



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 06:56 AM UTC

PDB ID : 6LQA / pdb_00006lqa
EMDB ID : EMD-0942
Title : voltage-gated sodium channel Nav1.5 with quinidine
Authors : Yan, N.; Li, Z.; Pan, X.; Huang, G.
Deposited on : 2020-01-13
Resolution : 3.30 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

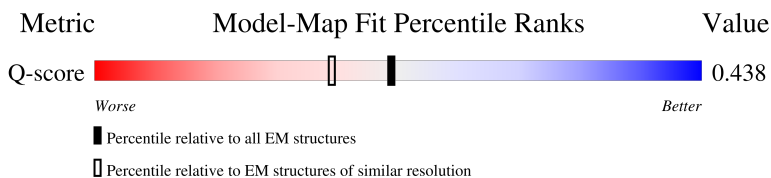
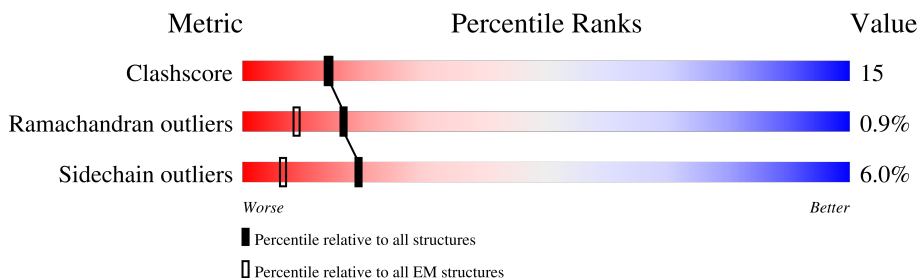
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	B	2059	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9387 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1151	Total	C	N	O	S	0	0
			9237	6115	1458	1591	73		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-42	MET	-	initiating methionine	UNP Q14524
B	-41	ALA	-	expression tag	UNP Q14524
B	-40	SER	-	expression tag	UNP Q14524
B	-39	TRP	-	expression tag	UNP Q14524
B	-38	SER	-	expression tag	UNP Q14524
B	-37	HIS	-	expression tag	UNP Q14524
B	-36	PRO	-	expression tag	UNP Q14524
B	-35	GLN	-	expression tag	UNP Q14524
B	-34	PHE	-	expression tag	UNP Q14524
B	-33	GLU	-	expression tag	UNP Q14524
B	-32	LYS	-	expression tag	UNP Q14524
B	-31	GLY	-	expression tag	UNP Q14524
B	-30	GLY	-	expression tag	UNP Q14524
B	-29	GLY	-	expression tag	UNP Q14524
B	-28	ALA	-	expression tag	UNP Q14524
B	-27	ARG	-	expression tag	UNP Q14524
B	-26	GLY	-	expression tag	UNP Q14524
B	-25	GLY	-	expression tag	UNP Q14524
B	-24	SER	-	expression tag	UNP Q14524
B	-23	GLY	-	expression tag	UNP Q14524
B	-22	GLY	-	expression tag	UNP Q14524
B	-21	GLY	-	expression tag	UNP Q14524
B	-20	SER	-	expression tag	UNP Q14524
B	-19	TRP	-	expression tag	UNP Q14524
B	-18	SER	-	expression tag	UNP Q14524
B	-17	HIS	-	expression tag	UNP Q14524
B	-16	PRO	-	expression tag	UNP Q14524
B	-15	GLN	-	expression tag	UNP Q14524

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	PHE	-	expression tag	UNP Q14524
B	-13	GLU	-	expression tag	UNP Q14524
B	-12	LYS	-	expression tag	UNP Q14524
B	-11	GLY	-	expression tag	UNP Q14524
B	-10	PHE	-	expression tag	UNP Q14524
B	-9	ASP	-	expression tag	UNP Q14524
B	-8	TYR	-	expression tag	UNP Q14524
B	-7	LYS	-	expression tag	UNP Q14524
B	-6	ASP	-	expression tag	UNP Q14524
B	-5	ASP	-	expression tag	UNP Q14524
B	-4	ASP	-	expression tag	UNP Q14524
B	-3	ASP	-	expression tag	UNP Q14524
B	-2	LYS	-	expression tag	UNP Q14524
B	-1	GLY	-	expression tag	UNP Q14524
B	0	THR	-	expression tag	UNP Q14524

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



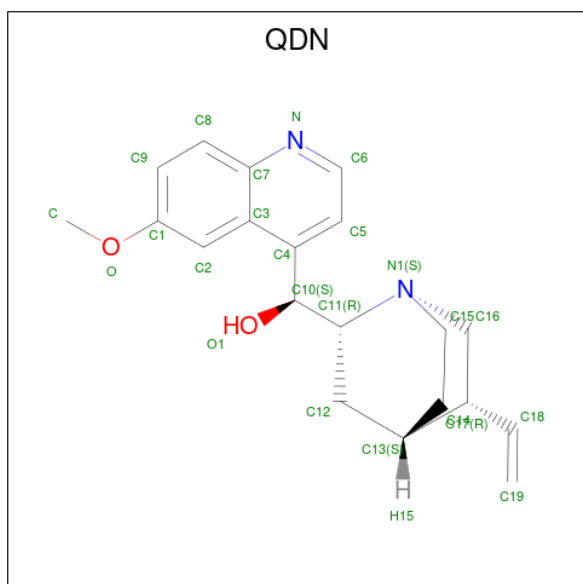
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 3 is Quinidine (CCD ID: QDN) (formula: $C_{20}H_{24}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			24	20	2	2	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	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	0.125	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	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: QDN, NAG

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	B	0.36	1/9462 (0.0%)	0.79	6/12835 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1331	ILE	C-N	5.05	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	739	TYR	N-CA-C	9.31	121.20	111.14
1	B	1260	ALA	N-CA-C	-7.50	106.07	114.62
1	B	870	ASP	N-CA-C	6.67	118.55	111.28
1	B	1296	MET	N-CA-C	5.76	117.55	111.28
1	B	771	LEU	CA-C-N	5.05	127.83	120.51
1	B	771	LEU	C-N-CA	5.05	127.83	120.51

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	B	9237	0	9413	291	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	126	0	117	1	0
3	B	24	0	24	5	0
All	All	9387	0	9554	293	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 15.

