



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:58 PM UTC

PDB ID : 8JAM / pdb_00008jam
EMDB ID : EMD-36122
Title : Cryo-EM structure of Omicron BA.1 RBD in complex with W328-6H2 (local refinement)
Authors : Nan, X.Y.; Li, Y.J.
Deposited on : 2023-05-06
Resolution : 3.92 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

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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

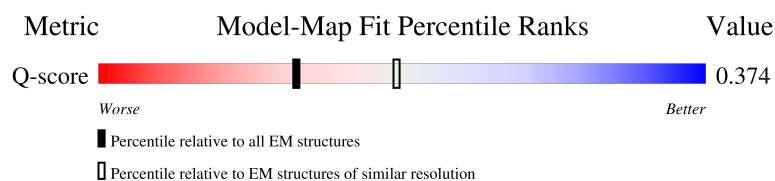
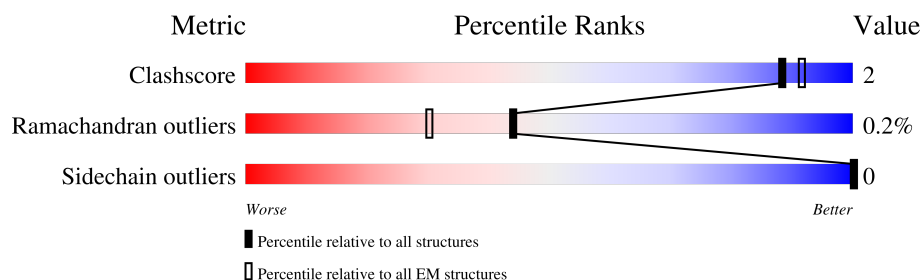
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.92 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	7646 (3.46 - 4.46)

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	1274	
2	H	107	
3	L	112	
4	A	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3369 atoms, of which 65 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	195	Total	C	N	O	S	0	0
			1560	1005	265	283	7		

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-258	VAL	ALA	conflict	UNP A0A7D8AJB5
B	?	-	HIS	deletion	UNP A0A7D8AJB5
B	?	-	VAL	deletion	UNP A0A7D8AJB5
B	-232	ILE	THR	conflict	UNP A0A7D8AJB5
B	-185	ASP	GLY	conflict	UNP A0A7D8AJB5
B	?	-	VAL	deletion	UNP A0A7D8AJB5
B	?	-	TYR	deletion	UNP A0A7D8AJB5
B	?	-	ASN	deletion	UNP A0A7D8AJB5
B	-119	ILE	LEU	conflict	UNP A0A7D8AJB5
B	-116	GLU	-	insertion	UNP A0A7D8AJB5
B	-115	PRO	-	insertion	UNP A0A7D8AJB5
B	-114	GLU	-	insertion	UNP A0A7D8AJB5
B	11	ASP	GLY	conflict	UNP A0A7D8AJB5
B	43	LEU	SER	conflict	UNP A0A7D8AJB5
B	45	PRO	SER	conflict	UNP A0A7D8AJB5
B	47	PHE	SER	conflict	UNP A0A7D8AJB5
B	89	ASN	LYS	conflict	UNP A0A7D8AJB5
B	112	LYS	ASN	conflict	UNP A0A7D8AJB5
B	118	SER	GLY	conflict	UNP A0A7D8AJB5
B	149	ASN	SER	conflict	UNP A0A7D8AJB5
B	150	LYS	THR	conflict	UNP A0A7D8AJB5
B	156	ALA	GLU	conflict	UNP A0A7D8AJB5
B	165	ARG	GLN	conflict	UNP A0A7D8AJB5
B	168	SER	GLY	conflict	UNP A0A7D8AJB5
B	170	ARG	GLN	conflict	UNP A0A7D8AJB5
B	173	TYR	ASN	conflict	UNP A0A7D8AJB5
B	177	HIS	TYR	conflict	UNP A0A7D8AJB5
B	219	LYS	THR	conflict	UNP A0A7D8AJB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	327	TYR	HIS	conflict	UNP A0A7D8AJB5
B	351	LYS	ASN	conflict	UNP A0A7D8AJB5
B	353	HIS	PRO	conflict	UNP A0A7D8AJB5
B	354	SER	ARG	conflict	UNP A0A7D8AJB5
B	355	GLY	ARG	conflict	UNP A0A7D8AJB5
B	357	GLY	ARG	conflict	UNP A0A7D8AJB5
B	379	CYS	TYR	conflict	UNP A0A7D8AJB5
B	436	LYS	ASN	conflict	UNP A0A7D8AJB5
B	468	TYR	ASP	conflict	UNP A0A7D8AJB5
B	489	PRO	PHE	conflict	UNP A0A7D8AJB5
B	528	LYS	ASN	conflict	UNP A0A7D8AJB5
B	555	CYS	THR	conflict	UNP A0A7D8AJB5
B	564	PRO	ALA	conflict	UNP A0A7D8AJB5
B	571	PRO	ALA	conflict	UNP A0A7D8AJB5
B	614	PRO	ALA	conflict	UNP A0A7D8AJB5
B	626	HIS	GLN	conflict	UNP A0A7D8AJB5
B	641	LYS	ASN	conflict	UNP A0A7D8AJB5
B	653	PHE	LEU	conflict	UNP A0A7D8AJB5
B	659	PRO	VAL	conflict	UNP A0A7D8AJB5
B	881	GLY	-	expression tag	UNP A0A7D8AJB5
B	882	SER	-	expression tag	UNP A0A7D8AJB5
B	883	GLY	-	expression tag	UNP A0A7D8AJB5
B	884	TYR	-	expression tag	UNP A0A7D8AJB5
B	885	ILE	-	expression tag	UNP A0A7D8AJB5
B	886	PRO	-	expression tag	UNP A0A7D8AJB5
B	887	GLU	-	expression tag	UNP A0A7D8AJB5
B	888	ALA	-	expression tag	UNP A0A7D8AJB5
B	889	PRO	-	expression tag	UNP A0A7D8AJB5
B	890	ARG	-	expression tag	UNP A0A7D8AJB5
B	891	ASP	-	expression tag	UNP A0A7D8AJB5
B	892	GLY	-	expression tag	UNP A0A7D8AJB5
B	893	GLN	-	expression tag	UNP A0A7D8AJB5
B	894	ALA	-	expression tag	UNP A0A7D8AJB5
B	895	TYR	-	expression tag	UNP A0A7D8AJB5
B	896	VAL	-	expression tag	UNP A0A7D8AJB5
B	897	ARG	-	expression tag	UNP A0A7D8AJB5
B	898	LYS	-	expression tag	UNP A0A7D8AJB5
B	899	ASP	-	expression tag	UNP A0A7D8AJB5
B	900	GLY	-	expression tag	UNP A0A7D8AJB5
B	901	GLU	-	expression tag	UNP A0A7D8AJB5
B	902	TRP	-	expression tag	UNP A0A7D8AJB5
B	903	VAL	-	expression tag	UNP A0A7D8AJB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	904	LEU	-	expression tag	UNP A0A7D8AJB5
B	905	LEU	-	expression tag	UNP A0A7D8AJB5
B	906	SER	-	expression tag	UNP A0A7D8AJB5
B	907	THR	-	expression tag	UNP A0A7D8AJB5
B	908	PHE	-	expression tag	UNP A0A7D8AJB5
B	909	LEU	-	expression tag	UNP A0A7D8AJB5
B	910	GLY	-	expression tag	UNP A0A7D8AJB5
B	911	ARG	-	expression tag	UNP A0A7D8AJB5
B	912	SER	-	expression tag	UNP A0A7D8AJB5
B	913	LEU	-	expression tag	UNP A0A7D8AJB5
B	914	GLU	-	expression tag	UNP A0A7D8AJB5
B	915	VAL	-	expression tag	UNP A0A7D8AJB5
B	916	LEU	-	expression tag	UNP A0A7D8AJB5
B	917	PHE	-	expression tag	UNP A0A7D8AJB5
B	918	GLN	-	expression tag	UNP A0A7D8AJB5
B	919	GLY	-	expression tag	UNP A0A7D8AJB5
B	920	PRO	-	expression tag	UNP A0A7D8AJB5
B	921	GLY	-	expression tag	UNP A0A7D8AJB5
B	922	SER	-	expression tag	UNP A0A7D8AJB5
B	923	GLY	-	expression tag	UNP A0A7D8AJB5
B	924	GLY	-	expression tag	UNP A0A7D8AJB5
B	925	LEU	-	expression tag	UNP A0A7D8AJB5
B	926	ASN	-	expression tag	UNP A0A7D8AJB5
B	927	ASP	-	expression tag	UNP A0A7D8AJB5
B	928	ILE	-	expression tag	UNP A0A7D8AJB5
B	929	PHE	-	expression tag	UNP A0A7D8AJB5
B	930	GLU	-	expression tag	UNP A0A7D8AJB5
B	931	ALA	-	expression tag	UNP A0A7D8AJB5
B	932	GLN	-	expression tag	UNP A0A7D8AJB5
B	933	LYS	-	expression tag	UNP A0A7D8AJB5
B	934	ILE	-	expression tag	UNP A0A7D8AJB5
B	935	GLU	-	expression tag	UNP A0A7D8AJB5
B	936	TRP	-	expression tag	UNP A0A7D8AJB5
B	937	HIS	-	expression tag	UNP A0A7D8AJB5
B	938	GLU	-	expression tag	UNP A0A7D8AJB5
B	939	GLY	-	expression tag	UNP A0A7D8AJB5
B	940	SER	-	expression tag	UNP A0A7D8AJB5
B	941	GLY	-	expression tag	UNP A0A7D8AJB5
B	942	HIS	-	expression tag	UNP A0A7D8AJB5
B	943	HIS	-	expression tag	UNP A0A7D8AJB5
B	944	HIS	-	expression tag	UNP A0A7D8AJB5
B	945	HIS	-	expression tag	UNP A0A7D8AJB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	946	HIS	-	expression tag	UNP A0A7D8AJB5
B	947	HIS	-	expression tag	UNP A0A7D8AJB5
B	948	HIS	-	expression tag	UNP A0A7D8AJB5
B	949	HIS	-	expression tag	UNP A0A7D8AJB5

