



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:35 AM UTC

PDB ID : 9D32 / pdb_00009d32
EMDB ID : EMD-46512
Title : Structure of the HKU5 RBD bound to the P. abramus ACE2 receptor
Authors : Park, Y.J.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2024-08-09
Resolution : 3.10 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
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

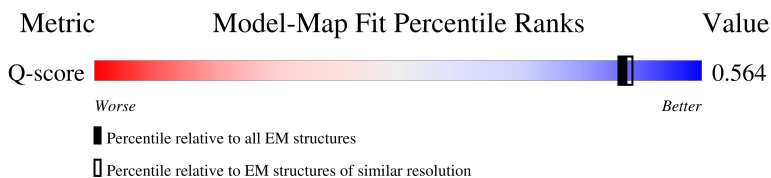
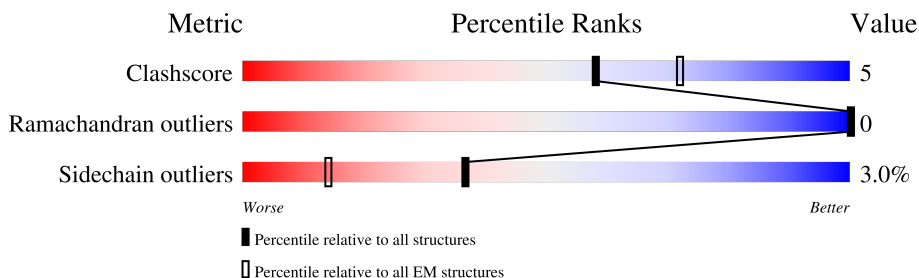
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	768	 8% 65% 10% 24%
2	B	267	 8% 65% 7% 27%
3	C	2	 50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6130 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	584	Total	C	N	O	S	0	0
			4570	2957	790	793	30		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP C7ECT9
A	-5	PRO	-	expression tag	UNP C7ECT9
A	-4	MET	-	expression tag	UNP C7ECT9
A	-3	GLY	-	expression tag	UNP C7ECT9
A	-2	SER	-	expression tag	UNP C7ECT9
A	-1	LEU	-	expression tag	UNP C7ECT9
A	0	GLN	-	expression tag	UNP C7ECT9
A	1	PRO	-	expression tag	UNP C7ECT9
A	2	LEU	-	expression tag	UNP C7ECT9
A	3	ALA	-	expression tag	UNP C7ECT9
A	4	THR	-	expression tag	UNP C7ECT9
A	5	LEU	-	expression tag	UNP C7ECT9
A	6	TYR	-	expression tag	UNP C7ECT9
A	7	LEU	-	expression tag	UNP C7ECT9
A	8	LEU	-	expression tag	UNP C7ECT9
A	9	GLY	-	expression tag	UNP C7ECT9
A	10	MET	-	expression tag	UNP C7ECT9
A	11	LEU	-	expression tag	UNP C7ECT9
A	12	VAL	-	expression tag	UNP C7ECT9
A	13	ALA	-	expression tag	UNP C7ECT9
A	14	SER	-	expression tag	UNP C7ECT9
A	15	VAL	-	expression tag	UNP C7ECT9
A	16	LEU	-	expression tag	UNP C7ECT9
A	725	LEU	-	expression tag	UNP C7ECT9
A	726	VAL	-	expression tag	UNP C7ECT9
A	727	PRO	-	expression tag	UNP C7ECT9
A	728	ARG	-	expression tag	UNP C7ECT9
A	729	GLY	-	expression tag	UNP C7ECT9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	730	SER	-	expression tag	UNP C7ECT9
A	731	SER	-	expression tag	UNP C7ECT9
A	732	SER	-	expression tag	UNP C7ECT9
A	733	GLY	-	expression tag	UNP C7ECT9
A	734	GLY	-	expression tag	UNP C7ECT9
A	735	SER	-	expression tag	UNP C7ECT9
A	736	GLY	-	expression tag	UNP C7ECT9
A	737	LEU	-	expression tag	UNP C7ECT9
A	738	ASN	-	expression tag	UNP C7ECT9
A	739	ASP	-	expression tag	UNP C7ECT9
A	740	ILE	-	expression tag	UNP C7ECT9
A	741	PHE	-	expression tag	UNP C7ECT9
A	742	GLU	-	expression tag	UNP C7ECT9
A	743	ALA	-	expression tag	UNP C7ECT9
A	744	GLN	-	expression tag	UNP C7ECT9
A	745	LYS	-	expression tag	UNP C7ECT9
A	746	ILE	-	expression tag	UNP C7ECT9
A	747	GLU	-	expression tag	UNP C7ECT9
A	748	TRP	-	expression tag	UNP C7ECT9
A	749	HIS	-	expression tag	UNP C7ECT9
A	750	GLU	-	expression tag	UNP C7ECT9
A	751	GLY	-	expression tag	UNP C7ECT9
A	752	GLY	-	expression tag	UNP C7ECT9
A	753	SER	-	expression tag	UNP C7ECT9
A	754	HIS	-	expression tag	UNP C7ECT9
A	755	HIS	-	expression tag	UNP C7ECT9
A	756	HIS	-	expression tag	UNP C7ECT9
A	757	HIS	-	expression tag	UNP C7ECT9
A	758	HIS	-	expression tag	UNP C7ECT9
A	759	HIS	-	expression tag	UNP C7ECT9
A	760	HIS	-	expression tag	UNP C7ECT9
A	761	HIS	-	expression tag	UNP C7ECT9