All (293) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:ARG:HD2	1:B:877:PRO:CG	1.51	1.39
1:B:801:MET:HA	1:B:801:MET:HE2	1.18	1.17
1:B:899:TRP:CD1	1:B:923:MET:HE1	1.82	1.14
1:B:1334:ILE:CD1	1:B:1469:ILE:HD11	1.83	1.08
1:B:869:ARG:HD2	1:B:877:PRO:HG2	1.31	1.07
1:B:869:ARG:HH11	1:B:869:ARG:HA	1.16	1.04
1:B:1292:GLY:C	1:B:1293:PHE:CD2	2.35	1.04
1:B:1758:ILE:O	1:B:1762:ILE:HD12	1.60	1.02
1:B:180:GLY:O	1:B:181:PHE:CD2	2.14	1.01
1:B:869:ARG:HG3	1:B:877:PRO:HD3	1.37	1.00
1:B:1292:GLY:O	1:B:1293:PHE:HD2	1.43	1.00
1:B:899:TRP:CG	1:B:923:MET:HE1	1.96	1.00
1:B:203:MET:HE2	1:B:218:LEU:HD11	1.42	0.99
1:B:405:VAL:HG11	3:B:2110:QDN:H13	1.43	0.97
1:B:802:SER:O	1:B:803:ASN:ND2	1.97	0.96
1:B:219:ARG:HD2	1:B:859:GLN:NE2	1.80	0.95
1:B:203:MET:CE	1:B:218:LEU:HD11	1.96	0.94
1:B:801:MET:HA	1:B:801:MET:CE	1.97	0.94
1:B:1292:GLY:C	1:B:1293:PHE:HD2	1.73	0.93
1:B:869:ARG:CG	1:B:877:PRO:HD3	1.98	0.93
1:B:869:ARG:HD2	1:B:877:PRO:HG3	1.48	0.92
1:B:869:ARG:HG3	1:B:877:PRO:CD	1.99	0.92
1:B:869:ARG:HD2	1:B:877:PRO:CD	2.01	0.90
1:B:907:MET:CE	1:B:916:LEU:HD23	2.00	0.90
1:B:1767:TYR:C	1:B:1767:TYR:HD2	1.80	0.90
1:B:219:ARG:O	1:B:222:ARG:HB3	1.73	0.89
1:B:1288:ALA:O	1:B:1294:ALA:HB3	1.74	0.88
1:B:219:ARG:HD2	1:B:859:GLN:HE22	1.37	0.87
1:B:1334:ILE:HD11	1:B:1469:ILE:CD1	2.04	0.87
1:B:803:ASN:ND2	1:B:803:ASN:O	2.09	0.85
1:B:219:ARG:CD	1:B:859:GLN:NE2	2.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:VAL:HG11	3:B:2110:QDN:C19	2.07	0.84
1:B:1334:ILE:CD1	1:B:1469:ILE:CD1	2.56	0.83
1:B:1767:TYR:HD2	1:B:1767:TYR:O	1.61	0.83
1:B:709:GLY:O	1:B:713:VAL:HG22	1.78	0.83
1:B:282:ARG:HD2	1:B:313:ASN:HA	1.59	0.83
1:B:736:LEU:HD21	1:B:745:PHE:HZ	1.44	0.83
1:B:1288:ALA:C	1:B:1294:ALA:HB3	2.05	0.82
1:B:1767:TYR:C	1:B:1767:TYR:CD2	2.55	0.81
1:B:710:VAL:O	1:B:713:VAL:HG23	1.81	0.80
1:B:869:ARG:CD	1:B:877:PRO:CG	2.48	0.79
1:B:869:ARG:HH11	1:B:869:ARG:CA	1.93	0.79
1:B:899:TRP:CD2	1:B:923:MET:HE1	2.19	0.78
1:B:710:VAL:O	1:B:714:VAL:HG23	1.83	0.78
1:B:1608:LEU:HD12	1:B:1608:LEU:O	1.83	0.77
1:B:1334:ILE:HD13	1:B:1469:ILE:HD11	1.65	0.77
1:B:899:TRP:NE1	1:B:923:MET:HE1	2.00	0.76
1:B:1292:GLY:O	1:B:1293:PHE:CD2	2.32	0.76
1:B:180:GLY:O	1:B:181:PHE:HD2	1.69	0.75
1:B:368:LEU:CD2	1:B:377:LEU:HD23	2.15	0.75
1:B:287:LEU:HB3	1:B:294:VAL:CG2	2.16	0.75
1:B:1288:ALA:HB1	1:B:1294:ALA:CB	2.15	0.75
1:B:868:LEU:HG	1:B:909:VAL:HG12	1.68	0.75
1:B:203:MET:HE2	1:B:218:LEU:CD1	2.17	0.74
1:B:899:TRP:CE2	1:B:923:MET:HE1	2.22	0.74
1:B:223:VAL:O	1:B:225:ARG:N	2.21	0.74
1:B:290:THR:OG1	1:B:294:VAL:HG13	1.87	0.73
1:B:807:LEU:HD12	1:B:807:LEU:N	2.03	0.72
1:B:1510:ILE:HG13	1:B:1511:PRO:HD2	1.69	0.72
1:B:1421:TRP:CD1	1:B:1421:TRP:H	2.08	0.72
1:B:368:LEU:HD23	1:B:377:LEU:HD23	1.71	0.71
1:B:736:LEU:HD23	1:B:736:LEU:O	1.89	0.71
1:B:869:ARG:CD	1:B:877:PRO:HG2	2.16	0.71
1:B:1457:GLY:O	1:B:1461:THR:HB	1.90	0.71
1:B:779:GLN:NE2	1:B:780:GLY:H	1.89	0.70
1:B:299:LEU:CD1	1:B:301:TRP:CZ3	2.74	0.70
1:B:806:VAL:O	1:B:809:SER:HB3	1.91	0.70
1:B:1734:ASN:HB3	1:B:1738:SER:O	1.92	0.70
1:B:299:LEU:HD12	1:B:301:TRP:CZ3	2.27	0.69
1:B:287:LEU:HD23	1:B:294:VAL:HG21	1.74	0.69
1:B:869:ARG:CD	1:B:877:PRO:CD	2.71	0.69
1:B:347:ASN:ND2	1:B:348:PRO:HD3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:GLN:CG	1:B:780:GLY:H	2.05	0.68
1:B:736:LEU:HD21	1:B:745:PHE:CZ	2.28	0.68
1:B:348:PRO:O	1:B:349:ASP:HB2	1.94	0.68
1:B:1288:ALA:O	1:B:1294:ALA:CB	2.43	0.67
1:B:779:GLN:CD	1:B:780:GLY:H	2.02	0.67
1:B:1334:ILE:HD11	1:B:1469:ILE:HD11	1.66	0.67
1:B:1288:ALA:HB1	1:B:1294:ALA:HB3	1.74	0.67
1:B:778:GLN:OE1	1:B:779:GLN:N	2.28	0.67
1:B:1760:PHE:O	1:B:1764:VAL:HG23	1.95	0.66
1:B:219:ARG:HG2	1:B:219:ARG:HH21	1.60	0.66
1:B:807:LEU:HD12	1:B:807:LEU:H	1.59	0.65
1:B:1334:ILE:HD11	1:B:1469:ILE:HD12	1.77	0.65
1:B:912:GLN:O	1:B:916:LEU:HB2	1.97	0.65
1:B:282:ARG:HD3	1:B:313:ASN:HD22	1.61	0.65
1:B:933:LEU:O	1:B:933:LEU:HD22	1.96	0.65
1:B:1684:TRP:CD1	1:B:1688:ILE:HG22	2.32	0.64
1:B:899:TRP:CZ3	1:B:903:MET:SD	2.90	0.64
1:B:1767:TYR:O	1:B:1767:TYR:CD2	2.49	0.64
1:B:903:MET:CE	1:B:916:LEU:HD22	2.28	0.64
1:B:282:ARG:CD	1:B:313:ASN:HA	2.28	0.63
1:B:869:ARG:CG	1:B:877:PRO:CD	2.68	0.63
1:B:1728:CYS:SG	1:B:1729:ASP:N	2.72	0.63
1:B:801:MET:SD	1:B:802:SER:N	2.72	0.63
1:B:217:ALA:O	1:B:220:THR:HG23	1.98	0.63
1:B:223:VAL:C	1:B:225:ARG:N	2.55	0.62
1:B:899:TRP:CD1	1:B:923:MET:CE	2.71	0.62
1:B:1462:LEU:HD13	1:B:1462:LEU:O	2.00	0.62
1:B:710:VAL:HG13	1:B:770:ALA:HA	1.81	0.61
1:B:1462:LEU:HD13	1:B:1466:ILE:HG12	1.81	0.61
1:B:869:ARG:CD	1:B:877:PRO:HD3	2.29	0.61
1:B:1421:TRP:H	1:B:1421:TRP:HD1	1.45	0.61
1:B:1510:ILE:CG1	1:B:1511:PRO:HD2	2.29	0.61
1:B:1365:ASN:HB2	1:B:1373:LEU:HD21	1.82	0.61
1:B:1504:LYS:O	1:B:1504:LYS:HG3	2.00	0.61
1:B:223:VAL:O	1:B:226:ALA:N	2.26	0.61
1:B:1504:LYS:C	1:B:1505:LYS:HG3	2.25	0.61
1:B:183:LEU:HD12	1:B:183:LEU:O	2.01	0.60
1:B:219:ARG:HH21	1:B:219:ARG:CG	2.15	0.60
1:B:710:VAL:HA	1:B:713:VAL:CG2	2.32	0.60
1:B:864:ASN:O	1:B:868:LEU:HD23	2.02	0.60
1:B:903:MET:HE1	1:B:916:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:TRP:HZ3	1:B:903:MET:SD	2.24	0.60
1:B:1752:PHE:O	1:B:1756:ILE:HG12	2.00	0.60
1:B:1457:GLY:O	1:B:1461:THR:CB	2.50	0.60
1:B:868:LEU:HG	1:B:909:VAL:CG1	2.33	0.59
1:B:219:ARG:CD	1:B:859:GLN:HE21	2.17	0.58
1:B:907:MET:HE1	1:B:916:LEU:HD23	1.84	0.58
1:B:1760:PHE:CE1	1:B:1764:VAL:CG2	2.86	0.58
1:B:899:TRP:CG	1:B:923:MET:CE	2.82	0.58
1:B:223:VAL:C	1:B:225:ARG:H	2.12	0.58
1:B:219:ARG:NH2	1:B:219:ARG:HB3	2.19	0.58
1:B:219:ARG:CD	1:B:859:GLN:HE22	2.06	0.58
1:B:347:ASN:HD22	1:B:348:PRO:HD3	1.68	0.58
1:B:368:LEU:HD23	1:B:377:LEU:CD2	2.33	0.58
1:B:1462:LEU:CD1	1:B:1466:ILE:HG12	2.33	0.58
1:B:804:LEU:O	1:B:805:SER:HB2	2.02	0.57
1:B:342:LEU:HA	2:B:2105:NAG:H83	1.86	0.57
1:B:180:GLY:O	1:B:181:PHE:CG	2.58	0.57
1:B:871:SER:OG	1:B:872:ASP:N	2.38	0.57
1:B:347:ASN:ND2	1:B:348:PRO:CD	2.68	0.56
1:B:295:GLU:HB2	1:B:301:TRP:HB3	1.87	0.56
1:B:293:SER:HB2	1:B:303:SER:HA	1.88	0.56
1:B:347:ASN:CG	1:B:348:PRO:HD2	2.30	0.56
1:B:290:THR:OG1	1:B:294:VAL:CG1	2.54	0.55
1:B:708:GLN:OE1	1:B:712:LEU:HD22	2.05	0.55
1:B:1293:PHE:CD2	1:B:1293:PHE:N	2.73	0.55
1:B:1421:TRP:CD1	1:B:1421:TRP:N	2.73	0.55
1:B:1732:LEU:HD22	1:B:1733:PRO:HD2	1.89	0.55
1:B:141:ILE:HG21	1:B:229:THR:HB	1.89	0.54
1:B:1375:TYR:CD2	1:B:1375:TYR:C	2.85	0.54
1:B:807:LEU:HA	1:B:810:PHE:CD2	2.42	0.54
1:B:1760:PHE:CD1	1:B:1764:VAL:HG23	2.43	0.54
1:B:809:SER:O	1:B:812:LEU:N	2.38	0.53
1:B:368:LEU:HD22	1:B:374:TRP:HB2	1.90	0.53
1:B:1465:PHE:C	1:B:1465:PHE:CD2	2.86	0.53
1:B:287:LEU:HB3	1:B:294:VAL:HG23	1.90	0.53
1:B:1417:THR:HG21	1:B:1713:TRP:HE1	1.73	0.53
