



Full wwPDB EM Validation Report ⓘ

Jul 10, 2026 – 01:21 PM JST

PDB ID : 20ZX / pdb_000020zx
EMDB ID : EMD-67439
Title : Cryo-EM structure of Gq-coupled LPAR5 in complex with LPA
Authors : Zhao, L.; Li, X.
Deposited on : 2025-12-04
Resolution : 2.96 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:

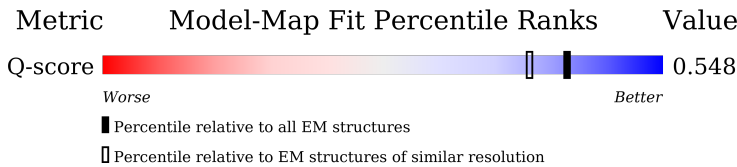
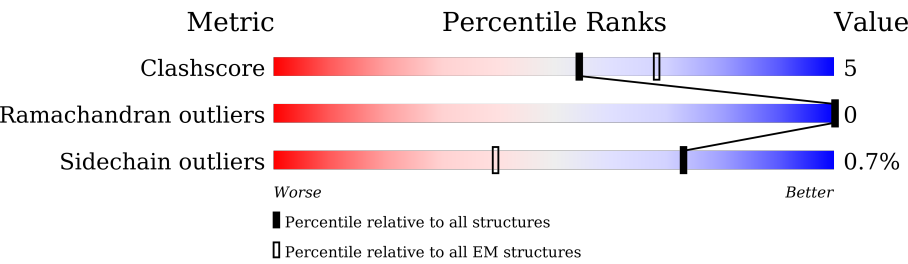
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	13155 (2.46 - 3.46)

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	371	5% 80% 10% 9%
2	G	70	14% 60% 14% 24%
3	R	372	• 70% 11% 19%
4	A	361	• 57% 6% 37%

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Mol	Chain	Length	Quality of chain
5	E	247	9% 86% 7% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9077 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(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	336	2583	1593	465	504	21	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P54311
B	2	GLY	-	expression tag	UNP P54311
B	3	SER	-	expression tag	UNP P54311
B	4	LEU	-	expression tag	UNP P54311
B	5	LEU	-	expression tag	UNP P54311
B	6	GLN	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	SER	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	GLY	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	GLY	-	expression tag	UNP P54311
B	357	GLY	-	expression tag	UNP P54311
B	358	SER	-	expression tag	UNP P54311
B	359	SER	-	expression tag	UNP P54311
B	360	GLY	-	expression tag	UNP P54311
B	361	VAL	-	expression tag	UNP P54311
B	362	SER	-	expression tag	UNP P54311
B	363	GLY	-	expression tag	UNP P54311
B	364	TRP	-	expression tag	UNP P54311
B	365	ARG	-	expression tag	UNP P54311
B	366	LEU	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	367	PHE	-	expression tag	UNP P54311
B	368	LYS	-	expression tag	UNP P54311
B	369	LYS	-	expression tag	UNP P54311
B	370	ILE	-	expression tag	UNP P54311
B	371	SER	-	expression tag	UNP P54311

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	53	Total	C	N	O	S	0	0
			410	257	73	77	3		

- Molecule 3 is a protein called Lysophosphatidic acid receptor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	300	Total	C	N	O	S	0	0
			2395	1572	429	379	15		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(324) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	229	Total	C	N	O	S	0	0
			1886	1192	335	351	8		

- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	231	Total	C	N	O	S	0	0
			1774	1125	294	345	10		

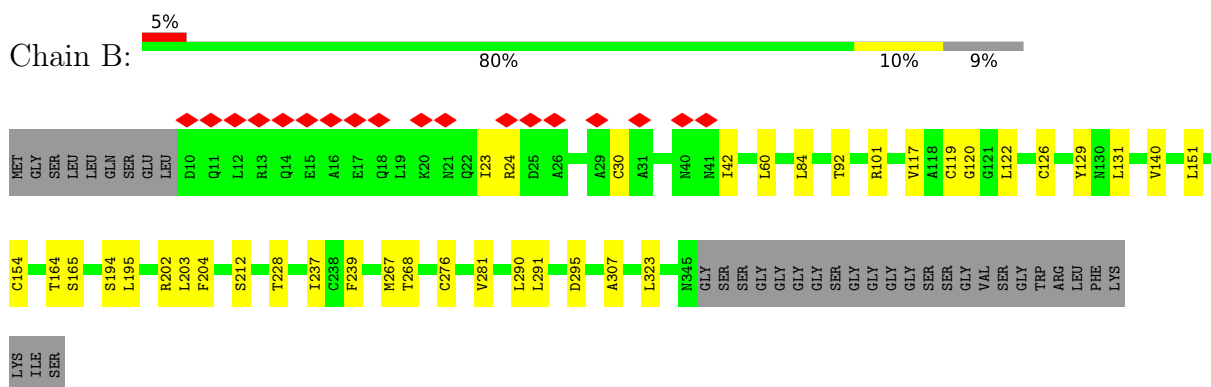
- Molecule 6 is [(2R)-2-oxidanyl-3-phosphonooxy-propyl] (Z)-octadec-9-enoate (CCD ID: UBL) (formula: C₂₁H₄₁O₇P) (labeled as "Ligand of Interest" by depositor).



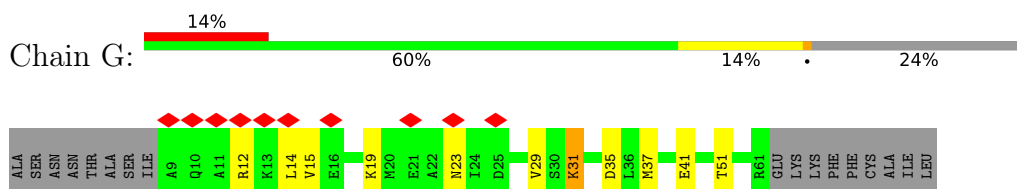
3 Residue-property plots

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.