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	194	Total	C	N	O	S	0	0
			1423	934	230	248	11		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	358	MET	-	expression tag	UNP S4WZQ4
B	359	GLY	-	expression tag	UNP S4WZQ4
B	360	ILE	-	expression tag	UNP S4WZQ4
B	361	LEU	-	expression tag	UNP S4WZQ4
B	362	PRO	-	expression tag	UNP S4WZQ4
B	363	SER	-	expression tag	UNP S4WZQ4
B	364	PRO	-	expression tag	UNP S4WZQ4
B	365	GLY	-	expression tag	UNP S4WZQ4
B	366	MET	-	expression tag	UNP S4WZQ4
B	367	PRO	-	expression tag	UNP S4WZQ4
B	368	ALA	-	expression tag	UNP S4WZQ4
B	369	LEU	-	expression tag	UNP S4WZQ4
B	370	LEU	-	expression tag	UNP S4WZQ4
B	371	SER	-	expression tag	UNP S4WZQ4
B	372	LEU	-	expression tag	UNP S4WZQ4
B	373	VAL	-	expression tag	UNP S4WZQ4
B	374	SER	-	expression tag	UNP S4WZQ4
B	375	LEU	-	expression tag	UNP S4WZQ4
B	376	LEU	-	expression tag	UNP S4WZQ4
B	377	SER	-	expression tag	UNP S4WZQ4
B	378	VAL	-	expression tag	UNP S4WZQ4
B	379	LEU	-	expression tag	UNP S4WZQ4
B	380	LEU	-	expression tag	UNP S4WZQ4
B	381	MET	-	expression tag	UNP S4WZQ4
B	382	GLY	-	expression tag	UNP S4WZQ4
B	383	CYS	-	expression tag	UNP S4WZQ4
B	384	VAL	-	expression tag	UNP S4WZQ4
B	385	ALA	-	expression tag	UNP S4WZQ4
B	386	GLU	-	expression tag	UNP S4WZQ4
B	387	THR	-	expression tag	UNP S4WZQ4
B	388	GLY	-	expression tag	UNP S4WZQ4
B	588	LEU	-	expression tag	UNP S4WZQ4
B	589	VAL	-	expression tag	UNP S4WZQ4
B	590	PRO	-	expression tag	UNP S4WZQ4
B	591	ARG	-	expression tag	UNP S4WZQ4
B	592	GLY	-	expression tag	UNP S4WZQ4
B	593	SER	-	expression tag	UNP S4WZQ4
B	594	SER	-	expression tag	UNP S4WZQ4
B	595	SER	-	expression tag	UNP S4WZQ4
B	596	GLY	-	expression tag	UNP S4WZQ4
B	597	GLY	-	expression tag	UNP S4WZQ4
B	598	SER	-	expression tag	UNP S4WZQ4
B	599	GLY	-	expression tag	UNP S4WZQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	600	LEU	-	expression tag	UNP S4WZQ4
B	601	ASN	-	expression tag	UNP S4WZQ4
B	602	ASP	-	expression tag	UNP S4WZQ4
B	603	ILE	-	expression tag	UNP S4WZQ4
B	604	PHE	-	expression tag	UNP S4WZQ4
B	605	GLU	-	expression tag	UNP S4WZQ4
B	606	ALA	-	expression tag	UNP S4WZQ4
B	607	GLN	-	expression tag	UNP S4WZQ4
B	608	LYS	-	expression tag	UNP S4WZQ4
B	609	ILE	-	expression tag	UNP S4WZQ4
B	610	GLU	-	expression tag	UNP S4WZQ4
B	611	TRP	-	expression tag	UNP S4WZQ4
B	612	HIS	-	expression tag	UNP S4WZQ4
B	613	GLU	-	expression tag	UNP S4WZQ4
B	614	GLY	-	expression tag	UNP S4WZQ4
B	615	GLY	-	expression tag	UNP S4WZQ4
B	616	SER	-	expression tag	UNP S4WZQ4
B	617	HIS	-	expression tag	UNP S4WZQ4
B	618	HIS	-	expression tag	UNP S4WZQ4
B	619	HIS	-	expression tag	UNP S4WZQ4
B	620	HIS	-	expression tag	UNP S4WZQ4
B	621	HIS	-	expression tag	UNP S4WZQ4
B	622	HIS	-	expression tag	UNP S4WZQ4
B	623	HIS	-	expression tag	UNP S4WZQ4
B	624	HIS	-	expression tag	UNP S4WZQ4

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

GLN
LYS
ILE
GLU
TRP
HIS
GLU
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	550684, 550684, 550684, 550684	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.930	Depositor
Minimum map value	-3.852	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.65	Depositor
Map size ($\text{\AA}$)	320.0, 320.0, 320.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN, FUC

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	0/4697	0.34	0/6379
2	B	0.17	0/1464	0.35	0/2005
All	All	0.17	0/6161	0.34	0/8384

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

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	4570	0	4270	46	0
2	B	1423	0	1246	11	0
3	C	24	0	22	0	0
4	A	84	0	78	0	0
4	B	28	0	26	0	0
5	A	1	0	0	0	0
All	All	6130	0	5642	55	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 (55) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:HD1	1:A:76:GLN:HG2	1.59	0.67
1:A:359:MET:HE2	1:A:361:THR:HG22	1.80	0.63
1:A:464:GLU:OE1	1:A:466:LYS:NZ	2.38	0.57
1:A:147:LEU:HG	1:A:163:VAL:HG13	1.89	0.54
1:A:393:ASN:HB2	1:A:561:LYS:HE2	1.89	0.54
1:A:142:PHE:HB2	1:A:147:LEU:HD13	1.90	0.54
1:A:407:MET:HE1	1:A:553:LEU:HD21	1.91	0.52
1:A:473:MET:HE1	1:A:499:PRO:HD2	1.92	0.51
1:A:481:ARG:NH2	1:A:488:GLU:OE2	2.45	0.50
2:B:410:ARG:NH2	2:B:528:GLY:O	2.33	0.49
1:A:52:THR:O	1:A:339:ARG:NH1	2.46	0.49
1:A:74:LYS:O	1:A:78:LYS:HG2	2.13	0.49
1:A:166:GLY:O	1:A:170:GLU:HB2	2.12	0.49
1:A:244:ARG:NH1	1:A:257:PRO:O	2.45	0.49
1:A:233:LYS:NZ	1:A:237:GLU:OE2	2.46	0.48
1:A:368:PHE:O	1:A:372:HIS:HD2	1.97	0.48
2:B:392:CYS:N	2:B:416:CYS:SG	2.86	0.48
1:A:481:ARG:HH21	1:A:488:GLU:CD	2.21	0.48
2:B:435:HIS:CE1	2:B:436:GLN:HG3	2.49	0.47
1:A:410:SER:OG	1:A:542:ASP:OD1	2.32	0.47
2:B:465:LEU:HD23	2:B:488:ARG:HD2	1.96	0.47
1:A:109:THR:O	1:A:111:GLU:N	2.48	0.46
2:B:547:SER:HA	2:B:555:THR:O	2.15	0.46
1:A:143:THR:O	1:A:147:LEU:HB2	2.15	0.46
2:B:403:PRO:HG3	2:B:409:LYS:HG3	1.97	0.46
1:A:238:GLN:HG3	1:A:598:ASN:HD22	1.81	0.46
1:A:328:ARG:HH22	2:B:461:MET:HE3	1.81	0.46
1:A:467:ILE:HG22	1:A:472:TRP:HD1	1.81	0.46
1:A:53:ASN:O	1:A:58:ASN:ND2	2.49	0.45
1:A:331:MET:HE1	1:A:341:VAL:HG11	1.98	0.45
1:A:283:PRO:HD3	1:A:439:LEU:HD23	1.98	0.45
2:B:402:PRO:HB3	2:B:568:MET:HE3	1.99	0.45
1:A:538:LEU:HD22	1:A:586:TYR:HD2	1.82	0.45
1:A:454:MET:HG3	1:A:455:LEU:N	2.31	0.44
2:B:434:CYS:HA	2:B:487:CYS:HA	2.00	0.44
1:A:392:ARG:NH2	2:B:520:LYS:HE3	2.32	0.44
1:A:244:ARG:HA	1:A:261:LEU:HD21	2.00	0.43
1:A:351:GLY:O	1:A:353:ASN:N	2.51	0.43
1:A:307:PHE:HE2	1:A:361:THR:HG21	1.84	0.42
1:A:33:ASN:O	1:A:37:GLU:HG2	2.20	0.42
1:A:304:GLU:O	1:A:308:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:LEU:HD12	1:A:594:LEU:HA	1.92	0.42
1:A:292:VAL:HB	1:A:422:LEU:HG	2.02	0.41
1:A:455:LEU:HD23	1:A:511:PHE:CD2	2.55	0.41
1:A:552:LYS:HE3	1:A:552:LYS:HB2	1.77	0.41
1:A:591:PHE:CE2	1:A:595:LYS:HD2	2.55	0.41
1:A:37:GLU:OE2	1:A:392:ARG:NH2	2.54	0.41
2:B:409:LYS:HE2	2:B:409:LYS:HB3	1.81	0.41
1:A:26:ARG:O	1:A:30:VAL:HG23	2.21	0.40
1:A:238:GLN:HE21	1:A:238:GLN:HB2	1.69	0.40
1:A:475:LYS:HD3	1:A:475:LYS:HA	1.87	0.40
1:A:246:LYS:HD3	1:A:281:THR:HA	2.02	0.40
1:A:477:TRP:HA	1:A:480:LYS:HB2	2.03	0.40
1:A:203:ARG:HD2	1:A:218:ARG:O	2.21	0.40
1:A:370:THR:O	1:A:374:GLU:HG2	2.21	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	582/768 (76%)	570 (98%)	12 (2%)	0	100	100
2	B	190/267 (71%)	186 (98%)	4 (2%)	0	100	100
All	All	772/1035 (75%)	756 (98%)	16 (2%)	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	436/683 (64%)	421 (97%)	15 (3%)	32	63
2	B	126/233 (54%)	124 (98%)	2 (2%)	55	75
All	All	562/916 (61%)	545 (97%)	17 (3%)	37	65