1:B:779:GLN:HG3	1:B:780:GLY:H	1.73	0.53
1:B:1288:ALA:CB	1:B:1294:ALA:HB3	2.38	0.53
1:B:402:PHE:O	1:B:406:ASN:ND2	2.42	0.52
1:B:282:ARG:NH2	1:B:297:ASP:OD1	2.42	0.52
1:B:293:SER:O	1:B:303:SER:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:GLN:CG	1:B:780:GLY:N	2.73	0.52
1:B:1288:ALA:HB1	1:B:1294:ALA:HB1	1.92	0.52
1:B:290:THR:HG21	1:B:294:VAL:HG11	1.91	0.51
1:B:1564:ASN:HD21	1:B:1629:ARG:HH12	1.59	0.51
1:B:219:ARG:HB3	1:B:219:ARG:CZ	2.41	0.51
1:B:290:THR:CG2	1:B:294:VAL:HG11	2.39	0.51
1:B:933:LEU:HD22	1:B:933:LEU:C	2.36	0.51
1:B:287:LEU:HD23	1:B:294:VAL:CG2	2.40	0.51
1:B:1288:ALA:CA	1:B:1294:ALA:HB3	2.40	0.51
1:B:402:PHE:CZ	1:B:1709:THR:HG22	2.45	0.51
1:B:739:TYR:CD1	1:B:739:TYR:C	2.88	0.51
1:B:1294:ALA:O	1:B:1299:ILE:HG21	2.11	0.51
1:B:1484:ASP:HB3	1:B:1487:MET:HG3	1.91	0.51
1:B:347:ASN:ND2	1:B:354:SER:OG	2.34	0.51
1:B:1510:ILE:CD1	1:B:1511:PRO:HD2	2.40	0.51
1:B:405:VAL:CG1	3:B:2110:QDN:C19	2.85	0.51
1:B:1522:PHE:HA	1:B:1525:VAL:HB	1.93	0.51
1:B:368:LEU:HD21	1:B:377:LEU:HD23	1.91	0.50
1:B:1542:MET:HE2	1:B:1633:ILE:HG23	1.93	0.50
1:B:1763:VAL:O	1:B:1763:VAL:HG12	2.10	0.50
1:B:869:ARG:HA	1:B:869:ARG:NH1	2.02	0.50
1:B:299:LEU:CD1	1:B:301:TRP:HZ3	2.25	0.50
1:B:349:ASP:OD2	1:B:904:TRP:CH2	2.65	0.50
1:B:1582:LEU:HB3	1:B:1585:TYR:HB2	1.94	0.50
1:B:1608:LEU:HD12	1:B:1608:LEU:C	2.37	0.50
1:B:268:GLY:O	1:B:272:PHE:HB2	2.11	0.49
1:B:218:LEU:O	1:B:218:LEU:HD12	2.11	0.49
1:B:939:LEU:O	1:B:943:SER:CB	2.60	0.49
1:B:282:ARG:HG3	1:B:313:ASN:O	2.12	0.49
1:B:295:GLU:OE1	1:B:295:GLU:HA	2.11	0.49
1:B:779:GLN:NE2	1:B:780:GLY:N	2.60	0.49
1:B:1572:THR:HG22	1:B:1599:VAL:HG13	1.94	0.49
1:B:1762:ILE:O	1:B:1765:ASN:HB2	2.12	0.49
1:B:1780:GLU:HG3	1:B:1781:GLU:HG2	1.93	0.49
1:B:708:GLN:OE1	1:B:708:GLN:HA	2.12	0.49
1:B:781:TRP:HZ3	1:B:784:PHE:CD2	2.31	0.49
1:B:722:THR:HG23	1:B:723:ILE:HD12	1.94	0.48
1:B:1375:TYR:CD1	1:B:1439:GLN:HG3	2.47	0.48
1:B:1760:PHE:CD1	1:B:1764:VAL:CG2	2.96	0.48
1:B:219:ARG:HD3	1:B:859:GLN:NE2	2.27	0.48
1:B:295:GLU:HB2	1:B:301:TRP:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLU:OE2	1:B:304:LEU:HA	2.14	0.48
1:B:347:ASN:HB3	1:B:351:GLY:HA2	1.94	0.48
1:B:302:GLU:OE1	1:B:302:GLU:HA	2.13	0.48
1:B:710:VAL:CG1	1:B:770:ALA:HA	2.43	0.48
1:B:347:ASN:CG	1:B:348:PRO:CD	2.87	0.47
1:B:1760:PHE:CD1	1:B:1760:PHE:C	2.91	0.47
1:B:287:LEU:HB3	1:B:294:VAL:HG21	1.95	0.47
1:B:301:TRP:CG	1:B:307:TYR:HD1	2.32	0.47
1:B:270:GLN:HE21	1:B:1630:ILE:HD11	1.79	0.47
1:B:219:ARG:CG	1:B:219:ARG:NH2	2.73	0.47
1:B:219:ARG:CZ	1:B:219:ARG:CB	2.91	0.47
1:B:803:ASN:ND2	1:B:803:ASN:C	2.73	0.46
1:B:868:LEU:C	1:B:869:ARG:NH1	2.73	0.46
1:B:881:MET:HE2	1:B:890:ILE:HG21	1.97	0.46
1:B:1554:PRO:O	1:B:1558:ASN:ND2	2.48	0.46
1:B:1589:ASN:OD1	1:B:1638:ARG:NH2	2.49	0.46
1:B:347:ASN:HD22	1:B:347:ASN:HA	1.51	0.46
1:B:1486:PHE:HE1	1:B:1765:ASN:OD1	1.98	0.46
1:B:869:ARG:HG3	1:B:877:PRO:HD2	1.91	0.46
1:B:1759:SER:O	1:B:1763:VAL:HG23	2.16	0.46
1:B:368:LEU:CD2	1:B:374:TRP:HB2	2.45	0.46
1:B:871:SER:O	1:B:872:ASP:HB2	2.16	0.46
1:B:804:LEU:O	1:B:805:SER:CB	2.64	0.46
1:B:939:LEU:O	1:B:943:SER:HB2	2.16	0.45
1:B:736:LEU:CD2	1:B:745:PHE:CZ	2.97	0.45
1:B:293:SER:O	1:B:303:SER:CA	2.64	0.45
1:B:1608:LEU:O	1:B:1610:ASP:N	2.50	0.45
1:B:879:TRP:NE1	1:B:1426:TYR:OH	2.38	0.45
1:B:1375:TYR:CE1	1:B:1439:GLN:HG3	2.52	0.45
1:B:899:TRP:CE3	1:B:903:MET:SD	3.09	0.45
1:B:173:LEU:HD23	1:B:176:ILE:HD11	1.98	0.45
1:B:781:TRP:O	1:B:782:ASN:CG	2.60	0.45
1:B:907:MET:HE2	1:B:916:LEU:HD23	1.94	0.45
1:B:1657:LEU:HD11	1:B:1766:MET:HE3	1.98	0.45
1:B:285:THR:HG22	1:B:296:ALA:HB3	1.98	0.45
1:B:383:ARG:HA	1:B:1691:MET:HE1	1.99	0.45
1:B:736:LEU:CD2	1:B:745:PHE:HZ	2.22	0.45
1:B:781:TRP:CZ3	1:B:784:PHE:CD2	3.05	0.45
1:B:778:GLN:O	1:B:779:GLN:HB3	2.16	0.44
1:B:347:ASN:HD21	1:B:354:SER:HG	1.60	0.44
1:B:1375:TYR:CD2	1:B:1375:TYR:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:PHE:HA	1:B:1460:PHE:HD2	1.82	0.44
1:B:1195:ARG:HH21	1:B:1196:LYS:HD3	1.83	0.44
1:B:223:VAL:O	1:B:224:LEU:C	2.60	0.44
1:B:806:VAL:O	1:B:809:SER:N	2.51	0.44
3:B:2110:QDN:C11	3:B:2110:QDN:H20	2.48	0.44
1:B:331:ASP:HB3	1:B:387:LYS:H	1.82	0.44
1:B:739:TYR:CD1	1:B:739:TYR:O	2.70	0.44
1:B:923:MET:HE2	1:B:923:MET:HB2	1.67	0.44
1:B:1267:PHE:O	1:B:1273:TRP:NE1	2.46	0.44
1:B:1252:LEU:O	1:B:1256:LEU:HB2	2.18	0.44
1:B:180:GLY:O	1:B:181:PHE:CB	2.65	0.44
1:B:830:LYS:O	1:B:834:ASN:HB2	2.18	0.44
1:B:293:SER:HB2	1:B:304:LEU:H	1.83	0.43
1:B:382:LEU:HD11	1:B:390:MET:HB3	2.00	0.43
1:B:1462:LEU:CD1	1:B:1466:ILE:CG1	2.96	0.43
1:B:282:ARG:HD3	1:B:297:ASP:OD1	2.19	0.43
3:B:2110:QDN:C2	3:B:2110:QDN:H3	2.48	0.43
1:B:779:GLN:CD	1:B:780:GLY:N	2.73	0.43
1:B:1462:LEU:CD1	1:B:1462:LEU:C	2.92	0.43
1:B:710:VAL:C	1:B:713:VAL:HG23	2.43	0.43
1:B:808:ARG:HG3	1:B:811:ARG:HH21	1.84	0.43
1:B:1288:ALA:O	1:B:1294:ALA:N	2.48	0.43
1:B:1401:ASN:ND2	1:B:1403:ASP:OD2	2.52	0.43
1:B:365:LEU:HA	1:B:368:LEU:HB2	2.01	0.42
1:B:710:VAL:HG13	1:B:711:LYS:N	2.34	0.42
1:B:1465:PHE:C	1:B:1465:PHE:HD2	2.25	0.42
1:B:1761:LEU:O	1:B:1764:VAL:HB	2.19	0.42
1:B:879:TRP:HZ3	1:B:889:LEU:HB3	1.84	0.42
1:B:1430:ASP:HB3	1:B:1438:PRO:HB2	1.99	0.42
1:B:295:GLU:HG3	1:B:307:TYR:CB	2.49	0.42
1:B:809:SER:HB2	1:B:1351:MET:SD	2.59	0.42
1:B:869:ARG:HA	1:B:869:ARG:HD3	1.74	0.42
1:B:1251:VAL:HG21	1:B:1283:LEU:HD21	2.02	0.42
1:B:1421:TRP:HD1	1:B:1421:TRP:N	2.13	0.42
1:B:1660:ILE:CG2	1:B:1762:ILE:HG23	2.49	0.42
1:B:807:LEU:H	1:B:807:LEU:CD1	2.20	0.41
1:B:1300:LYS:HA	1:B:1303:ARG:HG3	2.01	0.41
1:B:1510:ILE:HD12	1:B:1511:PRO:HD2	2.02	0.41
1:B:1630:ILE:HG23	1:B:1633:ILE:HD12	2.02	0.41
1:B:923:MET:O	1:B:927:ASN:HB2	2.19	0.41
1:B:1375:TYR:O	1:B:1375:TYR:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1762:ILE:O	1:B:1765:ASN:N	2.53	0.41
1:B:293:SER:HB2	1:B:304:LEU:N	2.36	0.41
1:B:347:ASN:CB	1:B:348:PRO:CD	2.98	0.41
1:B:1619:PRO:O	1:B:1623:ARG:NE	2.51	0.41
1:B:219:ARG:NH2	1:B:219:ARG:CB	2.84	0.41
1:B:294:VAL:HA	1:B:301:TRP:O	2.21	0.41
1:B:1760:PHE:HD1	1:B:1764:VAL:HG23	1.82	0.41
1:B:1629:ARG:HB2	1:B:1632:ARG:HH21	1.85	0.41
1:B:708:GLN:O	1:B:712:LEU:HD22	2.20	0.41
1:B:907:MET:CE	1:B:916:LEU:CD2	2.87	0.41
1:B:1734:ASN:CB	1:B:1738:SER:O	2.65	0.41
1:B:789:VAL:O	1:B:793:LEU:HB2	2.21	0.41
1:B:1462:LEU:HD13	1:B:1462:LEU:C	2.45	0.41
1:B:822:TRP:HD1	1:B:825:LEU:H	1.67	0.40
1:B:1486:PHE:CE1	1:B:1765:ASN:OD1	2.74	0.40
1:B:710:VAL:CG1	1:B:711:LYS:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1145/2059 (56%)	1046 (91%)	89 (8%)	10 (1%)	14 43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	PHE
1	B	224	LEU
1	B	182	CYS
1	B	358	PHE
1	B	350	HIS

