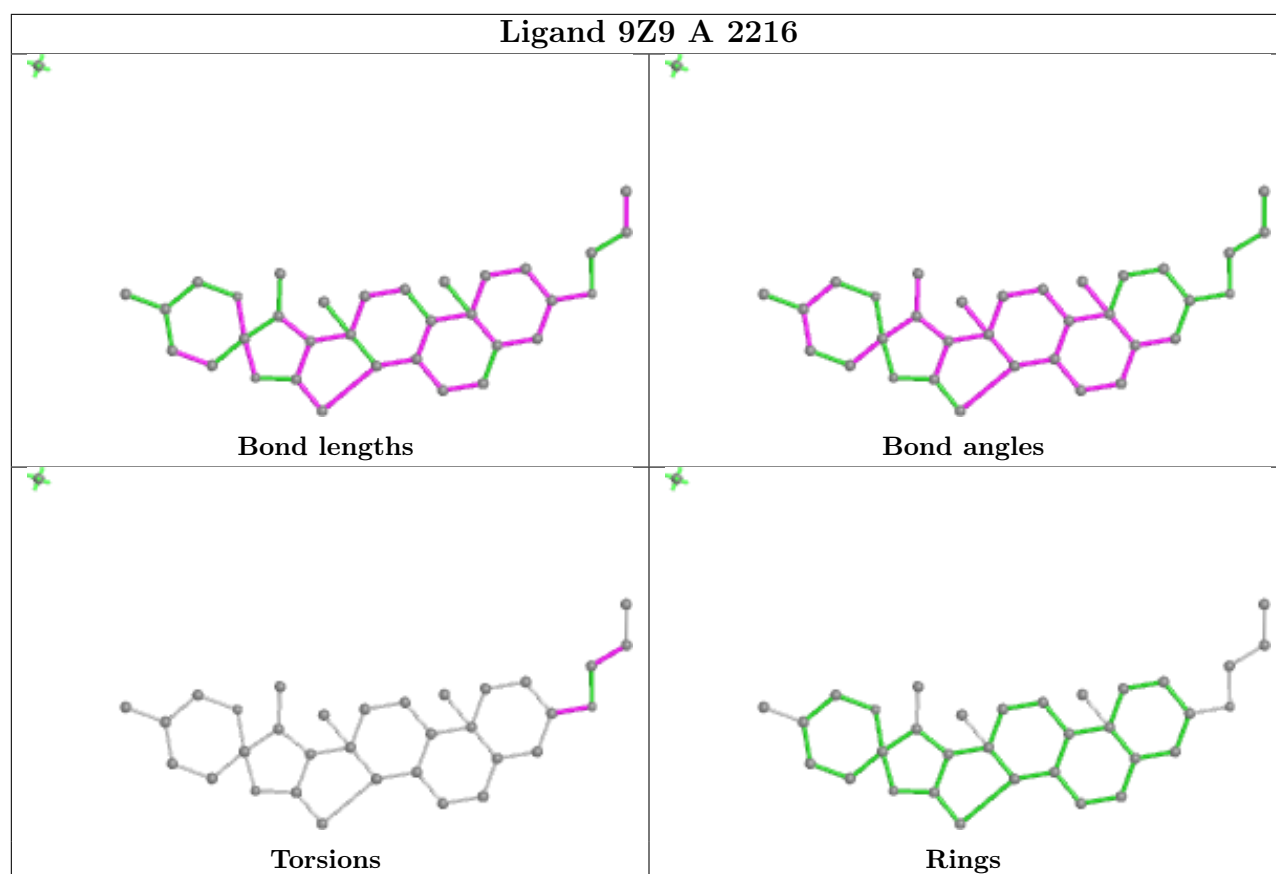


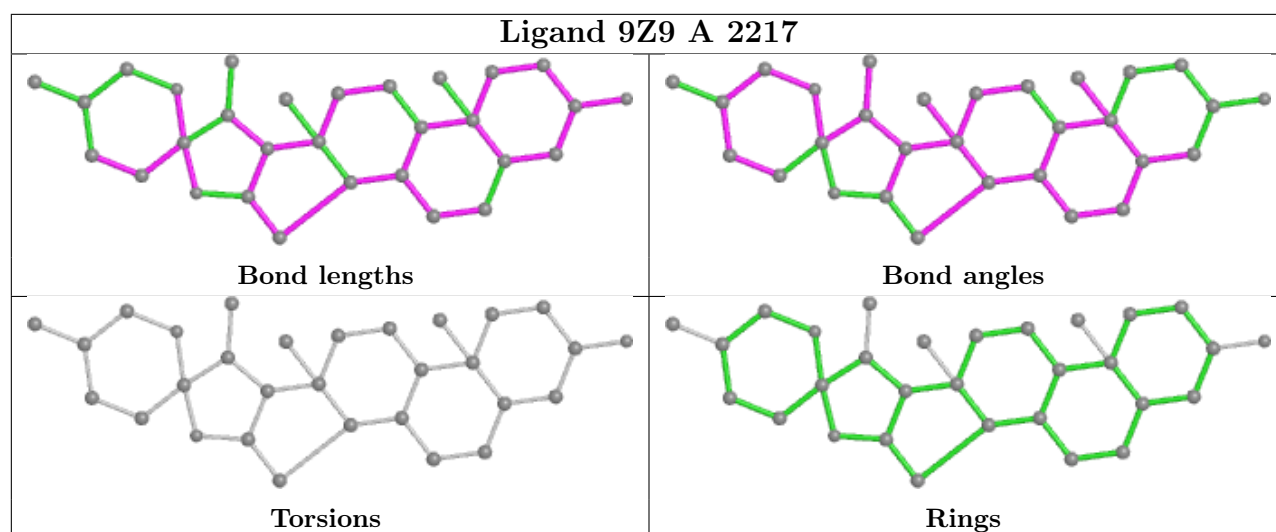












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

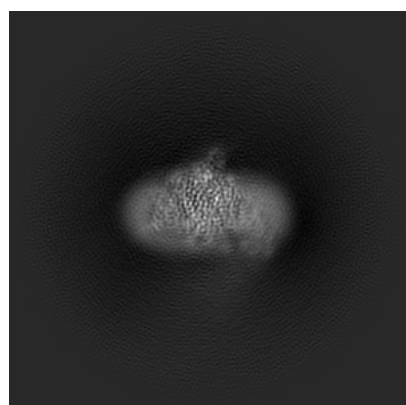
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31519. These allow visual inspection of the internal detail of the map and identification of artifacts.

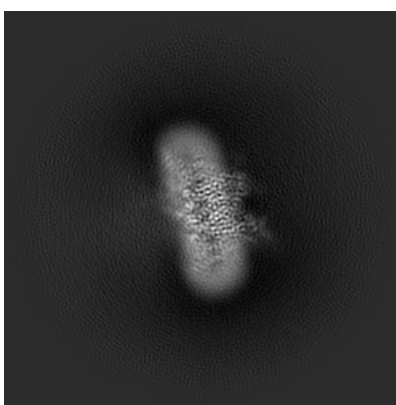
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

