



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:20 PM UTC

PDB ID : 7WRI / pdb_00007wri
EMDB ID : EMD-32727
Title : Cryo-EM structure of SARS-CoV-2 Omicron spike receptor-binding domain in complex with mouse ACE2
Authors : Han, P.; Xie, Y.; Qi, J.
Deposited on : 2022-01-26
Resolution : 3.03 Å(reported)
Based on initial model : 6LZG

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

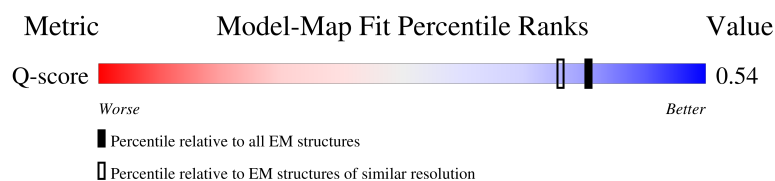
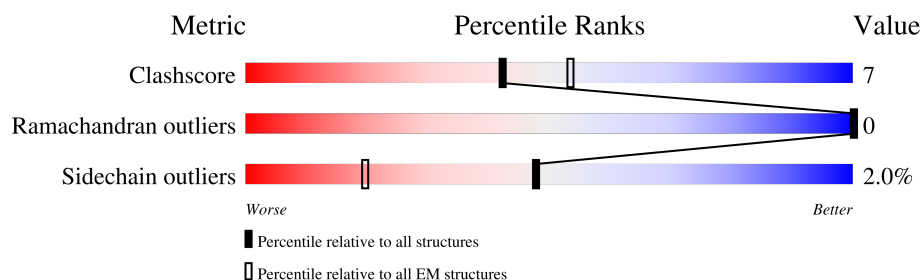
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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	13929 (2.53 - 3.53)

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	598	10% 81% 17% ..
2	B	1232	13% 84%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6431 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	595	Total	C	N	O	S	0	0
			4851	3091	815	916	29		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	195	Total	C	N	O	S	0	0
			1565	1009	264	284	8		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	70	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	96	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	143	ASP	TYR	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	ILE	LEU	variant	UNP P0DTC2
B	213	GLU	-	insertion	UNP P0DTC2
B	214	PRO	-	insertion	UNP P0DTC2
B	215	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	conflict	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1206	TYR	-	expression tag	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	SER	-	expression tag	UNP P0DTC2
B	1240	ALA	-	expression tag	UNP P0DTC2
B	1241	TRP	-	expression tag	UNP P0DTC2
B	1242	SER	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	PRO	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	PHE	-	expression tag	UNP P0DTC2
B	1247	GLU	-	expression tag	UNP P0DTC2
B	1248	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

ASN	PHE	ARG	VAL	GLN	PRO	THR	GLU	SER	ILE	VAL	ARG	PHE	PRO	ASN	ILE	T333	R334	L335	R346	V353	N354	R357	I358	A363	T369	N370	L371	A372	F375	K378	C379	T385	R386	T393	N394	V395	D398	V401	D428	C432	V433	N439	S443							
Y453	R454	L455	L461	E465	S469	K478	F490	R493	R509	V512	L518	P527	LYS	SER	THR	ASN	GLY	LEU	VAL	THR	ASN	THR	ASN	GLY	VAL	ASN	VAL	THR	ASN	PHE	ASN	GLY	LEU	GLY	THR	VAL	GLY	LEU	THR	GLN	SER	ASN	THR	LYS	PHE	LEU	PRO	PHE	GLN	
HIS	ALA	ASP	GLN	THR	THR	ARG	VAL	TYR	THR	VAL	THR	ALA	ASN	VAL	GLN	THR	ASN	ARG	ALA	GLY	THR	GLY	GLY	GLU	TYR	VAL	ASN	VAL	THR	ASN	THR	PRO	ASN	GLY	ALA	VAL	GLY	ALA	THR	TYR	SER	THR	LYS	PHE	VAL	PRO	VAL	ALA		
ARG	SER	VAL	ALA	SER	ILE	THR	THR	ILE	ALA	GLY	VAL	TYR	SER	GLY	THR	ALA	ASN	ALA	ALA	ALA	THR	ILE	GLY	GLU	ILE	PRO	ASN	THR	PHE	THR	ASN	THR	ILE	LEU	PRO	VAL	THR	LYS	THR	GLY	THR	VAL	TYR	GLN	GLY	VAL	THR	GLY		
ASP	SER	THR	GLY	SER	ASN	LEU	LEU	LEU	PHE	CYS	THR	ALA	THR	LEU	GLN	THR	ASN	ARG	ALA	THR	LEU	THR	GLY	GLN	ASP	PRO	ASN	GLN	THR	ILE	VAL	GLY	GLN	ILE	THR	VAL	TYR	GLY	THR	ASN	GLN	THR	VAL	THR	GLY	VAL	THR	GLN		
ILE	LEU	PRO	ASP	SER	PRO	LYS	ARG	GLY	THR	LEU	THR	ALA	GLY	LEU	PHE	ASN	VAL	ASN	VAL	THR	LEU	ILE	GLY	GLN	ASP	GLY	ASN	GLY	VAL	THR	GLY	ARG	GLN	ILE	TYR	VAL	THR	LYS	THR	GLY	THR	VAL	THR	GLY	VAL	THR	GLN			
LEU	THR	GLY	MET	ILE	ALA	GLN	TYR	THR	ALA	GLY	THR	THR	THR	LEU	SER	THR	GLY	GLY	TRP	THR	PHE	GLY	ALA	ILE	GLN	ILE	PRO	PHE	GLY	ALA	ARG	ALA	THR	ASN	ARG	ASP	ILE	GLN	THR	ASN	VAL	VAL	GLN	THR	GLY	VAL	THR	GLY		
ASN	GLN	PHE	ASN	SER	ALA	ILE	GLY	LYS	THR	GLY	THR	THR	PRO	THR	ASN	PRO	GLY	ALA	ALA	THR	GLY	GLY	ALA	GLY	ASN	HIS	ASN	ALA	ALA	THR	GLY	LEU	SER	ASN	GLY	THR	GLN	VAL	THR	ASN	THR	GLY	THR	GLY	VAL	THR	GLY			
ASP	PRO	PRO	GLY	ALA	VAL	GLN	ILE	ASP	ARG	LEU	THR	VAL	GLN	LEU	GLN	THR	GLY	LEU	GLY	THR	THR	VAL	ILE	ARG	ALA	ALA	ILE	ALA	ALA	ALA	THR	LYS	THR	GLY	GLY	GLY	VAL	GLY	GLY	THR	THR	GLY	THR	THR	GLY	VAL	THR	GLY		
LYS	GLY	TYR	HIS	MET	GLY	PHE	PRO	PHE	GLN	PRO	HIS	VAL	VAL	VAL	THR	VAL	THR	VAL	ILE	ASN	ASN	THR	VAL	ASN	PHE	THR	THR	ALA	ALA	THR	LYS	PHE	PRO	ARG	GLY	GLY	VAL	VAL	THR	ASN	ASN	GLY	THR	THR	THR	THR	THR	VAL		
THR	GLN	ARG	ASN	PHE	TYR	GLU	THR	ASN	THR	PHE	CYS	THR	VAL	ASN	VAL	VAL	SER	GLY	ASN	VAL	VAL	GLY	ASN	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
ASP	LEU	GLY	ASP	ILE	GLY	ILE	ASN	ALA	LYS	GLY	THR	PHE	VAL	THR	GLY	GLY	THR	ARG	LEU	GLY	VAL	ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLY	GLN	GLY	GLY	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ARG	LYS	ASP	GLY	TRP	VAL	LEU	THR	ALA	ALA	GLN	PHE	LEU	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	503967	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.766	Depositor
Minimum map value	-2.922	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.689	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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: ZN, 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	A	0.14	0/4986	0.33	2/6769 (0.0%)
2	B	0.14	0/1612	0.43	1/2195 (0.0%)
All	All	0.14	0/6598	0.36	3/8964 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASP	CB-CA-C	-7.61	97.55	109.34
2	B	432	CYS	CA-CB-SG	6.42	129.17	114.40
1	A	38	ASP	N-CA-C	-5.73	106.33	113.55