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Mol	Chain	Res	Type
1	B	779	GLN
1	B	1505	LYS
1	B	1685	GLU
1	B	1552	GLN
1	B	251	ALA

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	B	1013/1794 (56%)	952 (94%)	61 (6%)	17	46

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	182	CYS
1	B	183	LEU
1	B	218	LEU
1	B	219	ARG
1	B	220	THR
1	B	276	LEU
1	B	299	LEU
1	B	301	TRP
1	B	302	GLU
1	B	304	LEU
1	B	322	ASP
1	B	347	ASN
1	B	350	HIS
1	B	353	THR
1	B	365	LEU
1	B	368	LEU
1	B	371	GLN
1	B	407	LEU
1	B	712	LEU
1	B	713	VAL
1	B	723	ILE

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Mol	Chain	Res	Type
1	B	778	GLN
1	B	798	LEU
1	B	801	MET
1	B	802	SER
1	B	803	ASN
1	B	804	LEU
1	B	807	LEU
1	B	808	ARG
1	B	812	LEU
1	B	869	ARG
1	B	901	GLU
1	B	916	LEU
1	B	923	MET
1	B	933	LEU
1	B	1256	LEU
1	B	1293	PHE
1	B	1295	GLU
1	B	1296	MET
1	B	1373	LEU
1	B	1374	ASN
1	B	1375	TYR
1	B	1413	LEU
1	B	1421	TRP
1	B	1462	LEU
1	B	1464	LEU
1	B	1504	LYS
1	B	1505	LYS
1	B	1507	GLN
1	B	1508	LYS
1	B	1540	LEU
1	B	1559	ILE
1	B	1560	LEU
1	B	1576	ILE
1	B	1608	LEU
1	B	1654	LEU
1	B	1683	LYS
1	B	1732	LEU
1	B	1757	ILE
1	B	1759	SER
1	B	1767	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	ASN
1	B	214	ASN
1	B	270	GLN
1	B	278	HIS
1	B	313	ASN
1	B	347	ASN
1	B	420	ASN
1	B	730	ASN
1	B	740	ASN
1	B	826	ASN
1	B	859	GLN
1	B	932	ASN
1	B	1200	HIS
1	B	1204	HIS
1	B	1269	ASN
1	B	1483	GLN
1	B	1558	ASN
1	B	1659	ASN
1	B	1699	ASN
1	B	1734	ASN
1	B	1736	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](#)

10 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	NAG	B	2103	1	14,14,15	0.40	0	17,19,21	0.35	0
2	NAG	B	2101	1	14,14,15	0.28	0	17,19,21	0.42	0
2	NAG	B	2104	1	14,14,15	0.66	0	17,19,21	2.40	3 (17%)
2	NAG	B	2106	1	14,14,15	0.87	2 (14%)	17,19,21	0.63	1 (5%)
2	NAG	B	2108	1	14,14,15	0.39	0	17,19,21	0.80	1 (5%)
2	NAG	B	2105	1	14,14,15	0.50	0	17,19,21	0.61	0
2	NAG	B	2107	1	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
2	NAG	B	2102	1	14,14,15	0.46	0	17,19,21	0.68	1 (5%)
3	QDN	B	2110	-	27,27,27	1.83	9 (33%)	39,39,39	1.50	9 (23%)
2	NAG	B	2109	1	14,14,15	0.41	0	17,19,21	0.67	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
2	NAG	B	2103	1	-	2/6/23/26	0/1/1/1
2	NAG	B	2101	1	-	2/6/23/26	0/1/1/1
2	NAG	B	2104	1	-	6/6/23/26	0/1/1/1
2	NAG	B	2106	1	-	0/6/23/26	0/1/1/1
2	NAG	B	2108	1	-	2/6/23/26	0/1/1/1
2	NAG	B	2105	1	-	2/6/23/26	0/1/1/1
2	NAG	B	2107	1	-	2/6/23/26	0/1/1/1
2	NAG	B	2102	1	-	0/6/23/26	0/1/1/1
3	QDN	B	2110	-	-	4/12/33/33	0/5/4/4
2	NAG	B	2109	1	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2110	QDN	C17-C13	-3.29	1.48	1.54
3	B	2110	QDN	C14-C15	3.23	1.61	1.52
3	B	2110	QDN	C16-C17	3.01	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2110	QDN	C12-C11	2.77	1.59	1.53
3	B	2110	QDN	C6-N	2.64	1.37	1.32
3	B	2110	QDN	C4-C3	-2.57	1.38	1.43
3	B	2110	QDN	C14-C13	-2.56	1.47	1.53
2	B	2106	NAG	O5-C1	2.36	1.47	1.43
3	B	2110	QDN	C11-N1	-2.09	1.43	1.48
2	B	2106	NAG	C1-C2	2.08	1.55	1.52
3	B	2110	QDN	O-C1	2.04	1.41	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2104	NAG	C2-N2-C7	8.29	134.01	122.90
2	B	2104	NAG	C1-C2-N2	4.28	117.17	110.43
2	B	2107	NAG	C1-O5-C5	3.47	116.83	112.19
3	B	2110	QDN	C5-C6-N	-3.11	119.98	124.60
3	B	2110	QDN	C2-C3-C4	-2.87	120.30	123.73
2	B	2108	NAG	C1-O5-C5	2.75	115.87	112.19
3	B	2110	QDN	C16-C17-C13	2.74	111.35	107.23
3	B	2110	QDN	C3-C7-N	-2.53	120.14	122.82
3	B	2110	QDN	C12-C11-N1	2.43	113.07	110.50
2	B	2102	NAG	C1-O5-C5	2.42	115.43	112.19
3	B	2110	QDN	C12-C13-C17	-2.33	106.45	109.82
3	B	2110	QDN	C12-C11-C10	-2.21	111.43	113.91
2	B	2104	NAG	C8-C7-N2	2.08	119.57	116.12
3	B	2110	QDN	C4-C3-C7	2.08	120.08	117.47
3	B	2110	QDN	C6-N-C7	2.07	120.06	116.93
2	B	2106	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2105	NAG	O5-C5-C6-O6
3	B	2110	QDN	C9-C1-O-C
2	B	2101	NAG	O5-C5-C6-O6
3	B	2110	QDN	C2-C1-O-C
2	B	2103	NAG	O5-C5-C6-O6
2	B	2109	NAG	O5-C5-C6-O6
2	B	2105	NAG	C4-C5-C6-O6
2	B	2103	NAG	C4-C5-C6-O6
2	B	2101	NAG	C4-C5-C6-O6