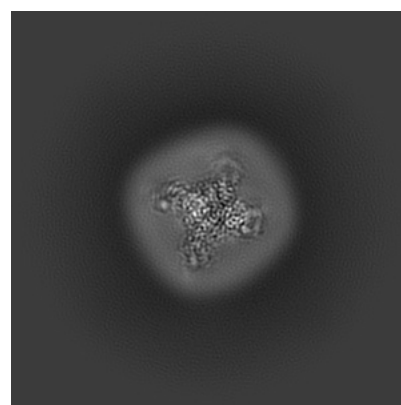
6.1.1 Primary map



X



Y

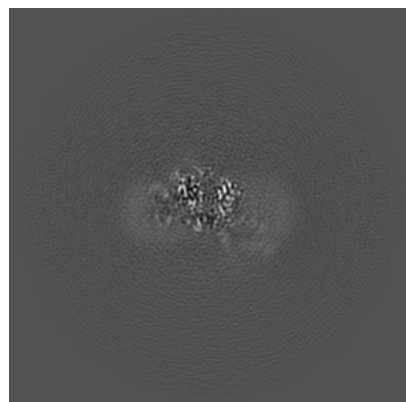


Z

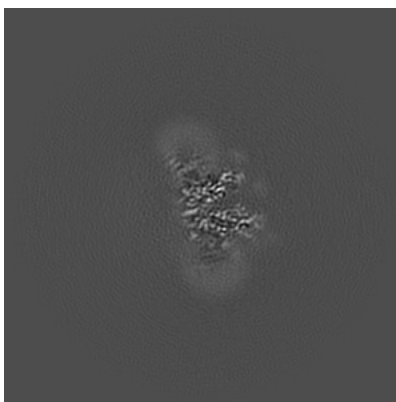
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

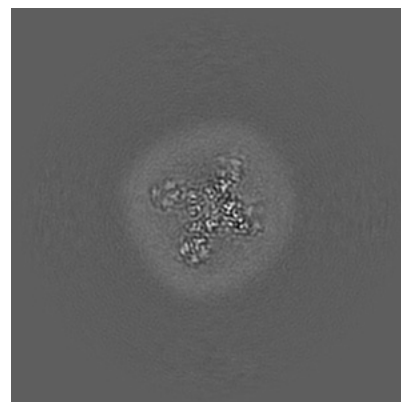
6.2.1 Primary map



X Index: 160



Y Index: 160

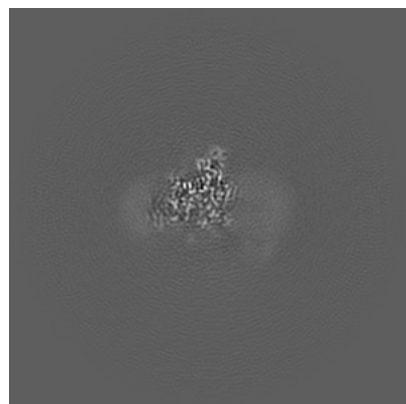


Z Index: 160

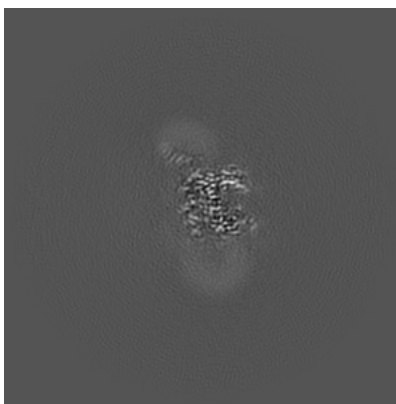
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

