



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:30 AM UTC

PDB ID : 7X8S / pdb_00007x8s
EMDB ID : EMD-33058
Title : Cryo-EM structure of the WB4-24-bound hGLP-1R-Gs complex
Authors : Cong, Z.T.; Zhou, Q.T.; Li, Y.; Chen, L.N.; Zhang, Z.C.; Liang, A.Y.; Liu, Q.;
Wu, X.Y.; Dai, A.T.; Xia, T.; Wu, W.; Zhang, Y.; Yang, D.H.; Wang, M.W.
Deposited on : 2022-03-14
Resolution : 3.09 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:

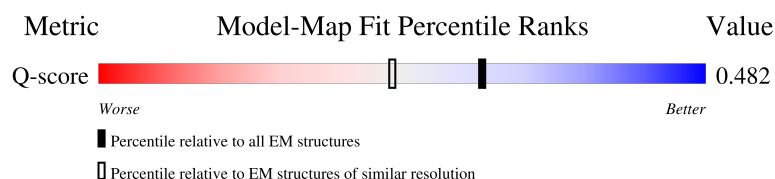
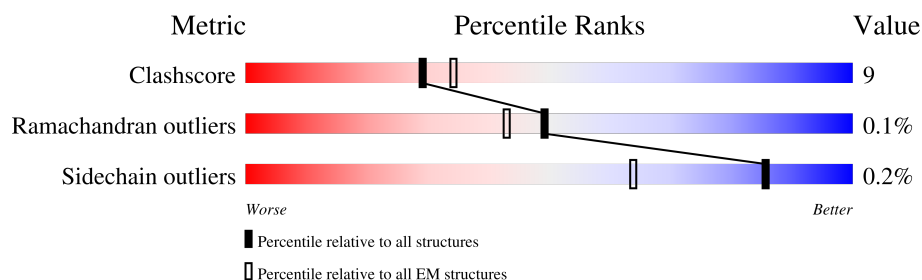
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.09 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	14003 (2.59 - 3.59)

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	394	
2	B	345	
3	G	70	
4	N	140	

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Mol	Chain	Length	Quality of chain
5	R	440	20%51%16%32%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8480 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	235	Total	C	N	O	S	0	0
			1933	1223	351	352	7		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	conflict	UNP P63092
A	226	ALA	GLY	conflict	UNP P63092
A	268	ALA	GLU	conflict	UNP P63092
A	271	LYS	ASN	conflict	UNP P63092
A	274	ASP	LYS	conflict	UNP P63092
A	280	LYS	ARG	variant	UNP P63092
A	284	ASP	THR	conflict	UNP P63092
A	285	THR	ILE	conflict	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2600	1604	467	508	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	54	Total	C	N	O	S	0	0
			418	263	74	78	3		

- Molecule 4 is a protein called Nanobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	126	Total	C	N	O	S	0	0
			961	599	168	188	6		

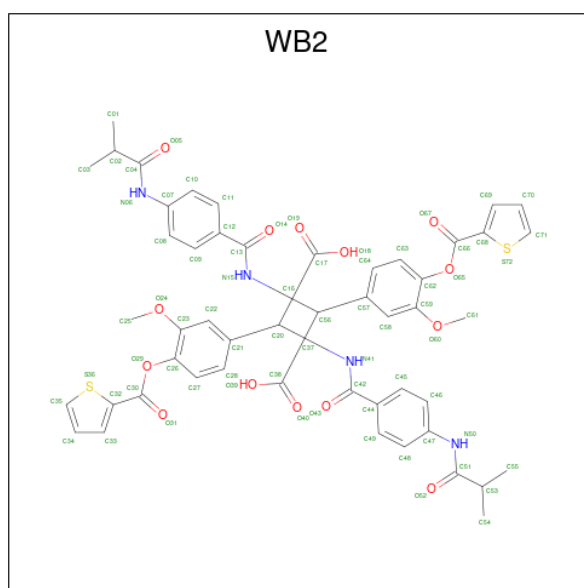
- Molecule 5 is a protein called Glucagon-like peptide 1 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	299	Total	C	N	O	S	0	0
			2496	1667	404	413	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	260	PHE	LEU	variant	UNP P43220

- Molecule 6 is 2,4-bis(3-methoxy-4-thiophen-2-ylcarbonyloxy-phenyl)-1,3-bis[[4-(2-methylpropanoylamino)phenyl]carbonylamino]cyclobutane-1,3-dicarboxylic acid (CCD ID: WB2) (formula: C₅₂H₄₈N₄O₁₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	N	O	S	0
			72	52	4	14	2	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125391	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.497	Depositor
Minimum map value	-3.937	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	274.176, 274.176, 274.176	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.071, 1.071, 1.071	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: WB2

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	0.17	0/1969	0.28	0/2648
2	B	0.18	0/2647	0.31	0/3589
3	G	0.08	0/424	0.22	0/572
4	N	0.16	0/981	0.40	0/1329
5	R	0.18	0/2565	0.37	1/3484 (0.0%)
All	All	0.17	0/8586	0.33	1/11622 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	379	LEU	N-CA-C	-5.14	106.51	112.89

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	1933	0	1913	41	0
2	B	2600	0	2505	53	0
3	G	418	0	431	7	0
4	N	961	0	928	20	0
5	R	2496	0	2524	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	72	0	0	0	0
All	All	8480	0	8301	156	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 9.