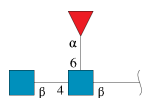
- Molecule 2 is a protein called H chain of W328-6H2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	107	Total	C	N	O	S	0	0
			822	527	136	155	4		

- Molecule 3 is a protein called L chain of W328-6H2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			856	544	139	169	4		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	3	Total	C	H	N	O	0	0
			75	22	37	2	14		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

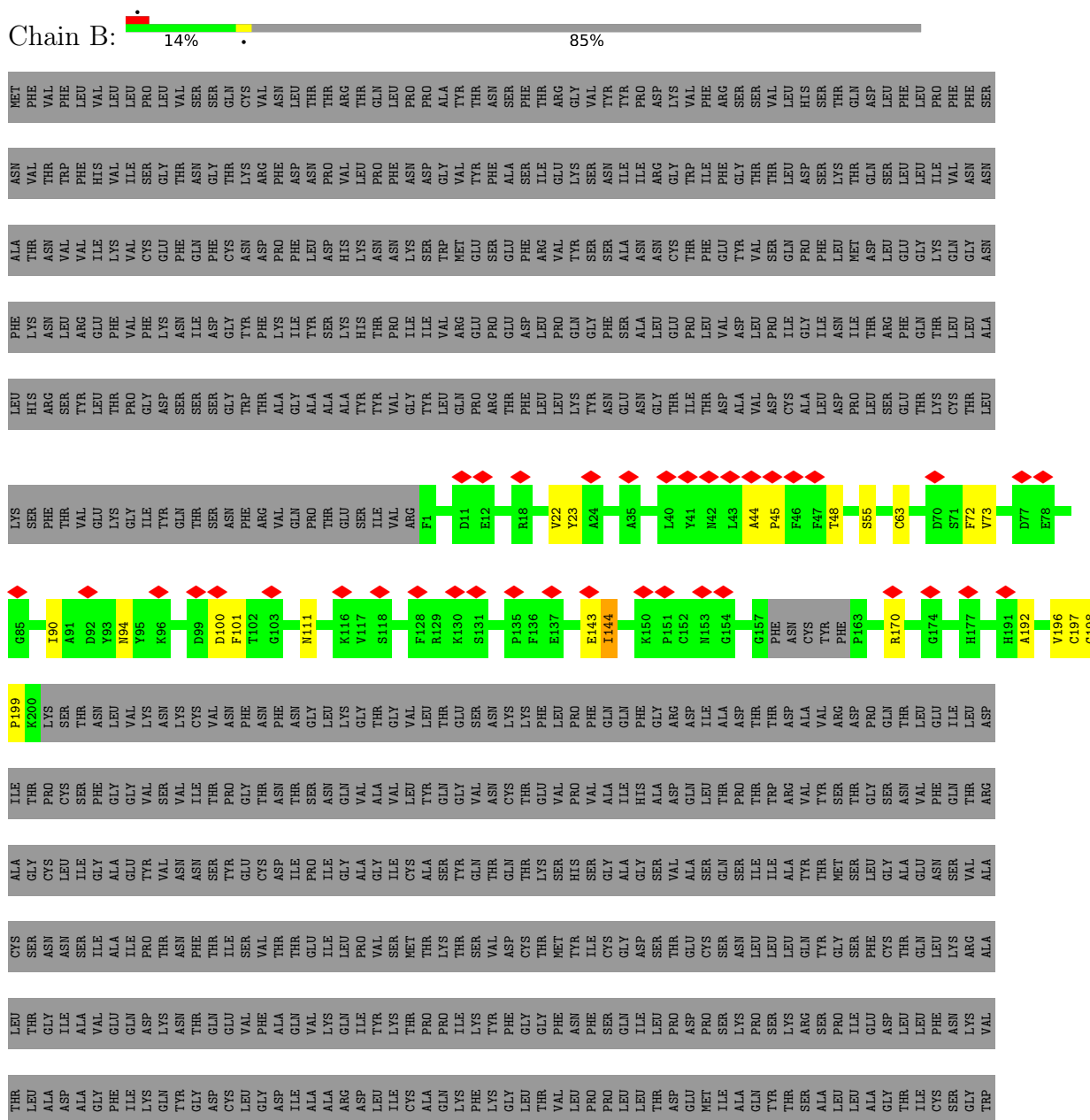


Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	B	1	Total	C	H	N	O	0
			28	8	14	1	5	