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	4851	0	4631	64	0
2	B	1565	0	1497	21	0
3	A	1	0	0	0	0
4	B	14	0	13	0	0
All	All	6431	0	6141	84	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 7.

All (84) 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)
2:B:379:CYS:HA	2:B:432:CYS:HB3	1.55	0.88
2:B:379:CYS:HA	2:B:432:CYS:CB	2.20	0.70
1:A:365:THR:OG1	1:A:368:ASN:ND2	2.26	0.68
2:B:490:PHE:O	2:B:493:ARG:NH1	2.27	0.68
1:A:161:ARG:NH2	1:A:267:LEU:O	2.30	0.64
1:A:204:ARG:HG2	1:A:222:LEU:HD23	1.79	0.63
1:A:392:LEU:HD13	1:A:563:SER:HB3	1.79	0.63
1:A:31:ASN:OD1	2:B:493:ARG:NH2	2.35	0.60
1:A:435:GLU:OE2	1:A:540:HIS:NE2	2.35	0.59
1:A:574:VAL:HG23	1:A:576:ALA:H	1.68	0.58
1:A:209:ALA:HB1	1:A:565:PRO:HB3	1.85	0.58
2:B:454:ARG:NH2	2:B:469:SER:O	2.36	0.58
2:B:378:LYS:O	2:B:432:CYS:HB2	2.04	0.57
1:A:268:GLY:O	1:A:277:ASN:ND2	2.38	0.56
1:A:60:GLN:NE2	1:A:64:GLU:OE2	2.39	0.55
1:A:318:VAL:HG12	1:A:551:GLY:HA3	1.88	0.55
1:A:20:LEU:HG	1:A:22:GLU:H	1.72	0.55
1:A:297:MET:HB3	1:A:302:TRP:HB2	1.88	0.55
1:A:543:ASP:N	1:A:543:ASP:OD1	2.40	0.54
2:B:358:ILE:HB	2:B:395:VAL:HB	1.89	0.54
1:A:143:LEU:HG	1:A:145:GLU:H	1.73	0.54
2:B:393:THR:HG21	2:B:518:LEU:HB2	1.89	0.54
1:A:229:THR:HG23	1:A:581:VAL:HG11	1.89	0.54
1:A:111:ASP:O	1:A:115:GLN:HG3	2.09	0.53
1:A:168:TRP:NE1	1:A:502:SER:OG	2.38	0.53
1:A:465:ARG:NH1	1:A:467:GLU:OE2	2.41	0.53
1:A:573:VAL:HG13	1:A:574:VAL:HG13	1.89	0.53
1:A:300:GLN:OE1	1:A:302:TRP:NE1	2.42	0.52
1:A:32:PHE:HD1	1:A:76:GLN:HG2	1.75	0.52
2:B:433:VAL:HG12	2:B:512:VAL:HG22	1.91	0.51
1:A:519:THR:O	1:A:522:GLN:HB3	2.11	0.51
1:A:429:GLN:HG2	1:A:430:GLU:H	1.75	0.51
1:A:228:ARG:NH2	1:A:579:MET:O	2.43	0.50
1:A:538:SER:HB2	1:A:541:LYS:HD3	1.92	0.50
1:A:213:ASP:OD1	1:A:213:ASP:N	2.38	0.49
1:A:388:GLN:HB2	1:A:393:ARG:HG2	1.94	0.48
1:A:389:PRO:HD2	1:A:392:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:LEU:HG	2:B:372:ALA:H	1.77	0.48
1:A:131:LYS:HD3	1:A:143:LEU:HB3	1.95	0.48
1:A:111:ASP:N	1:A:111:ASP:OD1	2.45	0.48
1:A:111:ASP:HA	1:A:114:LYS:NZ	2.29	0.47
2:B:461:LEU:HD22	2:B:465:GLU:HB3	1.96	0.47
2:B:439:ASN:O	2:B:443:SER:OG	2.26	0.47
1:A:264:ALA:N	1:A:488:VAL:O	2.48	0.46
1:A:315:PHE:HD2	1:A:320:LEU:HD12	1.80	0.46
1:A:351:LEU:HB2	1:A:355:ASP:HB3	1.96	0.46
1:A:70:SER:O	1:A:74:GLU:HG2	2.16	0.46
1:A:198:ASP:N	1:A:198:ASP:OD1	2.50	0.45
1:A:269:ASP:HB3	1:A:272:GLY:H	1.81	0.45
2:B:453:TYR:HE2	2:B:455:LEU:HD13	1.82	0.45
1:A:338:ASP:OD1	1:A:338:ASP:N	2.46	0.44
2:B:401:VAL:HG22	2:B:509:ARG:HG2	1.99	0.44
1:A:589:GLN:HB3	1:A:590:PRO:HD3	2.00	0.44
1:A:145:GLU:CD	1:A:147:GLY:H	2.26	0.44
1:A:275:TRP:HB2	1:A:444:LEU:HB3	2.00	0.44
2:B:353:TRP:CD1	2:B:353:TRP:H	2.35	0.44
1:A:457:GLU:HG2	1:A:513:ILE:HD13	2.00	0.43
1:A:109:SER:OG	1:A:110:ALA:N	2.51	0.43
1:A:217:TYR:OH	1:A:225:ASP:OD2	2.27	0.43
1:A:312:GLU:HA	1:A:376:MET:HE1	2.00	0.43
1:A:220:ASN:N	1:A:220:ASN:OD1	2.51	0.43
2:B:354:ASN:O	2:B:398:ASP:HA	2.19	0.43
1:A:161:ARG:HE	1:A:266:LEU:HA	1.82	0.42
1:A:218:ASN:HB3	1:A:221:GLN:HG3	2.02	0.42
2:B:478:LYS:HD2	2:B:478:LYS:HA	1.84	0.42
1:A:87:GLU:OE1	1:A:87:GLU:N	2.53	0.42
1:A:88:ILE:HB	1:A:94:LYS:HE3	2.02	0.42
1:A:174:LYS:NZ	1:A:496:THR:OG1	2.53	0.42
1:A:32:PHE:CD1	1:A:76:GLN:HG2	2.53	0.42
1:A:455:MET:HE3	1:A:455:MET:HB3	1.90	0.41
1:A:103:SER:HB2	1:A:106:SER:HB3	2.01	0.41
1:A:111:ASP:HA	1:A:114:LYS:HZ3	1.85	0.41
1:A:483:GLU:HG3	1:A:484:ILE:HG13	2.01	0.41
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.88	0.41
1:A:167:GLY:O	1:A:171:GLU:HG2	2.20	0.41
1:A:513:ILE:HD12	1:A:513:ILE:HA	1.98	0.41
1:A:134:ASN:OD1	1:A:134:ASN:N	2.54	0.41
1:A:143:LEU:H	1:A:143:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD13	1:A:186:LEU:HB3	2.02	0.40
2:B:379:CYS:CA	2:B:432:CYS:HB3	2.30	0.40
2:B:428:ASP:OD1	2:B:428:ASP:N	2.41	0.40
2:B:357:ARG:HH21	2:B:394:ASN:HD21	1.68	0.40
1:A:360:MET:HE2	1:A:362:THR:HG23	2.04	0.40
2:B:335:LEU:HD12	2:B:335:LEU:HA	1.92	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	593/598 (99%)	558 (94%)	35 (6%)	0	100	100
2	B	193/1232 (16%)	181 (94%)	12 (6%)	0	100	100
All	All	786/1830 (43%)	739 (94%)	47 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	520/522 (100%)	507 (98%)	13 (2%)	42	69
2	B	170/1076 (16%)	169 (99%)	1 (1%)	78	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	690/1598 (43%)	676 (98%)	14 (2%)	48 73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	90	THR
1	A	134	ASN
1	A	172	VAL
1	A	220	ASN
1	A	229	THR
1	A	342	VAL
1	A	365	THR
1	A	424	LEU
1	A	444	LEU
1	A	447	VAL
1	A	498	CYS
1	A	574	VAL
2	B	385	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	60	GLN
1	A	96	GLN
1	A	325	GLN
1	A	578	ASN
2	B	388	ASN
2	B	394	ASN
2	B	439	ASN
2	B	450	ASN

