



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:47 PM UTC

PDB ID : 7XSU / pdb_00007xsu
EMDB ID : EMD-33435
Title : Cardiac sodium channel in complex with LqhIII
Authors : Jiang, D.; Catterall, W.A.
Deposited on : 2022-05-15
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

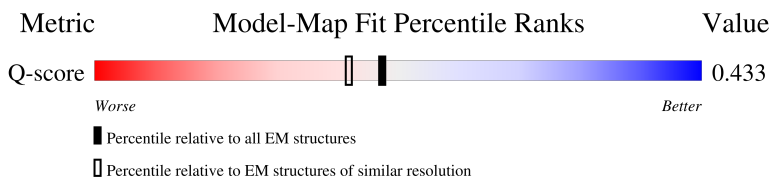
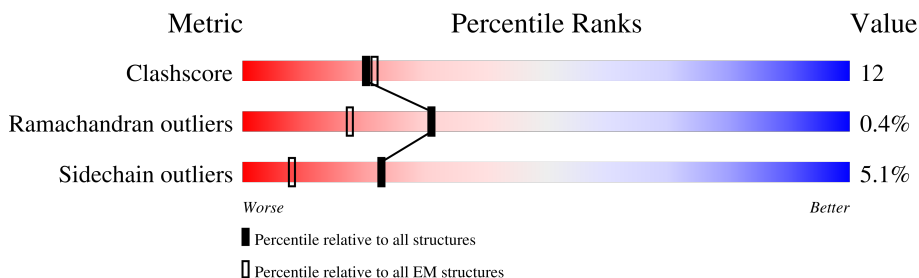
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	B	67	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8969 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,G protein/GFP fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1085	Total	C	N	O	S	0	0
			8247	5458	1304	1424	61		

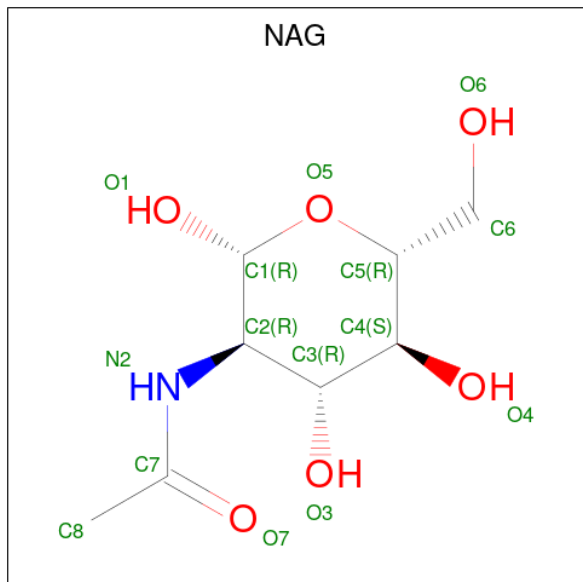
There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 a protein called Alpha-like toxin Lqh3.

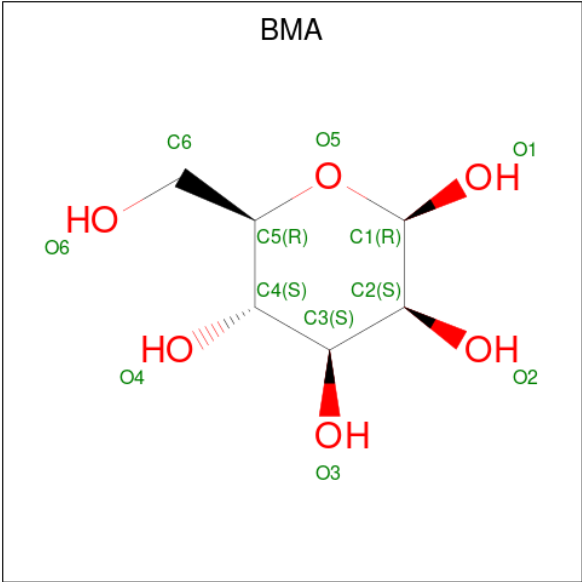
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	67	Total	C	N	O	S	0	0
			463	281	83	92	7		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



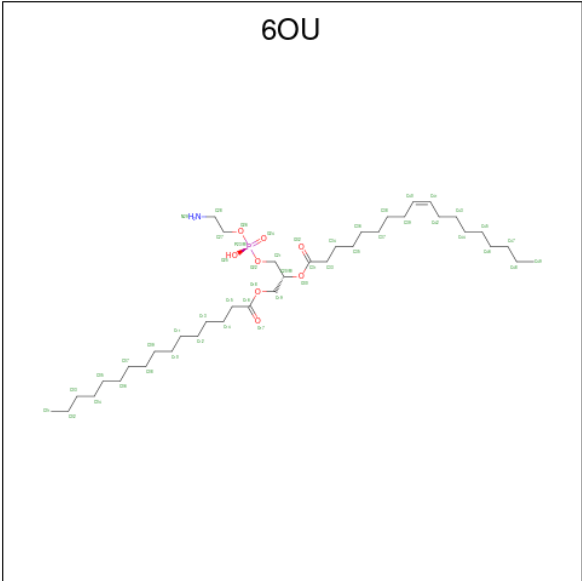
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			11	6	5	

- Molecule 5 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P).



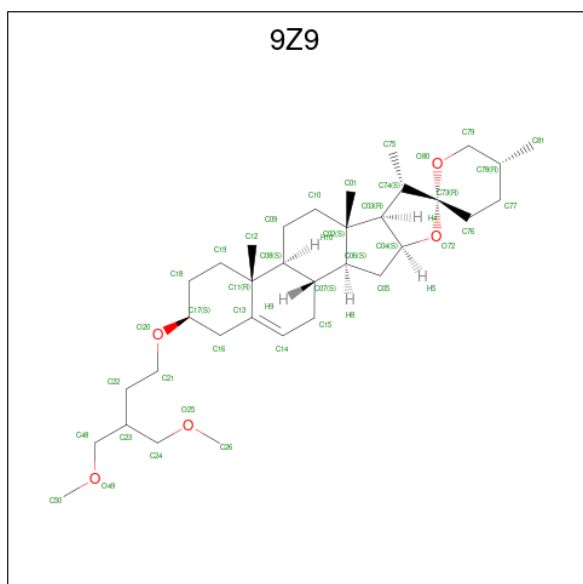
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
5	A	1	Total	C	N	O	P	0
			35	25	1	8	1	

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Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			15	12	3	
5	A	1	Total	C	O	0
			29	25	4	
5	A	1	Total	C	O	0
			17	15	2	
5	A	1	Total	C	O	0
			15	13	2	

- Molecule 6 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).

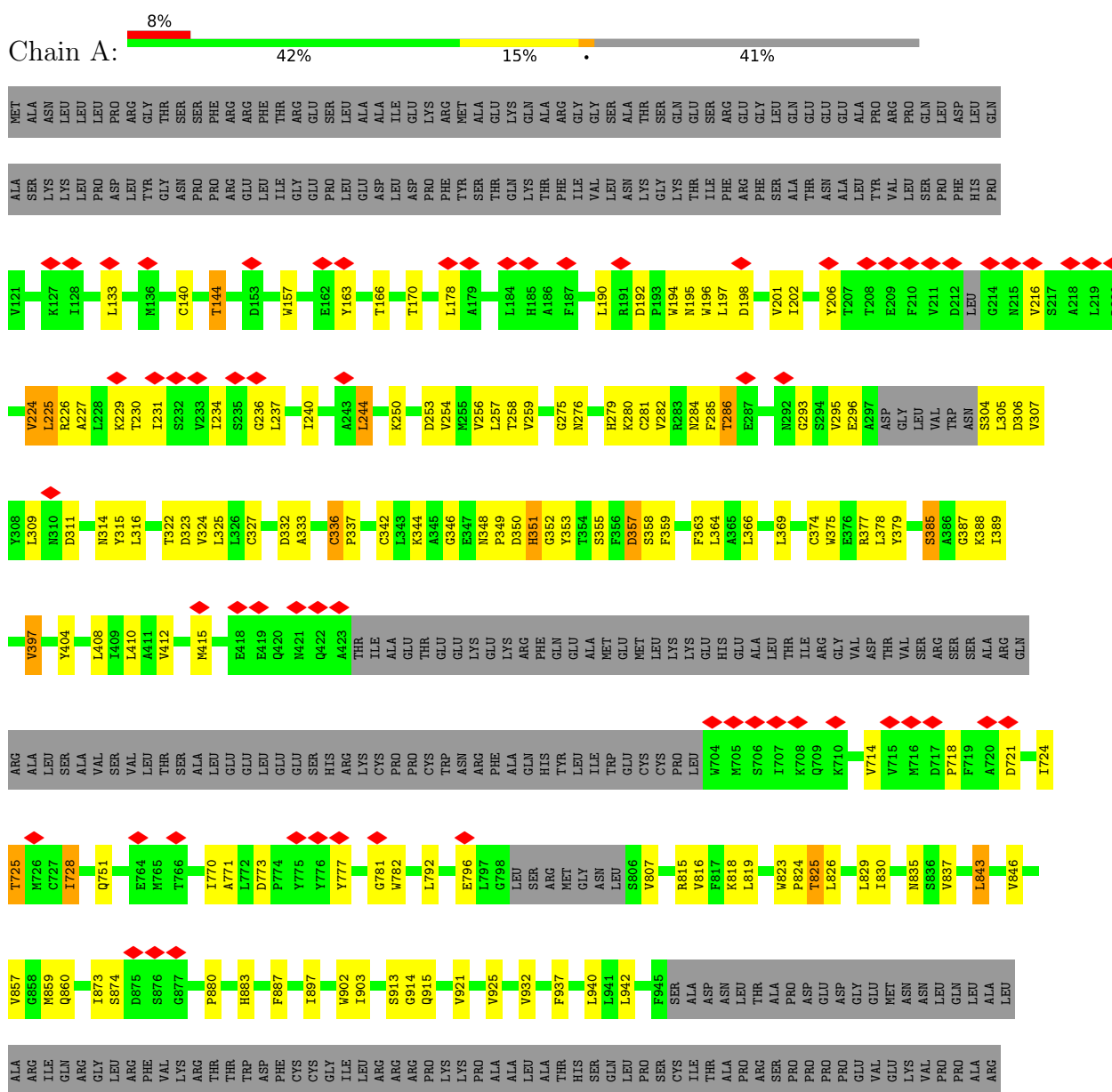


Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			32	29	3	

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: Sodium channel protein type 5 subunit alpha,G protein/GFP fusion protein





Opinion	Percentage
Best government	72%
Worst government	28%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198350	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.314	Depositor
Minimum map value	-2.786	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	270.336, 270.336, 270.336	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 9Z9, 6OU