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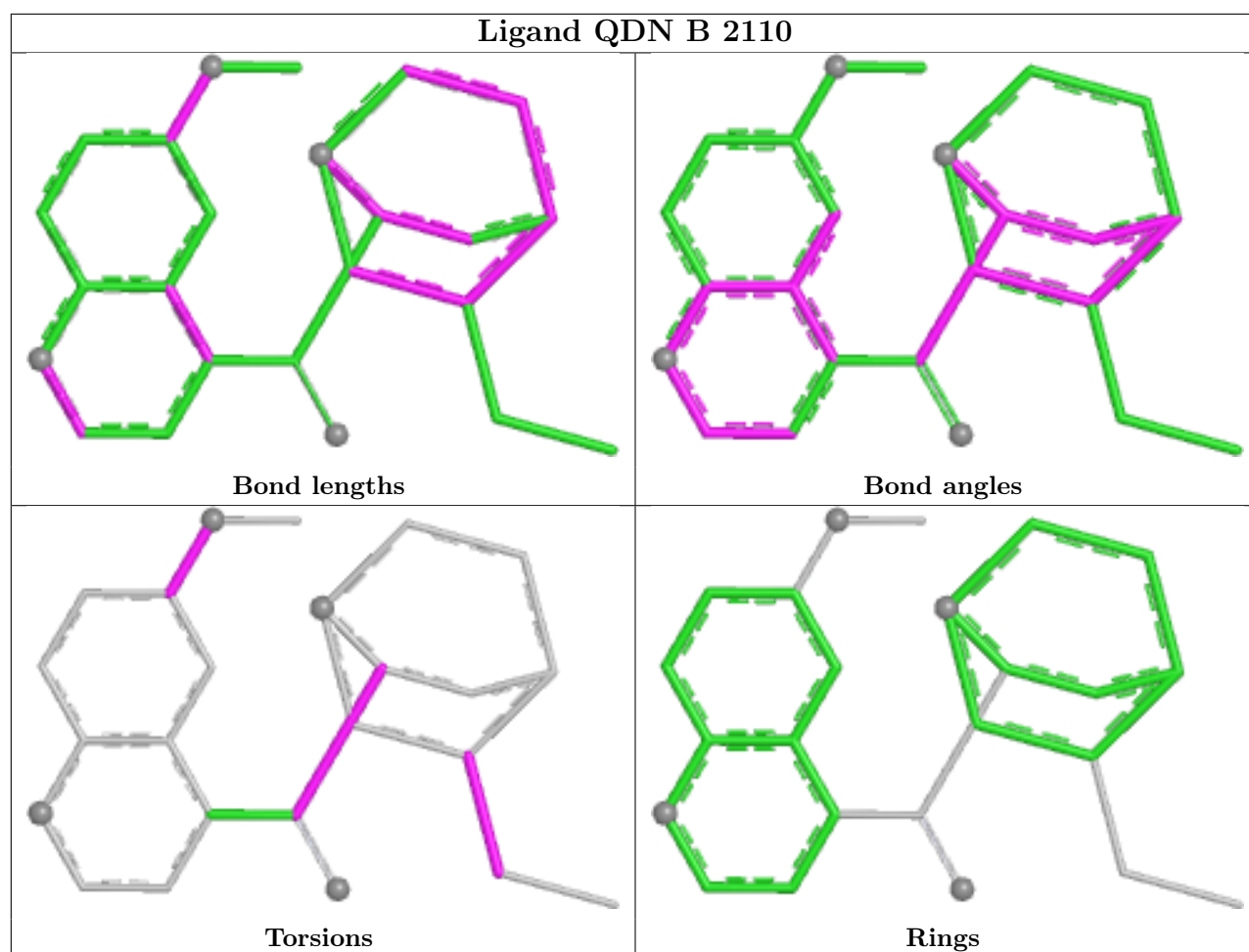
Mol	Chain	Res	Type	Atoms
2	B	2104	NAG	O5-C5-C6-O6
2	B	2107	NAG	O5-C5-C6-O6
2	B	2107	NAG	C4-C5-C6-O6
2	B	2104	NAG	C4-C5-C6-O6
2	B	2104	NAG	C8-C7-N2-C2
2	B	2104	NAG	O7-C7-N2-C2
2	B	2108	NAG	C4-C5-C6-O6
2	B	2108	NAG	O5-C5-C6-O6
2	B	2109	NAG	C4-C5-C6-O6
3	B	2110	QDN	C16-C17-C18-C19
2	B	2104	NAG	C1-C2-N2-C7
2	B	2104	NAG	C3-C2-N2-C7
3	B	2110	QDN	O1-C10-C11-C12

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2105	NAG	1	0
3	B	2110	QDN	5	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.

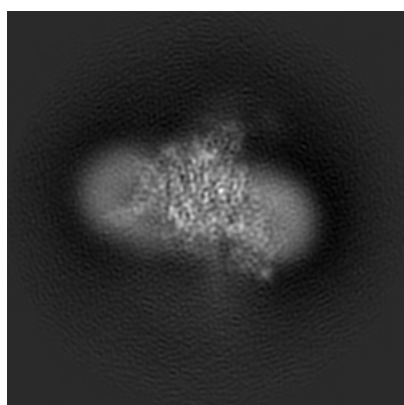
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0942. These allow visual inspection of the internal detail of the map and identification of artifacts.

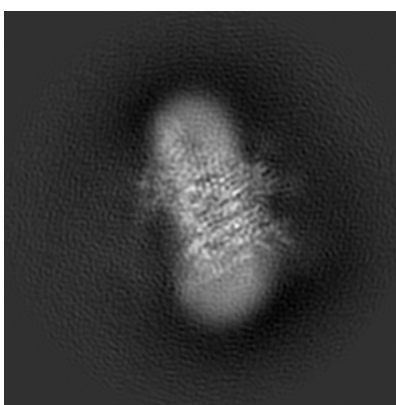
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

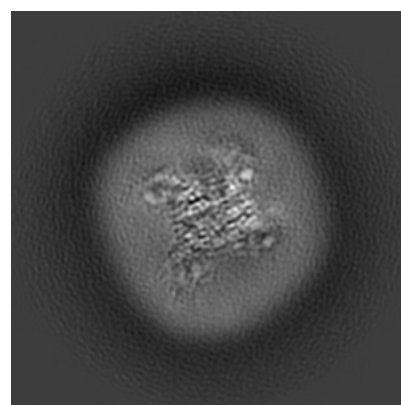
6.1.1 Primary map



X



Y

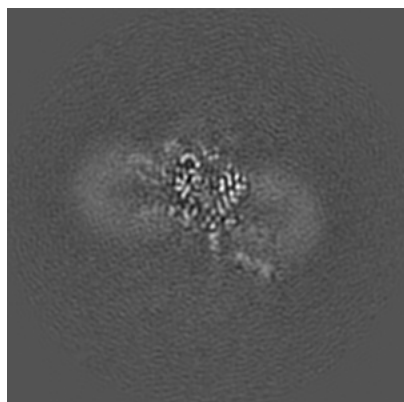


Z

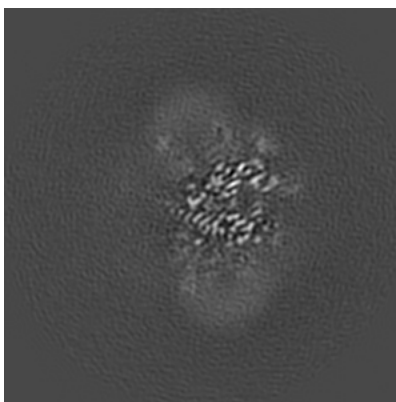
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