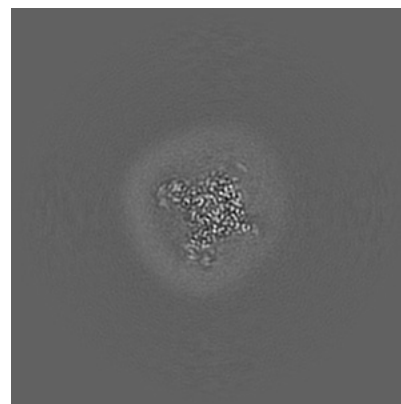
6.3.1 Primary map



X Index: 150



Y Index: 153

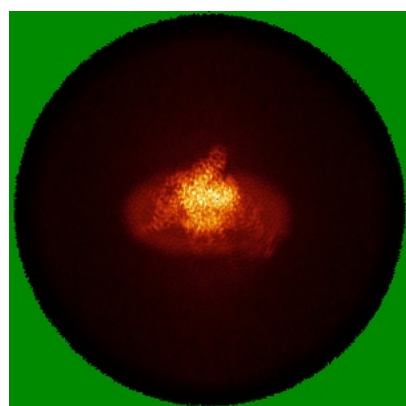


Z Index: 168

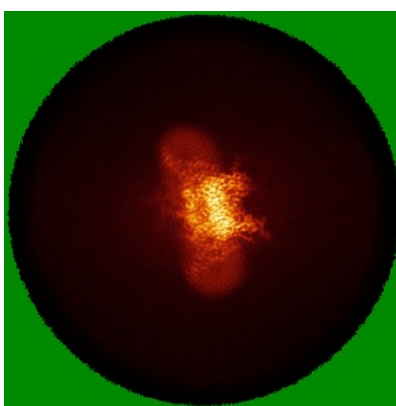
The images above show the largest variance slices of the map in three orthogonal directions.