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	0.59	0/8436	1.04	59/11493 (0.5%)
2	B	0.26	0/473	0.74	1/641 (0.2%)
All	All	0.58	0/8909	1.02	60/12134 (0.5%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	PRO	N-CA-C	17.67	148.87	112.47
1	A	1378	THR	N-CA-C	14.38	132.06	112.93
1	A	1379	ILE	N-CA-C	-13.52	100.95	111.90
1	A	350	ASP	N-CA-C	-12.21	95.77	112.12
1	A	1373	LEU	CA-C-N	11.88	132.29	120.52
1	A	1373	LEU	C-N-CA	11.88	132.29	120.52
1	A	349	PRO	CB-CA-C	-11.35	92.83	111.56
1	A	1641	GLY	N-CA-C	11.27	126.25	112.73
2	B	44	GLY	N-CA-C	9.44	122.87	112.29
1	A	285	PHE	N-CA-C	-9.28	95.43	108.23
1	A	1365	CYS	N-CA-C	8.50	121.56	110.43
1	A	1394	GLU	N-CA-C	8.04	120.04	111.28
1	A	286	THR	N-CA-CB	8.03	124.05	110.49
1	A	336	CYS	CA-C-N	7.61	127.56	120.03
1	A	336	CYS	C-N-CA	7.61	127.56	120.03
1	A	921	VAL	N-CA-C	7.58	117.65	110.53
1	A	902	TRP	N-CA-C	7.52	119.47	111.28
1	A	903	ILE	N-CA-C	7.41	118.18	110.62
1	A	385	SER	N-CA-C	7.38	119.12	111.14
1	A	1378	THR	CB-CA-C	-6.95	99.16	110.08
1	A	133	LEU	N-CA-C	-6.89	103.55	112.23
1	A	1554	GLN	N-CA-C	6.83	118.38	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	VAL	N-CA-C	-6.67	105.98	111.91
1	A	1358	PHE	N-CA-C	6.64	123.56	113.61
1	A	1680	ASN	N-CA-C	6.58	118.54	111.36
1	A	1614	ILE	N-CA-C	6.47	117.22	110.62
1	A	196	TRP	N-CA-C	-6.44	103.54	111.33
1	A	913	SER	N-CA-C	6.16	118.07	111.36
1	A	1430	ALA	N-CA-C	6.11	118.02	111.36
1	A	770	ILE	N-CA-C	6.04	116.82	110.72
1	A	1729	TYR	N-CA-C	6.02	117.84	111.28
1	A	284	ASN	N-CA-C	-5.95	101.23	110.10
1	A	1333	ILE	CB-CA-C	-5.94	108.06	114.35
1	A	1640	ARG	N-CA-C	5.91	117.80	111.36
1	A	1364	ARG	N-CA-C	5.82	123.20	110.80
1	A	1362	PHE	N-CA-C	5.68	118.25	111.71
1	A	1672	ILE	CB-CA-C	-5.67	104.49	112.14
1	A	1724	ASN	N-CA-C	5.65	118.43	109.96
1	A	1299	GLY	CA-C-N	5.63	127.53	121.00
1	A	1299	GLY	C-N-CA	5.63	127.53	121.00
1	A	1309	ALA	N-CA-C	-5.62	106.40	113.20
1	A	1688	ALA	CB-CA-C	-5.54	110.20	116.63
1	A	1376	ASN	N-CA-C	5.52	117.29	111.28
1	A	285	PHE	CB-CA-C	-5.49	102.55	113.80
1	A	397	VAL	N-CA-C	5.47	116.25	110.72
1	A	915	GLN	N-CA-C	5.43	117.20	111.28
1	A	357	ASP	CA-C-N	5.40	131.85	121.54
1	A	357	ASP	C-N-CA	5.40	131.85	121.54
1	A	286	THR	N-CA-C	-5.37	99.37	110.80
1	A	1550	GLU	N-CA-C	5.26	117.33	108.96
1	A	1426	ILE	CB-CA-C	-5.26	105.24	111.97
1	A	1697	GLN	N-CA-C	5.25	117.00	111.28
1	A	1262	ALA	N-CA-C	5.17	116.92	111.28
1	A	874	SER	N-CA-C	5.15	118.51	110.32
1	A	1722	ILE	CB-CA-C	-5.12	105.22	112.14
1	A	1337	MET	N-CA-C	5.07	116.81	111.28
1	A	914	GLY	N-CA-C	-5.05	105.10	111.72
1	A	1373	LEU	N-CA-C	5.02	116.02	109.64
1	A	781	GLY	N-CA-C	5.02	118.95	112.83
1	A	1754	PHE	N-CA-C	5.02	116.83	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8247	0	8073	199	0
2	B	463	0	405	8	0
3	A	70	0	65	7	0
4	A	11	0	10	0	0
5	A	146	0	0	1	0
6	A	32	0	0	3	0
All	All	8969	0	8553	213	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 12.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1283:VAL:HG21	1:A:1307:LEU:HD23	1.45	0.99
1:A:1283:VAL:HG21	1:A:1307:LEU:CD2	1.98	0.94
3:A:3001:NAG:H4	3:A:3002:NAG:H2	1.59	0.82
1:A:1283:VAL:CG2	1:A:1307:LEU:HD23	2.10	0.81
1:A:224:VAL:HG21	1:A:857:VAL:HG23	1.64	0.80
1:A:224:VAL:HG11	1:A:857:VAL:HG22	1.66	0.78
1:A:1675:ILE:HA	1:A:1678:MET:HE3	1.64	0.78
1:A:1668:LEU:O	1:A:1668:LEU:HD12	1.84	0.77
1:A:369:LEU:HD21	1:A:378:LEU:HD23	1.67	0.76
1:A:1623:LEU:HD23	1:A:1623:LEU:O	1.83	0.76
1:A:1774:LEU:CD2	6:A:3013:9Z9:C12	2.64	0.76
1:A:336:CYS:HB3	1:A:337:PRO:HD2	1.68	0.75
3:A:3001:NAG:H61	3:A:3002:NAG:H4	1.69	0.74
1:A:1292:THR:HG23	1:A:1293:LEU:HD13	1.69	0.74
1:A:721:ASP:HA	1:A:724:ILE:HG22	1.68	0.73
1:A:1774:LEU:HD21	6:A:3013:9Z9:C12	2.20	0.72
2:B:16:CYS:SG	2:B:17:PHE:N	2.61	0.72
1:A:1540:ILE:HG22	1:A:1632:ILE:HD11	1.73	0.71
1:A:1662:ILE:HG21	1:A:1768:MET:HB3	1.72	0.70
2:B:39:PHE:HA	2:B:45:LEU:HA	1.74	0.70
1:A:1708:GLN:HE21	1:A:1718:LEU:HD11	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ALA:O	1:A:230:THR:HG22	1.96	0.66
1:A:253:ASP:OD1	1:A:254:VAL:N	2.28	0.65
1:A:1316:LEU:HD23	1:A:1322:MET:HB3	1.80	0.63
1:A:1363:GLY:HA2	1:A:1399:LYS:HA	1.80	0.63
1:A:1441:GLN:HB2	1:A:1444:ASP:HB2	1.80	0.63
2:B:37:CYS:HA	2:B:47:CYS:HA	1.79	0.62
1:A:1336:ILE:O	1:A:1339:VAL:HG12	1.99	0.61
1:A:344:LYS:O	1:A:344:LYS:HD3	2.00	0.61
1:A:1445:ASN:O	1:A:1448:MET:HE2	2.01	0.60
1:A:296:GLU:HA	1:A:307:VAL:HG11	1.83	0.60
1:A:1602:ILE:HA	1:A:1605:ILE:HG22	1.82	0.59
1:A:258:THR:HG23	1:A:404:TYR:HE2	1.65	0.59
1:A:327:CYS:O	1:A:385:SER:HA	2.03	0.59
1:A:773:ASP:HB3	1:A:777:TYR:H	1.69	0.58
1:A:1610:LEU:O	1:A:1614:ILE:HG12	2.04	0.57
1:A:311:ASP:O	1:A:314:ASN:N	2.30	0.57
1:A:1623:LEU:HD23	1:A:1623:LEU:C	2.30	0.57
2:B:9:PRO:HA	2:B:10:GLU:C	2.29	0.57
1:A:1668:LEU:HD12	1:A:1668:LEU:C	2.29	0.56
1:A:280:LYS:HE2	1:A:324:VAL:HG11	1.88	0.56
1:A:410:LEU:HD21	1:A:1777:PHE:HE2	1.69	0.56
1:A:837:VAL:O	1:A:837:VAL:HG12	2.06	0.56
1:A:1283:VAL:HG21	1:A:1307:LEU:HD21	1.84	0.56
1:A:1774:LEU:HD23	6:A:3013:9Z9:C12	2.35	0.56
1:A:254:VAL:HG13	1:A:1648:LEU:HD22	1.87	0.56
1:A:1355:VAL:HG13	1:A:1359:ALA:HB2	1.88	0.56
1:A:1404:PHE:CD1	1:A:1404:PHE:N	2.74	0.56
1:A:1734:LEU:H	1:A:1742:GLY:HA2	1.71	0.55
1:A:244:LEU:HD21	1:A:932:VAL:HG12	1.88	0.55
1:A:281:CYS:SG	1:A:327:CYS:HB3	2.47	0.55
1:A:1201:TYR:CD2	1:A:1201:TYR:C	2.85	0.55
1:A:807:VAL:HG22	1:A:807:VAL:O	2.06	0.54
1:A:1461:PHE:CD2	1:A:1461:PHE:C	2.85	0.54
1:A:170:THR:HG22	1:A:202:ILE:HD12	1.90	0.54
1:A:1373:LEU:HD12	1:A:1373:LEU:O	2.07	0.54
1:A:190:LEU:HD22	1:A:195:ASN:HD22	1.72	0.54
1:A:937:PHE:C	1:A:937:PHE:CD1	2.85	0.54
1:A:1363:GLY:HA3	1:A:1397:TRP:CH2	2.42	0.54
1:A:275:GLY:HA3	1:A:1552:ASP:OD2	2.08	0.54
1:A:1323:ARG:O	1:A:1326:VAL:HG12	2.08	0.54
1:A:1526:ILE:HG22	1:A:1526:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:GLN:OE1	1:A:860:GLN:HA	2.08	0.54
1:A:887:PHE:CD2	1:A:887:PHE:C	2.86	0.54
1:A:1746:SER:HB3	1:A:1749:VAL:HG12	1.89	0.54
1:A:357:ASP:HB2	1:A:1552:ASP:HB2	1.90	0.53
2:B:32:GLY:HA3	2:B:49:CYS:SG	2.47	0.53
1:A:316:LEU:HD23	1:A:325:LEU:HD23	1.91	0.53
1:A:1752:LEU:HD12	1:A:1752:LEU:O	2.09	0.52
1:A:363:PHE:C	1:A:363:PHE:CD1	2.87	0.52
1:A:364:LEU:O	1:A:364:LEU:HD12	2.08	0.52
1:A:1416:GLN:HG2	1:A:1715:TRP:CZ2	2.44	0.52
1:A:829:LEU:HB2	1:A:1466:LEU:HD22	1.90	0.52
1:A:1436:TYR:CD2	1:A:1437:GLU:HG2	2.44	0.52
1:A:829:LEU:HD21	1:A:1346:PHE:CD2	2.44	0.52
1:A:1576:GLU:OE2	1:A:1576:GLU:HA	2.10	0.52
1:A:258:THR:HG23	1:A:404:TYR:CE2	2.45	0.52
1:A:1333:ILE:N	1:A:1334:PRO:HD2	2.26	0.51
1:A:293:GLY:HA3	1:A:304:SER:N	2.24	0.51
1:A:1731:ASP:OD2	1:A:1732:PRO:HD2	2.10	0.51
1:A:1268:TYR:CE1	1:A:1274:CYS:HB3	2.46	0.51
1:A:1282:ASP:HA	1:A:1285:LEU:HG	1.93	0.51
1:A:1365:CYS:SG	1:A:1366:ILE:N	2.84	0.50
1:A:1326:VAL:HG13	1:A:1327:ASN:N	2.26	0.50
1:A:1540:ILE:CG2	1:A:1632:ILE:HD11	2.39	0.50
1:A:336:CYS:CB	1:A:337:PRO:HD2	2.38	0.50
1:A:940:LEU:HB2	1:A:1465:ASN:HD21	1.77	0.50
1:A:323:ASP:OD2	1:A:377:ARG:NH2	2.37	0.50
1:A:1336:ILE:O	1:A:1339:VAL:CG1	2.60	0.50
1:A:276:ASN:OD1	1:A:279:HIS:NE2	2.41	0.50
1:A:224:VAL:HG11	1:A:857:VAL:CG2	2.37	0.50
1:A:332:ASP:HB3	1:A:388:LYS:H	1.77	0.50
1:A:714:VAL:HG23	1:A:771:ALA:CB	2.42	0.50
1:A:1730:CYS:SG	1:A:1731:ASP:N	2.85	0.49
1:A:250:LYS:HB3	1:A:415:MET:CE	2.42	0.49
1:A:1517:ASN:HB3	1:A:1520:GLN:HB3	1.95	0.49
1:A:782:TRP:HZ2	1:A:818:LYS:HA	1.77	0.49
1:A:1297:GLU:HA	1:A:1301:ILE:HD11	1.95	0.49
3:A:3004:NAG:HN2	3:A:3004:NAG:H5	1.77	0.49
1:A:256:VAL:HA	1:A:259:VAL:HG22	1.94	0.48
1:A:1373:LEU:HD12	1:A:1373:LEU:C	2.38	0.48
1:A:1671:PHE:CE1	1:A:1675:ILE:HD11	2.48	0.48
1:A:234:ILE:HG22	1:A:236:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:VAL:HG23	1:A:771:ALA:HB2	1.95	0.48
1:A:359:PHE:CD1	1:A:359:PHE:C	2.92	0.48
1:A:355:SER:OG	1:A:357:ASP:OD2	2.29	0.48
1:A:1431:VAL:O	1:A:1431:VAL:HG23	2.13	0.48
1:A:1204:VAL:HA	1:A:1209:PHE:CD2	2.48	0.48
1:A:1283:VAL:HG13	1:A:1304:LEU:HD12	1.96	0.48
1:A:823:TRP:HD1	1:A:824:PRO:HD2	1.79	0.47
1:A:170:THR:HG21	1:A:206:TYR:OH	2.14	0.47
1:A:1373:LEU:HB2	1:A:1374:PRO:HD2	1.95	0.47
1:A:1639:ILE:HG23	1:A:1639:ILE:O	2.13	0.47
2:B:4:GLY:HA2	2:B:48:TRP:CH2	2.50	0.47
1:A:410:LEU:HD22	1:A:1773:ILE:HG12	1.96	0.47
1:A:897:ILE:HG21	1:A:925:VAL:HG12	1.97	0.47
1:A:240:ILE:HD13	1:A:843:LEU:HD22	1.96	0.46
1:A:1282:ASP:HA	1:A:1285:LEU:CD2	2.45	0.46
1:A:1623:LEU:C	1:A:1623:LEU:CD2	2.88	0.46
1:A:244:LEU:CD2	1:A:932:VAL:HG12	2.45	0.46
1:A:1662:ILE:HG21	1:A:1768:MET:CB	2.42	0.46
1:A:351:HIS:HB3	1:A:353:TYR:CD2	2.51	0.46
1:A:140:CYS:O	1:A:144:THR:HG22	2.15	0.46
1:A:237:LEU:HD22	1:A:846:VAL:HG23	1.98	0.46
1:A:254:VAL:O	1:A:258:THR:OG1	2.29	0.46
1:A:792:LEU:HD23	1:A:792:LEU:HA	1.80	0.46
1:A:198:ASP:O	1:A:201:VAL:HG22	2.15	0.46
3:A:3001:NAG:C6	3:A:3002:NAG:H4	2.43	0.46
1:A:332:ASP:HB3	1:A:388:LYS:HB2	1.97	0.46
1:A:1427:MET:HE2	1:A:1452:PHE:HB3	1.98	0.46
1:A:1595:ILE:HA	1:A:1598:PHE:CD1	2.51	0.46
1:A:226:ARG:O	1:A:229:LYS:HB2	2.16	0.46
1:A:333:ALA:CA	1:A:387:GLY:HA2	2.46	0.45
1:A:825:THR:HB	1:A:1342:VAL:HG21	1.98	0.45
2:B:59:ILE:O	2:B:59:ILE:HG13	2.17	0.45
1:A:1448:MET:C	1:A:1450:ILE:N	2.73	0.45
1:A:363:PHE:CD1	1:A:363:PHE:O	2.70	0.44
1:A:1257:LEU:C	1:A:1257:LEU:HD12	2.42	0.44
1:A:389:ILE:O	1:A:389:ILE:HG12	2.17	0.44
1:A:728:ILE:HD11	1:A:816:VAL:HA	1.98	0.44
1:A:1408:GLY:O	5:A:3010:6OU:C13	2.65	0.44
1:A:1555:SER:HB3	1:A:1558:LYS:CB	2.47	0.44
2:B:66:HIS:ND1	2:B:66:HIS:N	2.64	0.44
1:A:1305:ARG:O	1:A:1308:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1426:ILE:N	1:A:1426:ILE:HD13	2.33	0.44
1:A:231:ILE:HG23	1:A:237:LEU:HB3	2.00	0.44
1:A:1382:ASN:CG	3:A:3001:NAG:H2	2.43	0.44
1:A:1746:SER:HA	1:A:1747:PRO:HD3	1.84	0.44
1:A:333:ALA:HA	1:A:387:GLY:HA2	1.98	0.43
1:A:348:ASN:CB	1:A:352:GLY:HA2	2.49	0.43
1:A:1404:PHE:H	1:A:1404:PHE:HD1	1.63	0.43
1:A:192:ASP:OD2	1:A:194:TRP:N	2.51	0.43
1:A:286:THR:HG22	1:A:286:THR:O	2.18	0.43
1:A:942:LEU:HD12	1:A:942:LEU:HA	1.82	0.43
1:A:282:VAL:HG22	1:A:315:TYR:CE1	2.54	0.43
1:A:1428:TYR:N	1:A:1428:TYR:CD1	2.86	0.43
1:A:1307:LEU:C	1:A:1309:ALA:H	2.26	0.43
1:A:1726:GLY:HA2	1:A:1727:PRO:HD3	1.86	0.43
1:A:830:ILE:HD13	1:A:830:ILE:HA	1.81	0.43
1:A:1693:MET:HE2	1:A:1693:MET:HB3	1.56	0.43
1:A:1723:LEU:HD21	1:A:1751:ILE:HD11	1.99	0.43
1:A:280:LYS:HD2	1:A:346:GLY:HA3	1.99	0.43
1:A:751:GLN:HA	1:A:751:GLN:OE1	2.18	0.42
1:A:295:VAL:C	1:A:307:VAL:HG21	2.44	0.42
1:A:796:GLU:CD	1:A:796:GLU:C	2.87	0.42
3:A:3004:NAG:H5	3:A:3004:NAG:N2	2.32	0.42
1:A:940:LEU:HB2	1:A:1465:ASN:ND2	2.35	0.42
1:A:1322:MET:HE3	1:A:1664:LEU:HG	2.01	0.42
1:A:1610:LEU:O	1:A:1610:LEU:HG	2.19	0.42
1:A:1656:LEU:N	1:A:1657:PRO:CD	2.82	0.42
1:A:1753:PHE:CD2	1:A:1753:PHE:C	2.97	0.42
1:A:195:ASN:N	1:A:195:ASN:OD1	2.51	0.42
1:A:364:LEU:HD12	1:A:364:LEU:C	2.44	0.42
1:A:1671:PHE:O	1:A:1671:PHE:HD1	2.01	0.42
1:A:1217:ILE:HD12	1:A:1315:ALA:HA	2.02	0.42
1:A:322:THR:HG23	1:A:322:THR:O	2.20	0.42
1:A:305:LEU:O	1:A:309:LEU:HB3	2.19	0.42
1:A:724:ILE:HD12	1:A:724:ILE:HA	1.92	0.42
1:A:369:LEU:CD2	1:A:375:TRP:HB2	2.49	0.42
1:A:1237:ILE:HG22	1:A:1241:LEU:HD23	2.01	0.42
1:A:1289:VAL:HA	1:A:1292:THR:HG22	2.02	0.42
1:A:1361:LYS:HB3	1:A:1433:SER:HB2	2.01	0.41
1:A:1361:LYS:HZ2	1:A:1436:TYR:HA	1.85	0.41
1:A:859:MET:HE2	1:A:859:MET:HB3	1.91	0.41
1:A:363:PHE:C	1:A:363:PHE:HD1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:THR:HG23	1:A:819:LEU:CD2	2.51	0.41
1:A:342:CYS:O	1:A:342:CYS:SG	2.79	0.41
1:A:1271:ASN:HD22	1:A:1271:ASN:HA	1.62	0.41
1:A:282:VAL:HG22	1:A:315:TYR:CD1	2.56	0.41
1:A:389:ILE:O	1:A:389:ILE:CG1	2.68	0.41
1:A:1562:LEU:HD13	1:A:1562:LEU:HA	1.94	0.41
1:A:1694:PHE:HB3	1:A:1705:CYS:SG	2.61	0.41
1:A:374:CYS:O	1:A:374:CYS:SG	2.79	0.41
1:A:1649:LEU:HD23	1:A:1649:LEU:HA	1.88	0.41
1:A:1699:PHE:CD2	1:A:1699:PHE:C	2.99	0.41
1:A:815:ARG:HG2	1:A:818:LYS:NZ	2.36	0.41
1:A:1231:LEU:HA	1:A:1231:LEU:HD23	1.59	0.41
1:A:224:VAL:O	1:A:225:LEU:C	2.63	0.40
1:A:1662:ILE:CG2	1:A:1768:MET:HB3	2.46	0.40
1:A:1674:SER:HB2	1:A:1702:SER:HB3	2.03	0.40
1:A:163:TYR:HA	1:A:166:THR:OG1	2.21	0.40
1:A:1254:LEU:O	1:A:1257:LEU:HG	2.22	0.40
1:A:1402:VAL:HG22	1:A:1412:LEU:HD21	2.03	0.40
1:A:880:PRO:HG2	1:A:883:HIS:HB3	2.02	0.40
1:A:1536:ILE:H	1:A:1536:ILE:HG13	1.53	0.40
1:A:1705:CYS:O	1:A:1708:GLN:HG2	2.22	0.40
1:A:1213:ILE:HD13	1:A:1213:ILE:HA	1.96	0.40
1:A:1292:THR:HG23	1:A:1293:LEU:CD1	2.45	0.40
1:A:1723:LEU:HD21	1:A:1751:ILE:CG1	2.50	0.40
1:A:1772:ILE:HD13	1:A:1772:ILE:HA	1.80	0.40
3:A:3004:NAG:H62	3:A:3005:NAG:H2	2.03	0.40
1:A:1373:LEU:HB2	1:A:1374:PRO:CD	2.51	0.40
1:A:1443:GLU:O	1:A:1444:ASP:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1071/1838 (58%)	1019 (95%)	47 (4%)	5 (0%)	24	54
2	B	65/67 (97%)	50 (77%)	15 (23%)	0	100	100
All	All	1136/1905 (60%)	1069 (94%)	62 (6%)	5 (0%)	31	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	718	PRO
1	A	225	LEU
1	A	1364	ARG
1	A	157	TRP
1	A	358	SER