All (156) 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)
4:N:19:ARG:HH21	4:N:82:GLN:HB2	1.49	0.76
4:N:20:LEU:HD12	4:N:81:LEU:HD23	1.68	0.75
2:B:155:ASN:ND2	2:B:170:ASP:OD1	2.20	0.74
1:A:283:ARG:HB3	1:A:356:ARG:HE	1.54	0.73
1:A:213:GLN:NE2	1:A:218:ASN:OD1	2.23	0.72
1:A:346:LEU:HD21	1:A:361:PRO:HG3	1.71	0.70
1:A:318:TYR:O	1:A:336:ARG:NH1	2.26	0.69
1:A:362:HIS:NE2	1:A:378:ASP:OD2	2.24	0.68
1:A:234:TRP:HB2	2:B:117:LEU:HD21	1.77	0.66
1:A:33:ASP:OD2	2:B:78:LYS:NZ	2.25	0.66
1:A:240:ASP:OD2	2:B:57:LYS:NZ	2.29	0.66
2:B:197:ARG:HD2	2:B:214:ARG:HH21	1.61	0.66
5:R:277:PRO:HA	5:R:280:PHE:CE1	2.31	0.66
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.77	0.65
2:B:212:ASP:HB3	2:B:215:GLU:HB2	1.80	0.63
5:R:412:GLU:HA	5:R:415:LYS:HE2	1.80	0.63
1:A:232:ARG:HG3	1:A:233:LYS:HD3	1.81	0.63
1:A:215:ASP:OD2	1:A:373:ARG:NH1	2.32	0.62
2:B:81:ILE:HD13	2:B:91:HIS:HB2	1.81	0.61
5:R:227:ARG:NH1	5:R:293:ASP:OD1	2.34	0.61
4:N:100:PRO:HD2	4:N:107:CYS:SG	2.41	0.60
5:R:224:LEU:HD23	5:R:227:ARG:HD2	1.81	0.60
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.83	0.60
4:N:52:SER:O	4:N:72:ARG:NH1	2.36	0.59
5:R:144:LEU:HD21	5:R:388:LEU:HD22	1.84	0.59
5:R:33:TRP:CD1	5:R:205:TYR:HH	2.20	0.59
4:N:110:VAL:O	4:N:118:ARG:NH2	2.36	0.59
5:R:172:LEU:O	5:R:177:ASN:ND2	2.24	0.58
2:B:260:GLU:OE2	2:B:263:THR:OG1	2.20	0.58
1:A:230:GLU:OE1	1:A:232:ARG:NH1	2.28	0.57
5:R:214:TRP:HA	5:R:217:LEU:HD13	1.86	0.56
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:NH1	4:N:109:ASP:OD2	2.37	0.56
1:A:304:GLY:O	1:A:307:LYS:NZ	2.39	0.56
5:R:293:ASP:HA	5:R:297:TRP:HE1	1.71	0.56
4:N:73:ASP:O	4:N:77:ASN:N	2.39	0.55
2:B:327:VAL:HG23	2:B:339:TRP:HB2	1.89	0.54
2:B:320:VAL:HG22	2:B:327:VAL:HG12	1.88	0.54
4:N:68:PHE:HA	4:N:82:GLN:O	2.07	0.54
2:B:54:HIS:NE2	2:B:72:SER:OG	2.34	0.54
5:R:293:ASP:OD1	5:R:297:TRP:NE1	2.41	0.53
4:N:22:CYS:HB3	4:N:79:LEU:HB3	1.91	0.53
1:A:30:LEU:HD21	2:B:80:ILE:HD11	1.91	0.53
1:A:53:LYS:HB3	1:A:247:VAL:HG11	1.89	0.53
2:B:318:LEU:HG	2:B:329:THR:HG22	1.91	0.53
4:N:39:GLN:HB2	4:N:45:LEU:HD13	1.91	0.52
5:R:37:GLN:HA	5:R:40:ARG:HG2	1.91	0.52
5:R:217:LEU:O	5:R:221:GLN:N	2.43	0.52
5:R:303:MET:HE2	5:R:303:MET:N	2.25	0.52
1:A:379:CYS:O	1:A:383:ILE:HG12	2.10	0.52
2:B:58:ILE:O	2:B:316:SER:OG	2.19	0.51
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.92	0.51
5:R:40:ARG:HA	5:R:43:ARG:HE	1.75	0.51
5:R:362:THR:O	5:R:365:VAL:HG22	2.10	0.51
2:B:279:SER:OG	3:G:48:ASP:OD2	2.28	0.51
1:A:229:ASP:N	1:A:229:ASP:OD1	2.41	0.51
2:B:46:ARG:HB2	2:B:48:ARG:NH1	2.26	0.51
1:A:19:GLN:O	1:A:23:ASN:ND2	2.43	0.51
2:B:60:ALA:HB3	2:B:73:ALA:HB3	1.92	0.50
2:B:93:ILE:HG12	2:B:133:VAL:HG11	1.93	0.50
1:A:330:GLU:OE2	1:A:338:LYS:NZ	2.42	0.50
2:B:161:SER:OG	2:B:163:ASP:OD1	2.15	0.50
5:R:407:ASN:O	5:R:411:LEU:HG	2.12	0.50
5:R:304:ASN:O	5:R:308:ILE:HG23	2.12	0.49
5:R:145:TYR:HA	5:R:148:TYR:CE2	2.46	0.49
5:R:282:VAL:HG23	5:R:283:PRO:HD3	1.94	0.49
1:A:318:TYR:OH	1:A:343:ASP:OD2	2.28	0.49
4:N:37:VAL:HG12	4:N:47:TRP:HA	1.94	0.49
5:R:34:GLU:O	5:R:37:GLN:HG3	2.12	0.49
5:R:278:LEU:HA	5:R:281:VAL:HG22	1.94	0.48
5:R:353:THR:O	5:R:357:ILE:HG13	2.12	0.48
3:G:18:GLN:HE21	3:G:22:GLU:HG3	1.79	0.48
4:N:51:ILE:HB	4:N:70:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:LYS:HD2	3:G:44:HIS:HE1	1.78	0.48
5:R:176:ARG:HG2	5:R:250:TYR:HE2	1.79	0.48
5:R:278:LEU:O	5:R:282:VAL:HG22	2.13	0.48
1:A:43:LEU:HD21	1:A:379:CYS:SG	2.54	0.48
2:B:96:ARG:HH11	2:B:96:ARG:HG2	1.78	0.48
5:R:283:PRO:HA	5:R:286:ILE:HG12	1.95	0.47
1:A:270:LEU:HD21	1:A:344:GLU:HB3	1.96	0.47
2:B:68:ARG:NH1	2:B:83:ASP:OD1	2.46	0.47
2:B:340:ASN:HD21	3:G:59:ASN:HD22	1.62	0.47