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

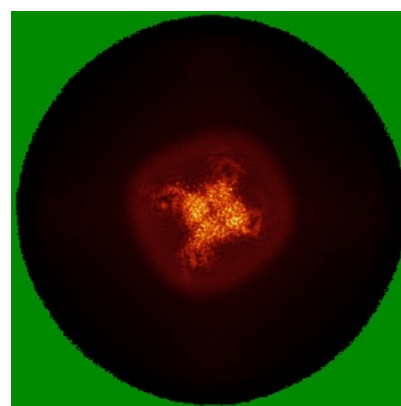
6.4.1 Primary map



X



Y

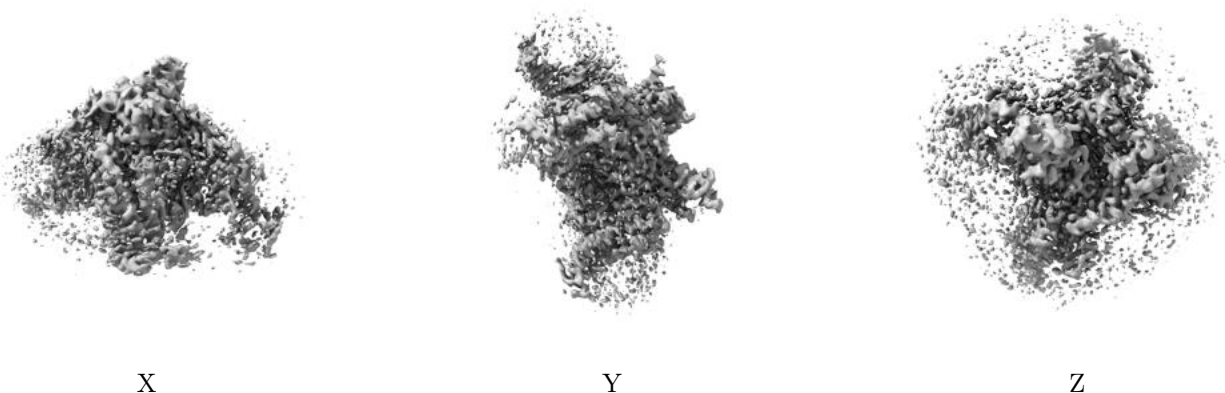


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

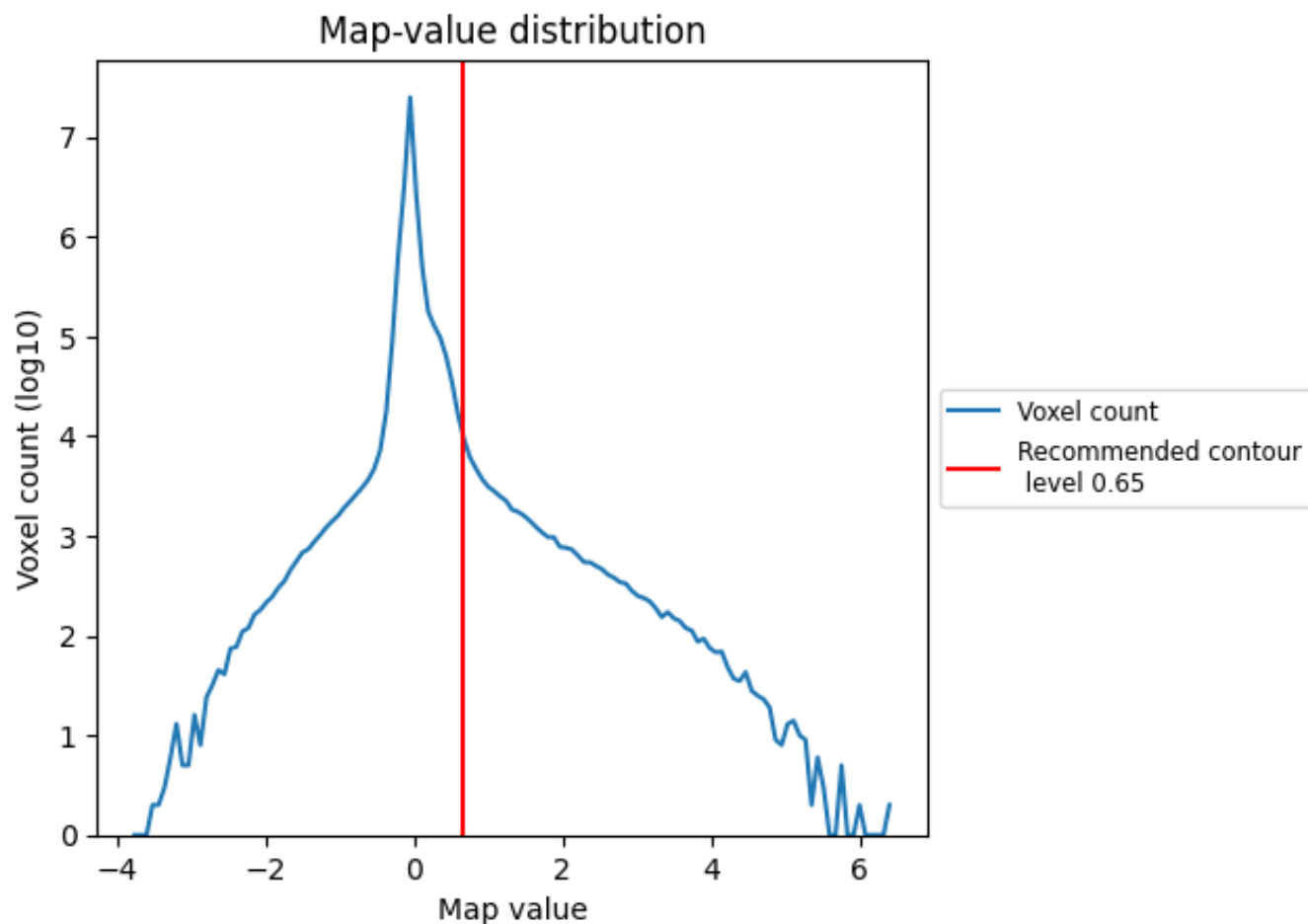
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