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	85	LEU
1	A	93	ILE
1	A	95	LEU
1	A	168	ARG
1	A	170	GLU
1	A	235	LEU
1	A	238	GLN
1	A	246	LYS
1	A	290	ILE
1	A	360	CYS
1	A	400	HIS
1	A	430	ASN
1	A	454	MET
1	A	594	LEU
2	B	474	VAL
2	B	562	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	63	ASN
1	A	76	GLN
1	A	372	HIS
1	A	598	ASN
2	B	436	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 ⓘ

2 monosaccharides 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$
3	NAG	C	1	1,3	14,14,15	0.71	0	17,19,21	0.87	0
3	FUC	C	2	3	10,10,11	0.71	0	14,14,16	1.25	2 (14%)

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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	FUC	C1-O5-C5	2.52	118.92	112.97
3	C	2	FUC	C1-C2-C3	2.40	113.13	109.64

There are no chirality outliers.

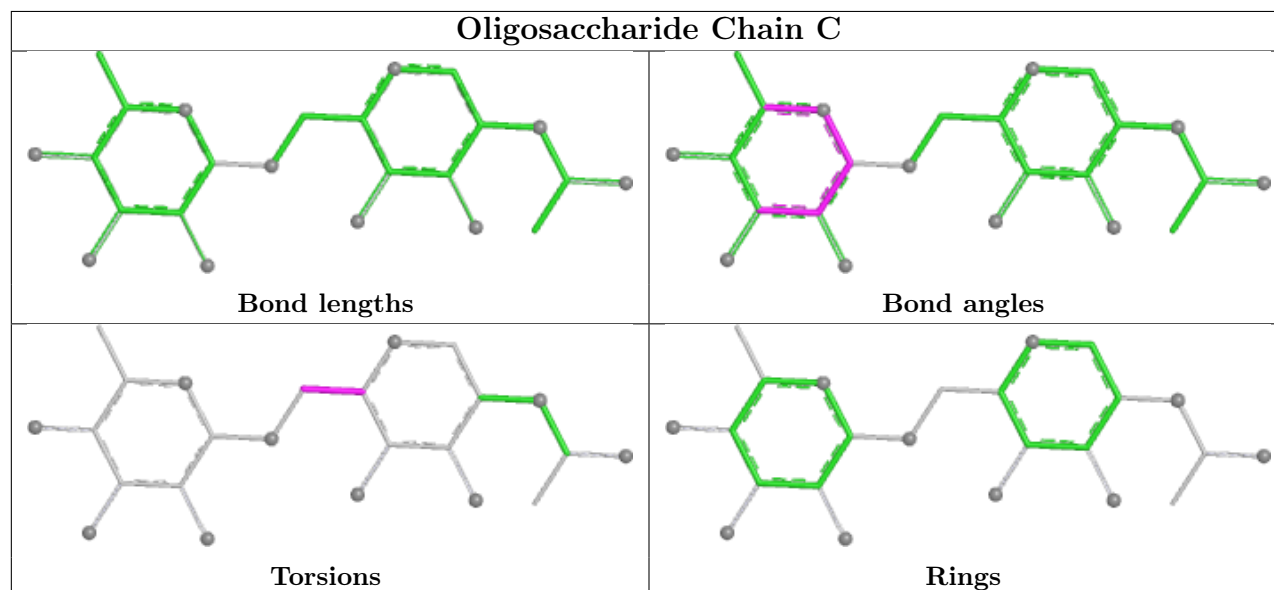
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6

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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	A	802	1	14,14,15	0.72	0	17,19,21	0.83	0
4	NAG	A	803	1	14,14,15	0.74	0	17,19,21	0.86	0
4	NAG	A	805	1	14,14,15	0.73	0	17,19,21	0.80	0
4	NAG	A	801	1	14,14,15	0.74	0	17,19,21	1.01	2 (11%)
4	NAG	A	804	1	14,14,15	0.75	0	17,19,21	0.94	1 (5%)
4	NAG	A	806	1	14,14,15	0.79	0	17,19,21	0.85	0
4	NAG	B	701	2	14,14,15	0.71	0	17,19,21	0.86	0
4	NAG	B	702	2	14,14,15	0.70	0	17,19,21	0.81	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	A	802	1	-	0/6/23/26	0/1/1/1
4	NAG	A	803	1	-	1/6/23/26	0/1/1/1
4	NAG	A	805	1	-	0/6/23/26	0/1/1/1
4	NAG	A	801	1	-	3/6/23/26	0/1/1/1
4	NAG	A	804	1	-	2/6/23/26	0/1/1/1
4	NAG	A	806	1	-	2/6/23/26	0/1/1/1
4	NAG	B	701	2	-	3/6/23/26	0/1/1/1
4	NAG	B	702	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	804	NAG	C1-O5-C5	2.15	115.07	112.19
4	A	801	NAG	C2-N2-C7	2.14	125.77	122.90
4	A	801	NAG	C1-O5-C5	2.11	115.01	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	NAG	O5-C5-C6-O6
4	A	804	NAG	C4-C5-C6-O6
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
4	B	701	NAG	C8-C7-N2-C2
4	B	701	NAG	O7-C7-N2-C2
4	B	701	NAG	O5-C5-C6-O6
4	A	801	NAG	O5-C5-C6-O6
4	A	803	NAG	O5-C5-C6-O6
4	A	806	NAG	O5-C5-C6-O6
4	A	806	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

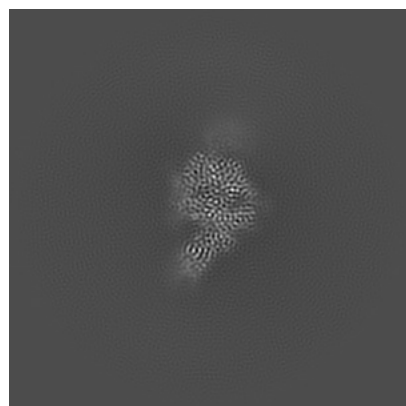
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46512. These allow visual inspection of the internal detail of the map and identification of artifacts.