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	NAG	B	1301	2	14,14,15	0.27	0	17,19,21	0.60	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
4	NAG	B	1301	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

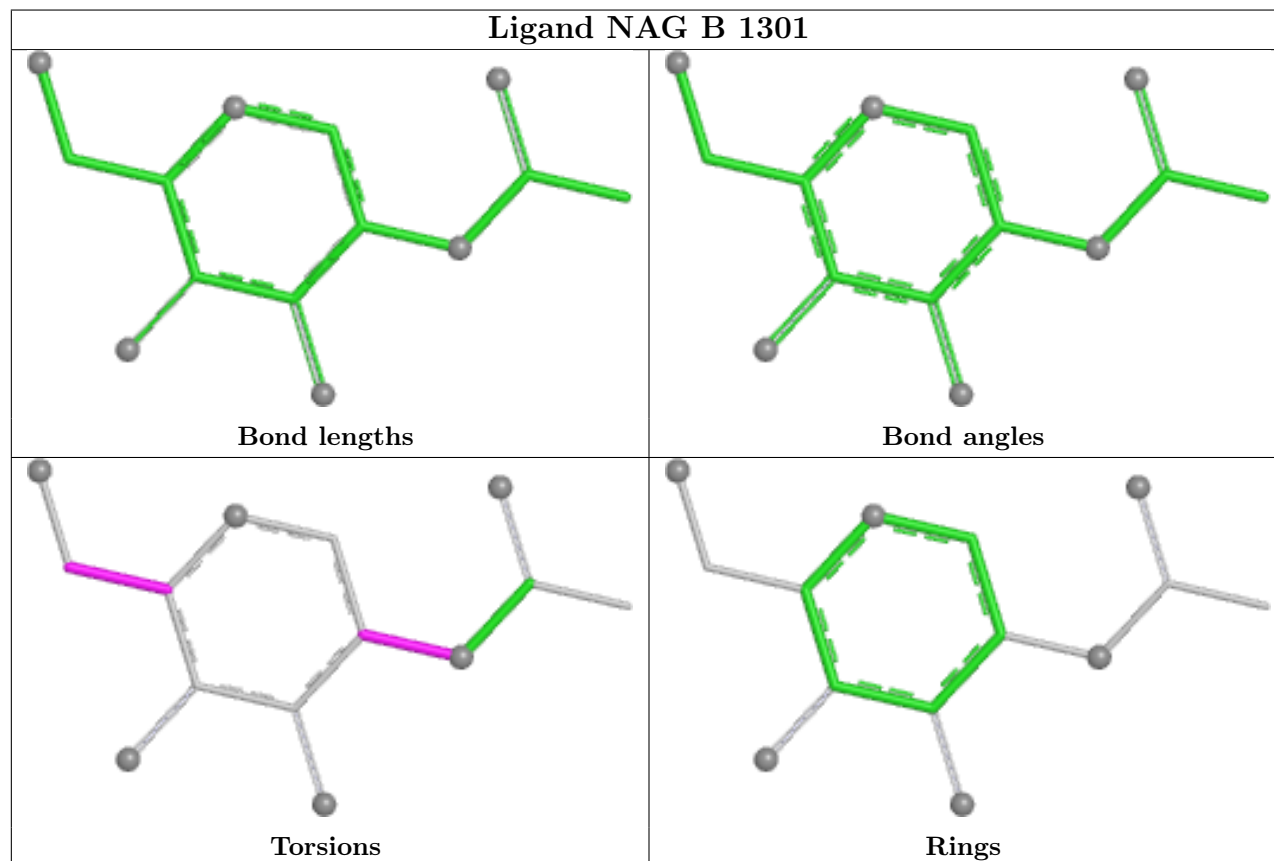
Mol	Chain	Res	Type	Atoms
4	B	1301	NAG	O5-C5-C6-O6
4	B	1301	NAG	C3-C2-N2-C7
4	B	1301	NAG	C1-C2-N2-C7