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	843/1612 (52%)	802 (95%)	41 (5%)	22	49
2	B	47/53 (89%)	43 (92%)	4 (8%)	10	33
All	All	890/1665 (54%)	845 (95%)	45 (5%)	23	48

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	THR
1	A	178	LEU
1	A	197	LEU
1	A	224	VAL
1	A	244	LEU
1	A	257	LEU
1	A	306	ASP
1	A	351	HIS
1	A	366	LEU
1	A	379	TYR
1	A	397	VAL

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Mol	Chain	Res	Type
1	A	408	LEU
1	A	412	VAL
1	A	725	THR
1	A	728	ILE
1	A	825	THR
1	A	826	LEU
1	A	835	ASN
1	A	843	LEU
1	A	873	ILE
1	A	1217	ILE
1	A	1253	VAL
1	A	1301	ILE
1	A	1304	LEU
1	A	1313	LEU
1	A	1345	ILE
1	A	1379	ILE
1	A	1402	VAL
1	A	1404	PHE
1	A	1426	ILE
1	A	1431	VAL
1	A	1474	ASN
1	A	1536	ILE
1	A	1538	PHE
1	A	1540	ILE
1	A	1619	PHE
1	A	1626	VAL
1	A	1647	THR
1	A	1665	LEU
1	A	1668	LEU
1	A	1722	ILE
2	B	27	CYS
2	B	29	GLU
2	B	41	VAL
2	B	65	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	827	ASN
1	A	865	ASN
1	A	1271	ASN
1	A	1356	ASN

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Mol	Chain	Res	Type
1	A	1381	ASN
1	A	1382	ASN
1	A	1406	ASN
1	A	1517	ASN
1	A	1680	ASN
1	A	1708	GLN
2	B	43	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 ⓘ

13 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
5	6OU	A	3012	-	14,14,48	1.46	3 (21%)	14,14,53	1.30	2 (14%)
5	6OU	A	3007	-	34,34,48	1.06	2 (5%)	37,39,53	1.31	3 (8%)
3	NAG	A	3002	-	14,14,15	0.31	0	17,19,21	0.85	0
3	NAG	A	3003	-	14,14,15	0.31	0	17,19,21	1.20	3 (17%)
5	6OU	A	3009	-	14,14,48	0.94	1 (7%)	14,14,53	1.29	1 (7%)
5	6OU	A	3008	-	34,34,48	1.06	3 (8%)	37,39,53	1.24	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	6OU	A	3011	-	16,16,48	1.36	3 (18%)	16,16,53	1.34	2 (12%)
3	NAG	A	3004	-	14,14,15	0.42	0	17,19,21	0.95	0
3	NAG	A	3005	-	14,14,15	0.35	0	17,19,21	1.10	2 (11%)
3	NAG	A	3001	-	14,14,15	0.30	0	17,19,21	1.03	2 (11%)
6	9Z9	A	3013	-	37,37,44	4.52	19 (51%)	58,60,68	3.92	29 (50%)
4	BMA	A	3006	-	11,11,12	0.25	0	15,15,17	0.76	0
5	6OU	A	3010	-	28,28,48	1.22	3 (10%)	30,30,53	1.43	3 (10%)