3 Residue-property plots

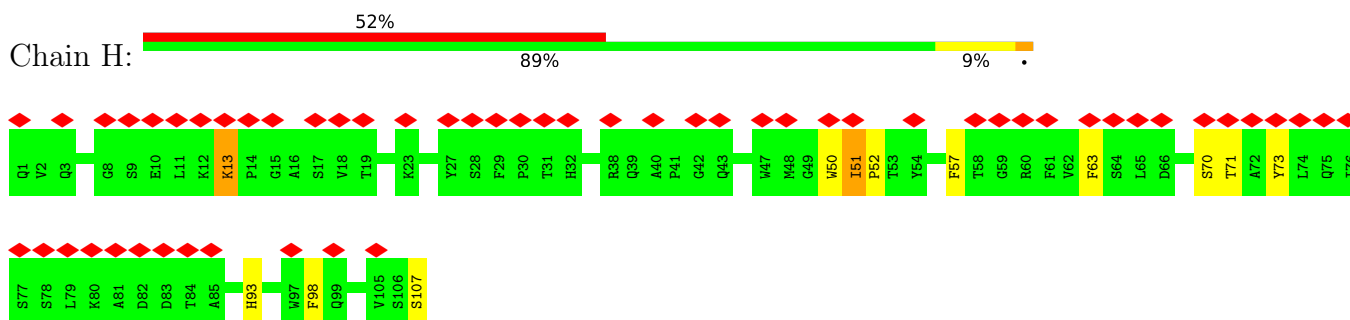
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

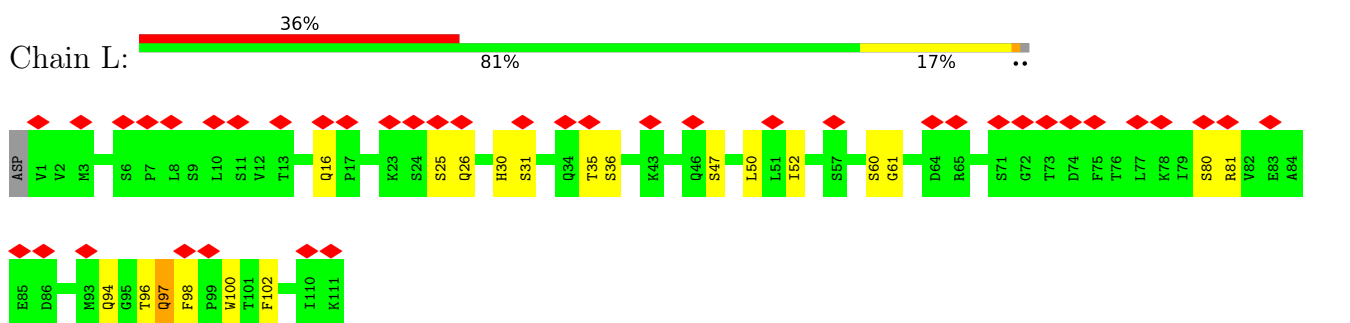


GLY	ASN	ASP	TTR	TTR	LYS	THR
PRO	GLU	VAL	VAL	VAL	LEU	PHE
GLY	GLU	VAL	PRO	GLR	GLN	GLY
SER	ALA	ILE	ALA	GLN	ASP	ALA
GLY	LYS	GLY	GLN	GLN	VAL	GLY
GLY	ASN	ILE	GLU	LEU	VAL	PRO
LEU	LEU	VAL	LYS	ILE	ASN	ALA
LEU	ASN	ASN	ASN	ARG	HIS	LEU
ASP	GLU	ASN	PHE	ALA	ASN	GLN
ILE	SER	THR	THR	ALA	ALA	ILE
PHE	LEU	VAL	THR	GLU	GLN	PRO
GLU	ILE	TTR	ALA	ILE	ALA	PHE
ALA	ASP	ASP	PRO	ARG	LEU	PRO
GLN	LEU	PRO	ALA	ALA	ASN	MET
LYS	GLN	GLN	ILE	SER	THR	GLY
ILE	GLU	GLN	CYS	ALA	LEU	MET
GLY	LEU	PRO	HIS	ASN	VAL	ALA
TTR	GLY	GLU	ASP	LEU	LYS	TTR
HIS	LYS	LEU	GLY	ALA	GLN	ARG
GLU	TTR	ASP	LYS	ALA	LEU	PHE
GLY	GLU	SER	ALA	THR	SER	GLY
SER	GLN	PHE	HIS	THR	SER	ASN
GLY	GLY	LYS	PHE	MET	LYS	ILE
HIS	SER	GLU	PRO	SER	PHE	GLY
HIS	GLY	GLU	ARG	GLU	GLY	VAL
HIS	TTR	LEU	GLY	CYS	ALA	THR
HIS	ILE	ASP	GLY	VAL	SER	GLN
HIS	PRO	PRO	VAL	LYS	LEU	ASN
HIS	GLU	TTR	PHE	GLY	SER	VAL
HIS	ALA	PHE	VAL	GLN	VAL	LEU
HIS	PRO	LYS	SER	SER	LEU	TTR
	ARG	ASN	LYS	LYS	ASN	GLU
	ASP	HIS	GLY	ARG	ASP	ASN
	GLY	THR	THR	VAL	ILE	GLN
	GLN	SER	HIS	ASP	PHE	LYS
	ALA	PRO	TTR	THR	SER	LEU
	TTR	ASP	PHE	CYS	ARG	ILE
	VAL	VAL	VAL	GLY	LEU	ALA
	ARG	ASP	THR	LYS	ASP	ASN
	LYS	LEU	GLN	LYS	GLN	ASN
	ASP	GLY	ARG	TTR	PRO	PHE
	GLY	ASP	ASN	HIS	GLU	ASN
	GLU	ILE	PHE	THR	ALA	SER
	TTR	SER	TTR	MET	GLY	ILE
	VAL	GLY	GLU	PHE	VAL	GLY
	LEU	ILE	PRO	THR	GLN	LYS
	LEU	ASN	GLN	PRO	ILE	ILE
	SER	ALA	ILE	GLN	ASP	GLN
	THR	VAL	ILE	ARG	ARG	THR
	PHE	VAL	THR	ALA	LEU	SER
	LEU	VAL	THR	PRO	ILE	ASP
	GLY	ASN	ASN	HIS	THR	LEU
	ARG	ILE	ASN	GLY	GLY	SER
	SER	GLN	THR	VAL	ARG	SER
	LEU	LYS	PHE	VAL	LEU	THR
	GLU	GLY	VAL	PHE	GLN	PRO
	VAL	ILE	SER	THR	THR	THR
	LEU	ASP	ASN	GLY	SER	GLY
	LEU	ASP	THR	HIS	THR	SER
	THR	VAL	THR	VAL	GLN	ALA
	PHE	ARG	GLY	HIS	LEU	ALA
	GLN	ILE	GLY	VAL	GLN	LEU
	THR	ASN	THR	THR	THR	GLY