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.

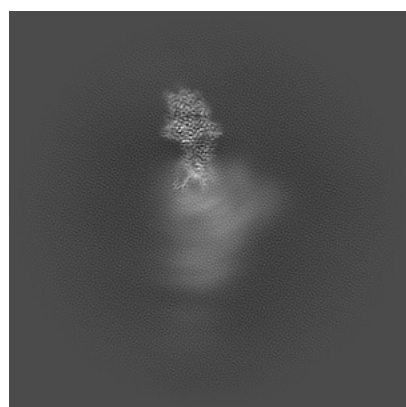
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32727. These allow visual inspection of the internal detail of the map and identification of artifacts.

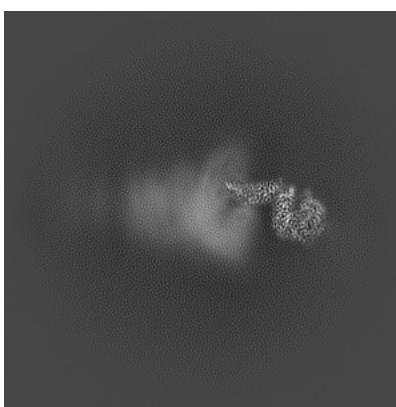
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

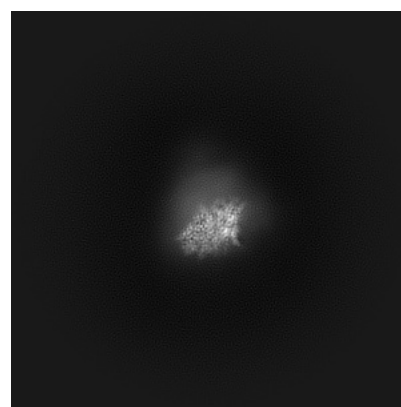
6.1.1 Primary map



X



Y



Z

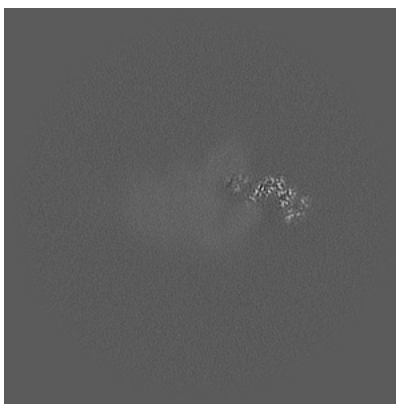
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

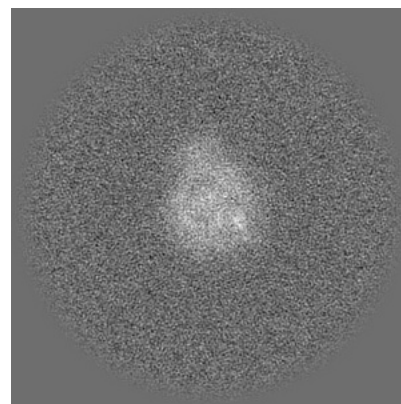
6.2.1 Primary map



X Index: 200



Y Index: 200

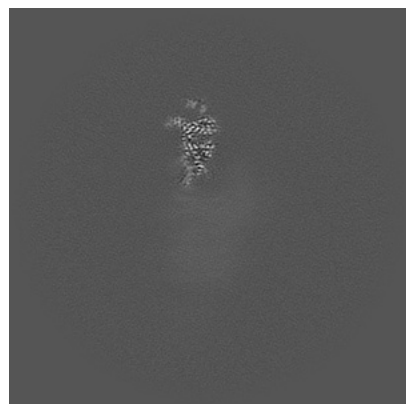


Z Index: 200

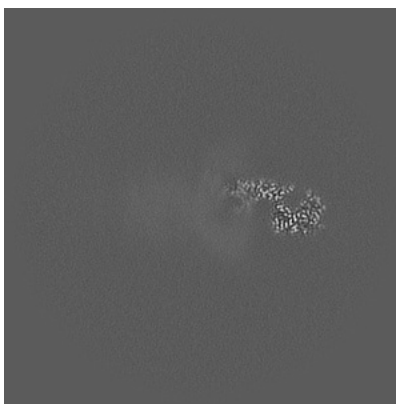
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

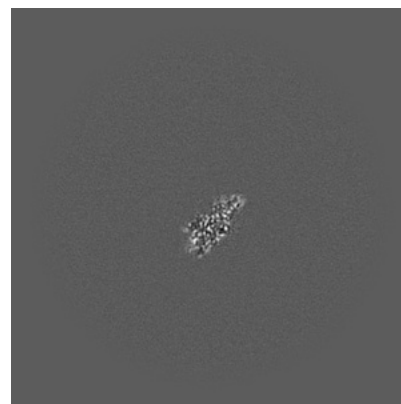
6.3.1 Primary map



X Index: 215



Y Index: 181

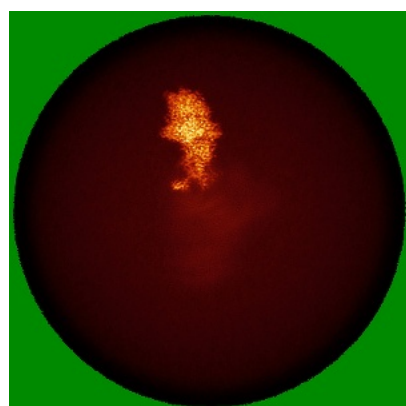


Z Index: 276

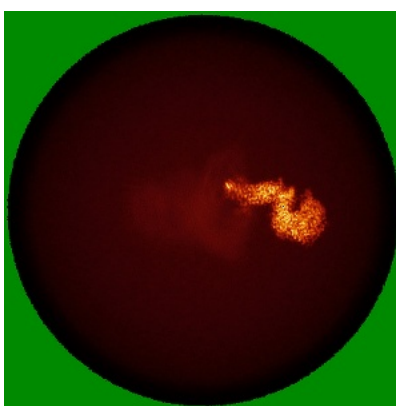
The images above show the largest variance slices of the map in three orthogonal directions.