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
5	6OU	A	3012	-	-	4/13/13/52	-
5	6OU	A	3007	-	-	15/38/38/52	-
3	NAG	A	3002	-	-	0/6/23/26	0/1/1/1
3	NAG	A	3003	-	-	3/6/23/26	0/1/1/1
5	6OU	A	3009	-	-	3/13/13/52	-
5	6OU	A	3008	-	-	16/38/38/52	-
5	6OU	A	3011	-	-	5/15/15/52	-
3	NAG	A	3004	-	-	2/6/23/26	0/1/1/1
3	NAG	A	3005	-	-	4/6/23/26	0/1/1/1
3	NAG	A	3001	-	-	4/6/23/26	0/1/1/1
6	9Z9	A	3013	-	-	3/3/91/100	0/6/6/6
4	BMA	A	3006	-	-	0/2/19/22	0/1/1/1
5	6OU	A	3010	-	-	9/29/29/52	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3013	9Z9	C14-C13	16.69	1.67	1.33
6	A	3013	9Z9	C10-C02	-8.68	1.39	1.54
6	A	3013	9Z9	O72-C04	-7.87	1.26	1.43
6	A	3013	9Z9	O72-C73	6.99	1.57	1.42
6	A	3013	9Z9	C10-C09	5.88	1.65	1.53
6	A	3013	9Z9	C75-C74	5.85	1.65	1.53
6	A	3013	9Z9	C02-C03	5.48	1.66	1.56
6	A	3013	9Z9	C73-C74	-5.41	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3013	9Z9	C15-C07	5.03	1.61	1.53
6	A	3013	9Z9	C03-C04	4.91	1.64	1.54
6	A	3013	9Z9	C03-C74	-4.81	1.40	1.54
5	A	3010	6OU	O30-C20	-4.52	1.39	1.47
5	A	3012	6OU	C08-C07	-4.06	1.31	1.51
5	A	3011	6OU	C08-C07	-4.05	1.31	1.51
6	A	3013	9Z9	O80-C73	3.89	1.48	1.42
6	A	3013	9Z9	C05-C06	3.58	1.61	1.54
6	A	3013	9Z9	O80-C79	3.03	1.48	1.43
6	A	3013	9Z9	C76-C77	-2.93	1.47	1.53
5	A	3007	6OU	O30-C31	2.91	1.42	1.34
5	A	3007	6OU	O18-C19	-2.90	1.38	1.45
6	A	3013	9Z9	C02-C06	-2.82	1.49	1.55
6	A	3013	9Z9	C16-C13	2.66	1.57	1.51
5	A	3008	6OU	O18-C16	2.57	1.40	1.33
5	A	3008	6OU	O30-C20	-2.56	1.40	1.46
5	A	3012	6OU	O18-C19	-2.46	1.39	1.45
5	A	3011	6OU	O18-C16	2.39	1.40	1.33
5	A	3009	6OU	O30-C31	2.32	1.40	1.33
6	A	3013	9Z9	C07-C08	2.31	1.58	1.53
5	A	3010	6OU	O18-C19	-2.31	1.40	1.45
5	A	3008	6OU	O30-C31	2.23	1.40	1.34
5	A	3011	6OU	O18-C19	-2.22	1.40	1.45
5	A	3010	6OU	O18-C16	2.11	1.39	1.33
6	A	3013	9Z9	C16-C17	2.04	1.56	1.52
5	A	3012	6OU	O18-C16	2.03	1.39	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3013	9Z9	O72-C73-C76	15.20	139.40	108.54
6	A	3013	9Z9	O80-C73-O72	-14.16	76.18	109.88
6	A	3013	9Z9	O80-C73-C76	-7.78	103.98	110.76
6	A	3013	9Z9	C16-C13-C11	-7.05	107.40	116.42
6	A	3013	9Z9	C15-C14-C13	-6.09	114.74	125.02
6	A	3013	9Z9	C77-C78-C79	5.23	114.94	108.59
6	A	3013	9Z9	C09-C08-C07	-5.00	104.81	111.78
6	A	3013	9Z9	C11-C13-C14	-4.90	115.77	122.93
6	A	3013	9Z9	C10-C02-C06	4.89	114.56	107.25
6	A	3013	9Z9	C01-C02-C06	-4.43	103.65	111.68
6	A	3013	9Z9	O80-C79-C78	4.29	117.68	112.17
5	A	3008	6OU	O30-C31-C33	4.19	120.54	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3007	6OU	O30-C31-C33	4.15	120.45	111.48
5	A	3010	6OU	O30-C31-C33	4.05	120.24	111.48
6	A	3013	9Z9	C73-C74-C03	4.00	109.26	103.37
6	A	3013	9Z9	C10-C02-C03	3.96	121.00	115.36
6	A	3013	9Z9	C01-C02-C10	-3.30	105.74	110.61
6	A	3013	9Z9	C75-C74-C73	-3.10	109.94	114.94
6	A	3013	9Z9	C12-C11-C08	-3.09	108.20	111.66
5	A	3008	6OU	O18-C16-C15	3.06	121.17	111.83
6	A	3013	9Z9	C05-C04-C03	-2.93	102.12	107.47
5	A	3007	6OU	C21-C20-C19	-2.85	105.14	111.78
5	A	3009	6OU	O30-C31-C33	2.83	120.46	111.83
6	A	3013	9Z9	O80-C73-C74	-2.83	98.84	107.26
6	A	3013	9Z9	C05-C06-C02	-2.80	100.53	103.85
6	A	3013	9Z9	C03-C02-C06	2.73	103.75	100.18
3	A	3005	NAG	C2-N2-C7	-2.63	119.37	122.90
5	A	3012	6OU	O18-C16-C15	2.58	121.89	112.14
5	A	3007	6OU	O18-C16-C15	2.56	119.64	111.83
3	A	3003	NAG	C2-N2-C7	2.55	126.31	122.90
6	A	3013	9Z9	C08-C07-C06	2.54	112.41	109.09
6	A	3013	9Z9	C06-C05-C04	-2.51	98.02	102.40
3	A	3003	NAG	C1-C2-N2	2.47	114.33	110.43
3	A	3001	NAG	C1-O5-C5	2.46	115.49	112.19
3	A	3001	NAG	C2-N2-C7	-2.45	119.61	122.90
6	A	3013	9Z9	C77-C76-C73	-2.45	108.10	111.93
6	A	3013	9Z9	C08-C11-C13	2.33	113.06	109.65
3	A	3005	NAG	C4-C3-C2	-2.31	107.63	111.02
5	A	3010	6OU	O18-C16-C15	2.29	118.81	111.83
6	A	3013	9Z9	C01-C02-C03	-2.27	106.64	111.58
3	A	3003	NAG	C1-O5-C5	2.22	115.16	112.19
6	A	3013	9Z9	C81-C78-C79	-2.22	107.62	111.03
6	A	3013	9Z9	C79-O80-C73	2.21	117.49	113.69
6	A	3013	9Z9	C10-C09-C08	-2.14	109.50	113.14
5	A	3012	6OU	C14-C15-C16	-2.10	106.01	113.69
5	A	3011	6OU	C08-C07-C06	2.08	124.86	114.37
5	A	3010	6OU	C21-C20-C19	-2.07	106.88	112.69
5	A	3011	6OU	O18-C16-C15	2.06	119.93	112.14
6	A	3013	9Z9	C02-C03-C74	-2.05	114.44	120.50

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3003	NAG	C1-C2-N2-C7
3	A	3003	NAG	C8-C7-N2-C2
3	A	3003	NAG	O7-C7-N2-C2
5	A	3007	6OU	C27-O26-P23-O22
5	A	3007	6OU	C27-O26-P23-O24
5	A	3007	6OU	O26-C27-C28-N29
5	A	3008	6OU	C21-O22-P23-O24
5	A	3008	6OU	O26-C27-C28-N29
5	A	3011	6OU	C06-C07-C08-C09
3	A	3004	NAG	O7-C7-N2-C2
3	A	3001	NAG	C8-C7-N2-C2
3	A	3001	NAG	O7-C7-N2-C2
3	A	3004	NAG	C8-C7-N2-C2
5	A	3008	6OU	C15-C16-O18-C19
5	A	3010	6OU	C15-C16-O18-C19
3	A	3005	NAG	C8-C7-N2-C2
5	A	3010	6OU	O17-C16-O18-C19
3	A	3005	NAG	O5-C5-C6-O6
5	A	3008	6OU	O17-C16-O18-C19
3	A	3005	NAG	O7-C7-N2-C2
5	A	3007	6OU	C31-C33-C34-C35
5	A	3010	6OU	C31-C33-C34-C35
5	A	3007	6OU	C15-C16-O18-C19
6	A	3013	9Z9	C22-C21-O20-C17
6	A	3013	9Z9	C16-C17-O20-C21
5	A	3007	6OU	O17-C16-O18-C19
5	A	3011	6OU	C10-C11-C12-C13
5	A	3012	6OU	C10-C11-C12-C13
5	A	3010	6OU	C06-C07-C08-C09
5	A	3008	6OU	O30-C20-C21-O22
5	A	3008	6OU	C10-C11-C12-C13
5	A	3009	6OU	C37-C38-C39-C40
5	A	3008	6OU	C19-C20-C21-O22
5	A	3009	6OU	C34-C35-C36-C37
6	A	3013	9Z9	C18-C17-O20-C21
5	A	3012	6OU	C07-C08-C09-C10
5	A	3010	6OU	C33-C34-C35-C36
5	A	3007	6OU	C35-C36-C37-C38
5	A	3007	6OU	C10-C11-C12-C13
5	A	3010	6OU	C10-C11-C12-C13
5	A	3010	6OU	C11-C12-C13-C14
5	A	3007	6OU	O18-C19-C20-O30
5	A	3011	6OU	C04-C05-C06-C07

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Mol	Chain	Res	Type	Atoms
5	A	3007	6OU	C38-C39-C40-C41
3	A	3005	NAG	C4-C5-C6-O6
5	A	3007	6OU	C08-C09-C10-C11
5	A	3010	6OU	C12-C13-C14-C15
5	A	3008	6OU	C33-C34-C35-C36
5	A	3008	6OU	O30-C31-C33-C34
5	A	3008	6OU	C35-C36-C37-C38
5	A	3007	6OU	C36-C37-C38-C39
5	A	3007	6OU	O18-C19-C20-C21
3	A	3001	NAG	C3-C2-N2-C7
5	A	3008	6OU	C27-O26-P23-O25
5	A	3011	6OU	C09-C10-C11-C12
5	A	3012	6OU	C15-C16-O18-C19
5	A	3010	6OU	C14-C15-C16-O18
5	A	3007	6OU	C34-C35-C36-C37
5	A	3008	6OU	C08-C09-C10-C11
3	A	3001	NAG	C1-C2-N2-C7
5	A	3008	6OU	C14-C15-C16-O18
5	A	3008	6OU	O32-C31-C33-C34
5	A	3008	6OU	C38-C39-C40-C41
5	A	3012	6OU	O17-C16-O18-C19
5	A	3008	6OU	C14-C15-C16-O17
5	A	3009	6OU	C31-C33-C34-C35
5	A	3007	6OU	O30-C31-C33-C34
5	A	3011	6OU	C14-C15-C16-O18