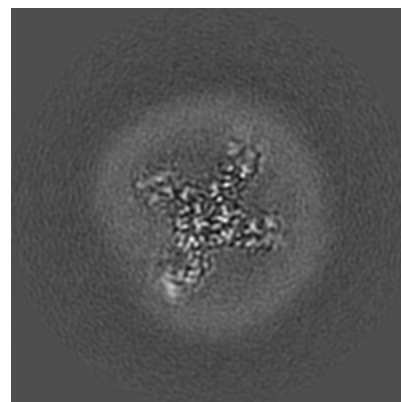
6.2.1 Primary map



X Index: 120



Y Index: 120

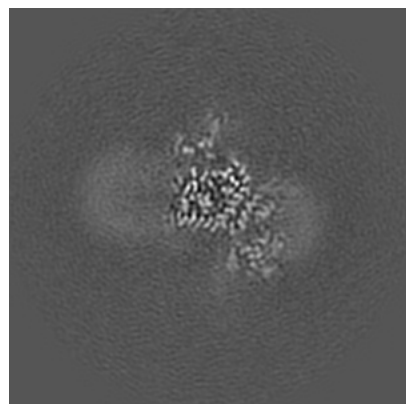


Z Index: 120

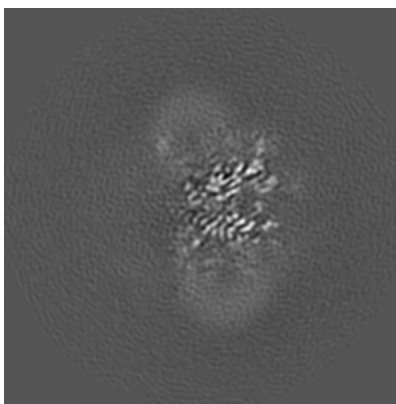
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

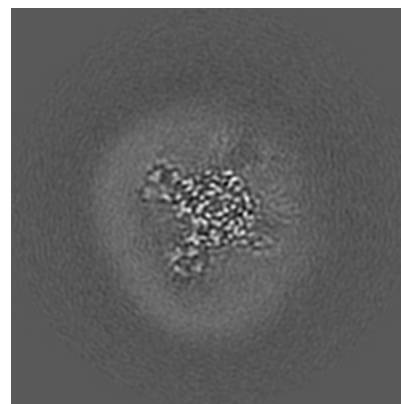
6.3.1 Primary map



X Index: 132



Y Index: 119

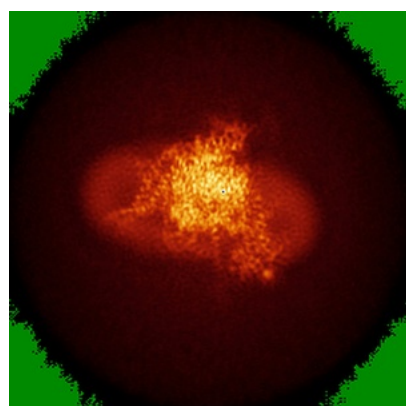


Z Index: 135

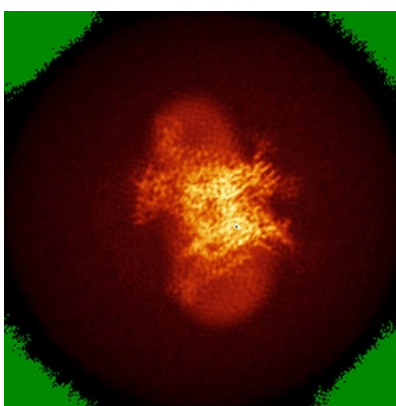
The images above show the largest variance slices of the map in three orthogonal directions.

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

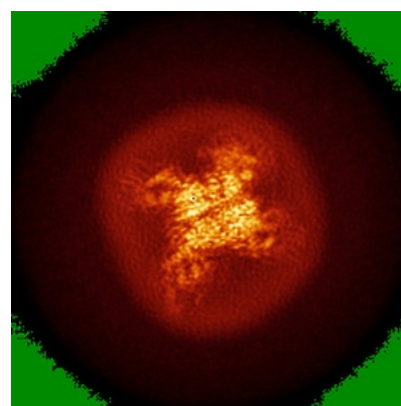
6.4.1 Primary map



X



Y

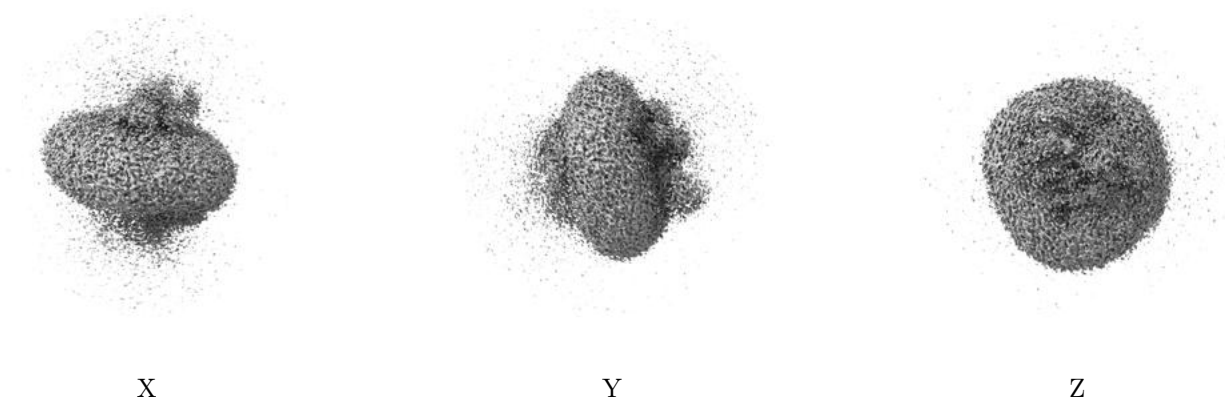


Z

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 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

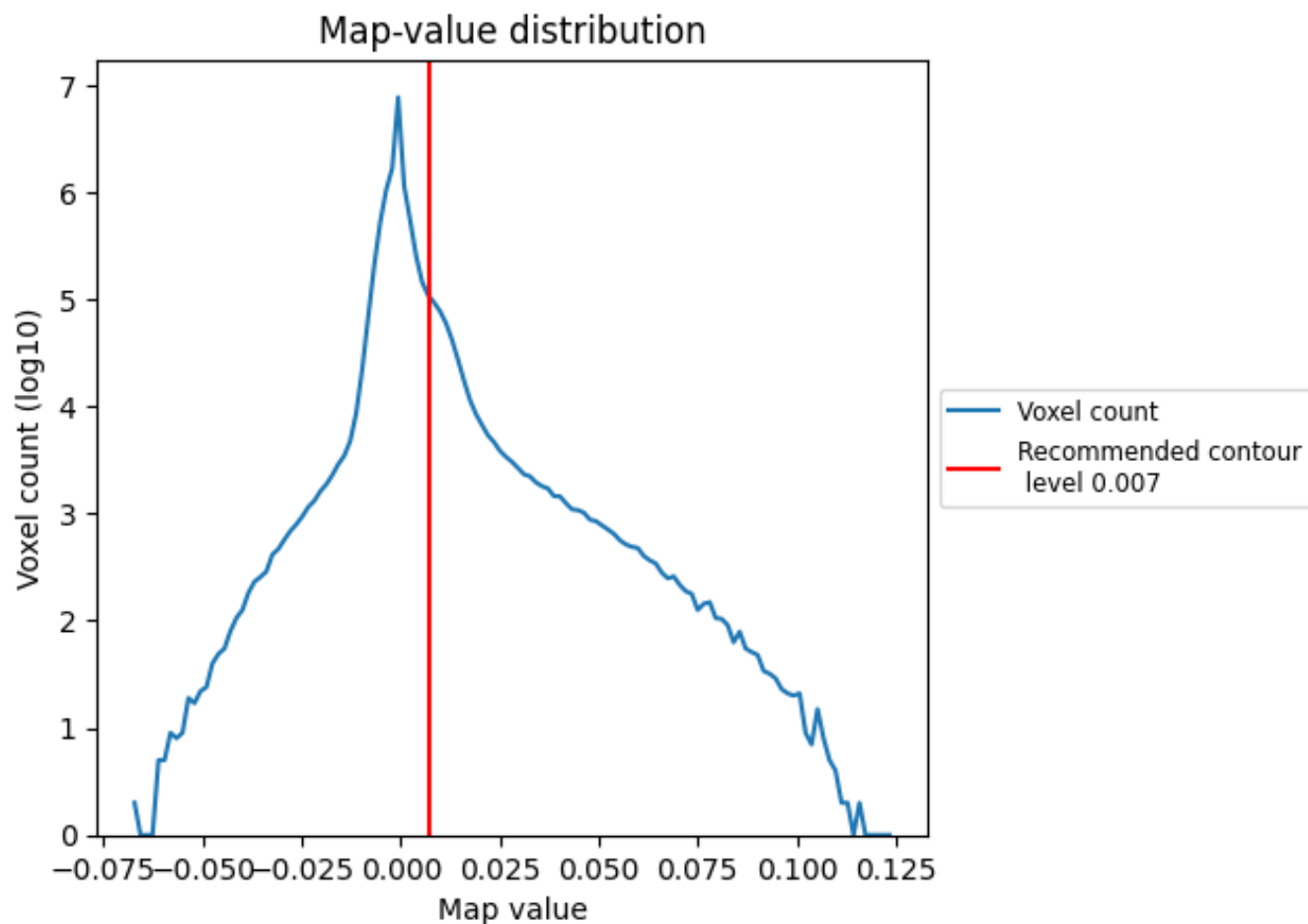
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