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

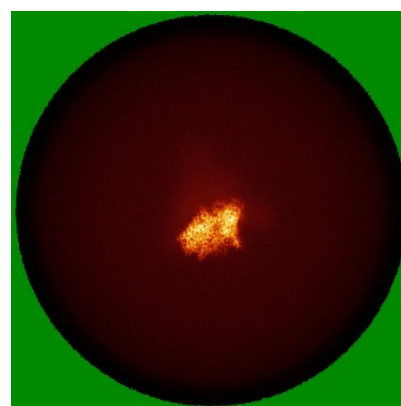
6.4.1 Primary map



X



Y

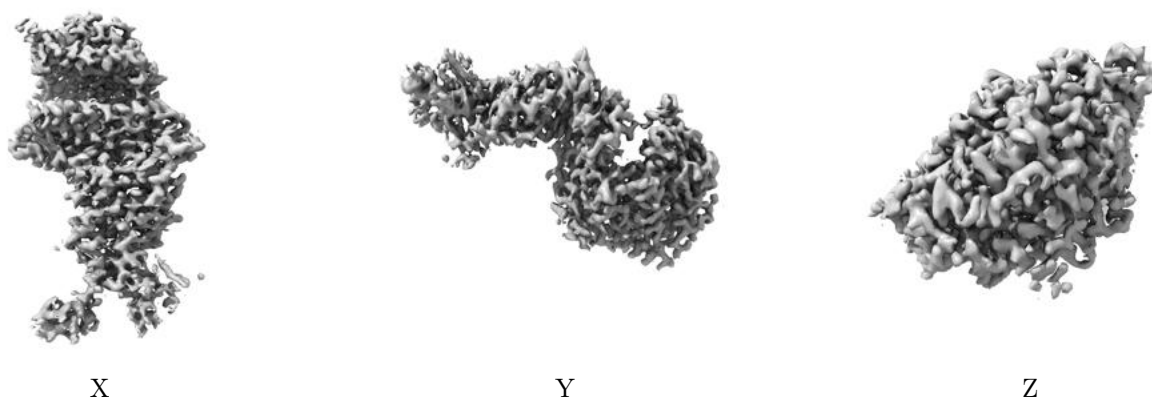


Z

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

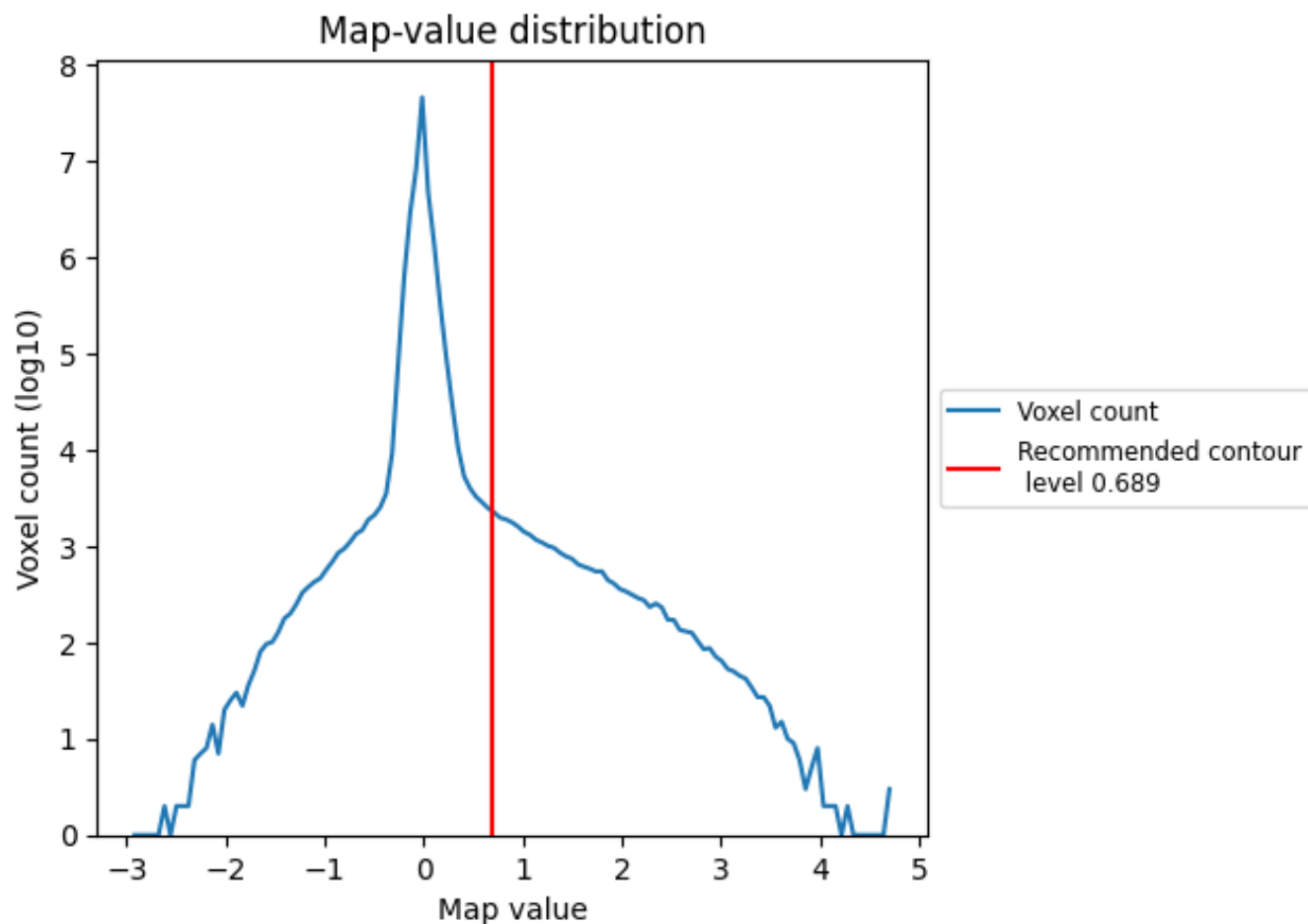
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