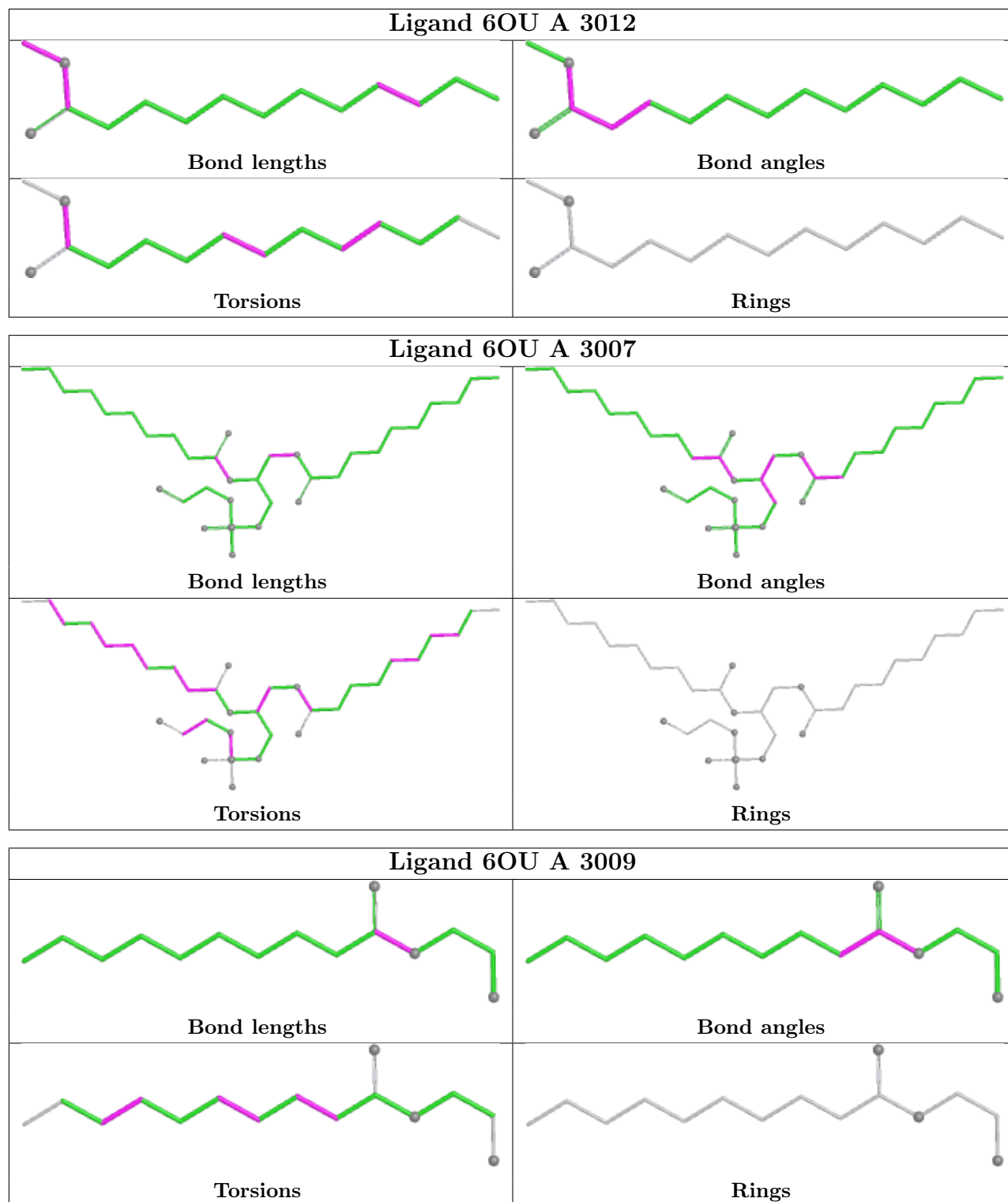
There are no ring outliers.

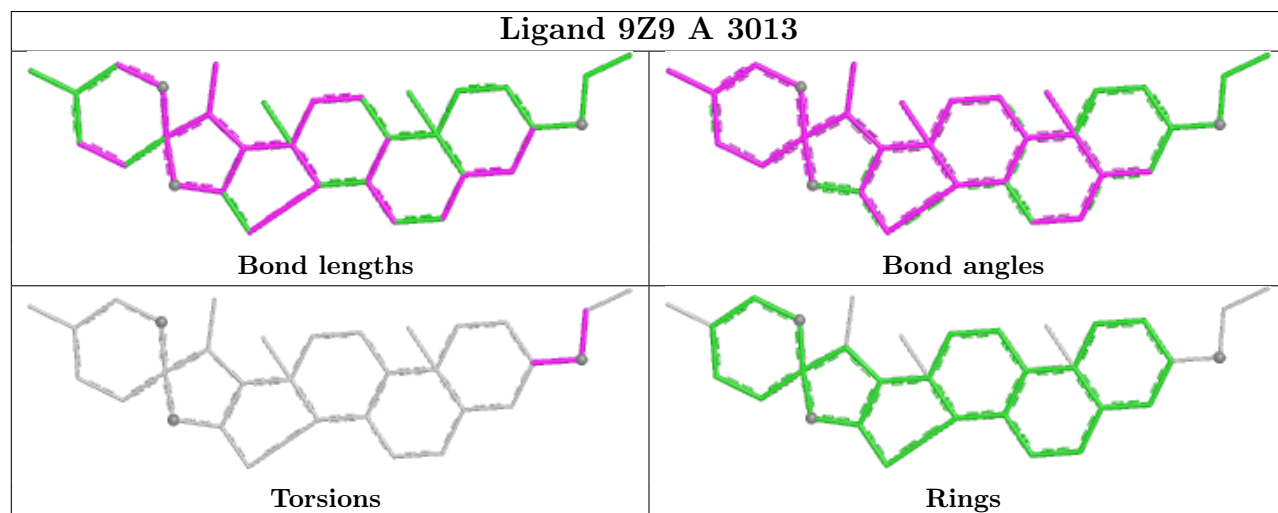
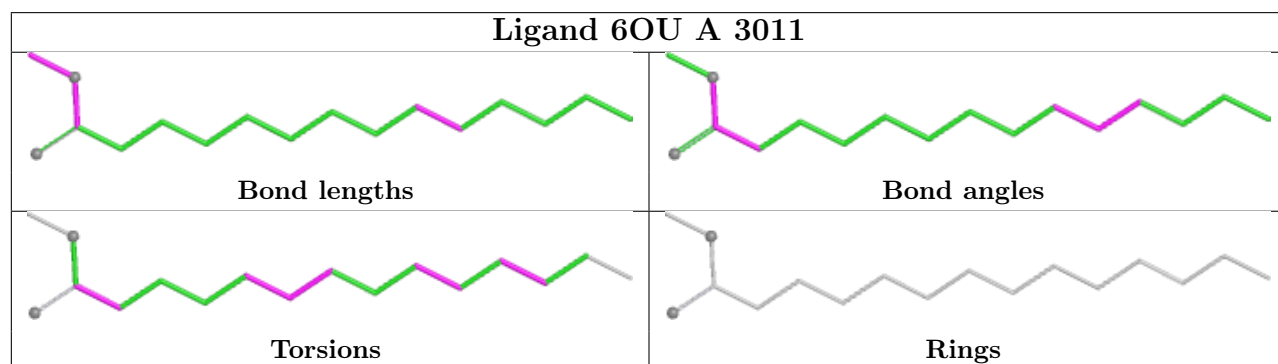
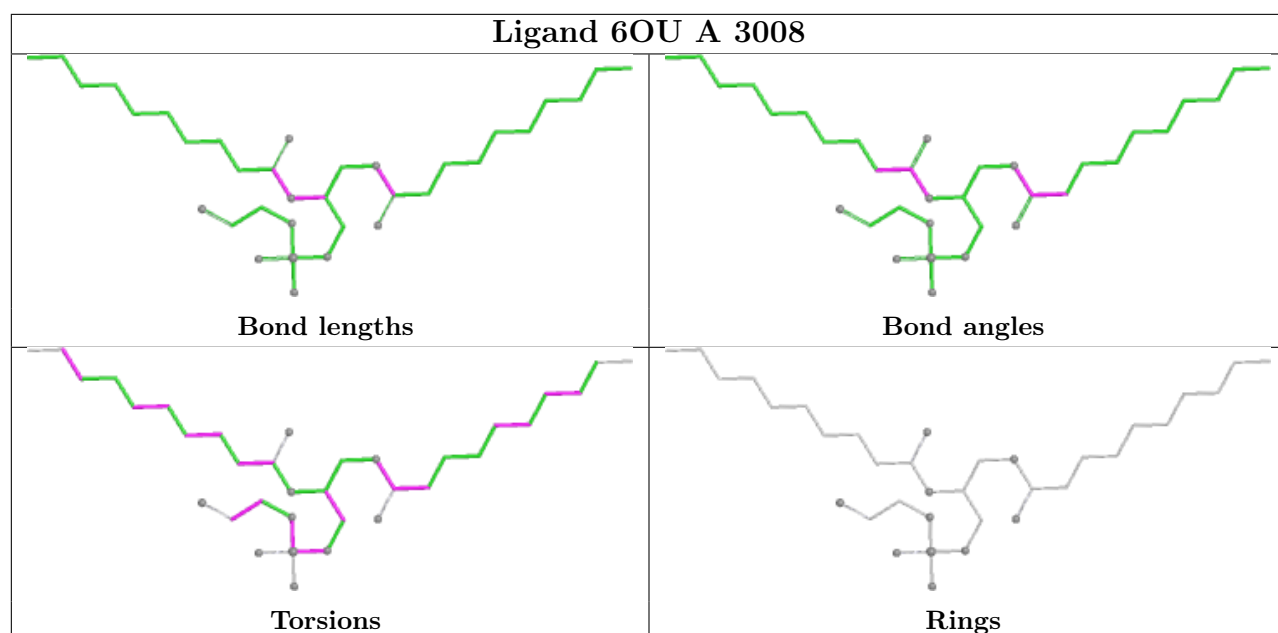
6 monomers are involved in 11 short contacts:

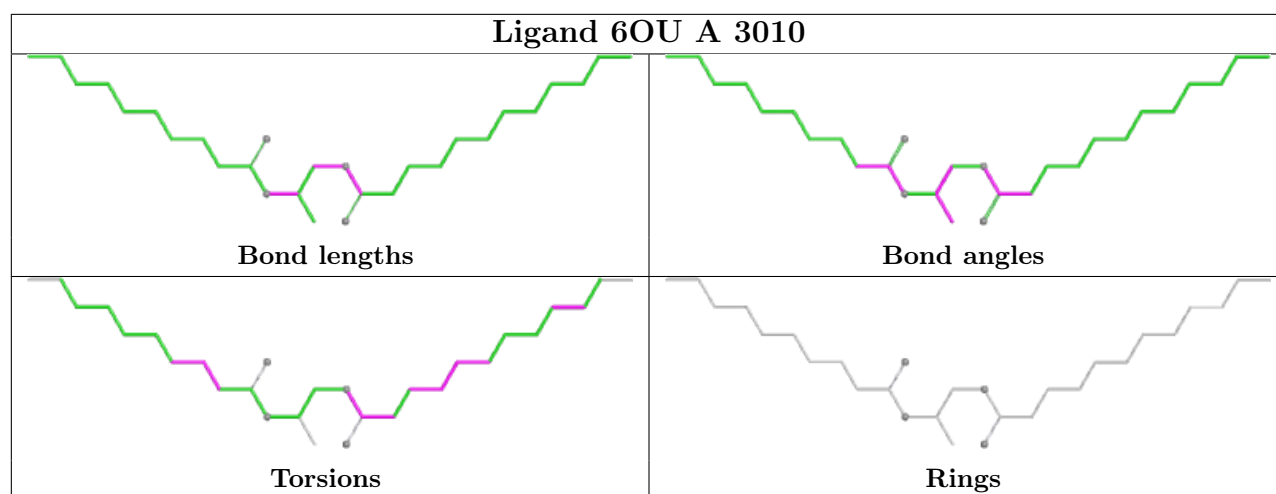
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	NAG	3	0
3	A	3004	NAG	3	0
3	A	3005	NAG	1	0
3	A	3001	NAG	4	0
6	A	3013	9Z9	3	0
5	A	3010	6OU	1	0

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.

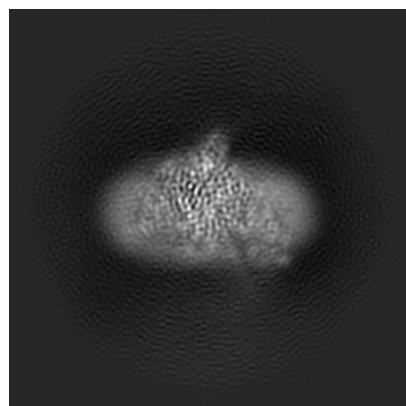
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33435. These allow visual inspection of the internal detail of the map and identification of artifacts.