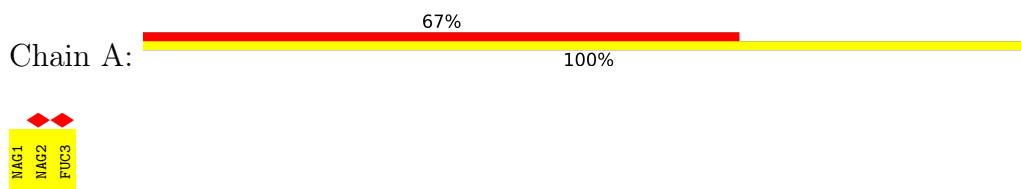
- Molecule 2: H chain of W328-6H2



- Molecule 3: L chain of W328-6H2



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[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, Not provided	
Number of particles used	44293	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.623	Depositor
Minimum map value	-1.704	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.586	Depositor
Map size (Å)	310.40002, 310.40002, 310.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9700001, 0.9700001, 0.9700001	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	1.07	0/1605	1.38	18/2183 (0.8%)
2	H	1.01	1/845 (0.1%)	1.39	11/1150 (1.0%)
3	L	1.09	0/878	1.54	16/1190 (1.3%)
All	All	1.06	1/3328 (0.0%)	1.42	45/4523 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	93	HIS	CB-CG	-5.60	1.42	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	100	TRP	N-CA-C	9.64	122.68	108.60
3	L	52	ILE	N-CA-C	8.59	120.14	108.11
3	L	97	GLN	N-CA-C	-8.57	101.43	112.23
3	L	94	GLN	N-CA-C	7.78	123.73	113.30
2	H	70	SER	N-CA-C	-7.40	101.16	111.52
1	B	192	ALA	N-CA-C	-7.23	101.62	108.13
1	B	198	GLY	CA-C-N	6.88	127.45	119.47
1	B	198	GLY	C-N-CA	6.88	127.45	119.47
3	L	102	PHE	CA-CB-CG	6.65	120.45	113.80
3	L	30	HIS	N-CA-C	-6.40	104.67	113.18
3	L	98	PHE	CA-C-N	6.30	127.72	119.84
3	L	98	PHE	C-N-CA	6.30	127.72	119.84
3	L	97	GLN	CA-C-N	6.26	129.37	120.49
3	L	97	GLN	C-N-CA	6.26	129.37	120.49
3	L	31	SER	N-CA-C	6.20	118.52	110.53
1	B	23	TYR	N-CA-C	-6.19	102.20	110.55
1	B	72	PHE	N-CA-C	6.16	117.60	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	ARG	CA-C-N	6.08	125.76	119.56
1	B	170	ARG	C-N-CA	6.08	125.76	119.56
1	B	73	VAL	N-CA-C	5.81	116.30	108.17
1	B	144	ILE	CA-C-N	5.73	128.23	120.38
1	B	144	ILE	C-N-CA	5.73	128.23	120.38
1	B	199	PRO	N-CA-C	5.69	122.07	113.81
2	H	63	PHE	CA-CB-CG	5.67	119.47	113.80
1	B	55	SER	CA-C-N	5.63	125.74	119.32
1	B	55	SER	C-N-CA	5.63	125.74	119.32
2	H	13	LYS	CA-C-N	5.61	125.54	119.76
2	H	13	LYS	C-N-CA	5.61	125.54	119.76
3	L	16	GLN	CA-C-N	5.56	125.48	119.76
3	L	16	GLN	C-N-CA	5.56	125.48	119.76
3	L	47	SER	CA-C-N	5.48	125.38	119.85
3	L	47	SER	C-N-CA	5.48	125.38	119.85
1	B	196	VAL	N-CA-C	5.47	115.98	107.28
2	H	51	ILE	CA-C-N	5.43	126.63	119.84
2	H	51	ILE	C-N-CA	5.43	126.63	119.84
2	H	73	TYR	CA-C-N	-5.38	113.81	121.50
2	H	73	TYR	C-N-CA	-5.38	113.81	121.50
2	H	57	PHE	CA-CB-CG	-5.18	108.62	113.80
1	B	111	ASN	CA-CB-CG	5.14	117.74	112.60
1	B	48	THR	N-CA-C	5.14	117.06	108.99
3	L	50	LEU	N-CA-C	5.13	117.86	109.59
2	H	71	THR	N-CA-C	-5.10	106.47	113.30
1	B	90	ILE	N-CA-C	-5.04	106.77	111.45
1	B	101	PHE	CA-CB-CG	5.03	118.83	113.80
2	H	98	PHE	N-CA-C	5.03	117.77	109.72

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	B	1560	0	1506	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	822	0	795	2	0
3	L	856	0	831	5	0
4	A	38	37	34	0	0
5	B	28	28	26	0	0
All	All	3304	65	3192	12	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 2.

All (12) 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:H:50:TRP:O	2:H:51:ILE:C	2.43	0.61
3:L:96:THR:OG1	3:L:97:GLN:N	2.35	0.58
3:L:35:THR:OG1	3:L:36:SER:N	2.41	0.53
2:H:13:LYS:NZ	2:H:107:SER:OXT	2.47	0.48
3:L:80:SER:OG	3:L:81:ARG:N	2.47	0.48
3:L:25:SER:OG	3:L:26:GLN:NE2	2.50	0.45
1:B:143:GLU:O	1:B:144:ILE:C	2.59	0.45
3:L:60:SER:OG	3:L:61:GLY:N	2.49	0.45
1:B:63:CYS:HA	1:B:197:CYS:HB3	2.00	0.44
1:B:44:ALA:N	1:B:45:PRO:CD	2.81	0.43
1:B:22:VAL:HG12	1:B:94:ASN:HB3	2.02	0.41
1:B:100:ASP:OD1	1:B:100:ASP:N	2.51	0.41

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	B	191/1274 (15%)	185 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/107 (98%)	97 (92%)	7 (7%)	1 (1%)	12	44
3	L	109/112 (97%)	99 (91%)	10 (9%)	0	100	100
All	All	405/1493 (27%)	381 (94%)	23 (6%)	1 (0%)	44	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	52	PRO

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	B	170/1110 (15%)	170 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
3	L	98/99 (99%)	98 (100%)	0	100	100
All	All	356/1297 (27%)	356 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	1	GLN
2	H	3	GLN
3	L	26	GLN
3	L	46	GLN

5.3.3 RNA [i](#)

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 ⓘ

3 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	$\# Z > 2$
4	NAG	A	1	1,4	14,14,15	1.67	2 (14%)	17,19,21	1.08	1 (5%)
4	NAG	A	2	4	14,14,15	1.96	4 (28%)	17,19,21	0.96	1 (5%)
4	FUC	A	3	4	10,10,11	1.79	3 (30%)	14,14,16	0.83	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	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	A	2	4	-	1/6/23/26	0/1/1/1
4	FUC	A	3	4	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	NAG	C1-C2	4.76	1.58	1.52
4	A	1	NAG	C1-C2	4.68	1.58	1.52
4	A	2	NAG	O5-C5	3.17	1.49	1.43
4	A	3	FUC	C2-C3	2.96	1.57	1.52
4	A	3	FUC	O5-C5	2.79	1.49	1.43
4	A	1	NAG	O5-C5	2.52	1.48	1.43
4	A	2	NAG	C3-C2	2.45	1.57	1.52
4	A	3	FUC	C4-C5	2.43	1.58	1.52
4	A	2	NAG	C4-C5	2.23	1.57	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2	NAG	C8-C7-N2	2.41	120.12	116.12
4	A	1	NAG	C8-C7-N2	2.09	119.58	116.12

There are no chirality outliers.