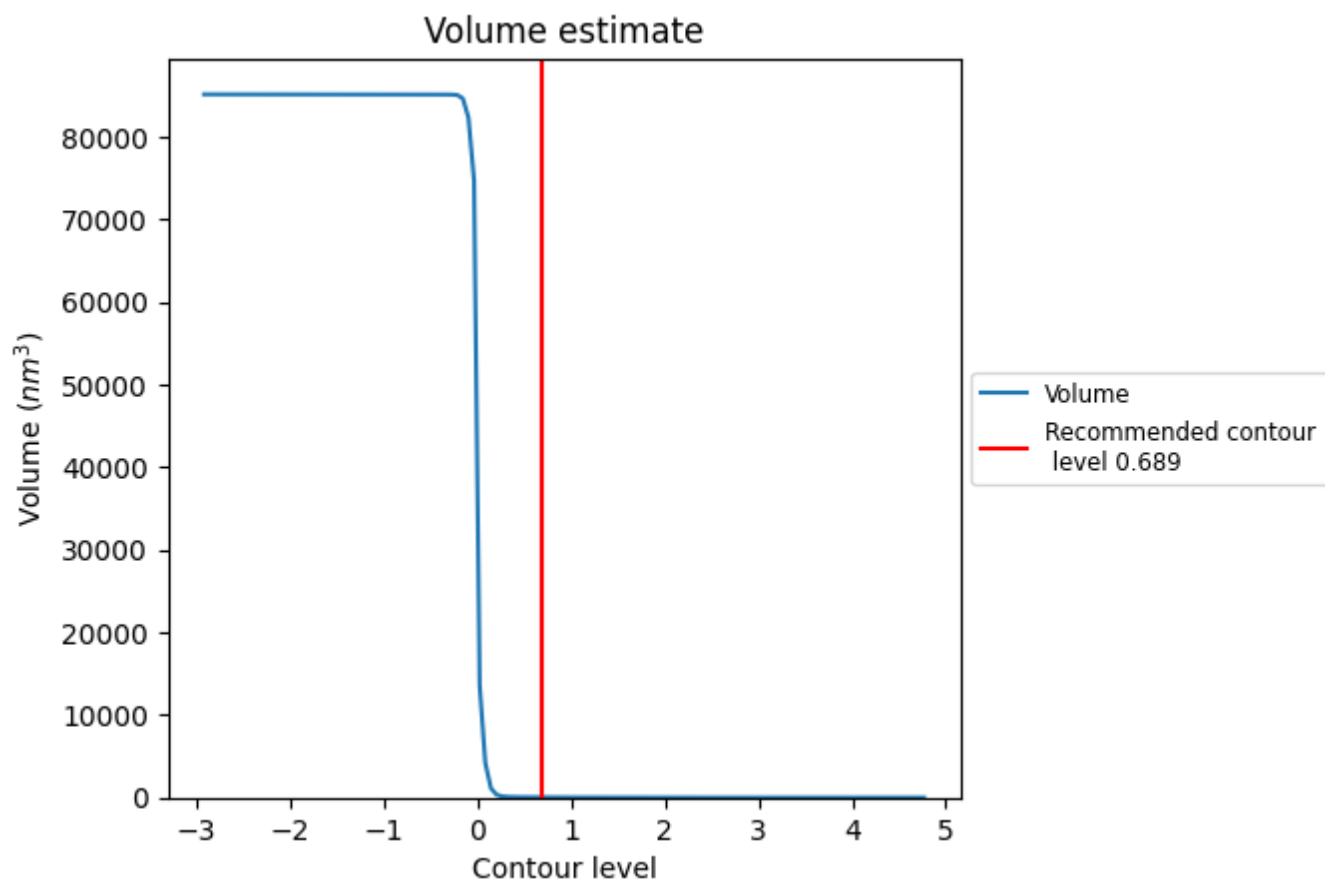
This section contains the results of statistical analysis of the map.

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.

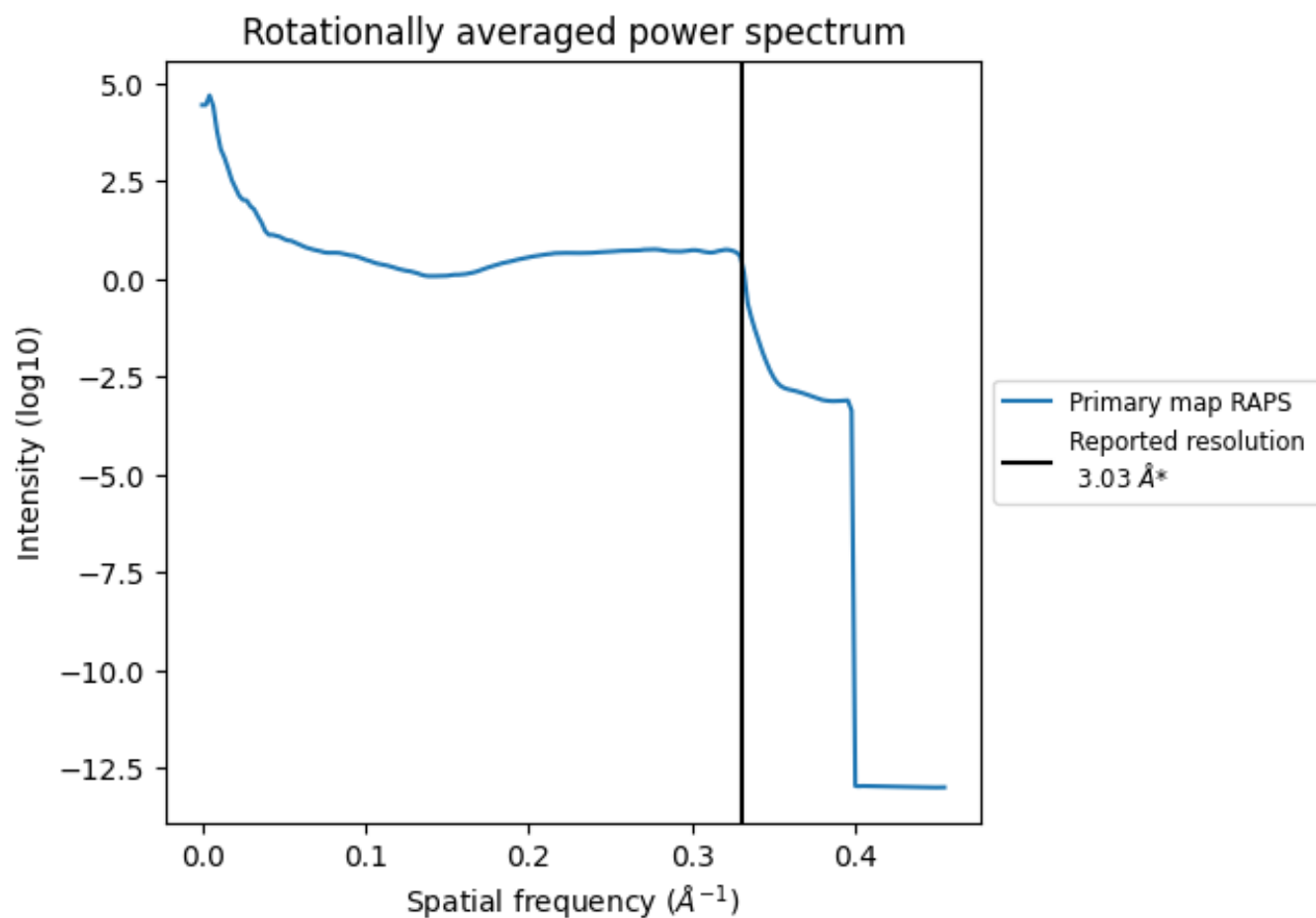
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm³; this corresponds to an approximate mass of 33 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 ⓘ