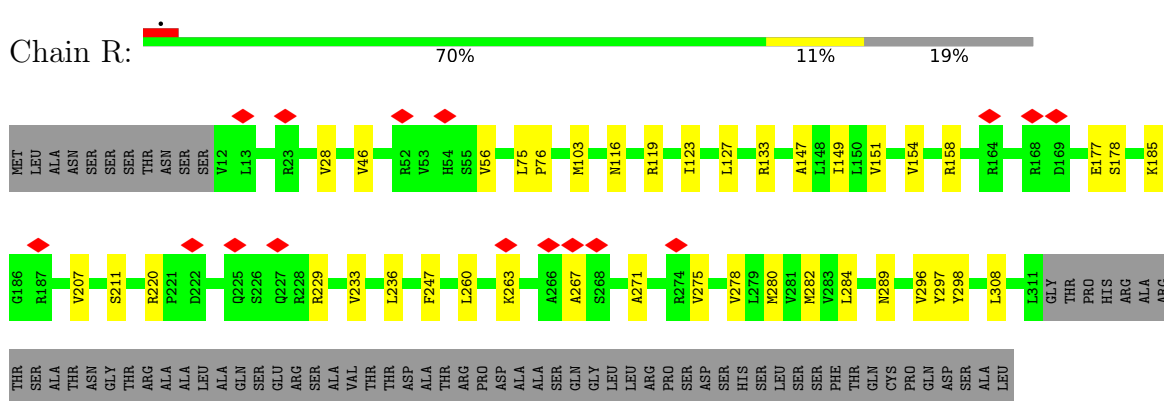
- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

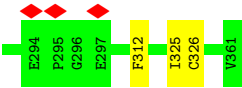
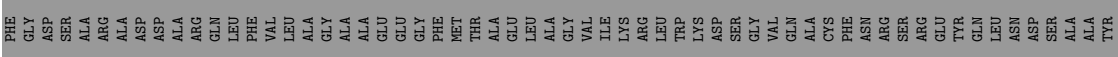
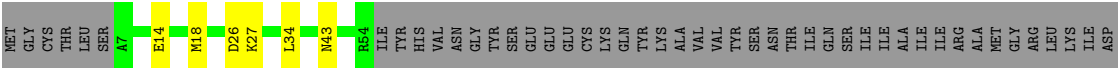


- Molecule 3: Lysophosphatidic acid receptor 5

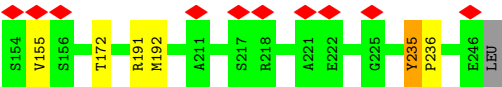
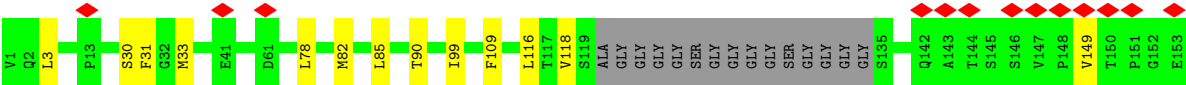
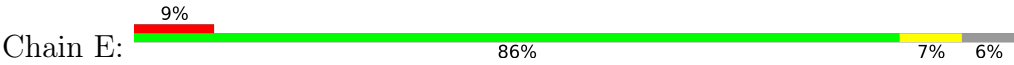


- Molecule 4: Guanine nucleotide-binding protein G(324) subunit alpha





● Molecule 5: scFv16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102163	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	18000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.128	Depositor
Minimum map value	-1.376	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	262.80002, 262.80002, 262.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7300001, 0.7300001, 0.7300001	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: UBL

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	0.13	0/2630	0.27	0/3566
2	G	0.15	0/416	0.28	0/561
3	R	0.14	0/2456	0.30	0/3350
4	A	0.13	0/1920	0.27	0/2583
5	E	0.11	0/1818	0.26	0/2465
All	All	0.13	0/9240	0.28	0/12525

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2583	0	2486	29	0
2	G	410	0	420	9	0
3	R	2395	0	2516	27	0
4	A	1886	0	1878	17	0
5	E	1774	0	1709	16	0
6	R	29	0	0	2	0
All	All	9077	0	9009	92	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 5.