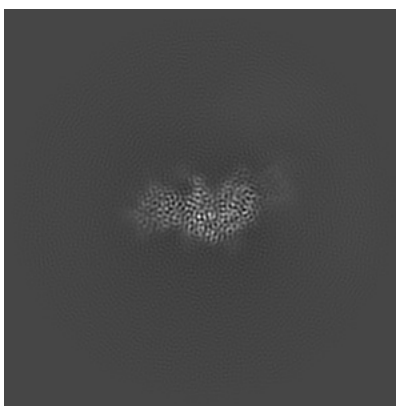
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

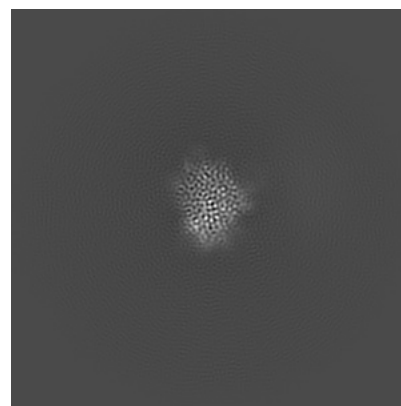
6.1.1 Primary map



X

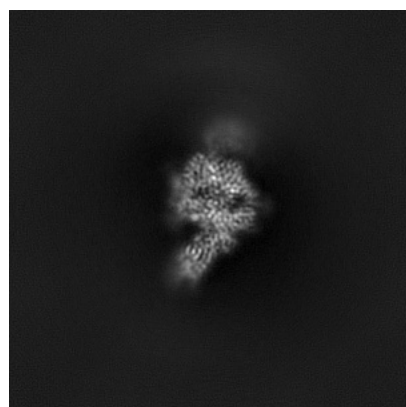


Y

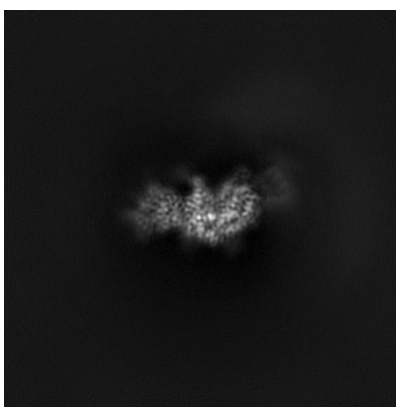


Z

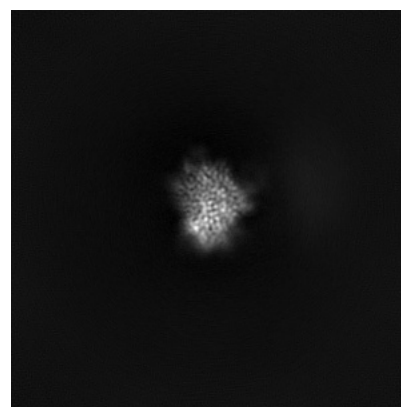
6.1.2 Raw map



X



Y

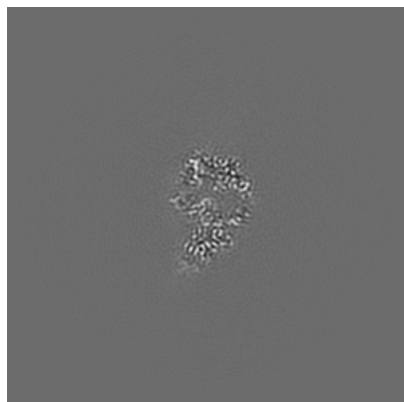


Z

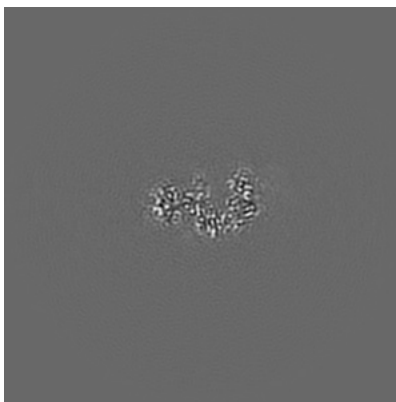
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

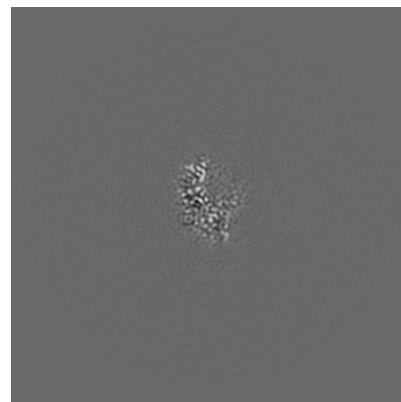
6.2.1 Primary map



X Index: 160

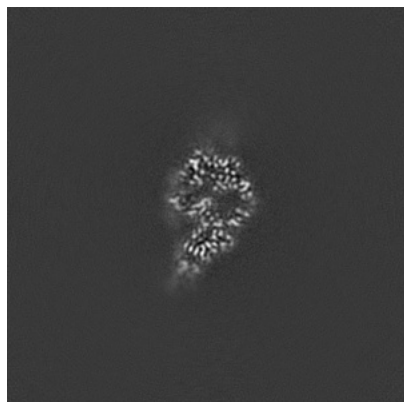


Y Index: 160

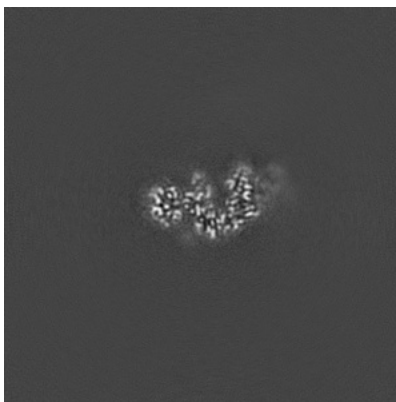


Z Index: 160

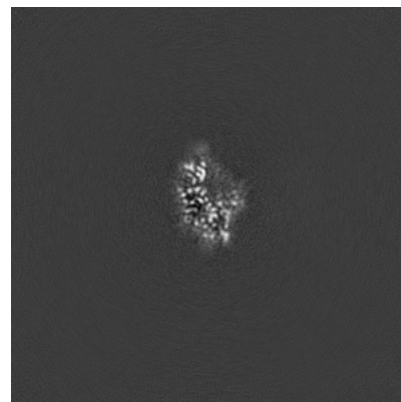
6.2.2 Raw map



X Index: 160



Y Index: 160

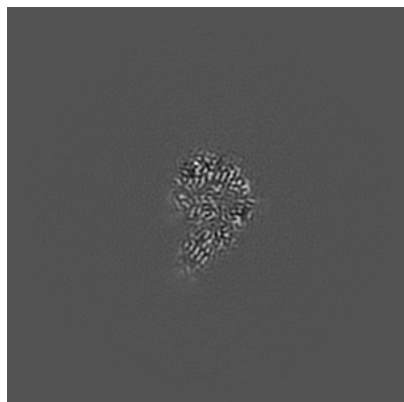


Z Index: 160

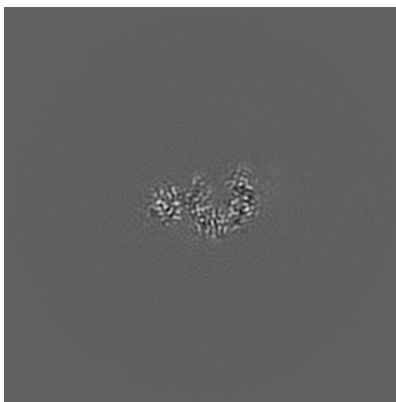
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