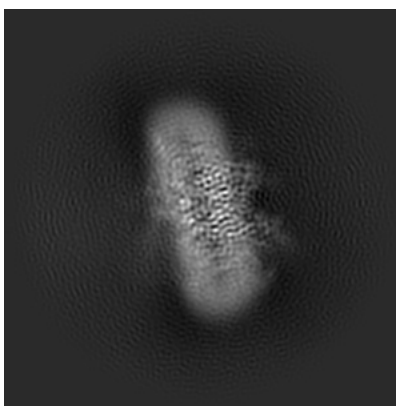
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

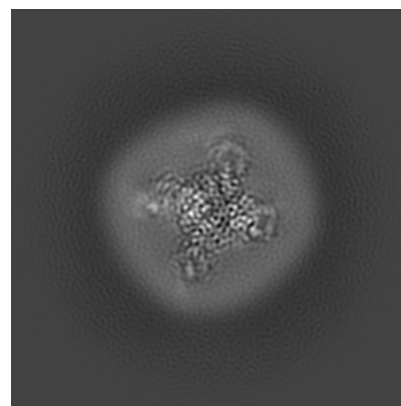
6.1.1 Primary map



X

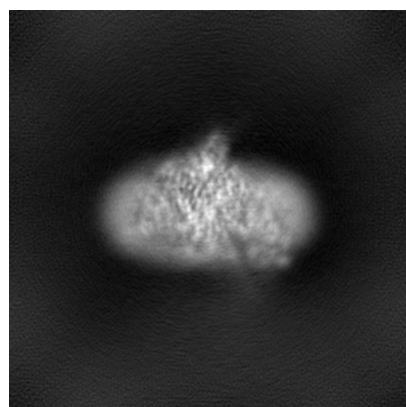


Y

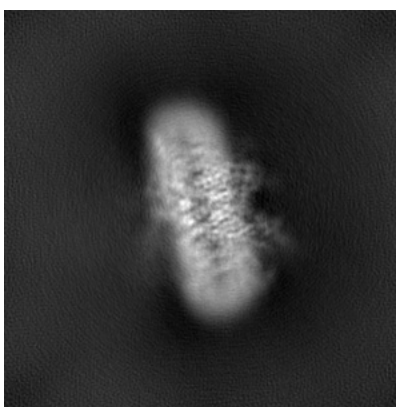


Z

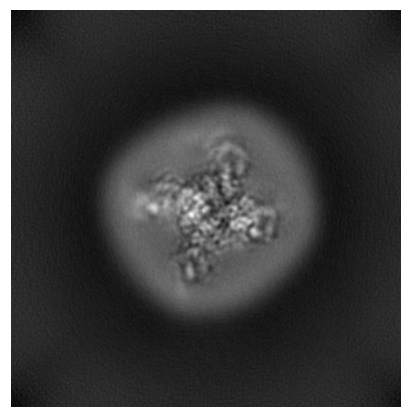
6.1.2 Raw map



X



Y

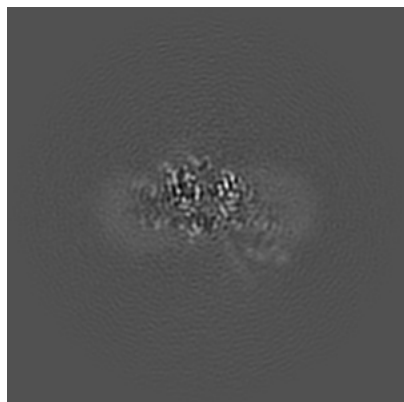


Z

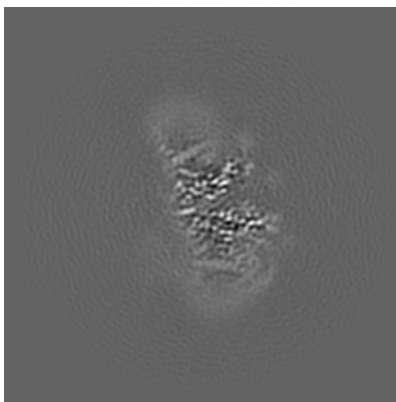
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

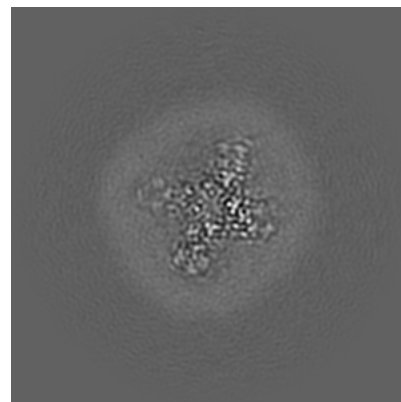
6.2.1 Primary map



X Index: 128

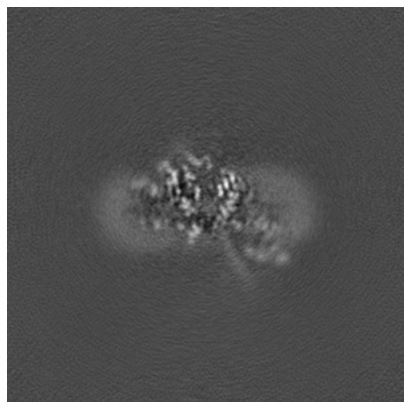


Y Index: 128

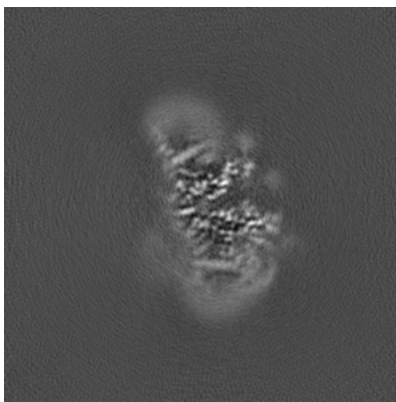


Z Index: 128

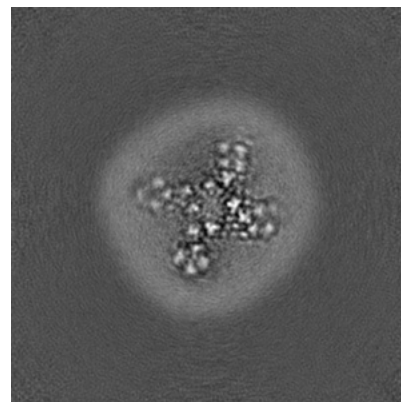
6.2.2 Raw map



X Index: 128



Y Index: 128

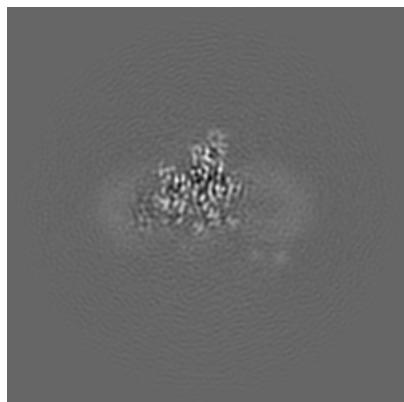


Z Index: 128

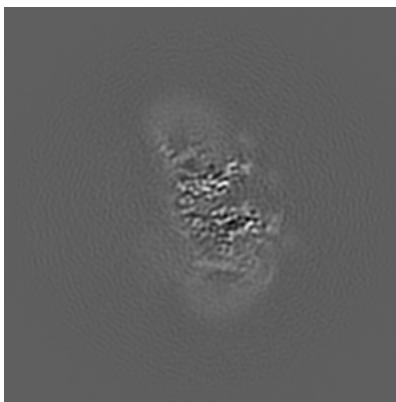
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

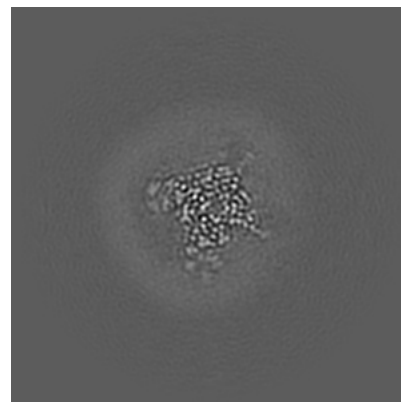
6.3.1 Primary map



X Index: 118

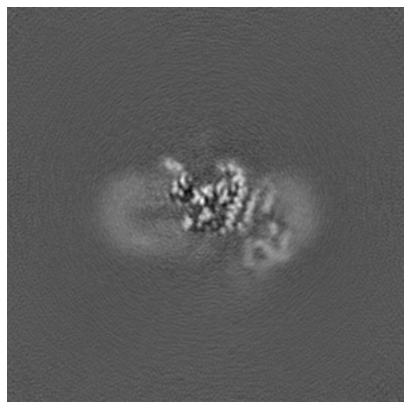


Y Index: 129

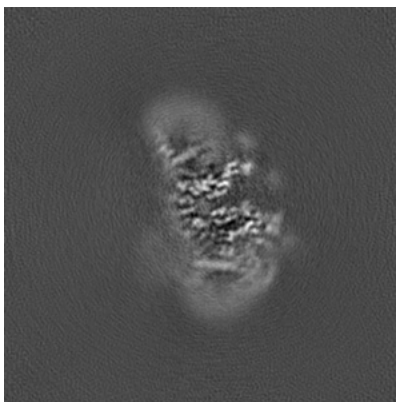


Z Index: 139

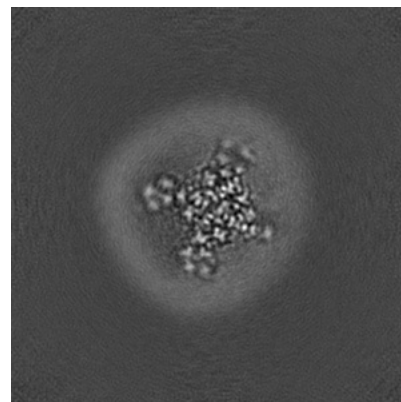
6.3.2 Raw map



X Index: 137



Y Index: 129

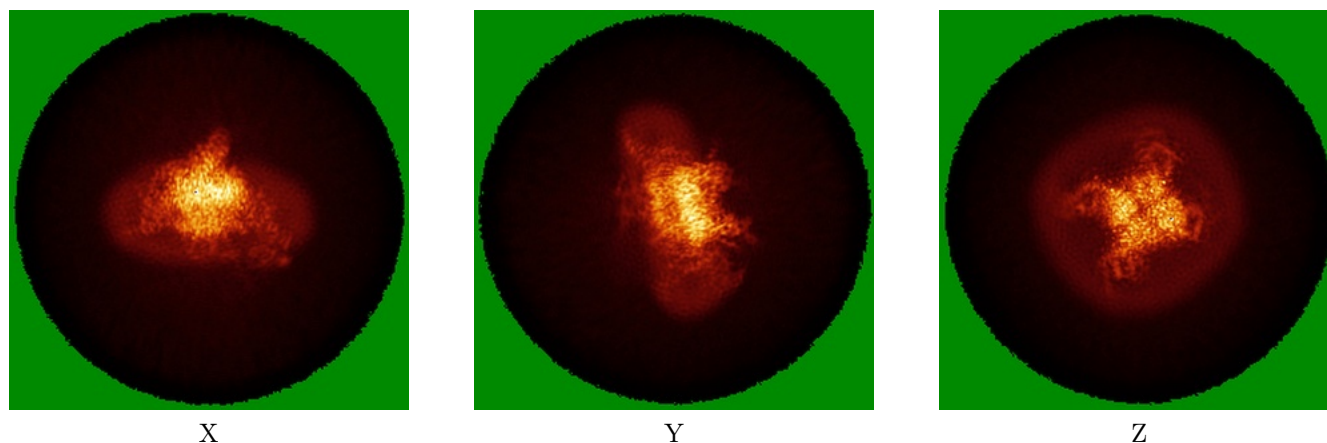


Z Index: 135

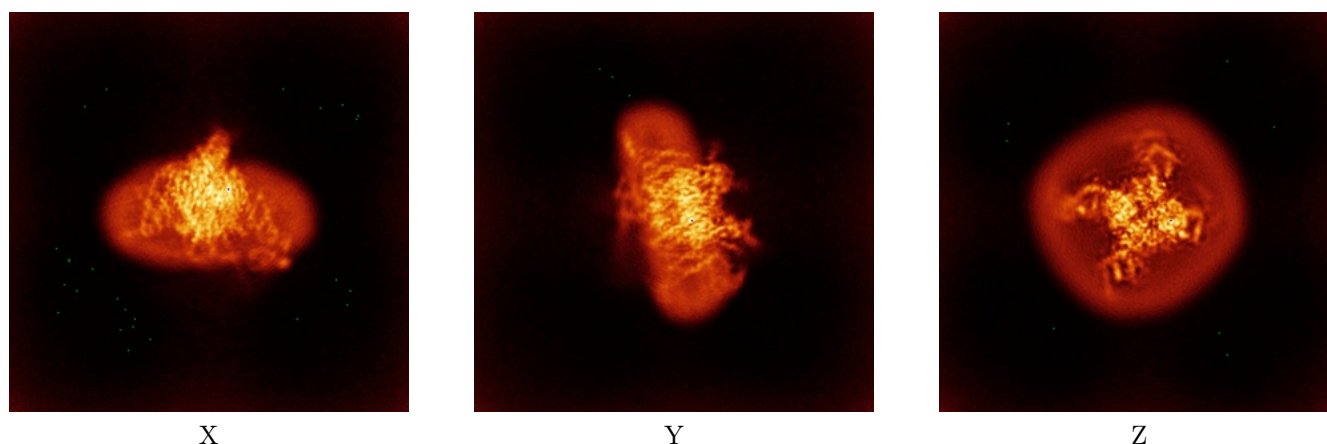
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