2:B:137:ARG:NH1	2:B:171:ILE:O	2.47	0.47
1:A:364:THR:OG1	1:A:371:ASN:OD1	2.21	0.47
5:R:146:ILE:O	5:R:150:VAL:HG23	2.14	0.47
1:A:20:ARG:HA	1:A:23:ASN:HD22	1.80	0.47
2:B:155:ASN:HD21	2:B:172:GLU:HG3	1.80	0.47
1:A:20:ARG:NH1	2:B:88:ASN:OD1	2.47	0.46
5:R:359:LEU:HB2	5:R:402:TYR:CE2	2.51	0.46
2:B:164:THR:HG22	2:B:185:GLY:C	2.41	0.46
4:N:15:GLY:HA2	4:N:85:SER:HA	1.98	0.46
2:B:163:ASP:O	2:B:164:THR:OG1	2.30	0.46
2:B:183:HIS:NE2	2:B:201:SER:OG	2.39	0.46
1:A:354:ASP:OD2	1:A:356:ARG:NH1	2.49	0.46
4:N:61:THR:HG22	4:N:64:VAL:HG22	1.97	0.46
5:R:247:GLU:HG2	5:R:359:LEU:HD11	1.98	0.46
2:B:266:HIS:HB3	2:B:269:ILE:HG12	1.97	0.45
5:R:33:TRP:HA	5:R:36:VAL:HG22	1.98	0.45
2:B:215:GLU:HB3	2:B:217:MET:SD	2.57	0.45
2:B:124:TYR:CE2	2:B:135:VAL:HG22	2.52	0.45
2:B:331:SER:HB3	2:B:333:ASP:OD1	2.16	0.45
2:B:333:ASP:O	2:B:334:SER:OG	2.30	0.45
1:A:13:ARG:HA	1:A:13:ARG:HD3	1.82	0.44
1:A:33:ASP:HA	1:A:36:VAL:HG12	1.99	0.44
2:B:280:LYS:NZ	3:G:47:GLU:O	2.41	0.44
4:N:91:THR:HA	4:N:124:VAL:O	2.17	0.44
4:N:24:ALA:HB1	4:N:27:PHE:CZ	2.52	0.44
5:R:293:ASP:HA	5:R:297:TRP:NE1	2.31	0.44
5:R:227:ARG:HB3	5:R:297:TRP:CZ3	2.52	0.44
2:B:286:LEU:HG	2:B:296:VAL:HG22	2.00	0.44
1:A:342:ARG:NH2	1:A:343:ASP:OD1	2.51	0.43
1:A:27:GLU:O	1:A:31:GLN:HG2	2.18	0.43
2:B:201:SER:HG	2:B:211:TRP:HE1	1.65	0.43
1:A:51:SER:HA	1:A:249:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:336:LYS:HD3	5:R:336:LYS:HA	1.80	0.43
5:R:367:PHE:CE2	5:R:383:LYS:HE2	2.52	0.43
4:N:91:THR:HG23	4:N:125:THR:HA	1.99	0.43
1:A:16:GLU:OE1	1:A:16:GLU:N	2.49	0.43
1:A:310:ASP:OD1	1:A:311:TYR:N	2.52	0.43
2:B:326:ALA:HB1	2:B:338:ILE:HG23	2.01	0.43
5:R:330:ILE:O	5:R:334:LYS:HG2	2.18	0.43
4:N:94:TYR:O	4:N:121:GLY:HA2	2.19	0.42
2:B:162:GLY:HA2	2:B:186:ASP:HB2	2.02	0.42
2:B:311:HIS:CE1	2:B:337:LYS:HG3	2.54	0.42
5:R:145:TYR:O	5:R:149:THR:OG1	2.34	0.42
1:A:224:VAL:HG21	1:A:234:TRP:CZ3	2.55	0.42
5:R:284:TRP:HD1	5:R:308:ILE:HD11	1.85	0.42
2:B:99:TRP:HB3	2:B:117:LEU:HD12	2.00	0.42
2:B:283:ARG:HD2	2:B:283:ARG:HA	1.85	0.42
2:B:273:ILE:HG13	2:B:289:TYR:CE2	2.55	0.42
5:R:416:SER:HA	5:R:419:ARG:HG2	2.02	0.42
2:B:198:LEU:HD23	2:B:210:LEU:HD11	2.01	0.42
4:N:34:MET:HE2	4:N:34:MET:HB3	1.92	0.42
5:R:227:ARG:O	5:R:231:LEU:HD23	2.20	0.42
5:R:317:ILE:HA	5:R:320:ASN:HD21	1.84	0.42
5:R:393:PHE:O	5:R:397:MET:HG3	2.19	0.42
3:G:28:ILE:HD12	3:G:32:LYS:HB3	2.01	0.41
5:R:282:VAL:CG2	5:R:283:PRO:HD3	2.50	0.41
2:B:284:LEU:HD12	2:B:284:LEU:HA	1.87	0.41
1:A:233:LYS:HE2	2:B:204:CYS:SG	2.59	0.41
1:A:252:SER:OG	1:A:265:ARG:HB3	2.20	0.41
1:A:228:ARG:NH2	1:A:230:GLU:OE2	2.43	0.41
1:A:247:VAL:HG21	1:A:292:ASN:HD22	1.85	0.41
4:N:68:PHE:CD1	4:N:83:MET:HA	2.55	0.41
1:A:233:LYS:NZ	2:B:228:ASP:OD2	2.40	0.41
2:B:180:PHE:HB3	2:B:211:TRP:CE3	2.56	0.41
1:A:42:ARG:HB3	1:A:222:PHE:HE2	1.86	0.41
5:R:159:LEU:HD11	5:R:395:GLY:O	2.20	0.41
5:R:390:PHE:O	5:R:394:GLN:HG2	2.21	0.41
5:R:292:GLU:HB3	5:R:294:GLU:OE1	2.21	0.41
1:A:322:GLU:N	1:A:322:GLU:OE2	2.54	0.40
5:R:170:ARG:HD2	5:R:170:ARG:HA	1.96	0.40
2:B:225:HIS:CD2	2:B:243:THR:HG1	2.32	0.40
5:R:410:GLN:O	5:R:414:ARG:HG2	2.20	0.40
3:G:17:GLU:O	3:G:21:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:243:TRP:CZ3	5:R:246:VAL:HG11	2.56	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	229/394 (58%)	221 (96%)	8 (4%)	0	100	100
2	B	336/345 (97%)	323 (96%)	13 (4%)	0	100	100
3	G	52/70 (74%)	49 (94%)	3 (6%)	0	100	100
4	N	124/140 (89%)	120 (97%)	4 (3%)	0	100	100
5	R	291/440 (66%)	283 (97%)	7 (2%)	1 (0%)	36	67
All	All	1032/1389 (74%)	996 (96%)	35 (3%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	R	380	ARG