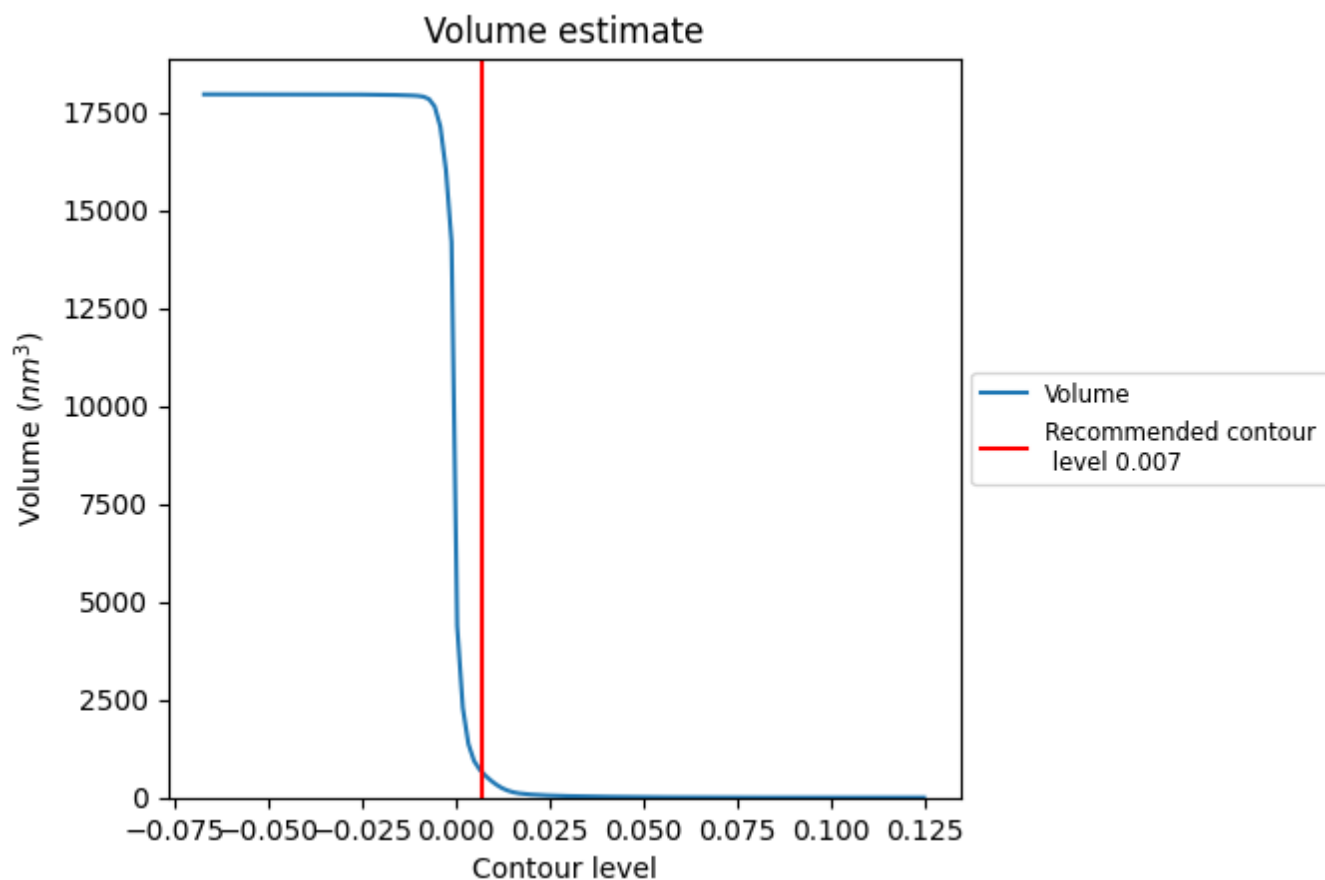
This section contains the results of statistical analysis of the map.

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.

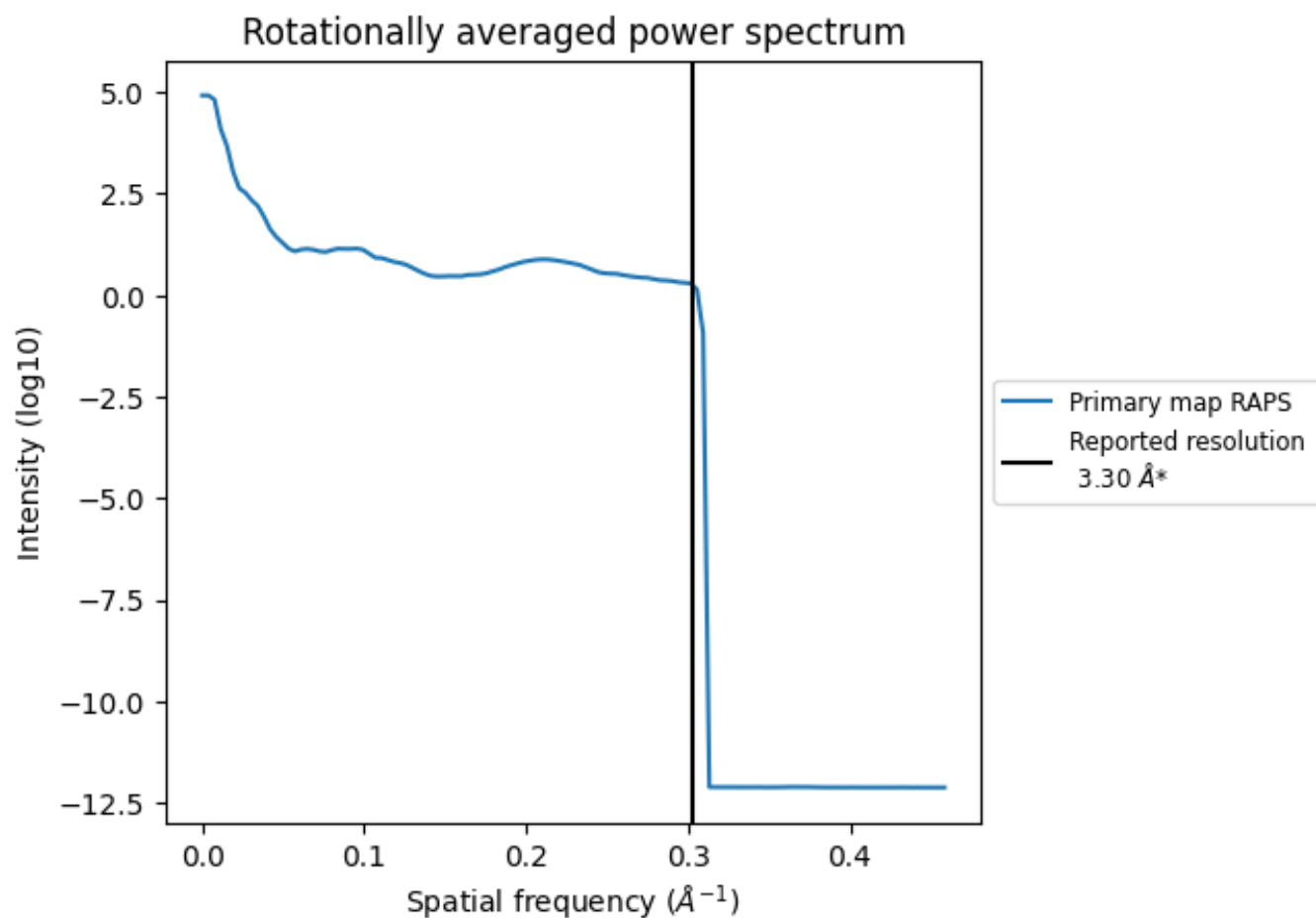
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 649 nm³; this corresponds to an approximate mass of 586 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 0.303 Å⁻¹