All (92) 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)
3:R:178:SER:HA	6:R:401:UBL:O1	1.85	0.77
1:B:84:LEU:HD11	1:B:119:CYS:HB3	1.72	0.72
1:B:281:VAL:HG13	1:B:290:LEU:HD11	1.73	0.70
1:B:126:CYS:HB2	1:B:151:LEU:HD21	1.74	0.70
5:E:3:LEU:HD12	5:E:109:PHE:HD2	1.59	0.68
1:B:120:GLY:HA3	1:B:151:LEU:HD23	1.76	0.67
5:E:149:VAL:HG21	5:E:155:VAL:HG22	1.82	0.62
2:G:51:THR:HG23	2:G:51:THR:O	1.99	0.62
5:E:90:THR:HG22	5:E:118:VAL:H	1.65	0.61
1:B:202:ARG:C	1:B:203:LEU:HD12	2.27	0.60
3:R:103:MET:HE3	3:R:103:MET:HA	1.84	0.59
2:G:12:ARG:O	2:G:15:VAL:HG22	2.03	0.59
1:B:42:ILE:HD11	2:G:37:MET:HE3	1.85	0.57
1:B:212:SER:OG	1:B:228:THR:HG22	2.05	0.56
3:R:185:LYS:HE2	3:R:263:LYS:HD2	1.88	0.56
1:B:151:LEU:HD11	1:B:164:THR:HB	1.89	0.55
3:R:28:VAL:HG21	3:R:284:LEU:HD13	1.87	0.55
1:B:30:CYS:O	2:G:29:VAL:HG23	2.07	0.54
5:E:33:MET:HB3	5:E:78:LEU:HD22	1.90	0.54
4:A:229:ASP:O	4:A:229:ASP:OD1	2.25	0.54
5:E:30:SER:O	5:E:99:ILE:HG22	2.07	0.53
2:G:23:ASN:OD1	2:G:23:ASN:C	2.51	0.53
1:B:92:THR:HG22	1:B:92:THR:O	2.07	0.53
3:R:260:LEU:CD1	3:R:275:VAL:HG21	2.39	0.53
5:E:116:LEU:O	5:E:118:VAL:HG23	2.11	0.51
3:R:185:LYS:CE	3:R:263:LYS:HD2	2.41	0.50
5:E:82:MET:CB	5:E:85:LEU:HD11	2.41	0.50
5:E:3:LEU:HD12	5:E:109:PHE:CD2	2.45	0.50
2:G:31:LYS:O	2:G:35:ASP:OD1	2.30	0.50
3:R:271:ALA:O	3:R:275:VAL:HG23	2.12	0.49
3:R:116:ASN:ND2	3:R:207:VAL:HG22	2.27	0.48
1:B:291:LEU:HD12	1:B:291:LEU:N	2.28	0.48
2:G:51:THR:O	2:G:51:THR:CG2	2.61	0.48
4:A:186:GLU:HA	4:A:186:GLU:OE2	2.13	0.48
1:B:60:LEU:HD13	4:A:27:LYS:HA	1.95	0.48
5:E:82:MET:HB3	5:E:85:LEU:HD11	1.96	0.47
1:B:117:VAL:HG23	1:B:131:LEU:HD11	1.96	0.47
3:R:116:ASN:HD22	3:R:207:VAL:HG22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:46:VAL:CG2	3:R:308:LEU:HD21	2.44	0.47
3:R:229:ARG:O	3:R:233:VAL:HG23	2.15	0.47
1:B:122:LEU:HD21	4:A:211:TRP:HB2	1.97	0.47
4:A:215:PHE:O	4:A:218:VAL:HG22	2.14	0.47
5:E:149:VAL:HG21	5:E:155:VAL:CG2	2.45	0.47
1:B:151:LEU:HD12	1:B:165:SER:O	2.15	0.46
3:R:280:MET:HE1	6:R:401:UBL:OBC	2.16	0.46
1:B:92:THR:O	1:B:92:THR:CG2	2.63	0.46
3:R:127:LEU:CD2	4:A:34:LEU:HD11	2.46	0.46
3:R:103:MET:HB3	3:R:149:ILE:HG23	1.97	0.46
3:R:278:VAL:O	3:R:282:MET:HG2	2.16	0.46
1:B:267:MET:SD	1:B:307:ALA:HB2	2.56	0.46
4:A:281:GLU:HA	4:A:281:GLU:OE2	2.16	0.46
1:B:154:CYS:HB3	1:B:164:THR:HG22	1.97	0.46
1:B:276:CYS:HB2	1:B:295:ASP:HB2	1.98	0.46
1:B:194:SER:OG	1:B:237:ILE:HG22	2.16	0.45
4:A:325:ILE:HG22	4:A:326:CYS:N	2.32	0.45
4:A:43:ASN:OD1	4:A:43:ASN:C	2.59	0.45
5:E:235:TYR:N	5:E:236:PRO:HD2	2.31	0.45
1:B:60:LEU:HD11	4:A:26:ASP:OD1	2.17	0.45
5:E:172:THR:CG2	5:E:192:MET:HE3	2.47	0.45
1:B:154:CYS:CB	1:B:164:THR:HG22	2.48	0.44
4:A:14:GLU:O	4:A:18:MET:HG2	2.18	0.44
1:B:129:TYR:CE2	1:B:140:VAL:HG22	2.53	0.44
3:R:56:VAL:HG21	3:R:133:ARG:O	2.18	0.44
3:R:296:VAL:HG23	3:R:297:TYR:N	2.33	0.44
1:B:202:ARG:HB3	1:B:203:LEU:HD12	1.99	0.44
3:R:247:PHE:HZ	3:R:289:ASN:HD22	1.66	0.44
1:B:195:LEU:HD11	1:B:204:PHE:CD1	2.53	0.43
1:B:267:MET:HG3	1:B:268:THR:N	2.34	0.43
4:A:229:ASP:OD1	4:A:229:ASP:C	2.61	0.43
5:E:31:PHE:CD2	5:E:99:ILE:HG23	2.54	0.43
1:B:23:ILE:HG22	1:B:24:ARG:N	2.33	0.43
3:R:298:TYR:N	3:R:298:TYR:CD1	2.87	0.43
2:G:19:LYS:HB3	2:G:19:LYS:HE2	1.89	0.42
3:R:119:ARG:HG2	3:R:123:ILE:HD12	2.01	0.42
4:A:237:LEU:HD23	4:A:312:PHE:CE1	2.55	0.42
5:E:191:ARG:O	5:E:192:MET:CG	2.68	0.42
3:R:177:GLU:O	3:R:178:SER:C	2.63	0.42
2:G:14:LEU:C	2:G:14:LEU:HD13	2.45	0.41
3:R:147:ALA:O	3:R:151:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:211:SER:HA	3:R:236:LEU:HD11	2.03	0.41
3:R:260:LEU:HD22	3:R:267:ALA:HB3	2.02	0.41
3:R:260:LEU:HD11	3:R:275:VAL:HG21	2.01	0.41
4:A:235:GLU:HA	4:A:235:GLU:OE2	2.20	0.41
1:B:323:LEU:O	1:B:323:LEU:HD12	2.21	0.41
5:E:90:THR:HG22	5:E:118:VAL:N	2.34	0.41
3:R:154:VAL:O	3:R:158:ARG:HG3	2.21	0.40
4:A:198:MET:HG3	4:A:199:PHE:N	2.36	0.40
4:A:225:VAL:HG11	4:A:312:PHE:CZ	2.56	0.40
1:B:101:ARG:NH1	1:B:140:VAL:HG21	2.36	0.40
5:E:82:MET:HB2	5:E:85:LEU:HD11	2.04	0.40
3:R:75:LEU:N	3:R:76:PRO:CD	2.85	0.40
4:A:266:GLU:HA	4:A:266:GLU:OE2	2.22	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	334/371 (90%)	318 (95%)	16 (5%)	0	100	100
2	G	51/70 (73%)	50 (98%)	1 (2%)	0	100	100
3	R	298/372 (80%)	290 (97%)	8 (3%)	0	100	100
4	A	225/361 (62%)	222 (99%)	3 (1%)	0	100	100
5	E	227/247 (92%)	218 (96%)	9 (4%)	0	100	100
All	All	1135/1421 (80%)	1098 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	279/302 (92%)	278 (100%)	1 (0%)	84	92
2	G	43/57 (75%)	41 (95%)	2 (5%)	23	49
3	R	258/316 (82%)	257 (100%)	1 (0%)	84	92
4	A	206/315 (65%)	204 (99%)	2 (1%)	68	82
5	E	195/198 (98%)	194 (100%)	1 (0%)	81	90
All	All	981/1188 (83%)	974 (99%)	7 (1%)	73	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239	PHE
2	G	31	LYS
2	G	41	GLU
3	R	220	ARG
4	A	184	ILE
4	A	229	ASP
5	E	235	TYR

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

Mol	Chain	Res	Type
1	B	180	GLN
3	R	116	ASN
3	R	160	HIS
3	R	289	ASN
4	A	197	HIS
4	A	245	ASN
5	E	38	GLN
5	E	179	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	UBL	R	401	-	28,28,28	1.29	4 (14%)	31,32,32	1.36	4 (12%)

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	UBL	R	401	-	-	11/28/28/28	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	401	UBL	CAT-CAS	3.54	1.52	1.31
6	R	401	UBL	PAC-O1	-2.48	1.45	1.54
6	R	401	UBL	PAC-OAA	2.45	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	401	UBL	OAJ-CAI	-2.44	1.39	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	401	UBL	OAJ-CAK-CAL	2.72	120.43	111.91
6	R	401	UBL	CAR-CAS-CAT	-2.25	107.49	124.73
6	R	401	UBL	CAU-CAT-CAS	-2.19	107.90	124.73
6	R	401	UBL	O1-PAC-OAB	-2.09	102.50	110.68