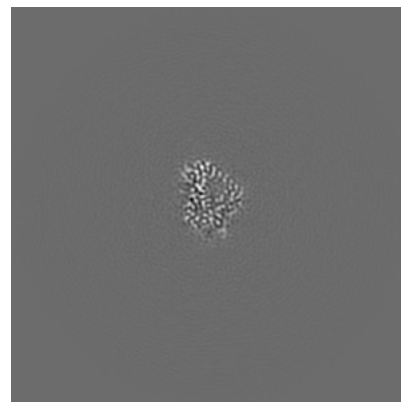
6.3.1 Primary map



X Index: 155

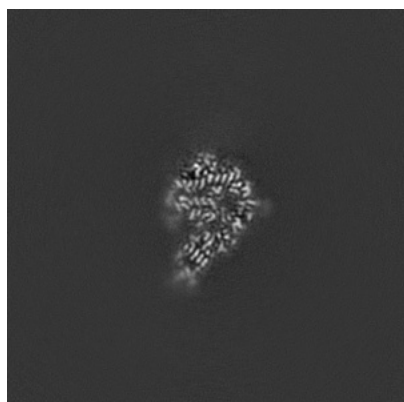


Y Index: 161

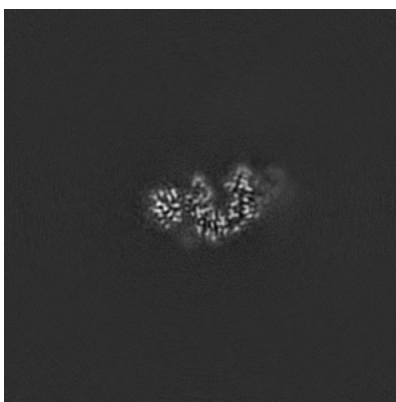


Z Index: 156

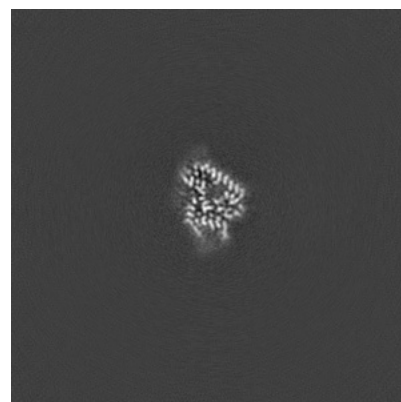
6.3.2 Raw map



X Index: 155



Y Index: 161

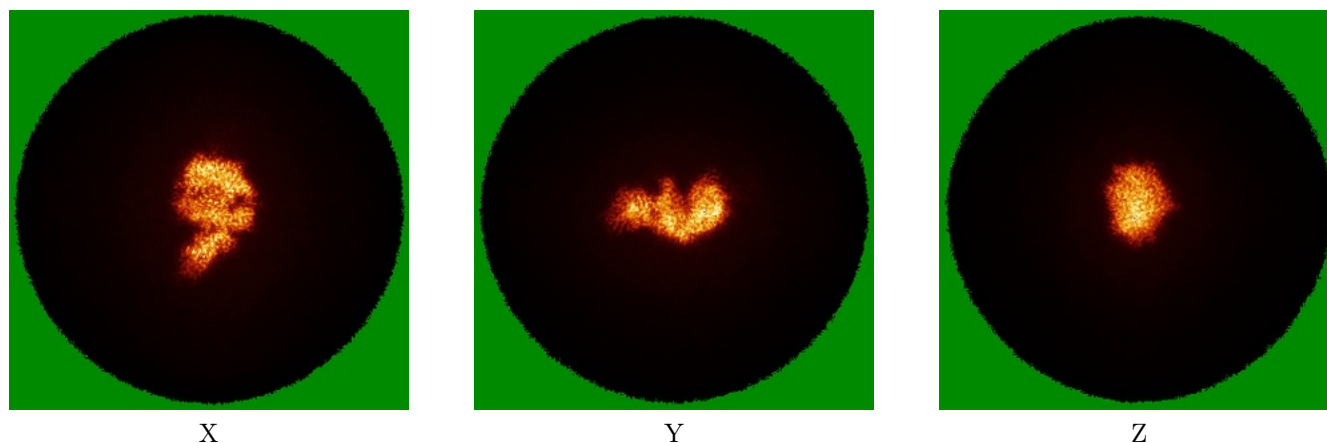


Z Index: 155

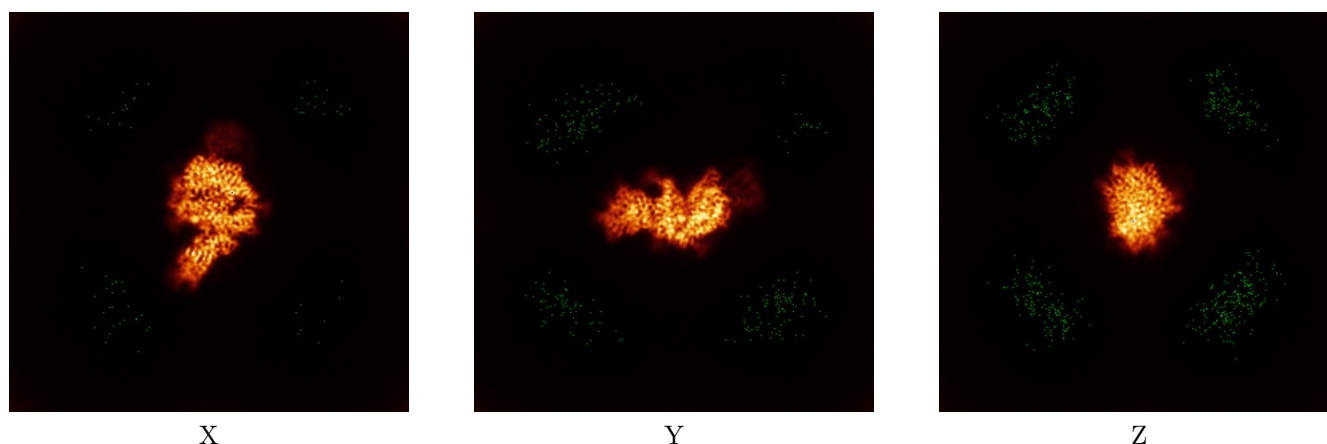
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