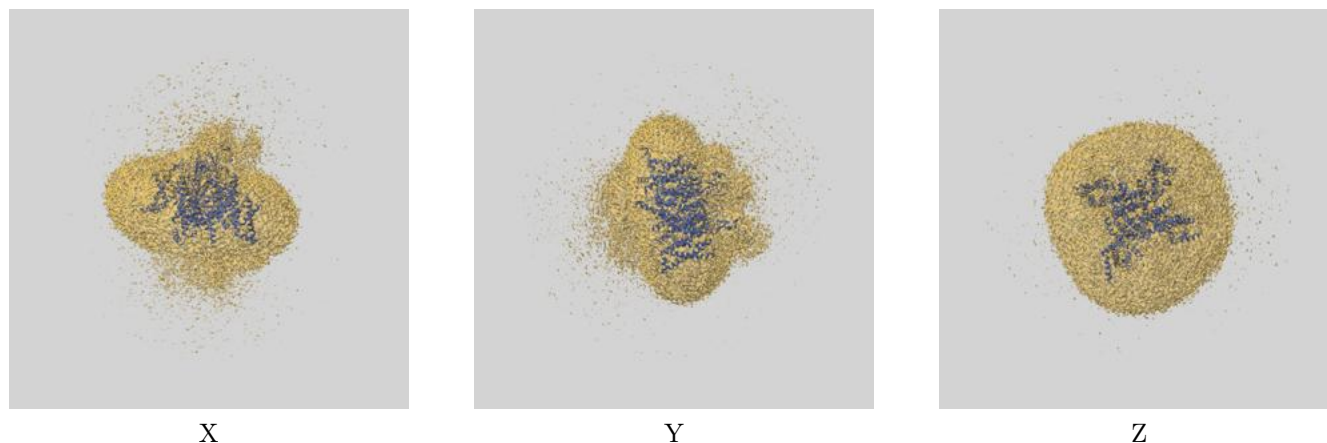
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

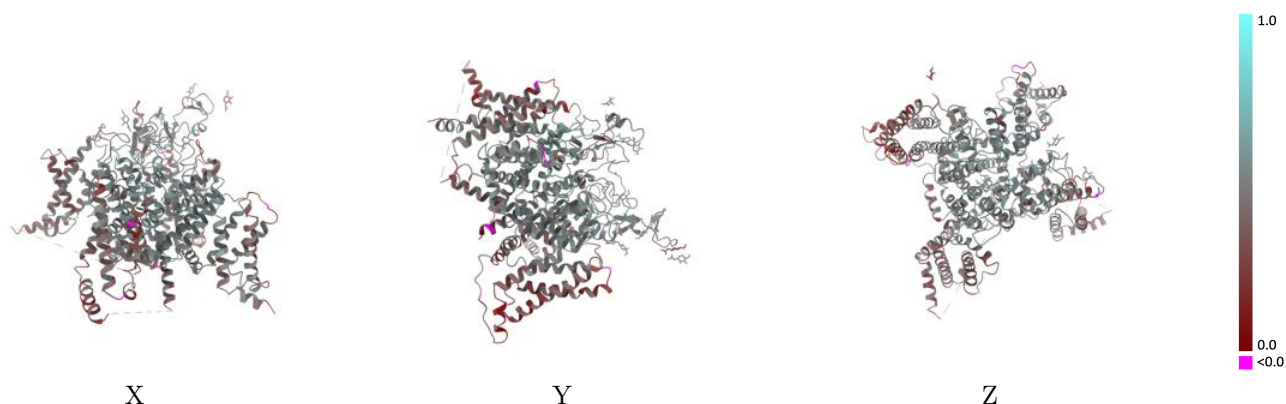
This section contains information regarding the fit between EMDB map EMD-0942 and PDB model 6LQA. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



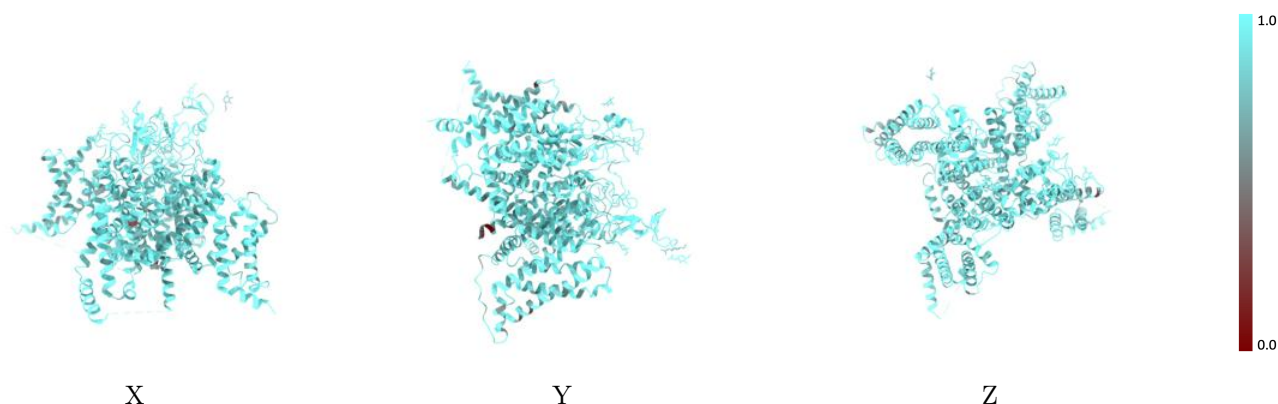
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



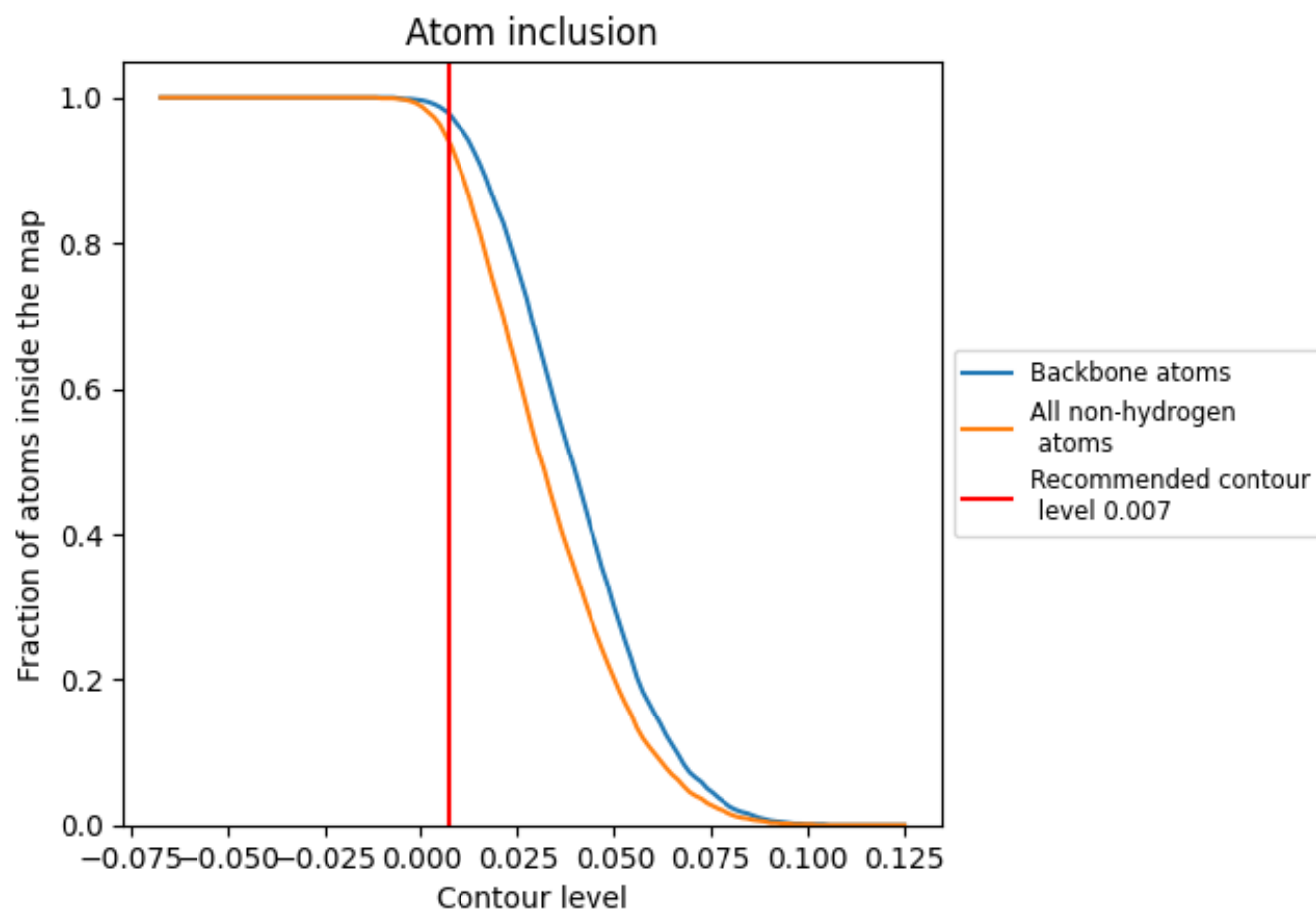
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9420	0.4380
B	0.9420	0.4380