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	401	UBL	CAG-OAF-PAC-OAA
6	R	401	UBL	CAG-OAF-PAC-OAB
6	R	401	UBL	CAW-CAX-CAY-CAZ
6	R	401	UBL	CAL-CAK-OAJ-CAI
6	R	401	UBL	OAE-CAK-OAJ-CAI
6	R	401	UBL	CAL-CAM-CAN-CAO
6	R	401	UBL	CAO-CAP-CAQ-CAR
6	R	401	UBL	CAX-CAY-CAZ-CBA
6	R	401	UBL	CAK-CAL-CAM-CAN
6	R	401	UBL	CAG-OAF-PAC-O1
6	R	401	UBL	CAS-CAT-CAU-CAV

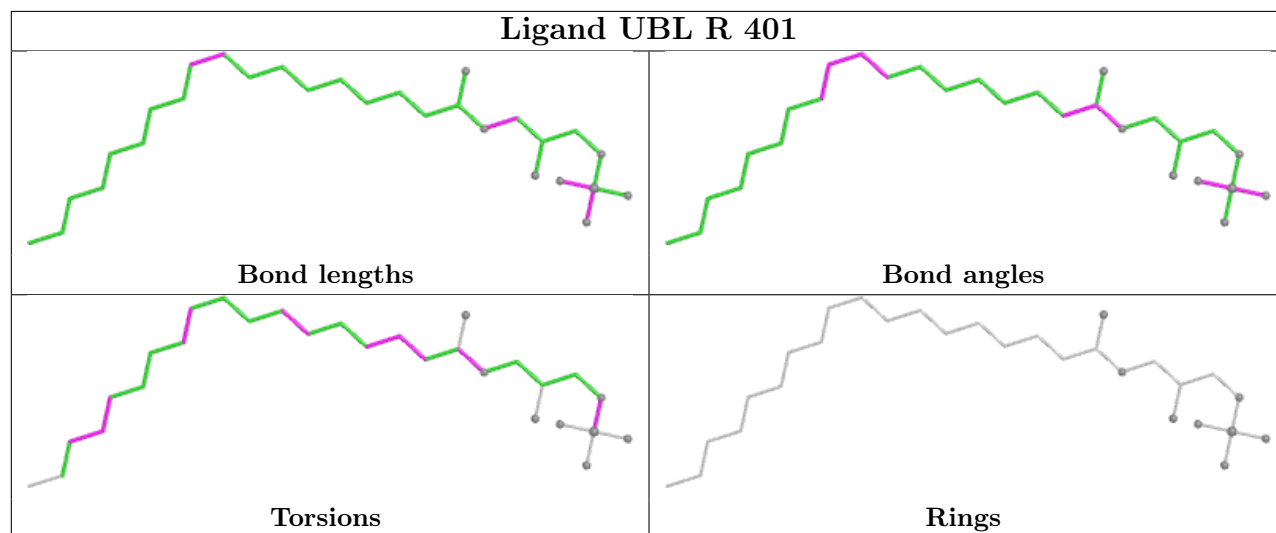
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	401	UBL	2	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.

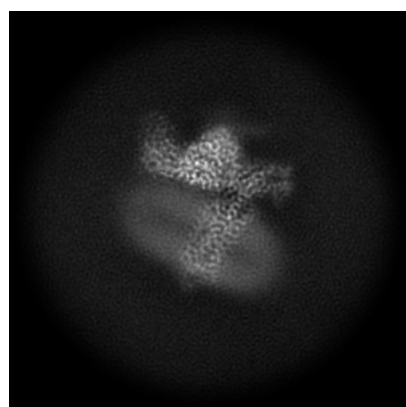
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67439. These allow visual inspection of the internal detail of the map and identification of artifacts.

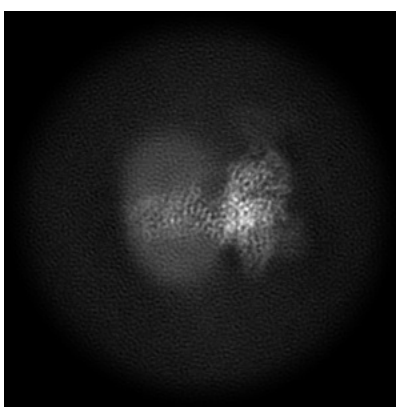
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

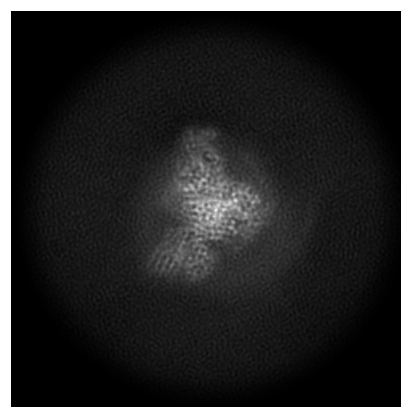
6.1.1 Primary map



X



Y

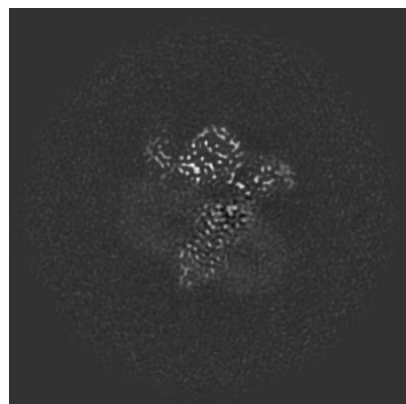


Z

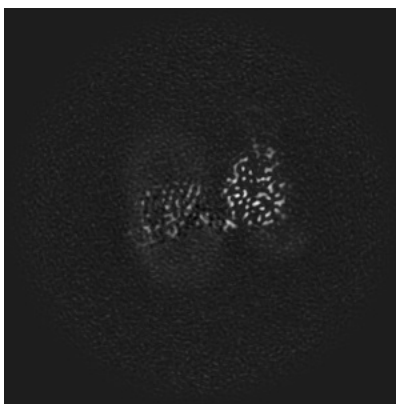
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