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/349 (59%)	205 (100%)	0	100	100
2	B	281/287 (98%)	281 (100%)	0	100	100
3	G	44/57 (77%)	44 (100%)	0	100	100
4	N	104/116 (90%)	104 (100%)	0	100	100
5	R	269/392 (69%)	267 (99%)	2 (1%)	76	82
All	All	903/1201 (75%)	901 (100%)	2 (0%)	85	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	378	THR
5	R	379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
2	B	230	ASN
2	B	340	ASN
4	N	3	GLN
5	R	300	ASN
5	R	302	ASN
5	R	363	HIS
5	R	394	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
6	WB2	R	501	-	74,78,78	2.08	19 (25%)	98,114,114	2.42	34 (34%)

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
6	WB2	R	501	-	-	24/72/98/98	0/7/7/7

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	WB2	C37-C38	7.12	1.65	1.53
6	R	501	WB2	C16-C17	6.64	1.64	1.53
6	R	501	WB2	C51-N50	4.70	1.46	1.35
6	R	501	WB2	C57-C56	4.51	1.58	1.51
6	R	501	WB2	C04-N06	4.21	1.45	1.35
6	R	501	WB2	C42-N41	3.52	1.41	1.34
6	R	501	WB2	C21-C20	3.31	1.56	1.51
6	R	501	WB2	C12-C13	2.83	1.56	1.50
6	R	501	WB2	C13-N15	2.81	1.39	1.34
6	R	501	WB2	C66-C68	2.80	1.55	1.48
6	R	501	WB2	O29-C30	2.77	1.43	1.35
6	R	501	WB2	C30-C32	2.49	1.55	1.48
6	R	501	WB2	C58-C57	2.46	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	WB2	C53-C51	2.35	1.58	1.52
6	R	501	WB2	C47-N50	2.34	1.46	1.41
6	R	501	WB2	C28-C27	2.15	1.42	1.38
6	R	501	WB2	C22-C21	2.08	1.42	1.39
6	R	501	WB2	C28-C21	2.06	1.42	1.39
6	R	501	WB2	C07-N06	2.01	1.45	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	WB2	O29-C30-C32	9.63	126.30	110.56
6	R	501	WB2	O65-C66-C68	9.13	125.47	110.56
6	R	501	WB2	C28-C21-C22	-5.09	112.83	118.74
6	R	501	WB2	C44-C42-N41	4.77	125.60	116.87
6	R	501	WB2	C64-C57-C58	-4.54	113.47	118.74
6	R	501	WB2	O43-C42-C44	-4.37	112.25	120.90
6	R	501	WB2	O29-C30-O31	-3.68	113.66	123.74
6	R	501	WB2	C59-C58-C57	3.64	125.49	119.86
6	R	501	WB2	C23-C22-C21	3.43	125.15	119.86
6	R	501	WB2	C17-C16-N15	-3.15	105.84	111.66
6	R	501	WB2	C53-C51-N50	3.09	122.07	114.62
6	R	501	WB2	O60-C59-C62	3.01	119.49	115.40
6	R	501	WB2	C11-C12-C09	-2.99	114.76	118.57
6	R	501	WB2	O65-C66-O67	-2.98	115.58	123.74
6	R	501	WB2	C27-C26-C23	-2.97	115.77	119.71
6	R	501	WB2	C33-C32-S36	-2.81	104.68	111.23
6	R	501	WB2	C10-C07-C08	-2.78	115.36	119.04
6	R	501	WB2	C35-S36-C32	2.77	97.31	92.33
6	R	501	WB2	C58-C57-C56	2.68	126.10	119.81
6	R	501	WB2	C69-C68-S72	-2.68	104.99	111.23
6	R	501	WB2	C02-C04-N06	2.68	121.07	114.62
6	R	501	WB2	O52-C51-C53	-2.67	117.89	122.38
6	R	501	WB2	C07-N06-C04	-2.62	121.39	127.37
6	R	501	WB2	C54-C53-C51	2.55	114.85	109.66
6	R	501	WB2	C26-O29-C30	2.54	124.03	118.24
6	R	501	WB2	C12-C13-N15	2.53	121.50	116.87
6	R	501	WB2	C48-C47-C46	-2.44	115.81	119.04
6	R	501	WB2	O19-C17-C16	-2.25	117.32	123.10
6	R	501	WB2	O29-C26-C27	2.13	124.03	118.89
6	R	501	WB2	C27-C28-C21	2.12	123.30	121.18
6	R	501	WB2	C66-C68-S72	2.12	126.94	121.19
6	R	501	WB2	C10-C11-C12	2.10	123.04	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	WB2	C47-N50-C51	-2.09	122.59	127.37
6	R	501	WB2	O05-C04-N06	-2.07	119.55	123.92

There are no chirality outliers.

All (24) torsion outliers are listed below:

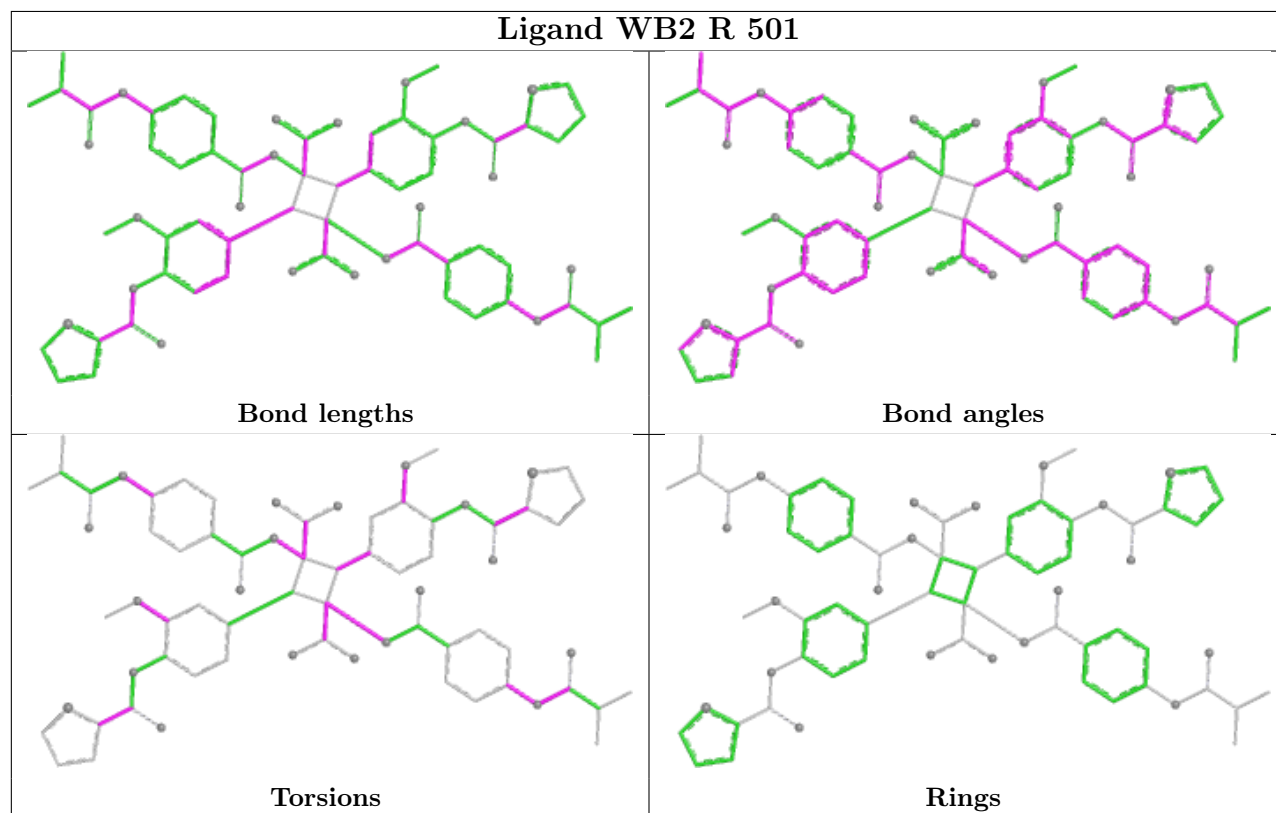
Mol	Chain	Res	Type	Atoms
6	R	501	WB2	N15-C16-C17-O19
6	R	501	WB2	O29-C30-C32-C33
6	R	501	WB2	O29-C30-C32-S36
6	R	501	WB2	O65-C66-C68-C69
6	R	501	WB2	O65-C66-C68-S72
6	R	501	WB2	O67-C66-C68-C69
6	R	501	WB2	O67-C66-C68-S72
6	R	501	WB2	O05-C04-N06-C07
6	R	501	WB2	C62-C59-O60-C61
6	R	501	WB2	C02-C04-N06-C07
6	R	501	WB2	O31-C30-C32-S36
6	R	501	WB2	O31-C30-C32-C33
6	R	501	WB2	C58-C59-O60-C61
6	R	501	WB2	C10-C07-N06-C04
6	R	501	WB2	C46-C47-N50-C51
6	R	501	WB2	C22-C23-O24-C25
6	R	501	WB2	C08-C07-N06-C04
6	R	501	WB2	C48-C47-N50-C51
6	R	501	WB2	C26-C23-O24-C25
6	R	501	WB2	C16-C56-C57-C58
6	R	501	WB2	C16-C56-C57-C64
6	R	501	WB2	C20-C16-N15-C13
6	R	501	WB2	N41-C37-C38-O40
6	R	501	WB2	C20-C37-N41-C42

There are no ring outliers.

No monomer is involved in short contacts.

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.

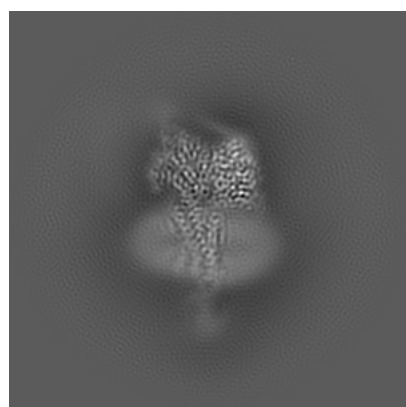
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33058. These allow visual inspection of the internal detail of the map and identification of artifacts.

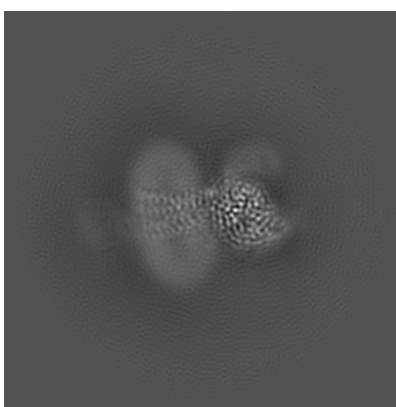
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

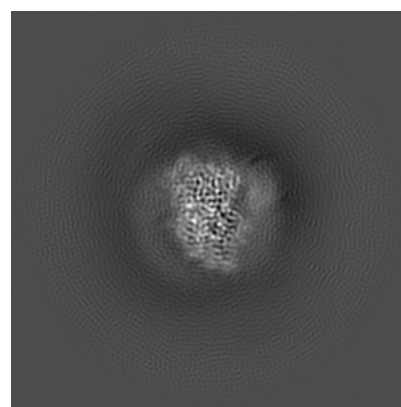
6.1.1 Primary map



X



Y

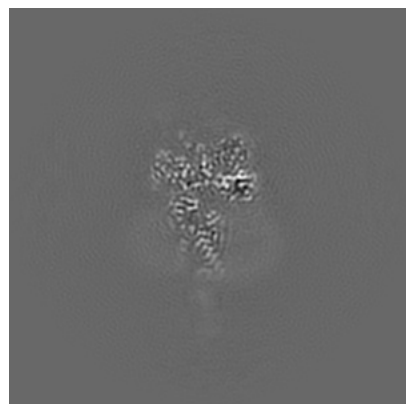


Z

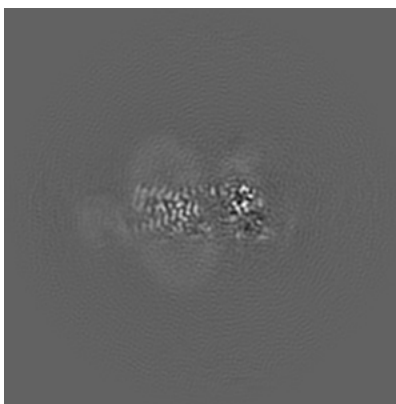
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