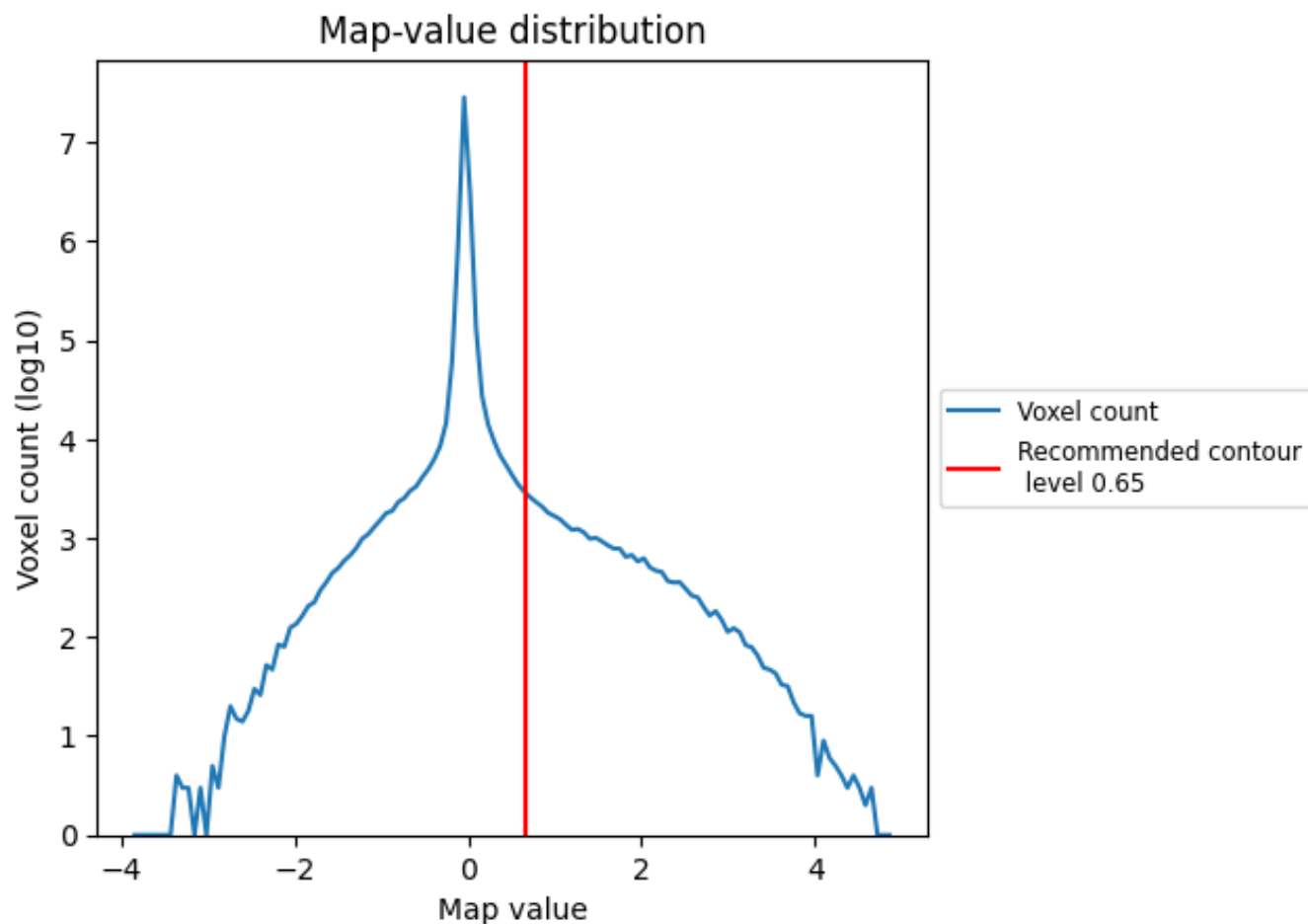
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

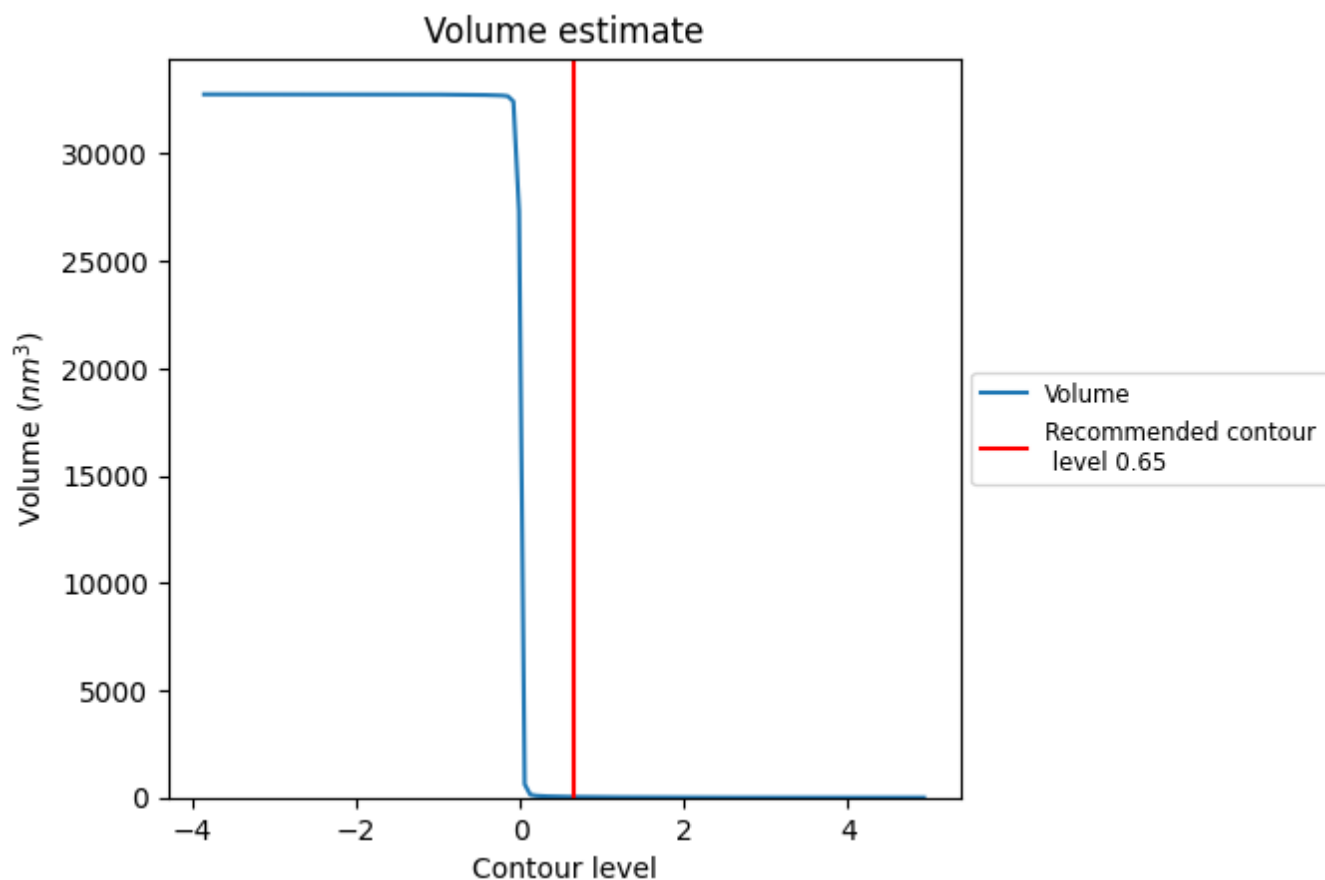
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