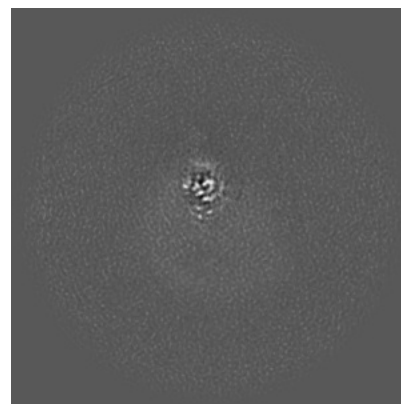
6.2.1 Primary map



X Index: 180



Y Index: 180

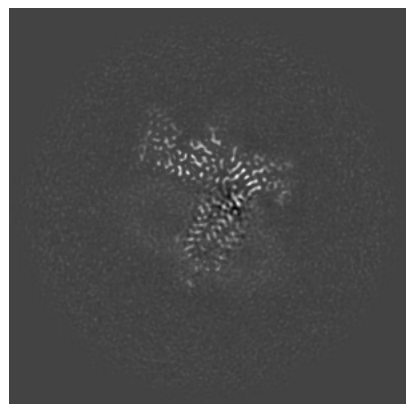


Z Index: 180

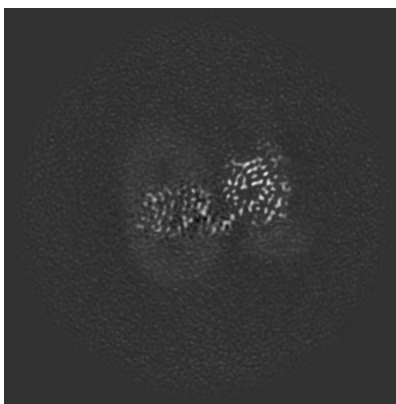
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

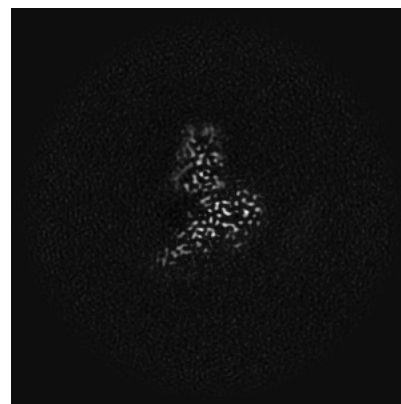
6.3.1 Primary map



X Index: 170



Y Index: 188

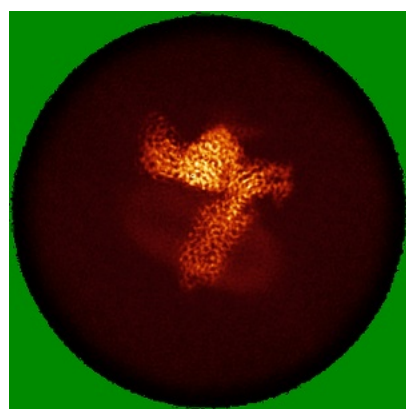


Z Index: 212

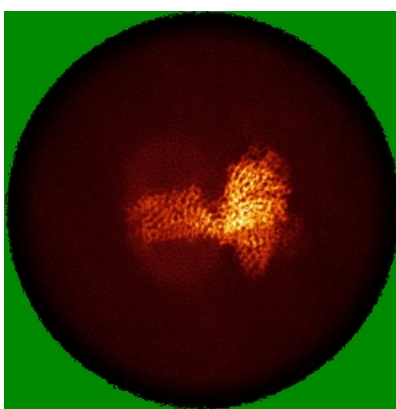
The images above show the largest variance slices of the map in three orthogonal directions.