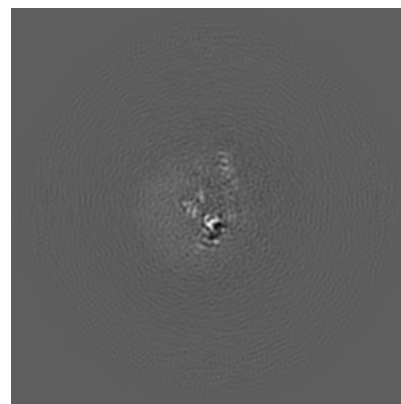
6.2.1 Primary map



X Index: 128



Y Index: 128

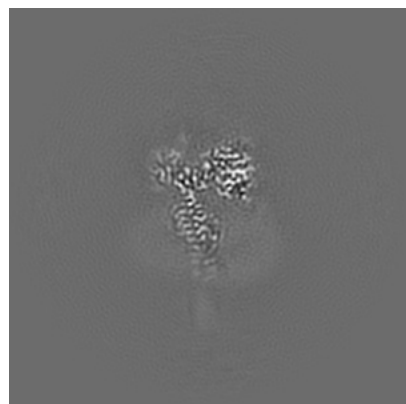


Z Index: 128

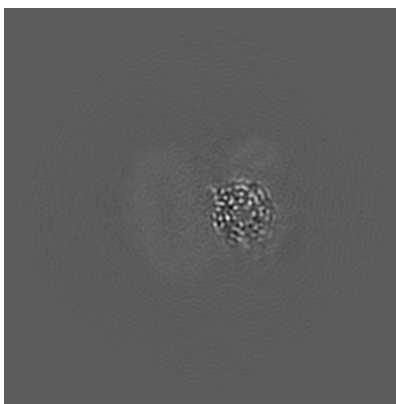
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

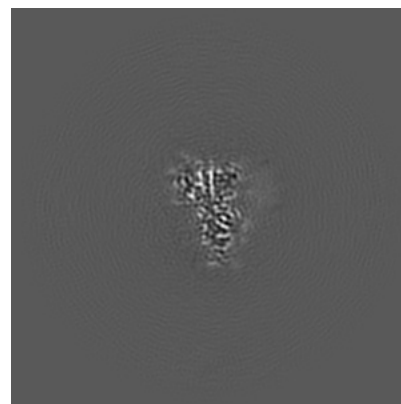
6.3.1 Primary map



X Index: 132



Y Index: 146

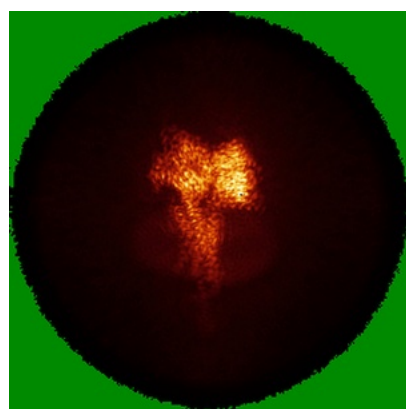


Z Index: 147

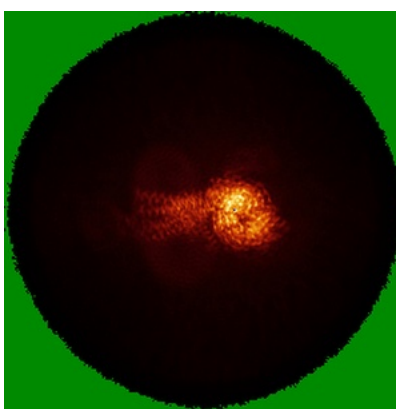
The images above show the largest variance slices of the map in three orthogonal directions.

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

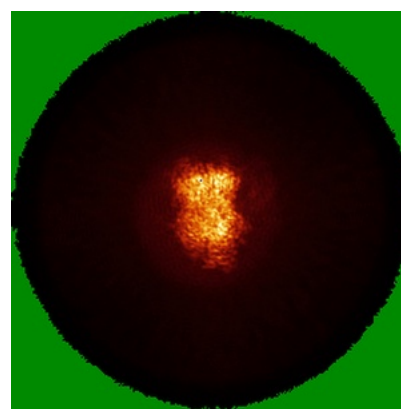
6.4.1 Primary map



X



Y



Z

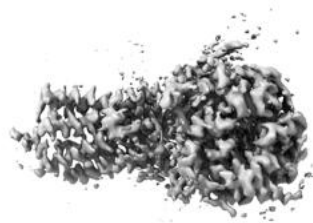
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

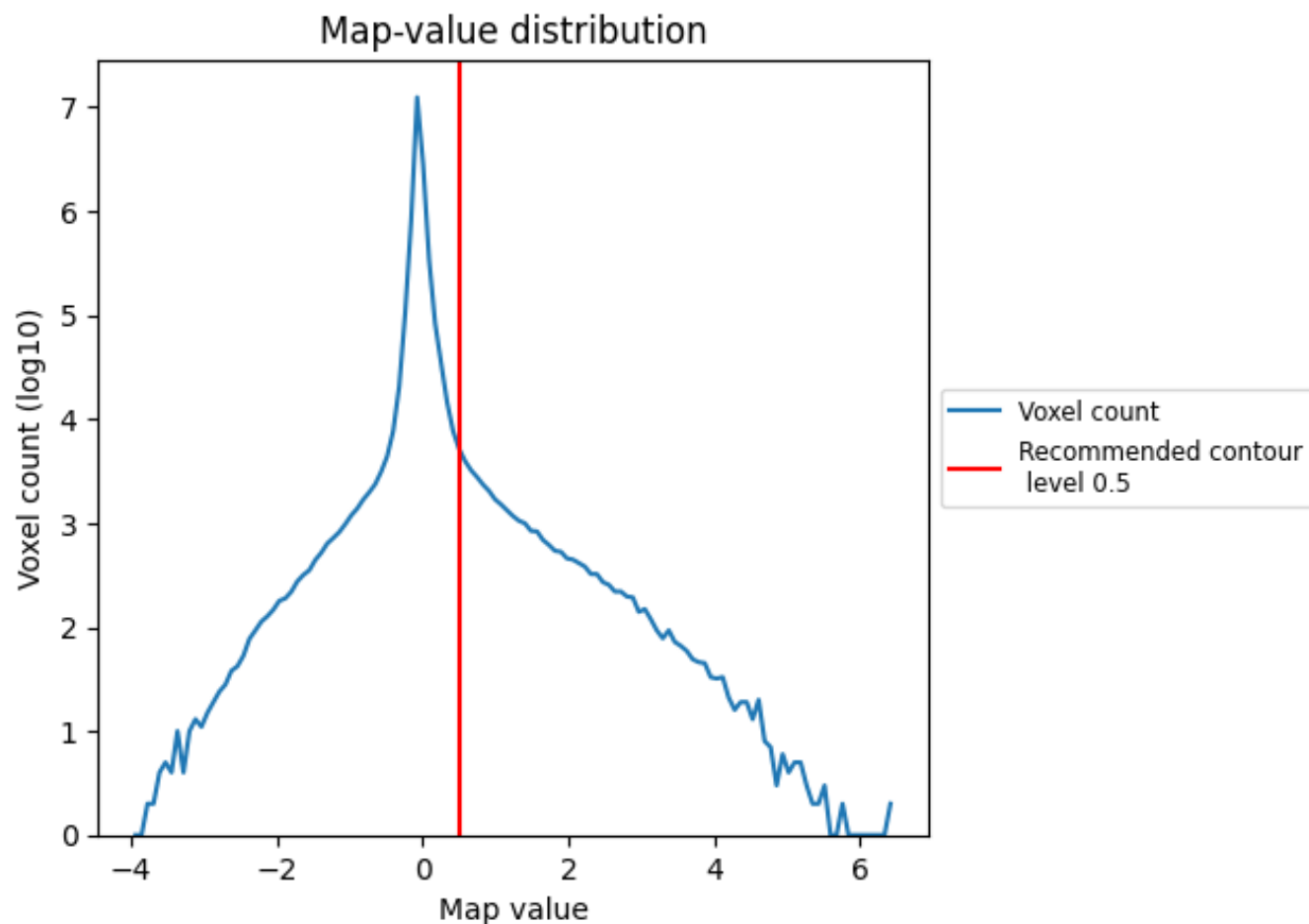
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