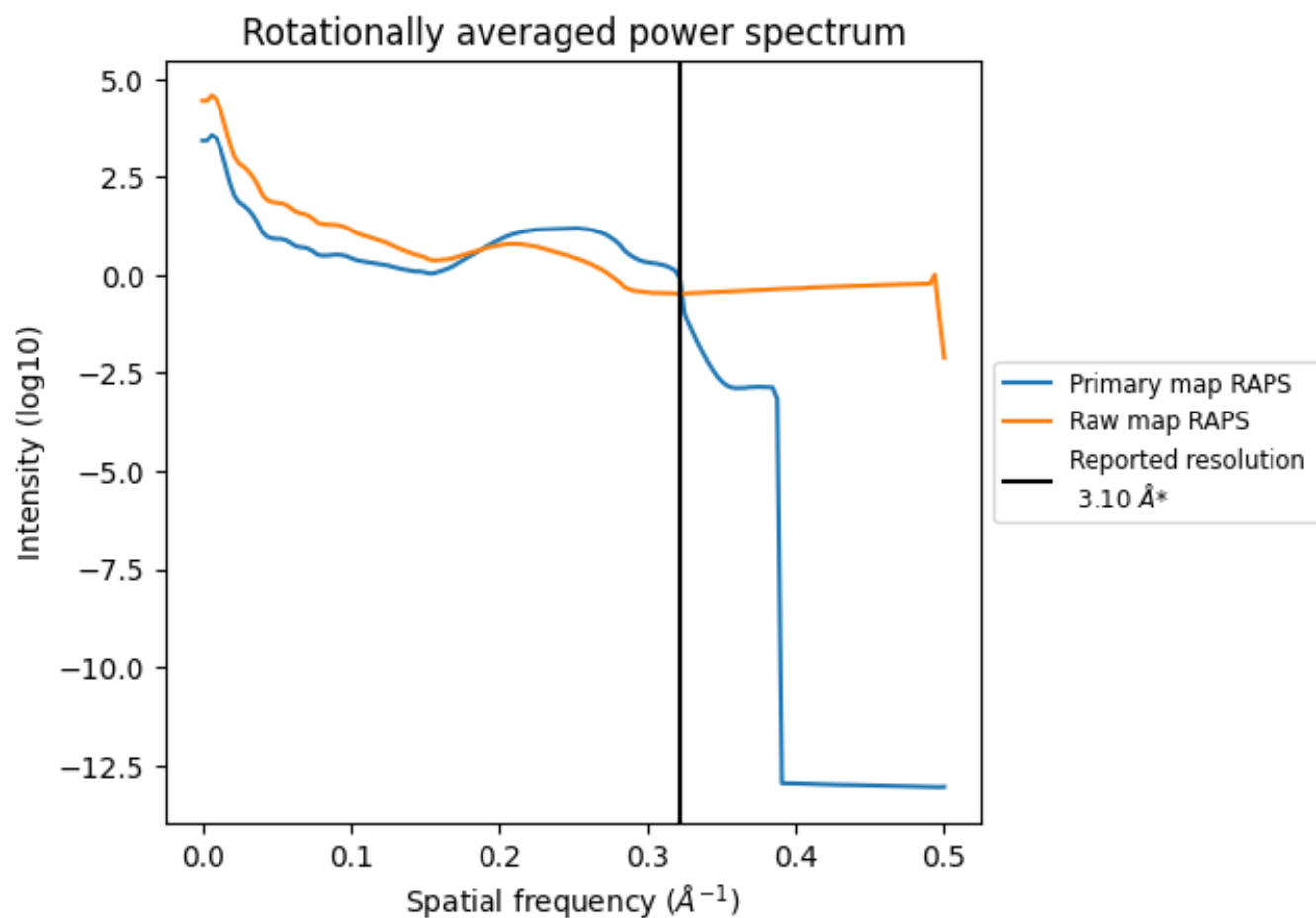
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 32 nm^3 ; this corresponds to an approximate mass of 29 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 ⓘ