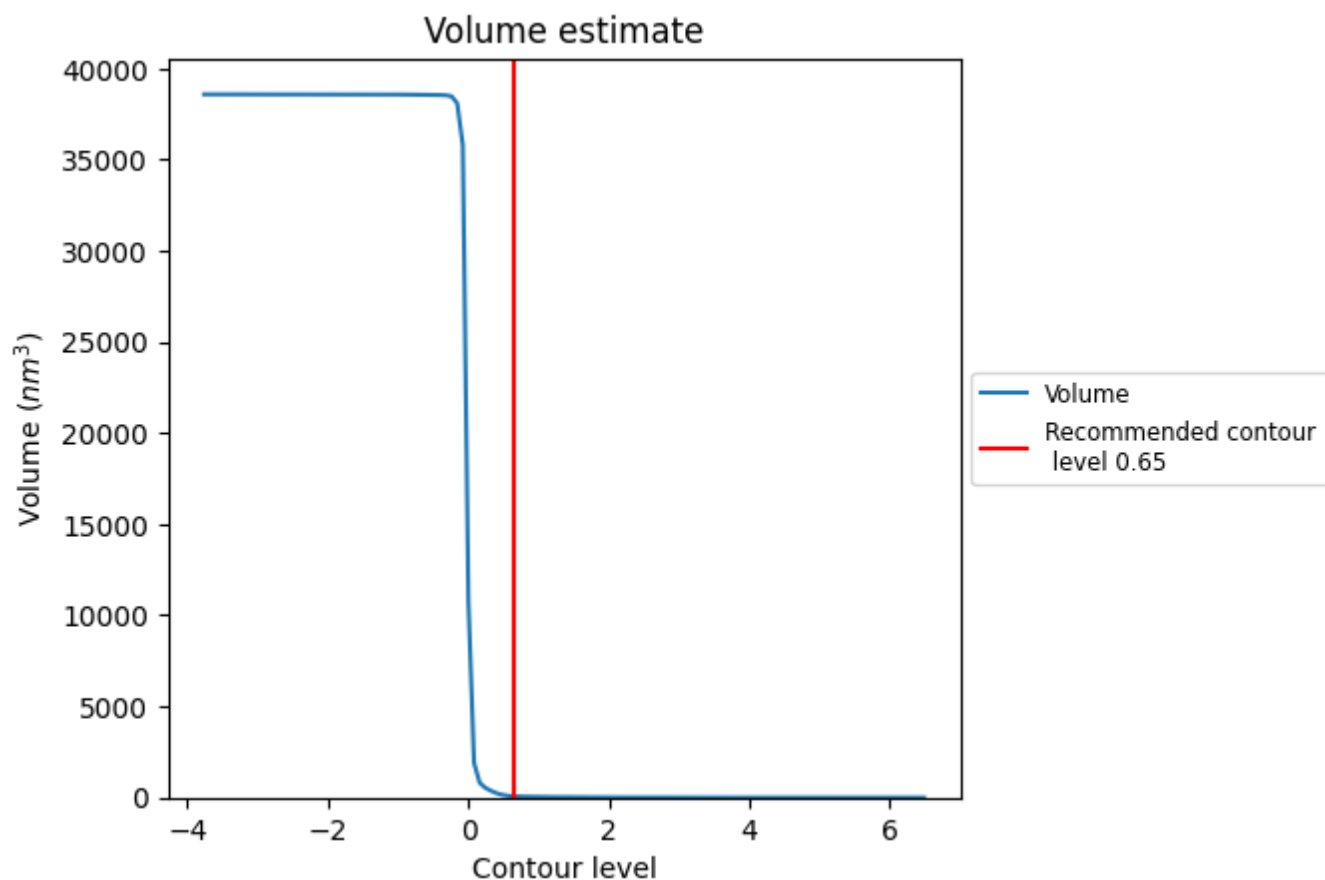
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

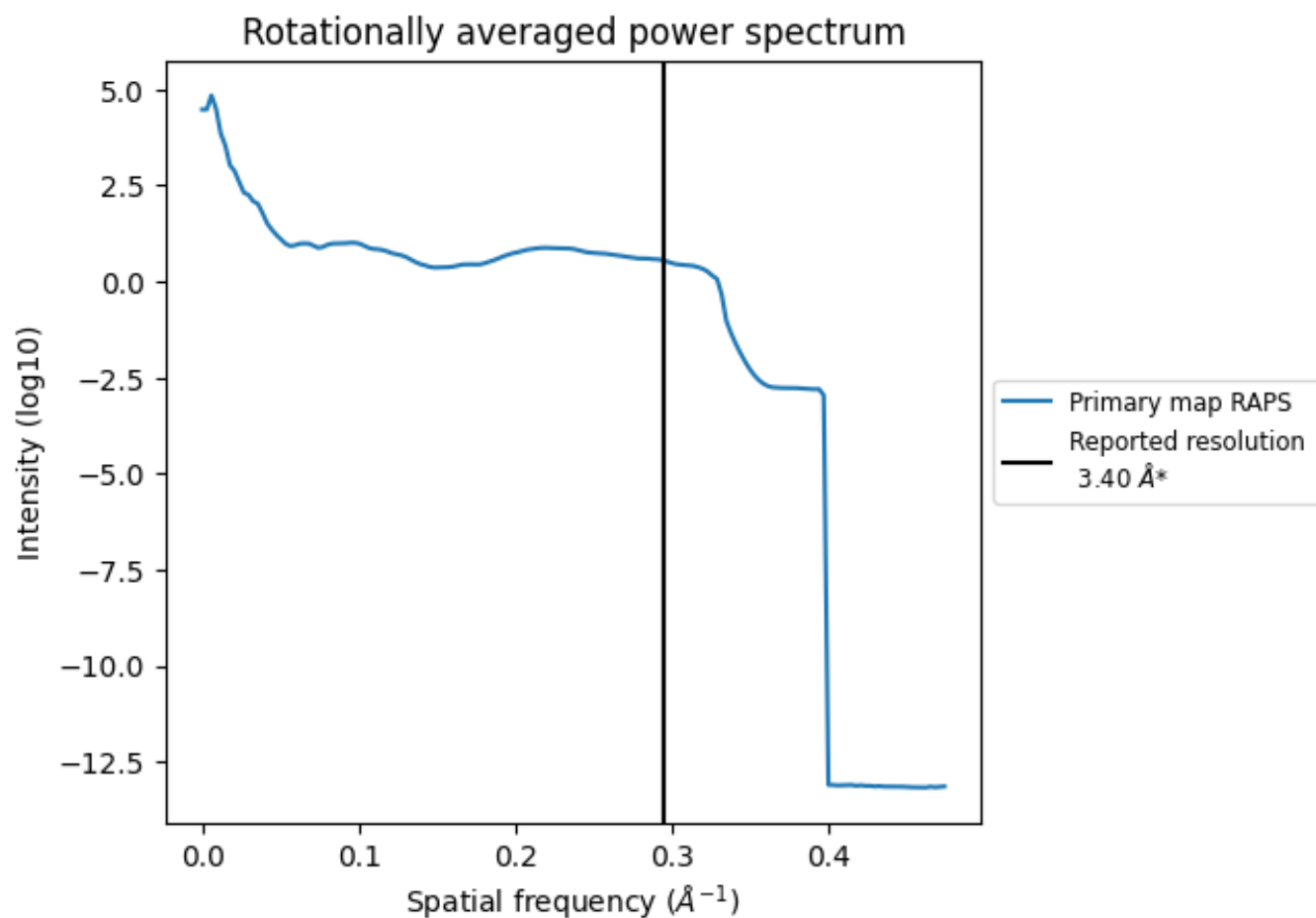
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm³; this corresponds to an approximate mass of 63 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 ⓘ