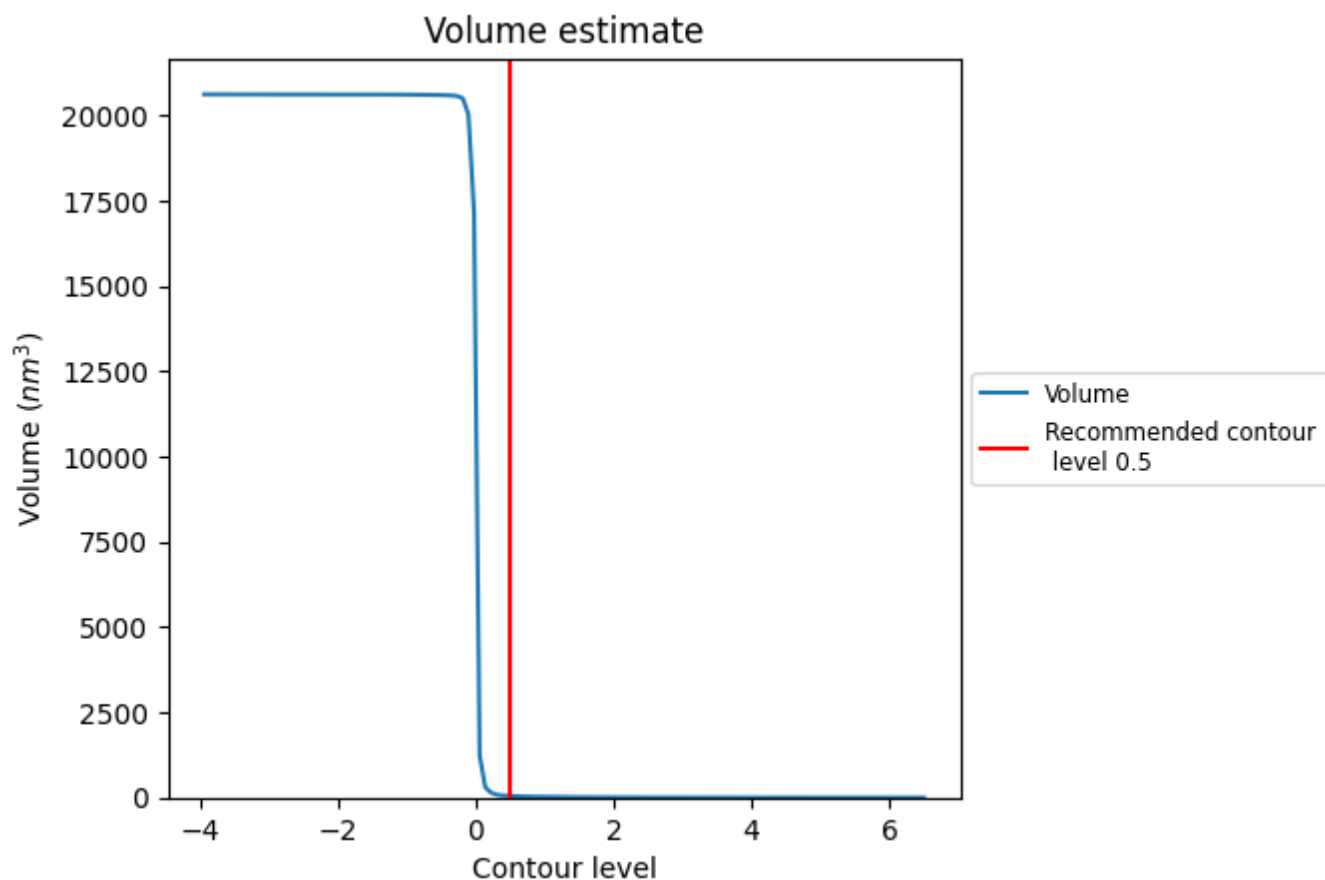
This section contains the results of statistical analysis of the map.

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.