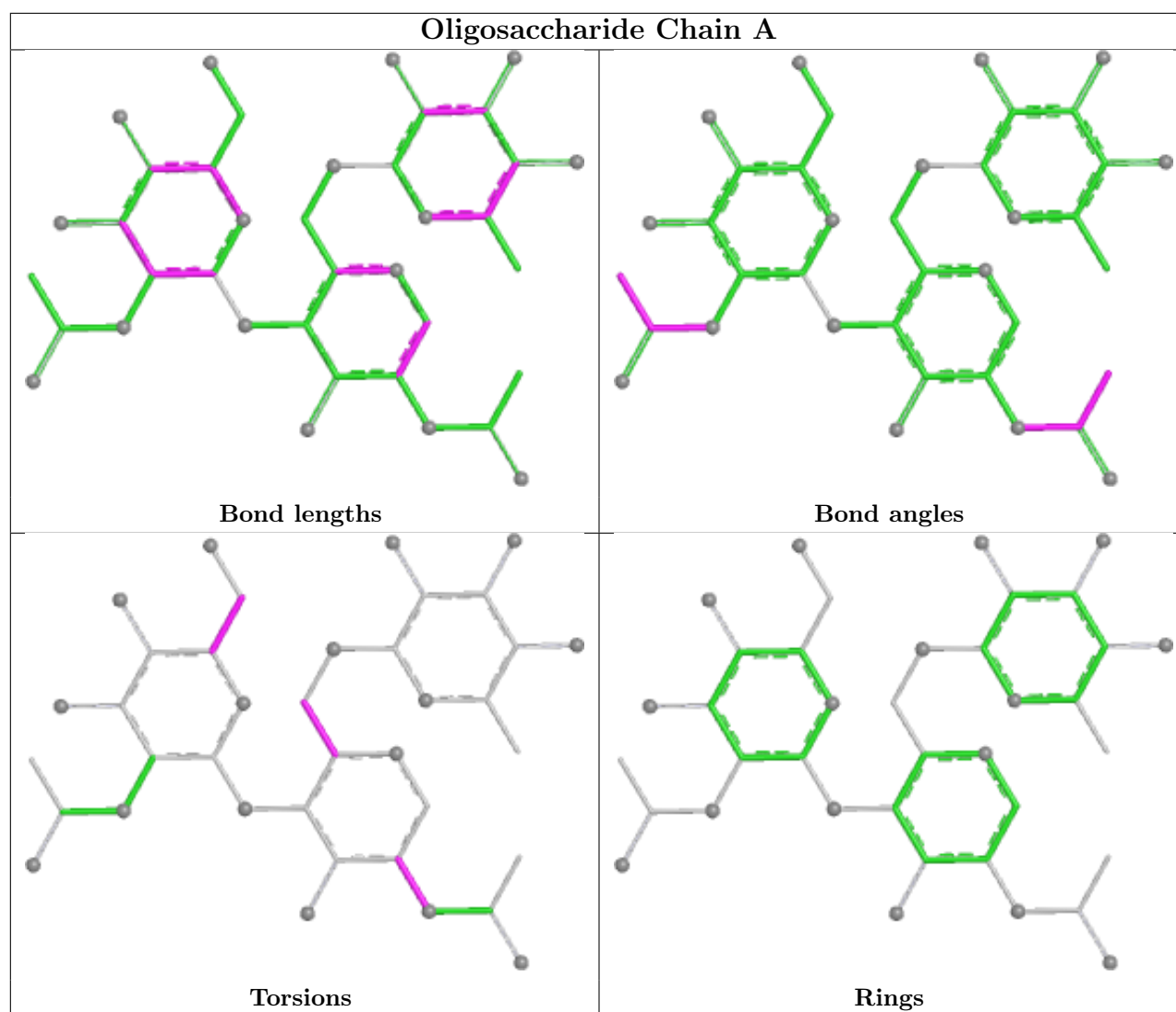
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C1-C2-N2-C7
4	A	2	NAG	O5-C5-C6-O6
4	A	1	NAG	C3-C2-N2-C7
4	A	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	B	1001	1	14,14,15	2.28	5 (35%)	17,19,21	1.18	3 (17%)
5	NAG	B	1002	1	14,14,15	2.48	5 (35%)	17,19,21	1.05	1 (5%)

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
5	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1002	1	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1002	NAG	C1-C2	6.87	1.61	1.52
5	B	1001	NAG	C1-C2	6.26	1.60	1.52
5	B	1002	NAG	O5-C5	3.58	1.50	1.43
5	B	1001	NAG	O5-C5	3.00	1.49	1.43
5	B	1002	NAG	O5-C1	2.87	1.48	1.43
5	B	1001	NAG	O5-C1	2.60	1.48	1.43
5	B	1002	NAG	C3-C2	2.58	1.57	1.52
5	B	1001	NAG	C3-C2	2.44	1.57	1.52
5	B	1001	NAG	C4-C5	2.13	1.57	1.53
5	B	1002	NAG	C4-C5	2.08	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	NAG	C8-C7-N2	2.57	120.38	116.12
5	B	1001	NAG	O7-C7-C8	-2.40	117.77	122.05
5	B	1001	NAG	C1-O5-C5	2.18	115.10	112.19
5	B	1002	NAG	C8-C7-N2	2.12	119.63	116.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

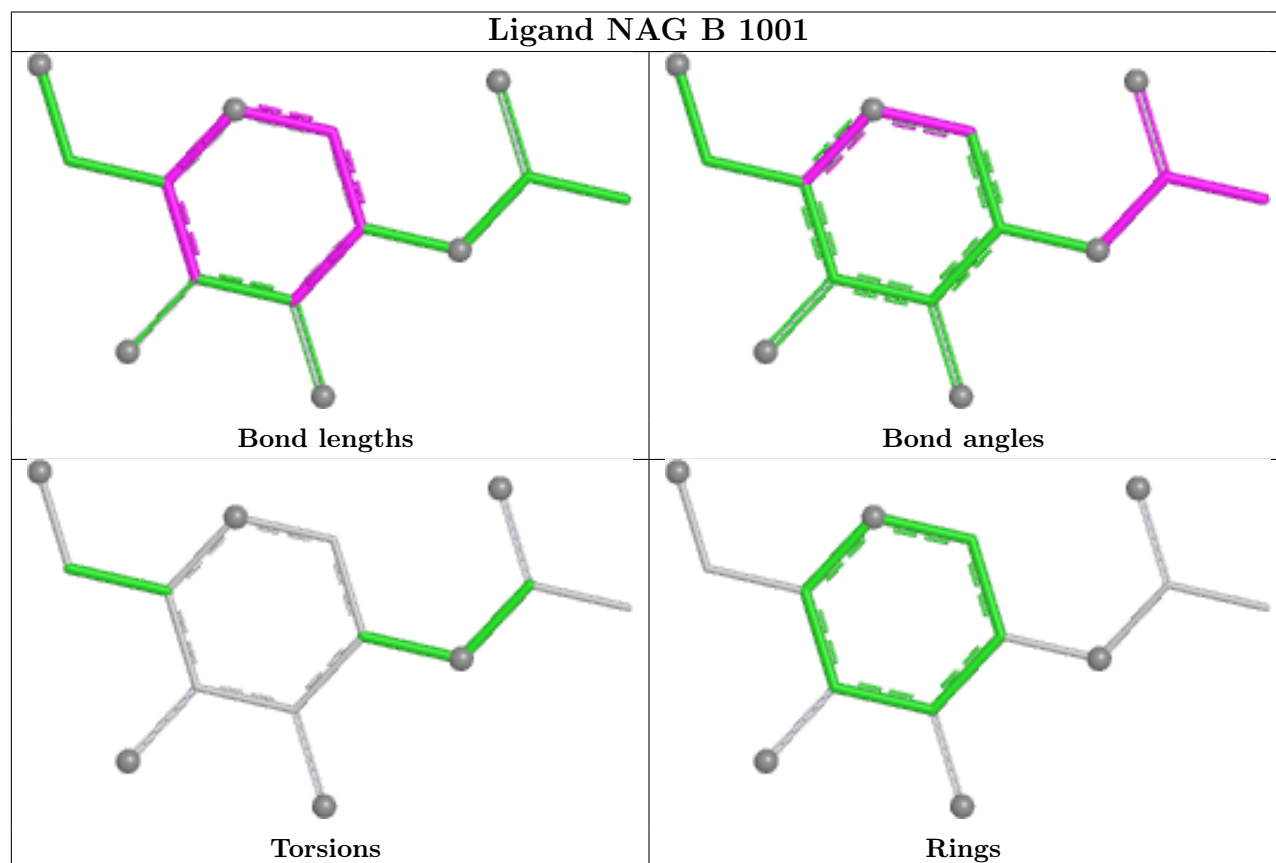
Mol	Chain	Res	Type	Atoms
5	B	1002	NAG	O5-C5-C6-O6