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

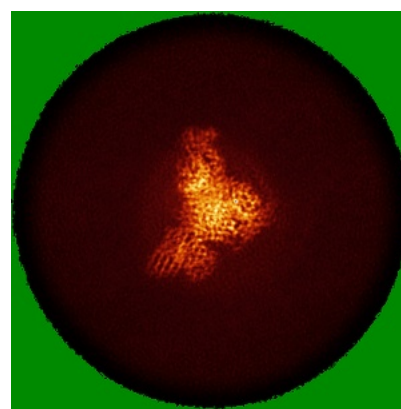
6.4.1 Primary map



X



Y

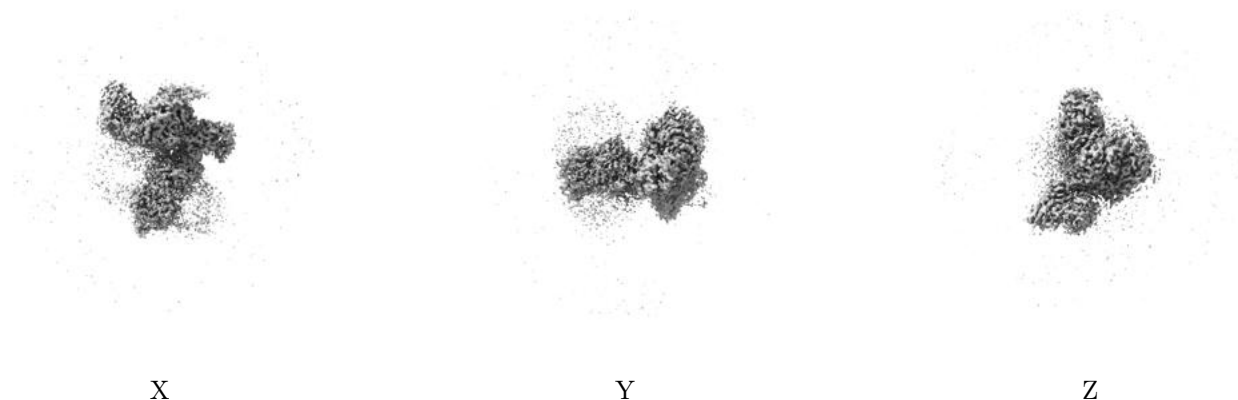


Z

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

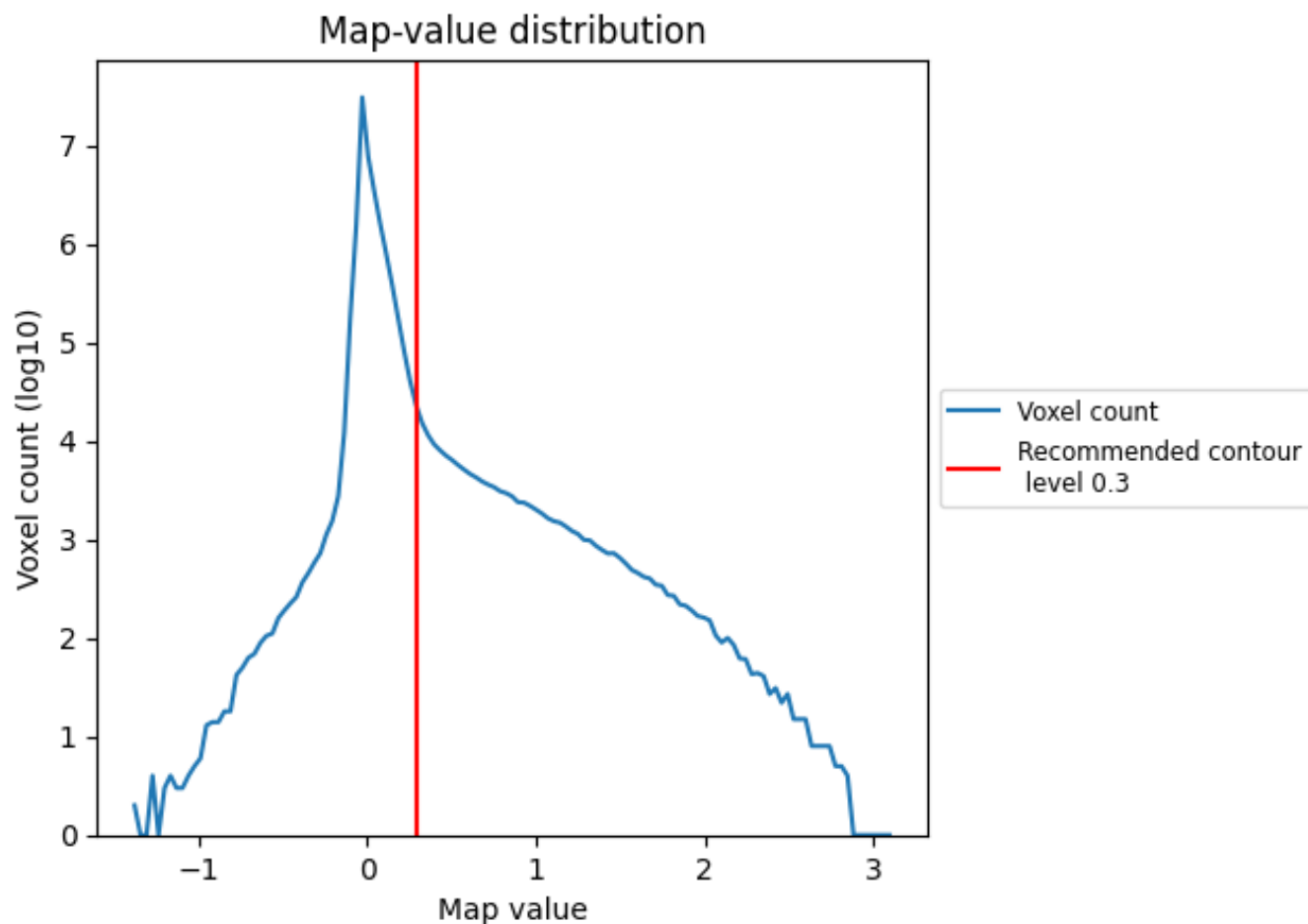
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

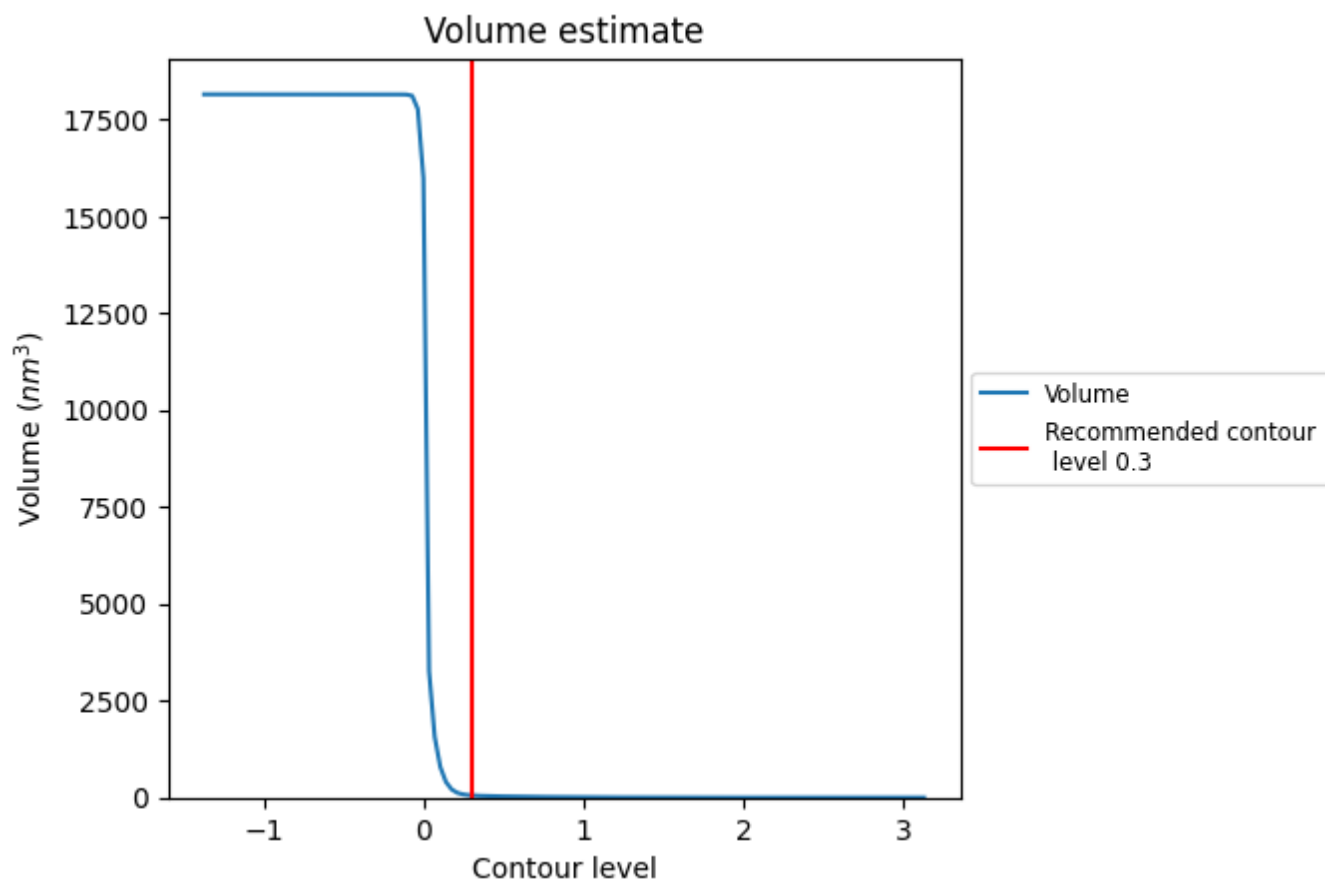
This section contains the results of statistical analysis of the map.

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.