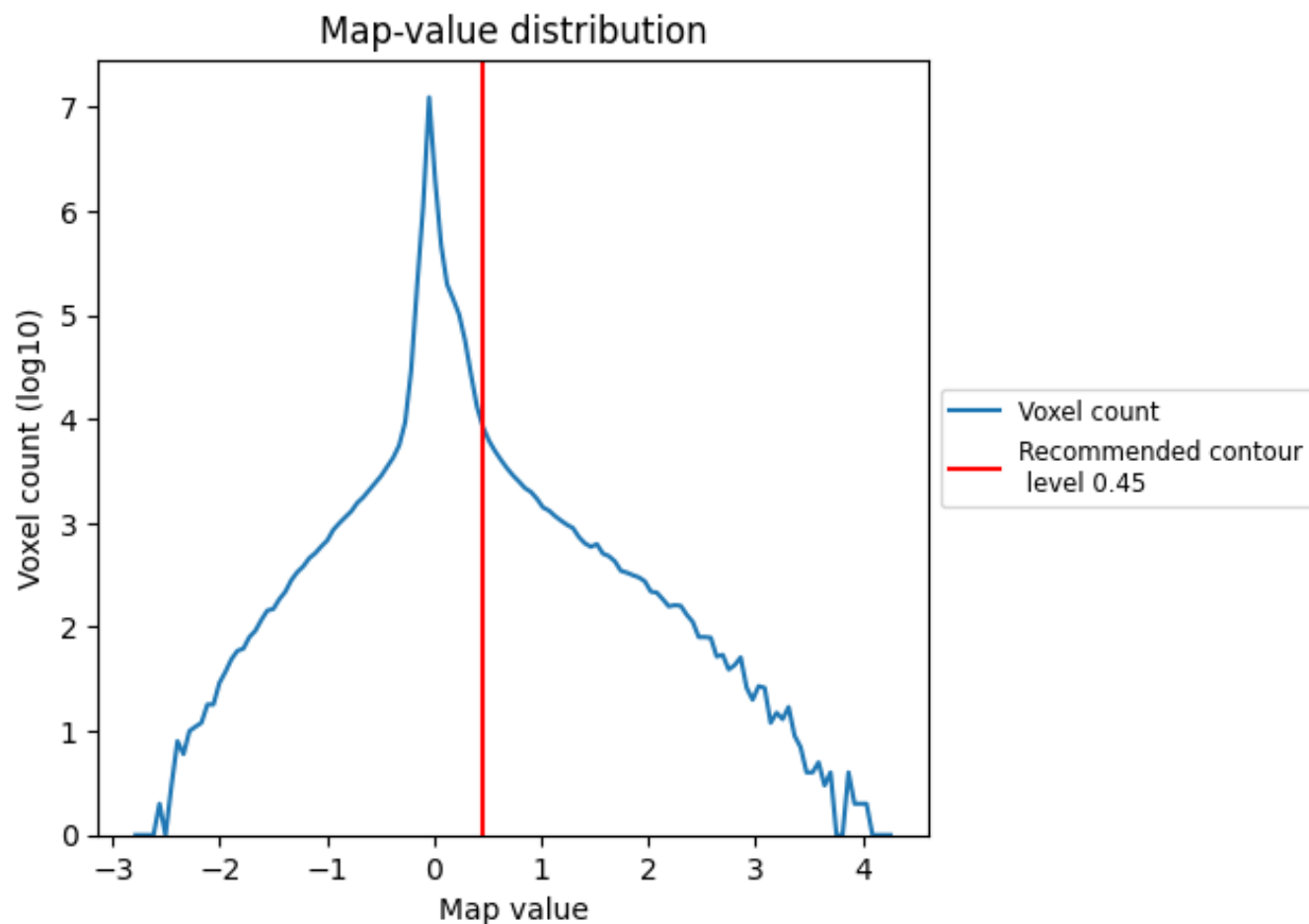
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

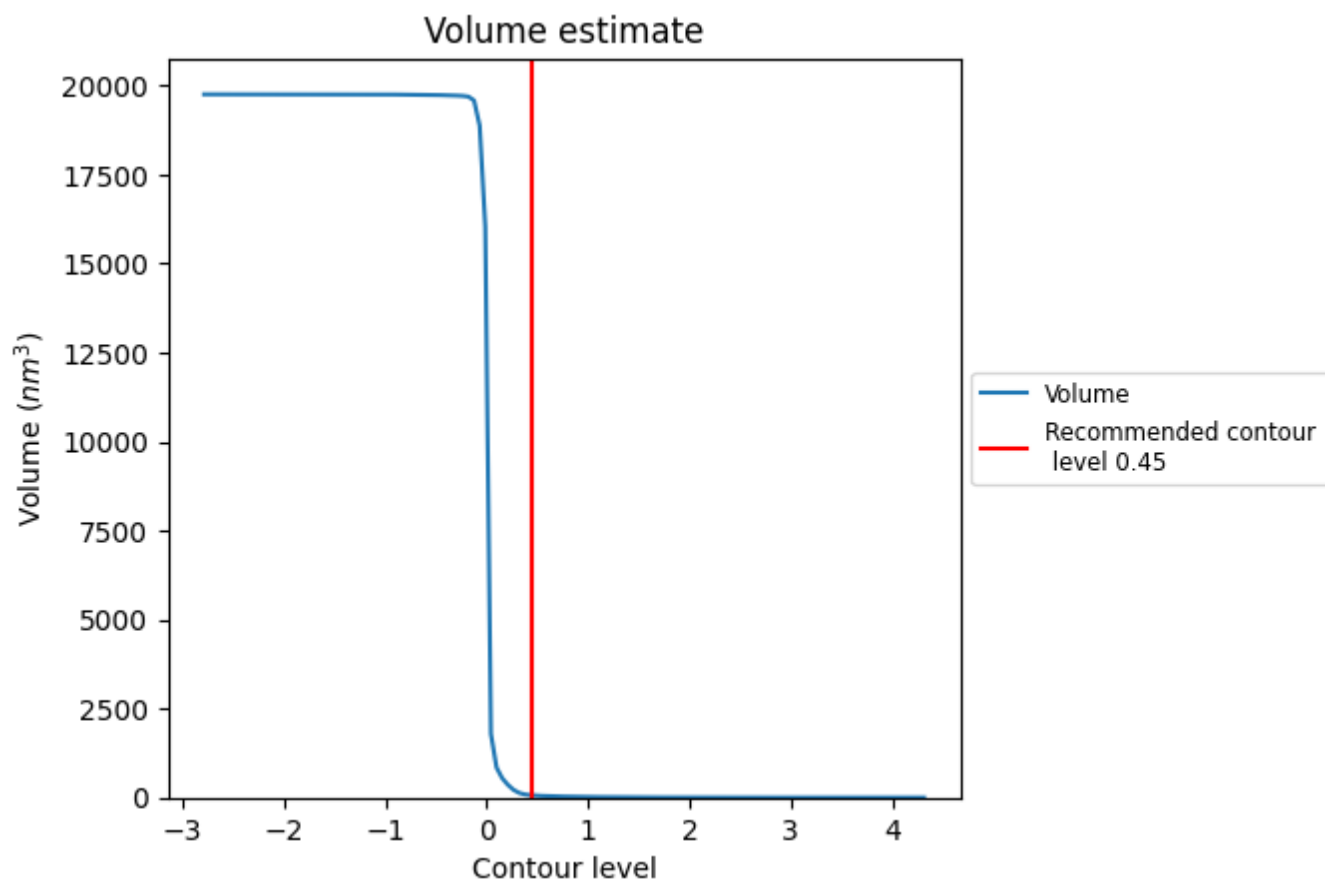
This section contains the results of statistical analysis of the map.

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.

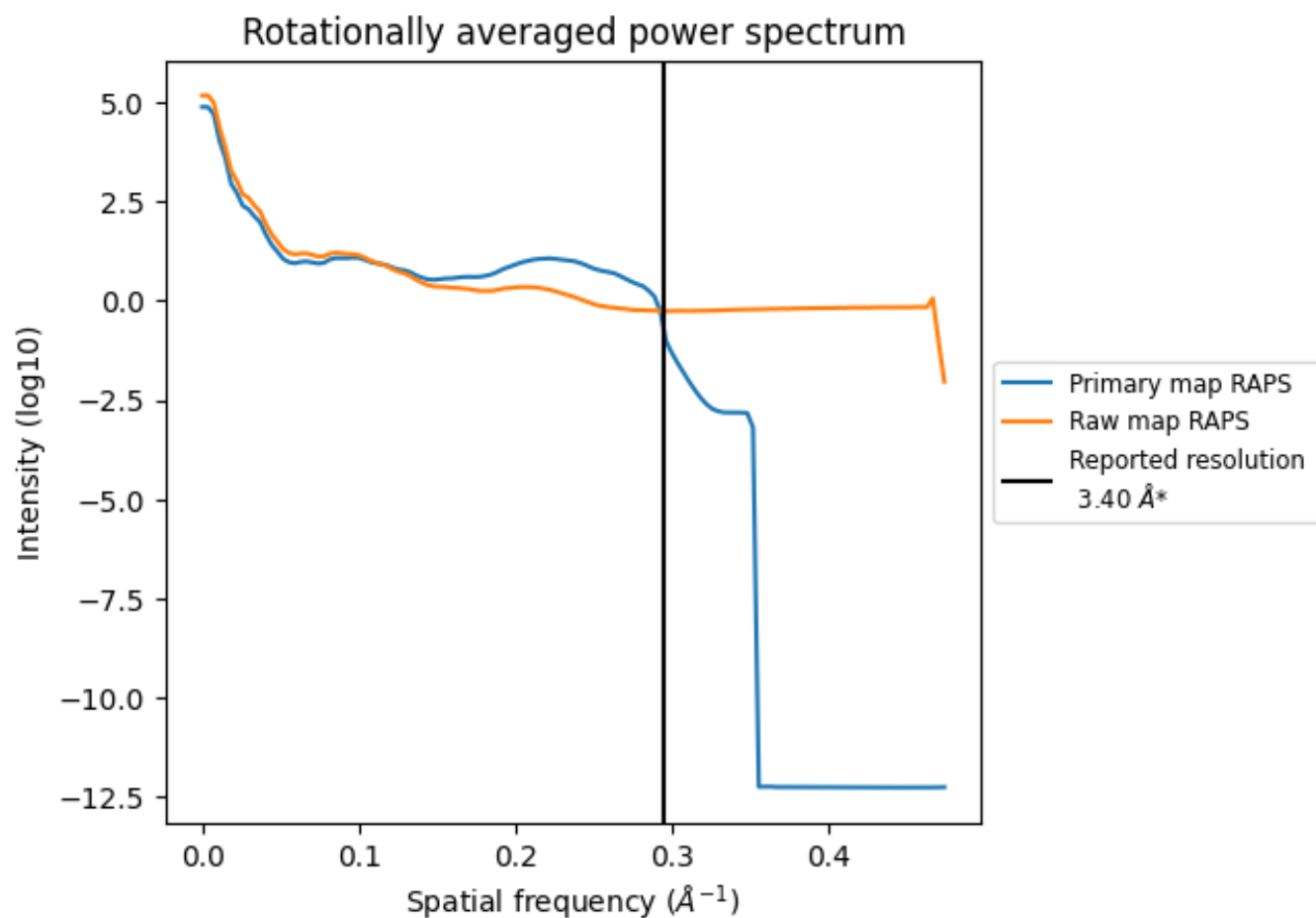
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm^3 ; this corresponds to an approximate mass of 57 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 ⓘ