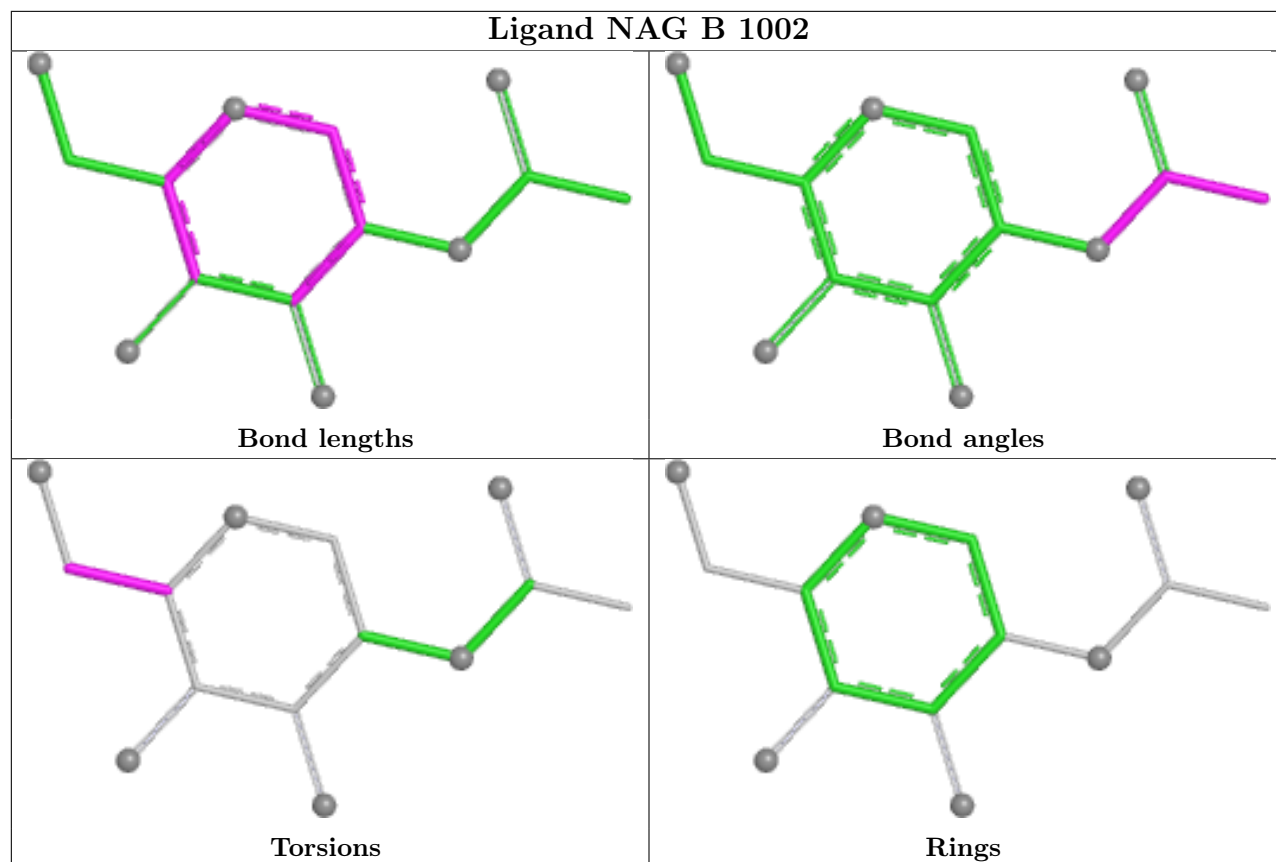
There are no ring outliers.

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 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.

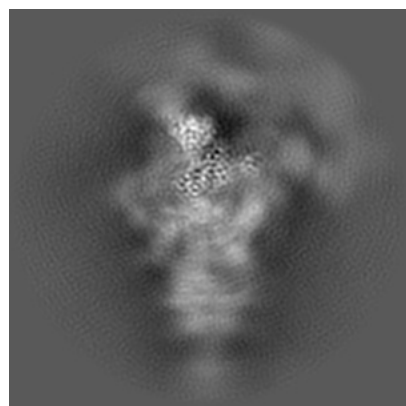
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36122. These allow visual inspection of the internal detail of the map and identification of artifacts.

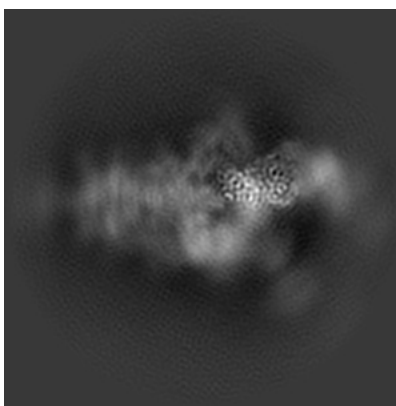
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