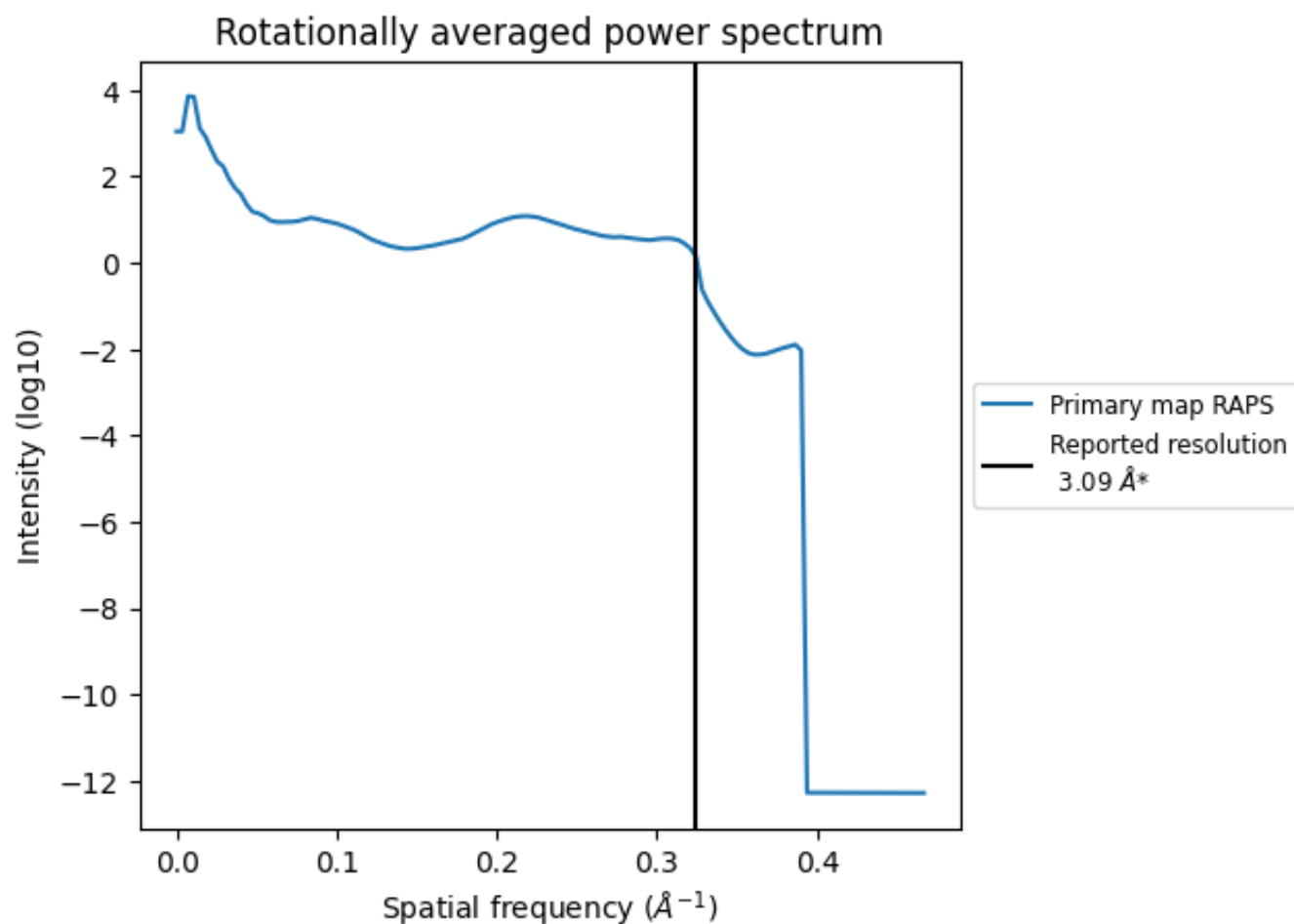
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm^3 ; this corresponds to an approximate mass of 41 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 0.324 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 EMD map EMD-33058 and PDB model 7X8S. 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](#)

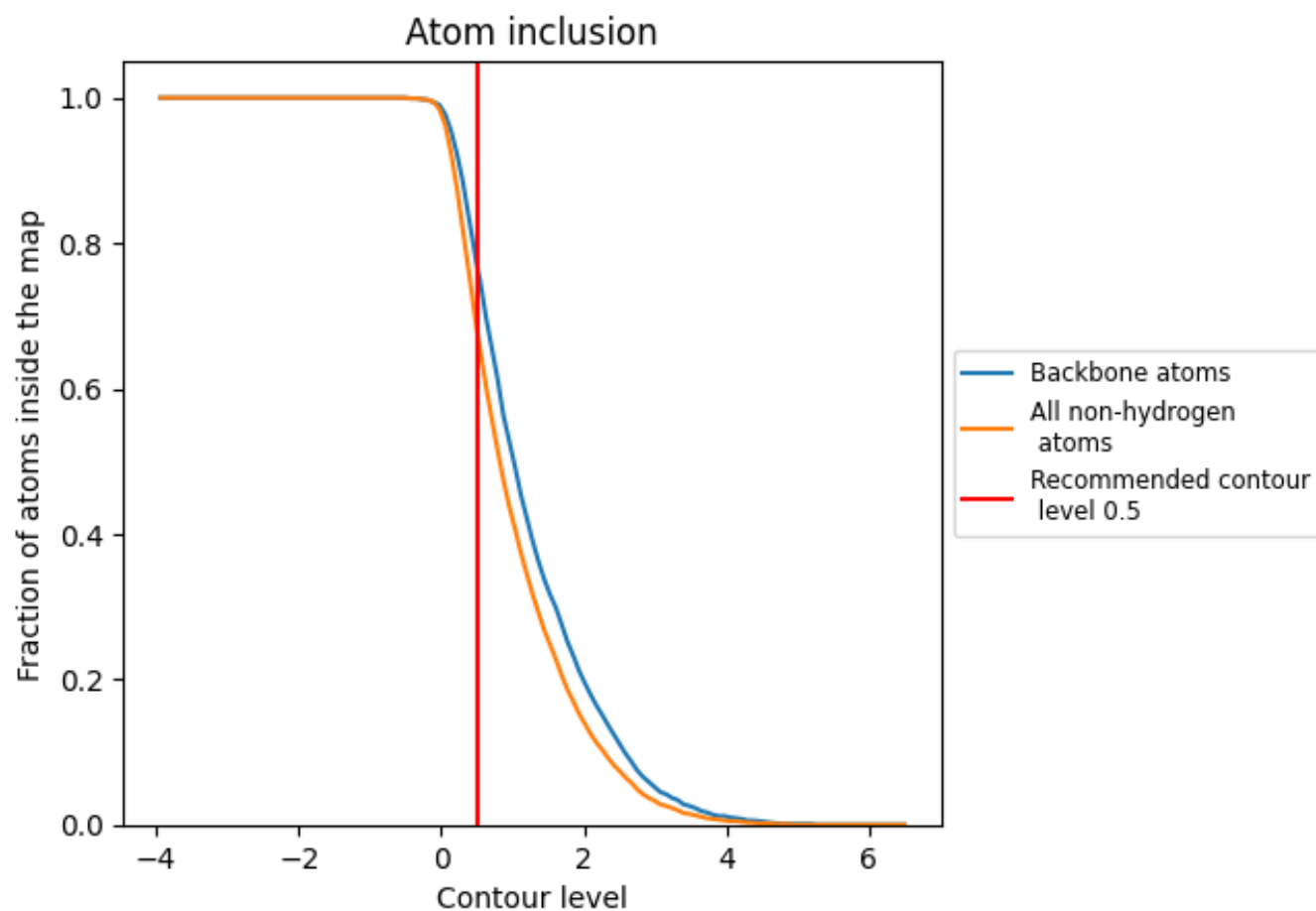


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 68% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6800	0.4820
A	0.7870	0.5220
B	0.7620	0.5210
G	0.3380	0.3610
N	0.7500	0.4980
R	0.5470	0.4270