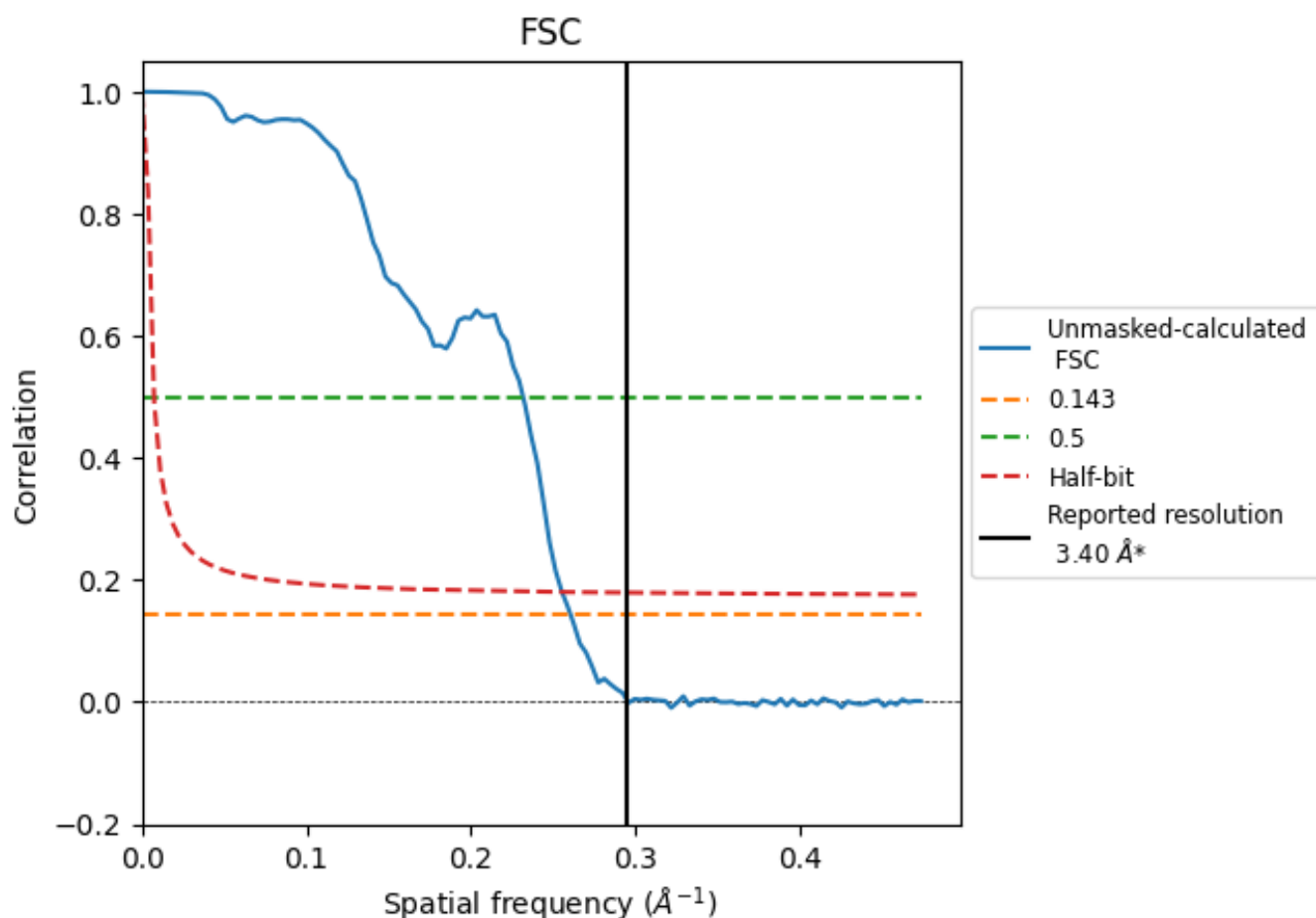


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.84	4.32	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 3.4 by more than 10 %

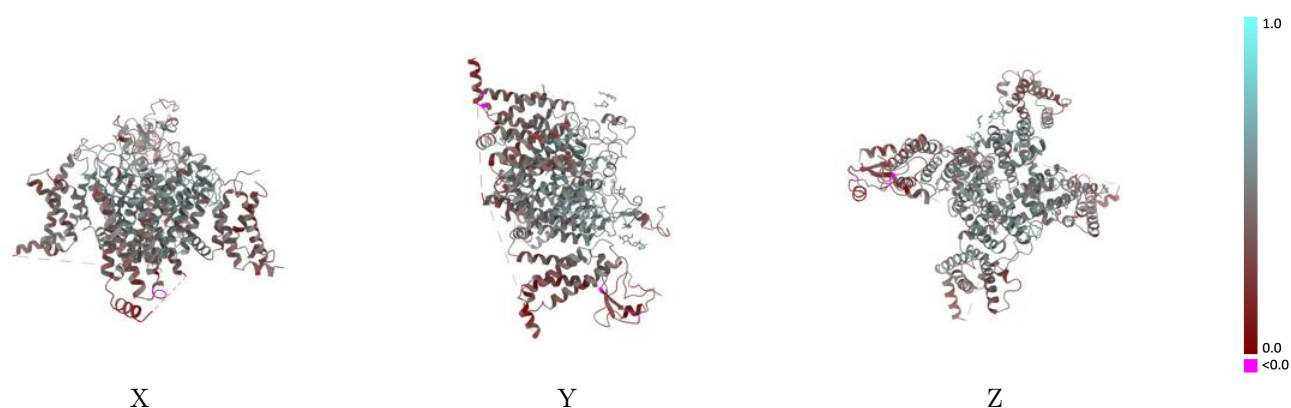
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-33435 and PDB model 7XSU. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

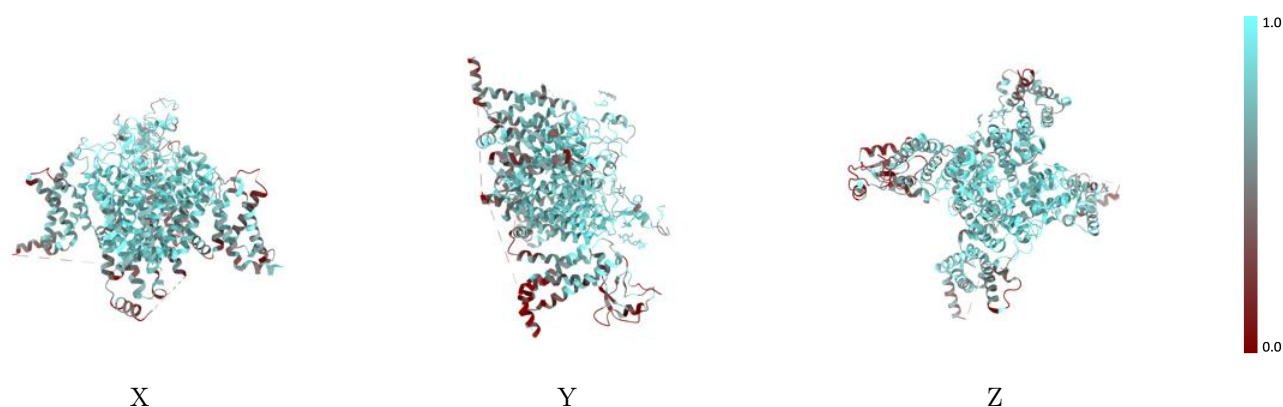
This section was not generated.

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



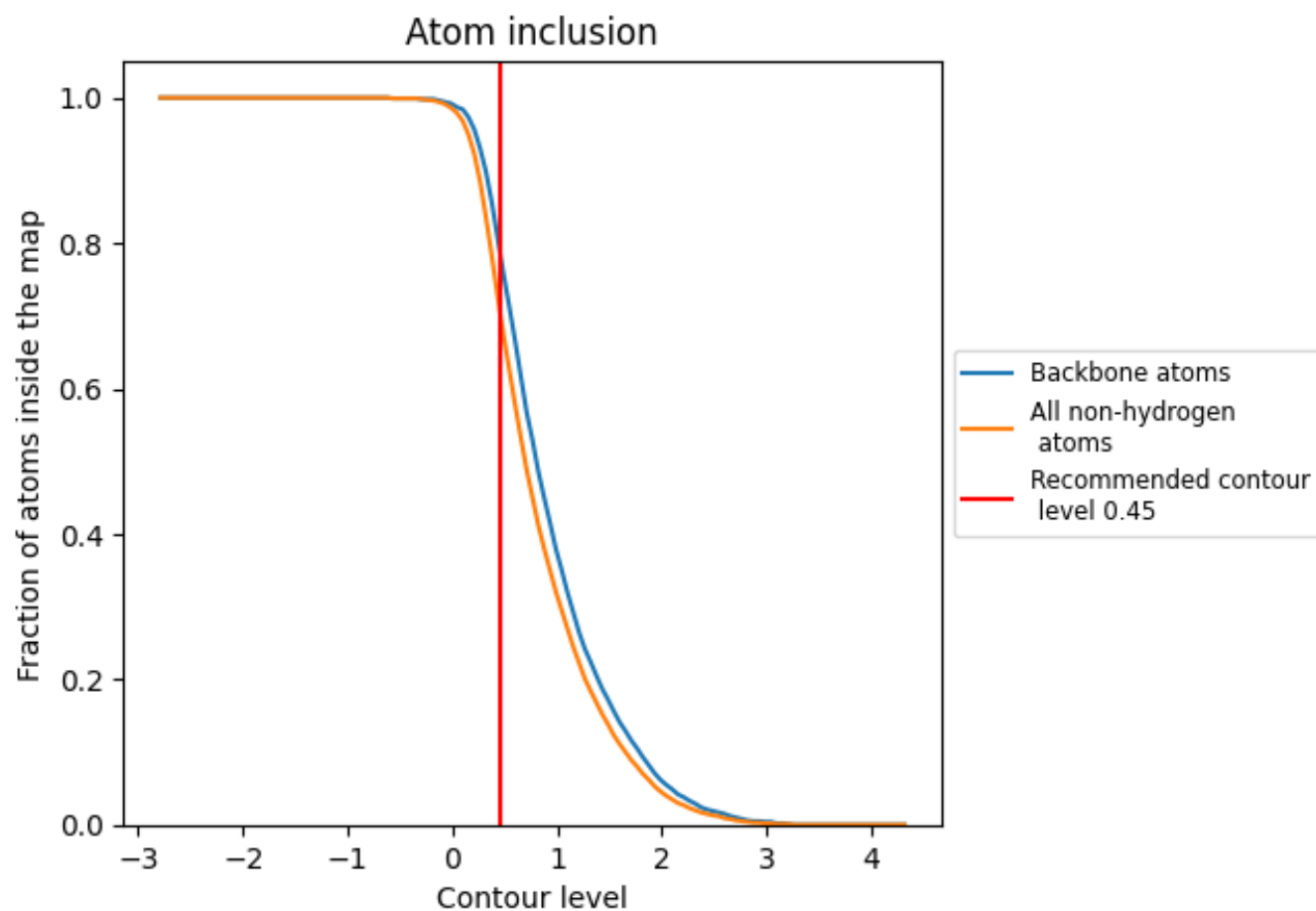
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.4330
A	0.7250	0.4420
B	0.3950	0.2840