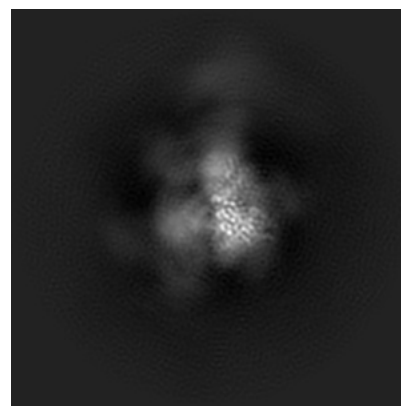
6.1.1 Primary map



X

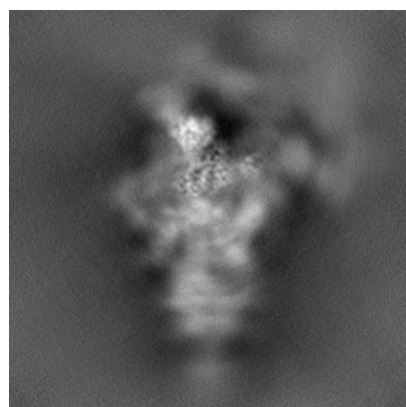


Y

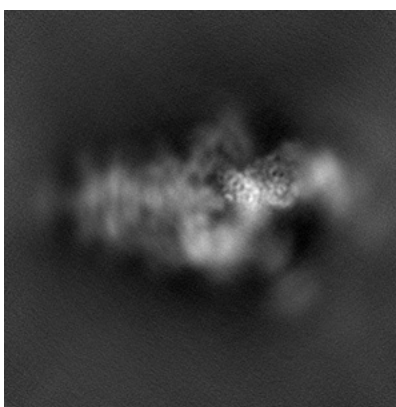


Z

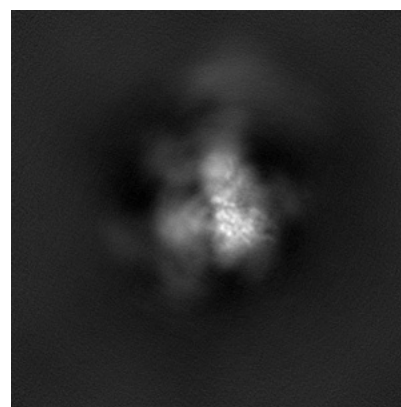
6.1.2 Raw map



X



Y

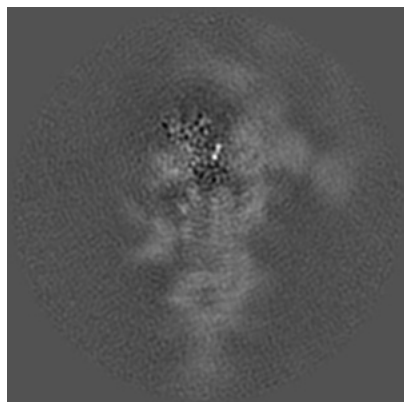


Z

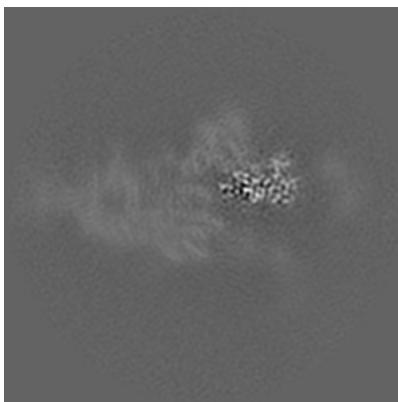
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

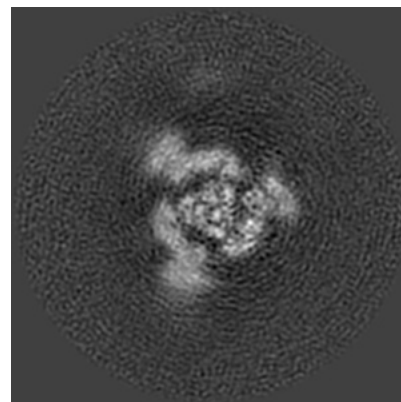
6.2.1 Primary map



X Index: 160

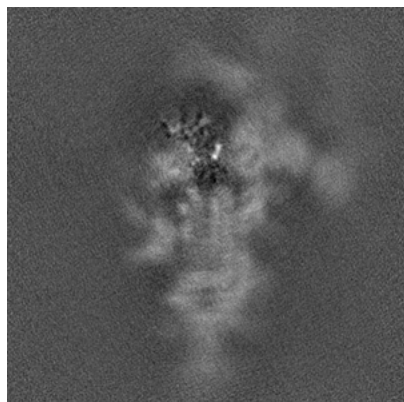


Y Index: 160

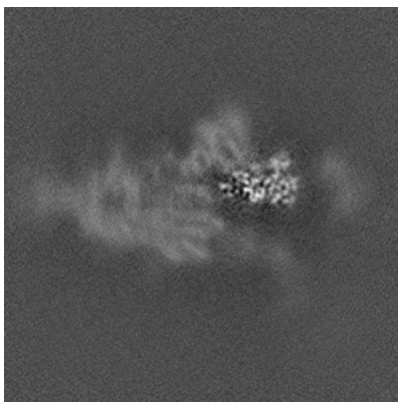


Z Index: 160

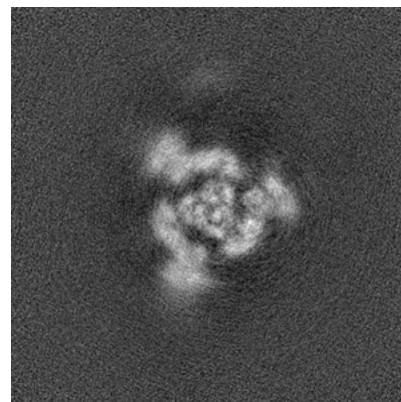
6.2.2 Raw map



X Index: 160



Y Index: 160

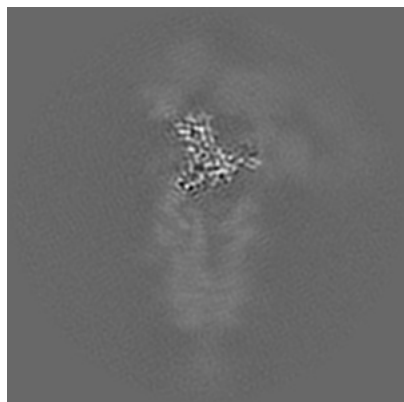


Z Index: 160

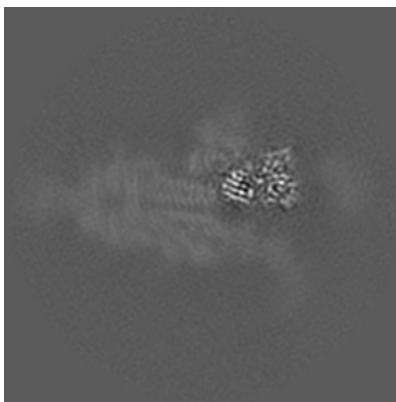
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