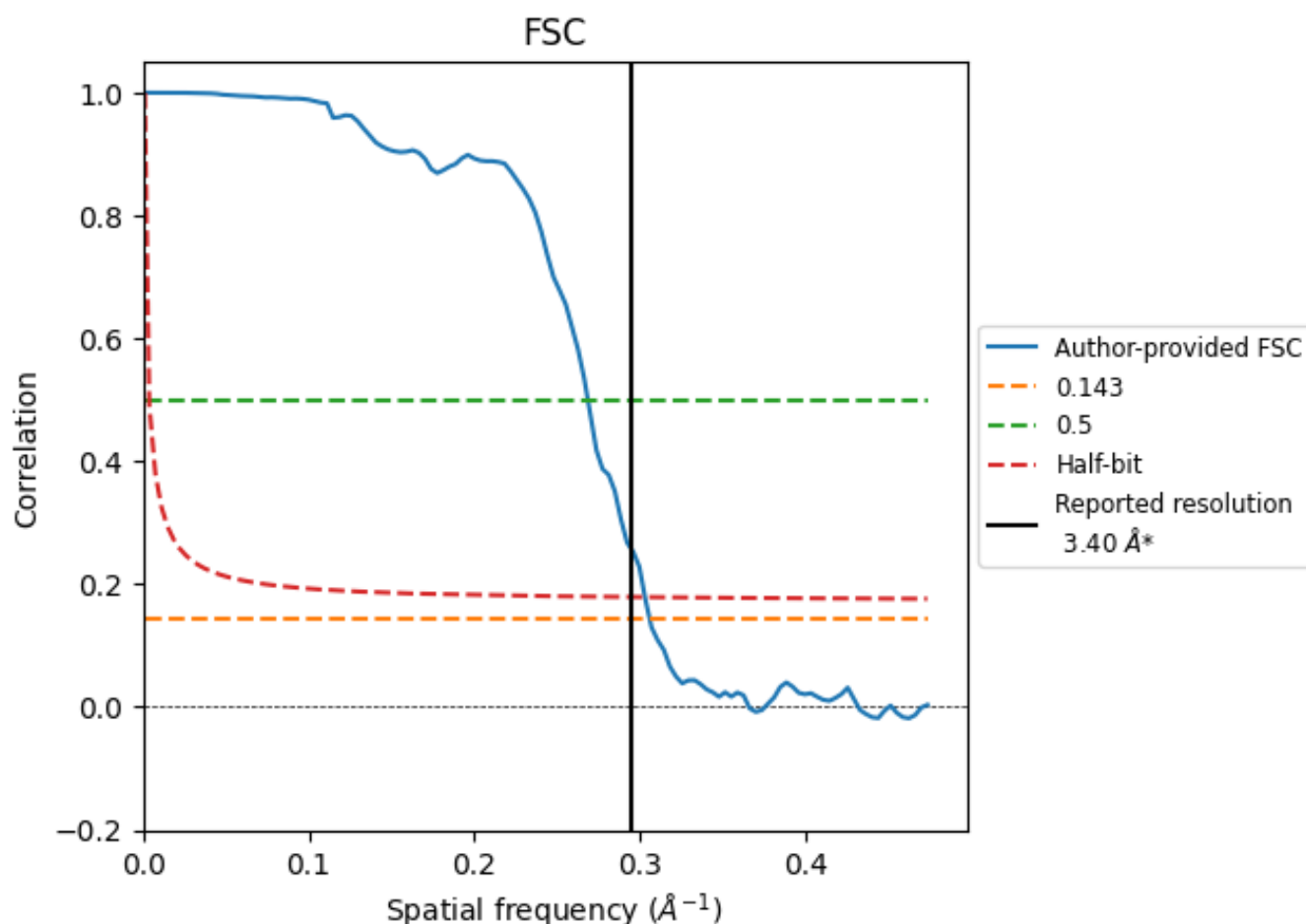


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

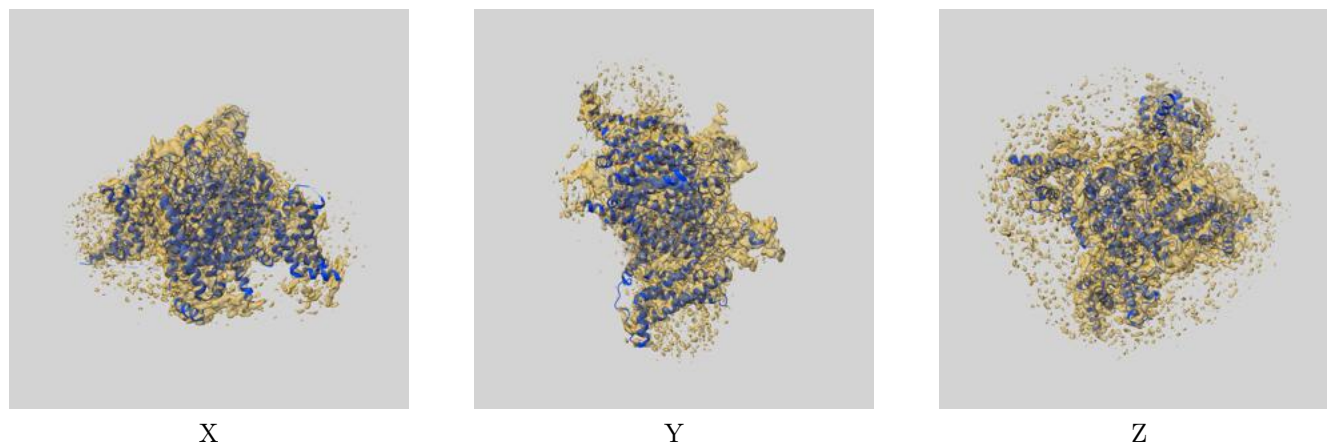
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.27	3.72	3.30
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

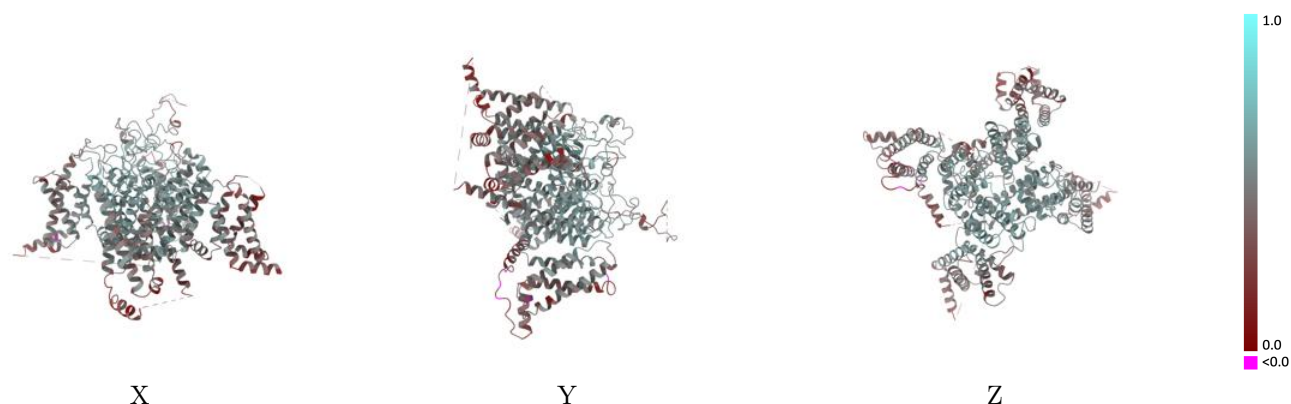
This section contains information regarding the fit between EMDB map EMD-31519 and PDB model 7FBS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