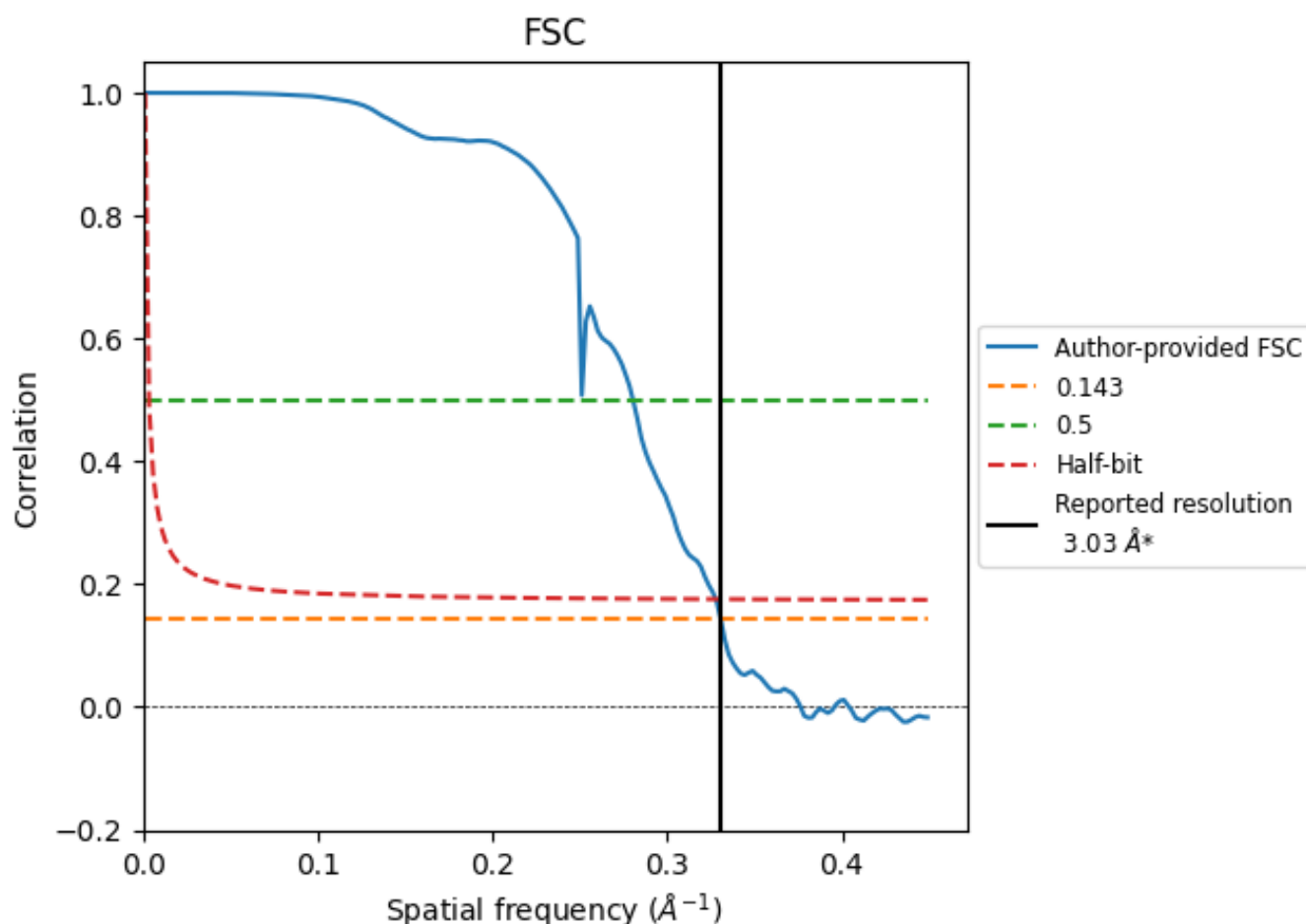


*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.02	3.57	3.05
Unmasked-calculated*	-	-	-

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

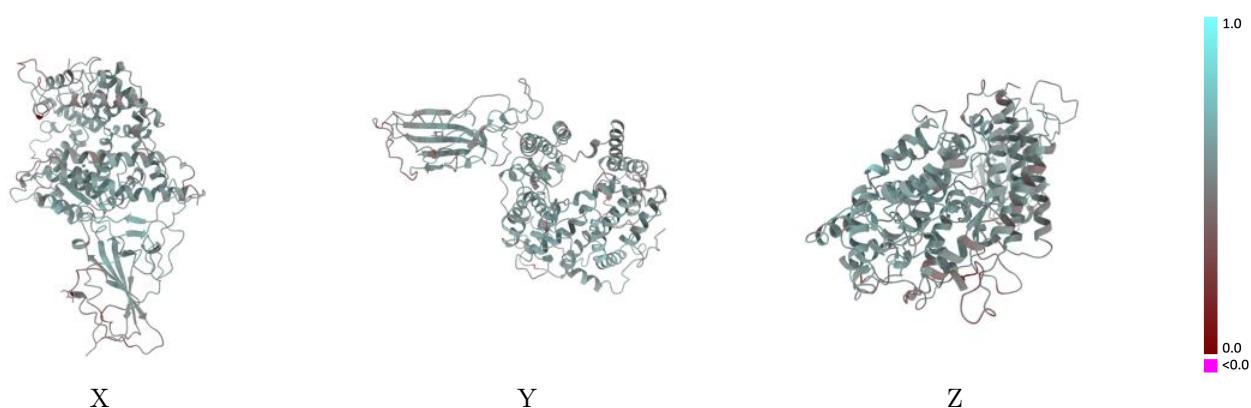
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-32727 and PDB model 7WRI. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