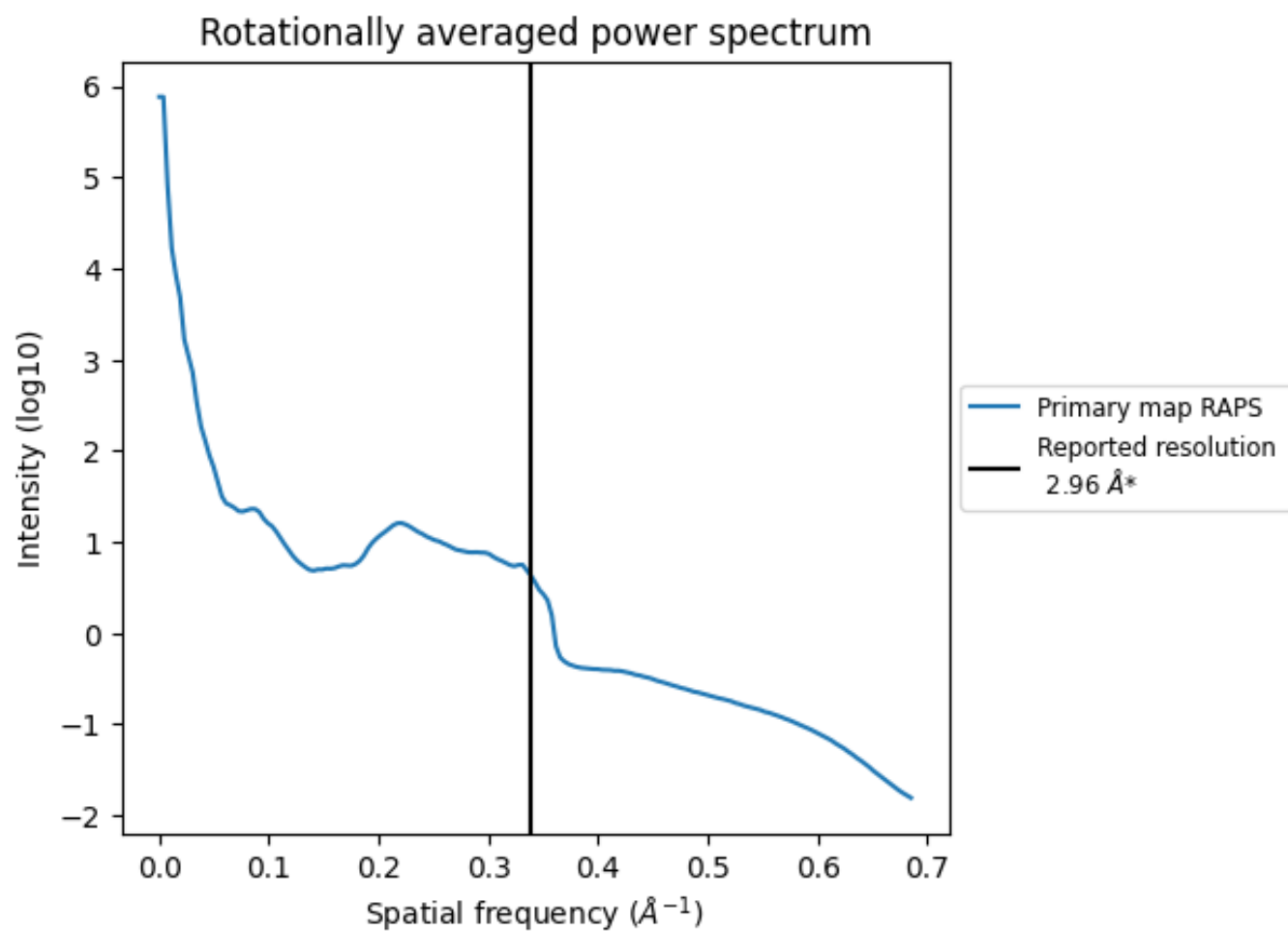
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm^3 ; this corresponds to an approximate mass of 51 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 0.338 Å⁻¹

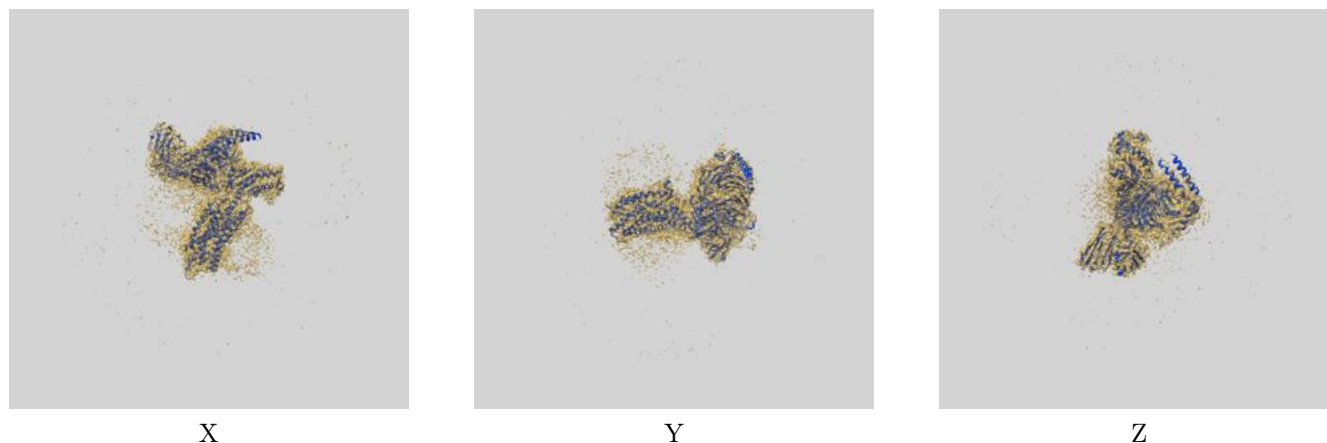
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

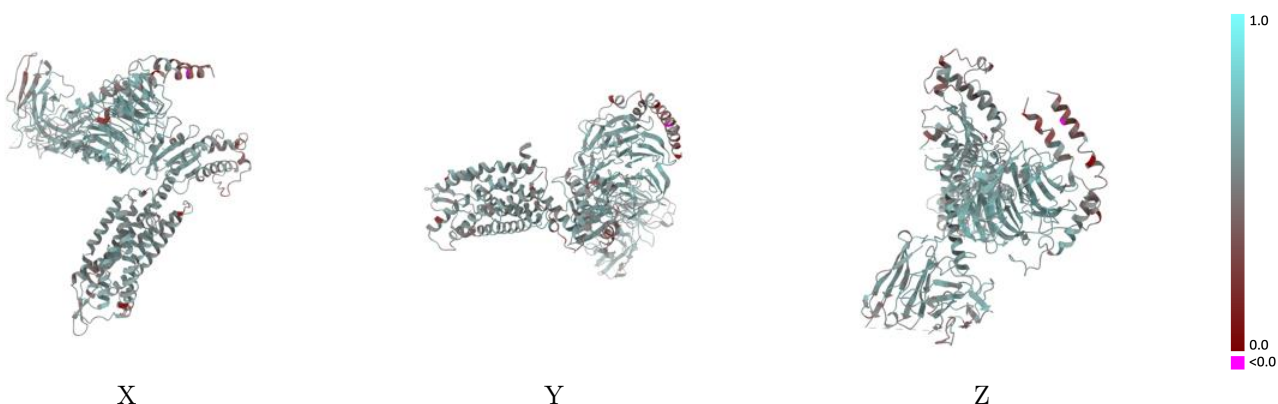
This section contains information regarding the fit between EMDB map EMD-67439 and PDB model 20ZX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