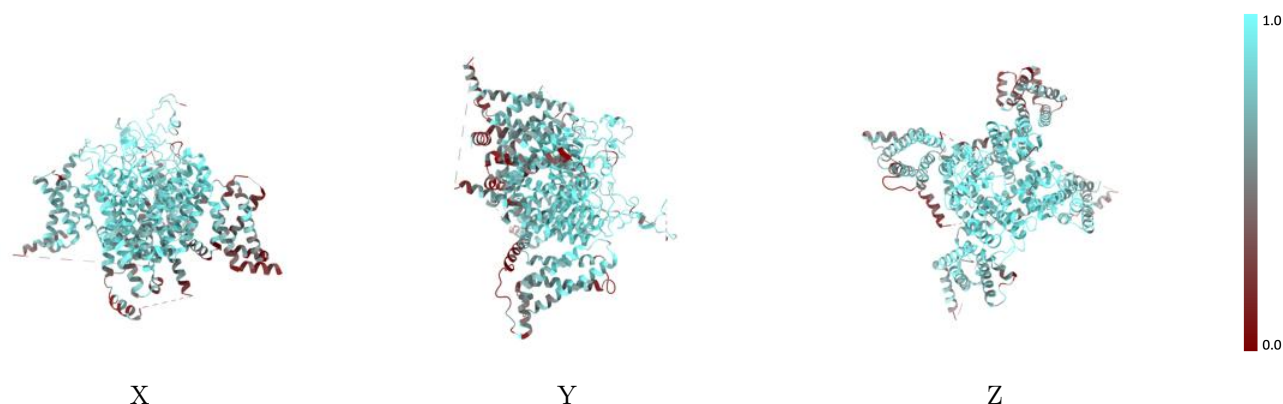
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



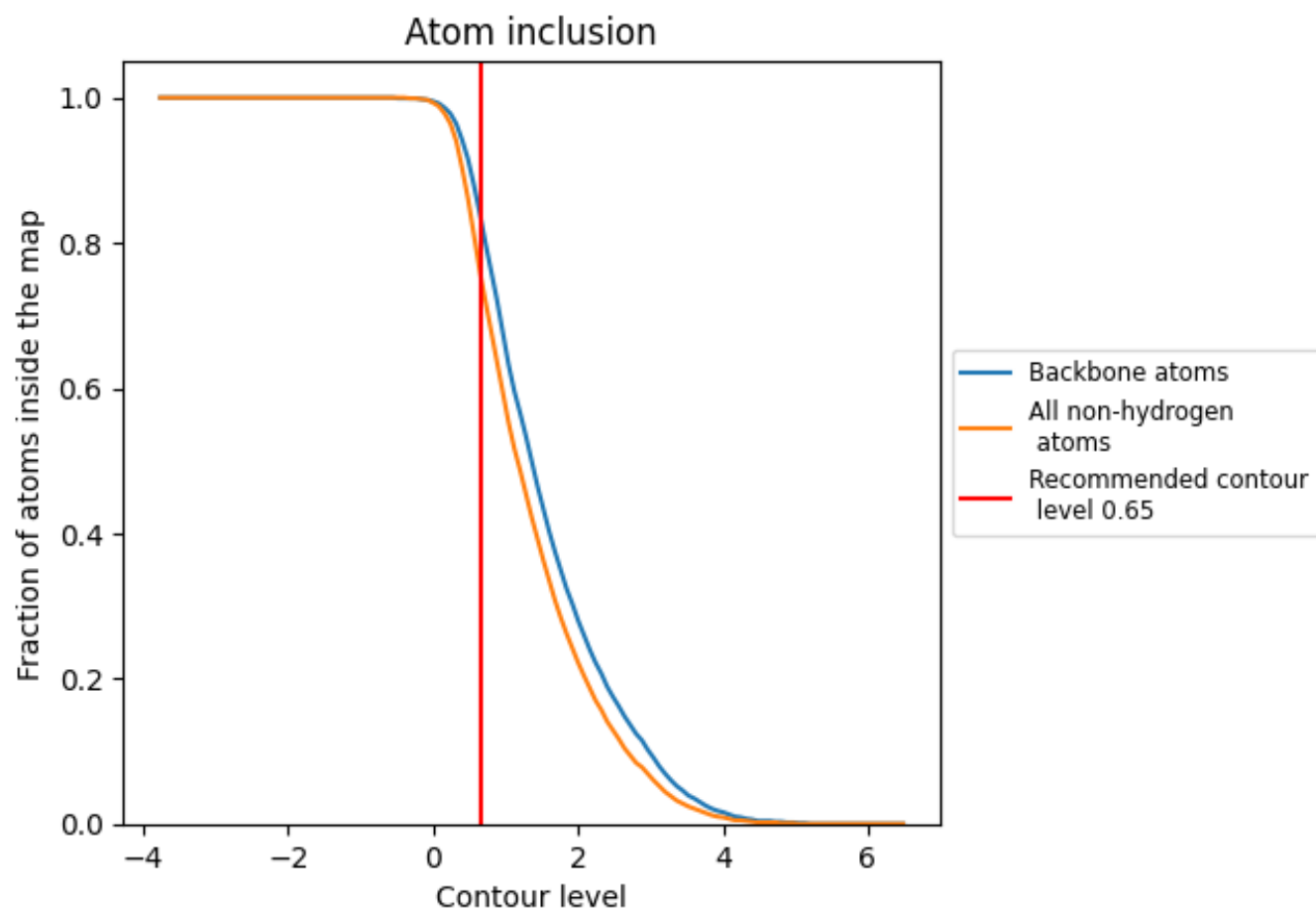
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7580	<div><div></div></div> 0.4770
A	<div><div></div></div> 0.7580	<div><div></div></div> 0.4770