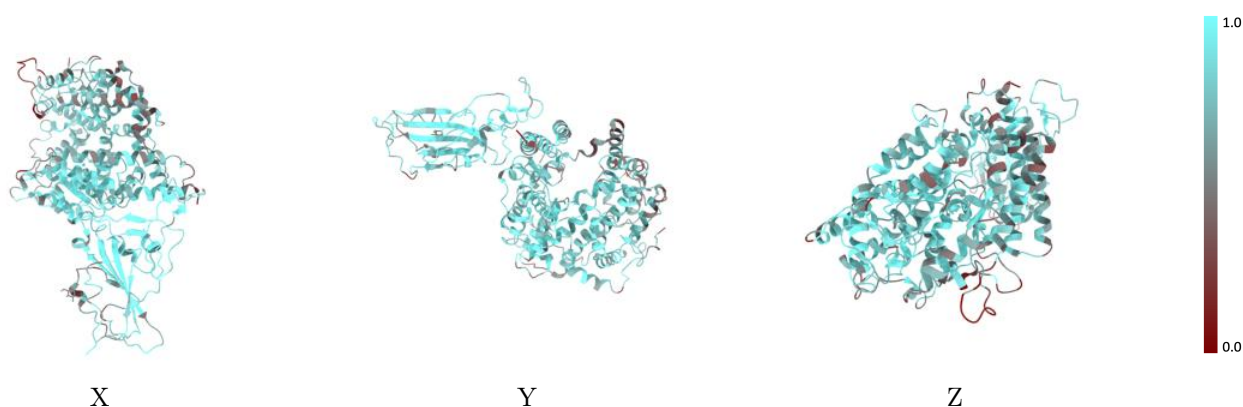
This section was not generated.

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



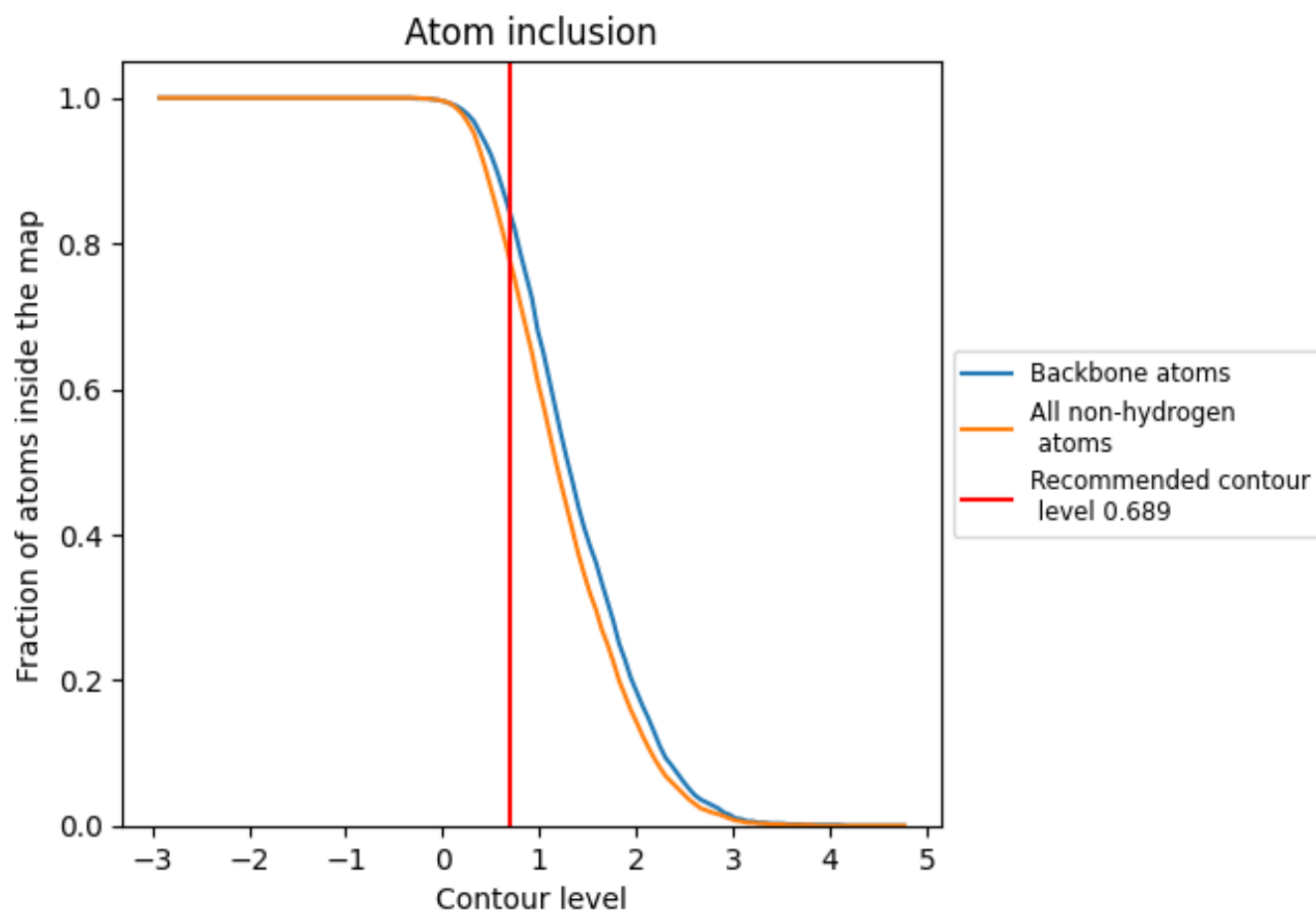
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.689).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.689) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.5400
A	0.7670	0.5450
B	0.8140	0.5230