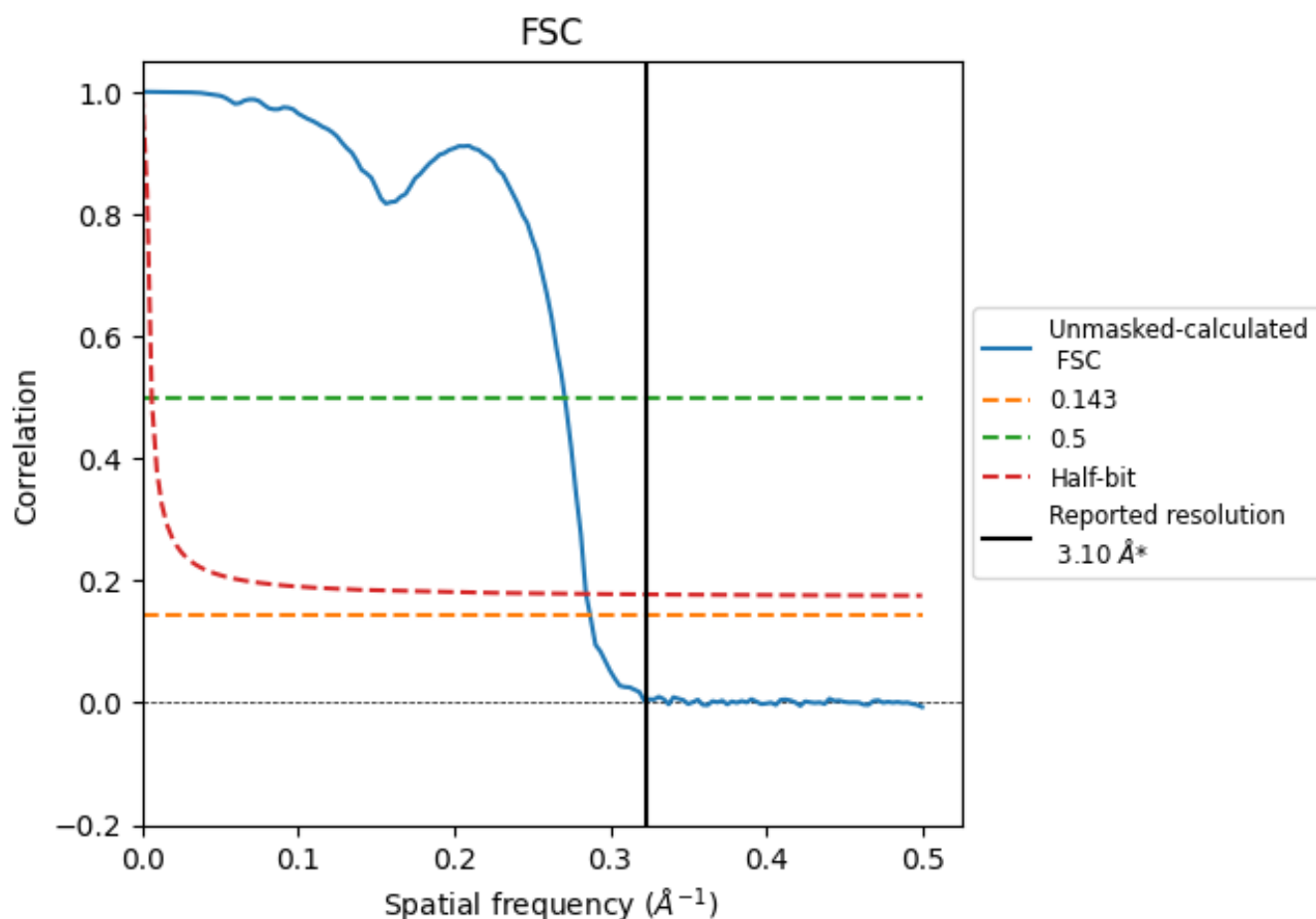


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	3.69	3.51

*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-46512 and PDB model 9D32. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

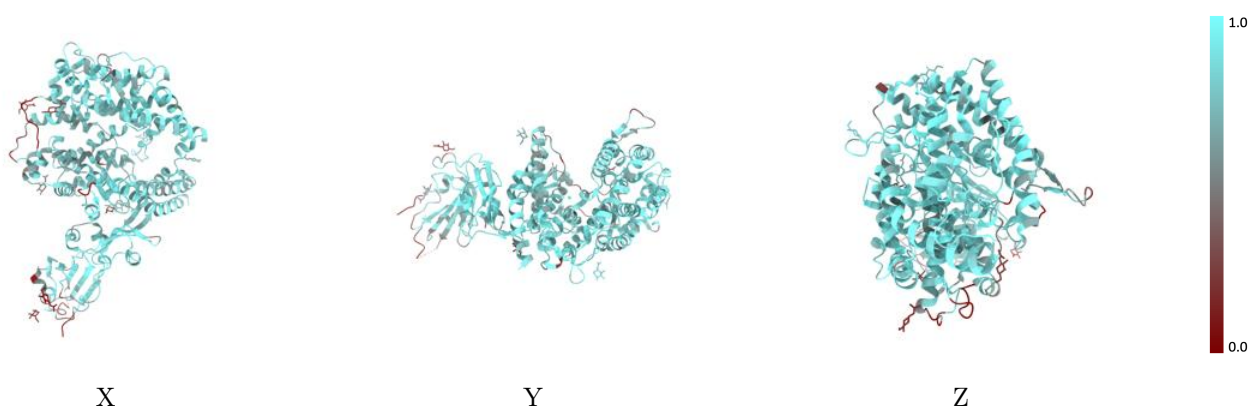
This section was not generated.

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



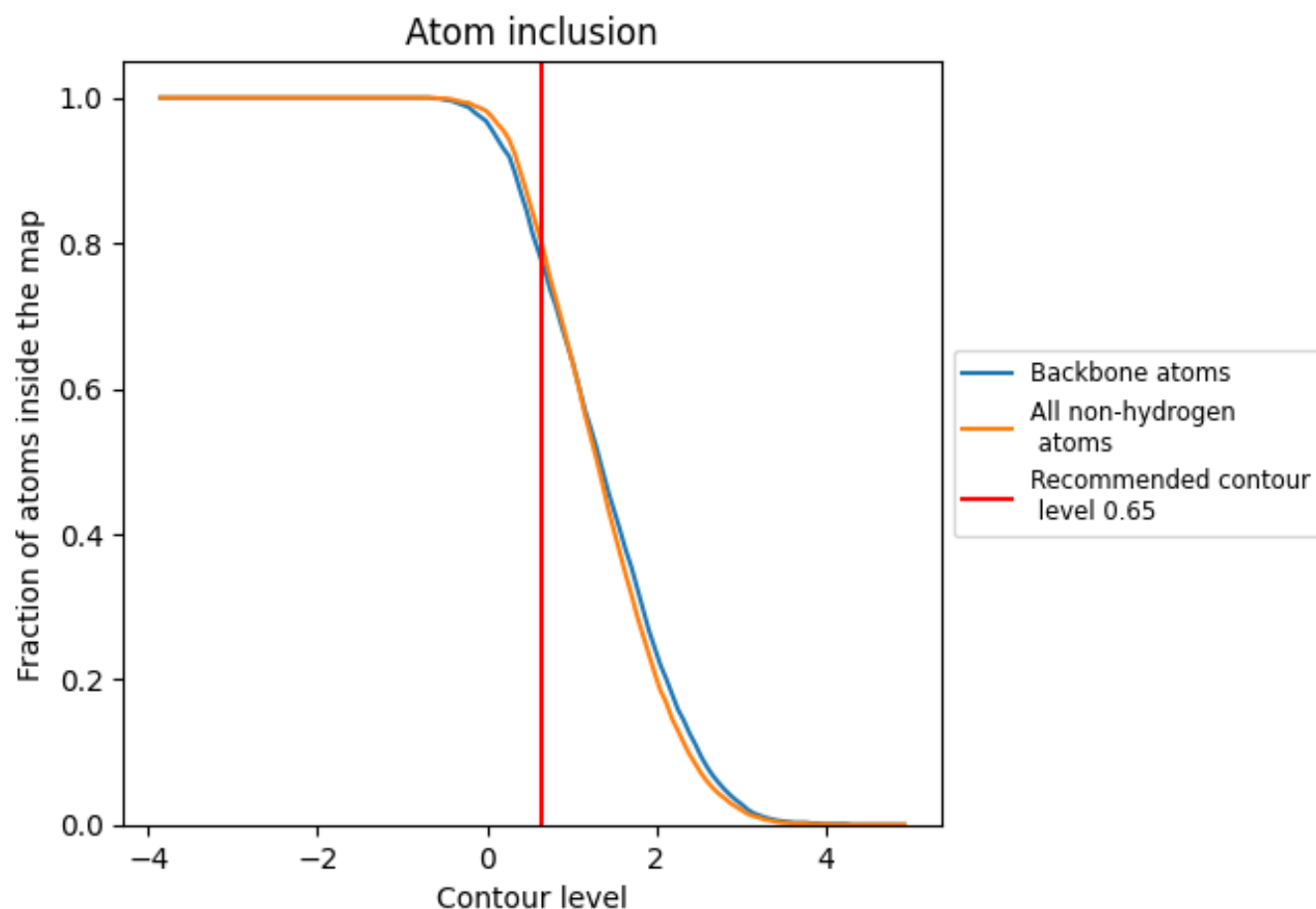
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 80% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.5640
A	0.8130	0.5690
B	0.7570	0.5520
C	0.3750	0.3260