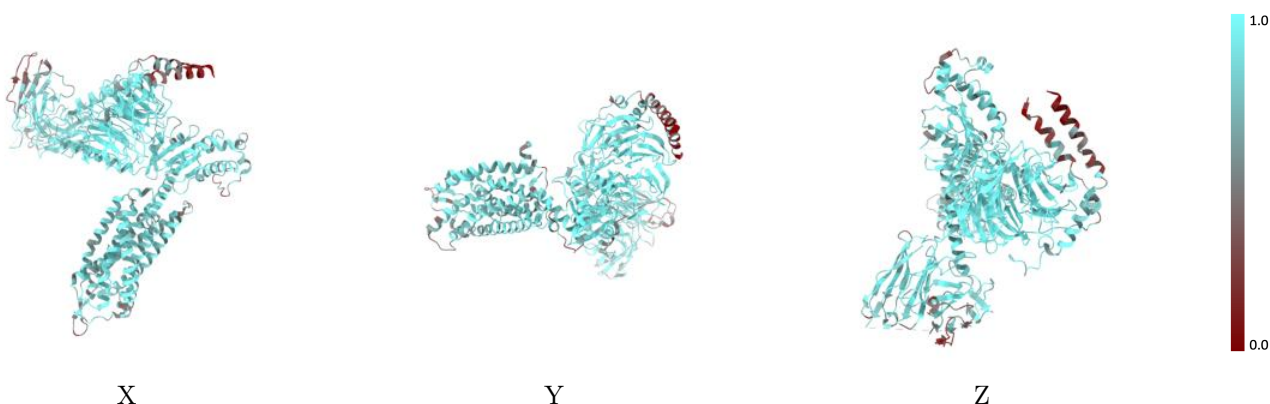
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



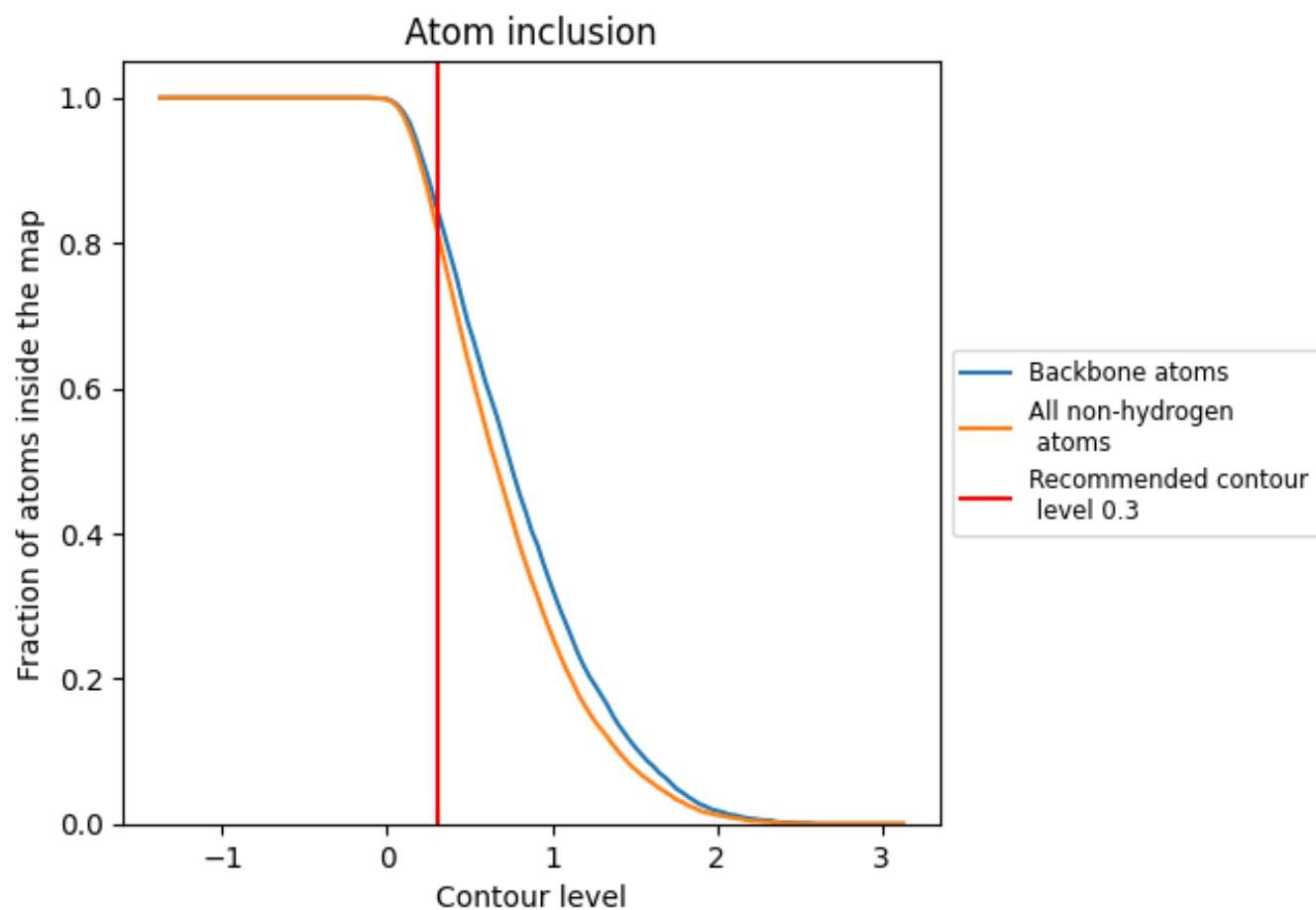
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.5480
A	0.8420	0.5320
B	0.8920	0.5870
E	0.7590	0.5440
G	0.6650	0.4950
R	0.7960	0.5300