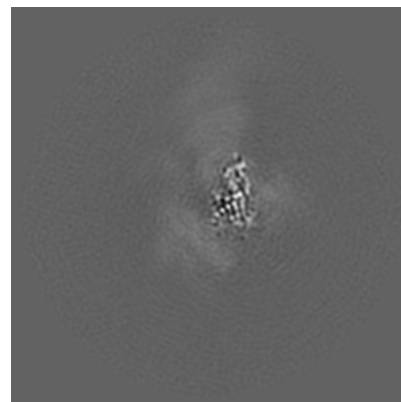
6.3.1 Primary map



X Index: 179

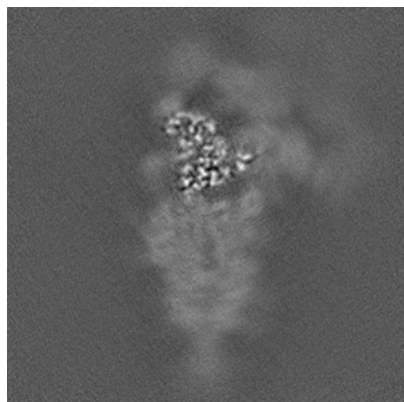


Y Index: 155

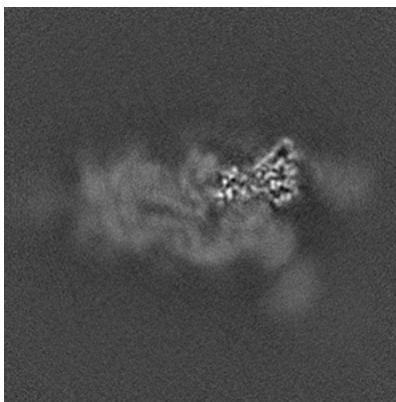


Z Index: 194

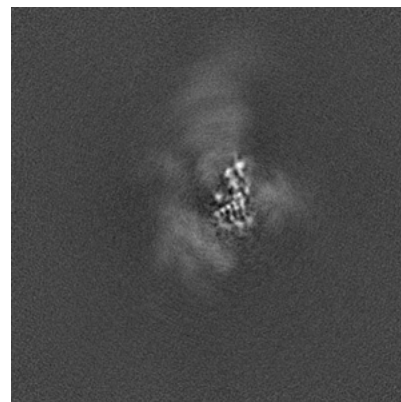
6.3.2 Raw map



X Index: 172



Y Index: 144

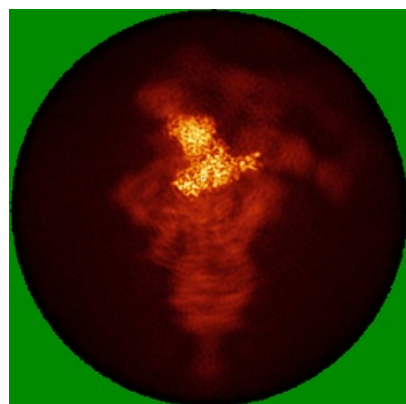


Z Index: 193

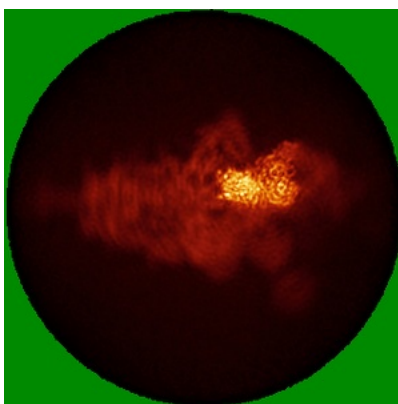
The images above show the largest variance slices of the map in three orthogonal directions.

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

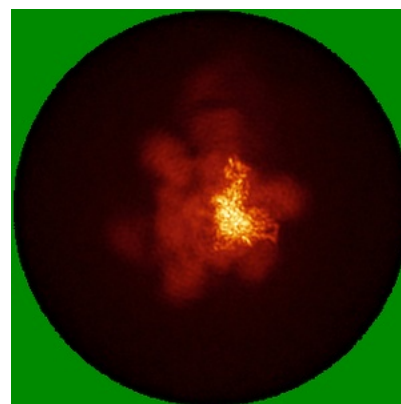
6.4.1 Primary map



X

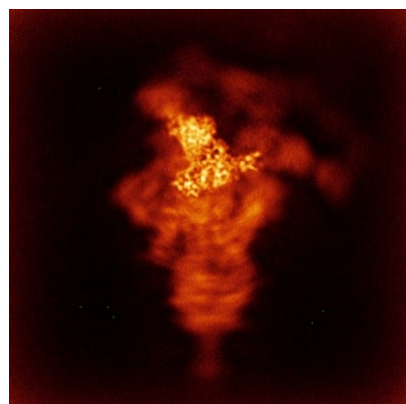


Y

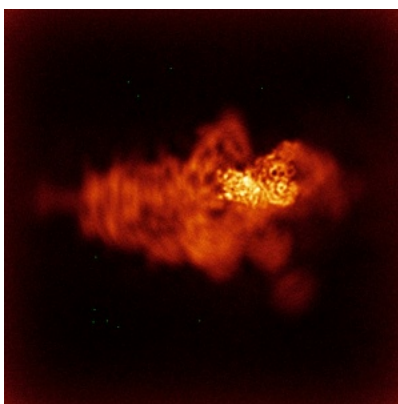


Z

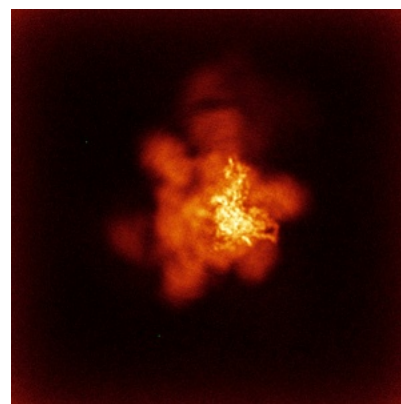
6.4.2 Raw map



X



Y

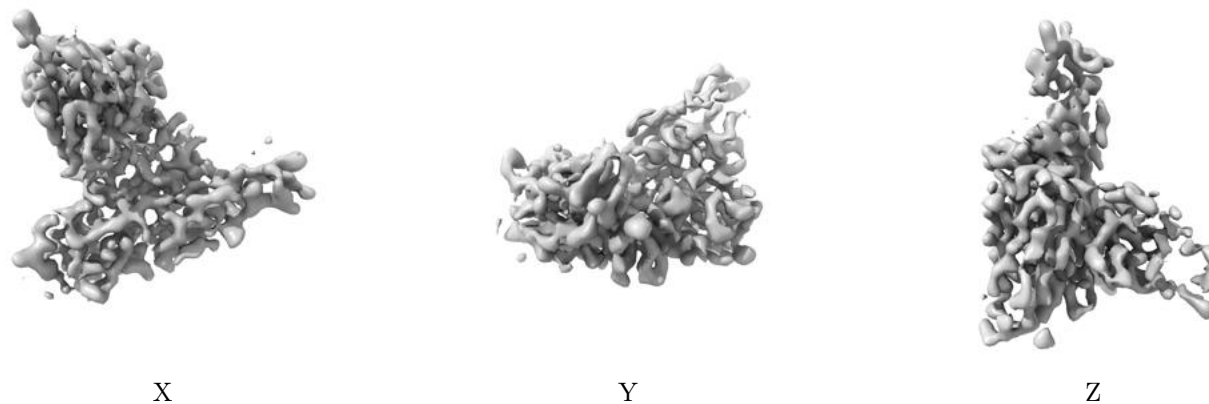


Z

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.

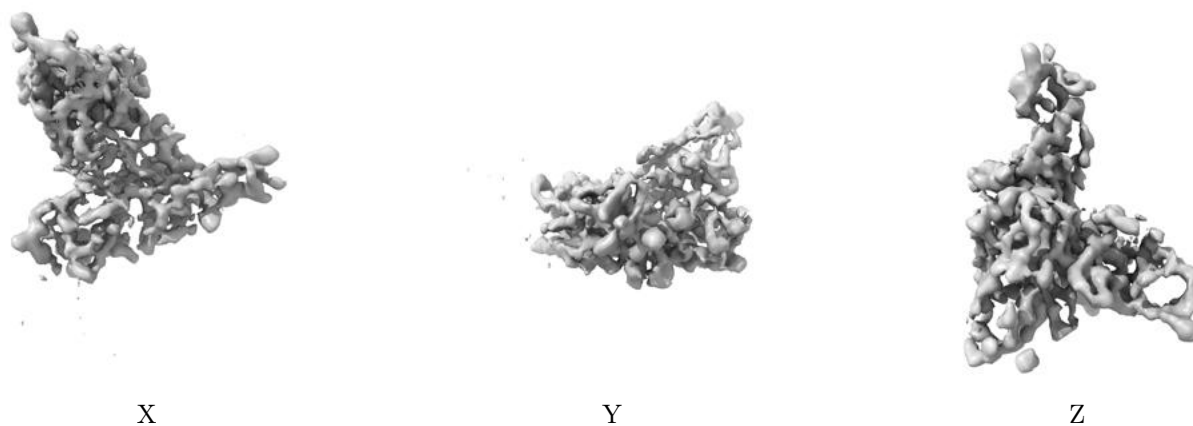
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.586. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

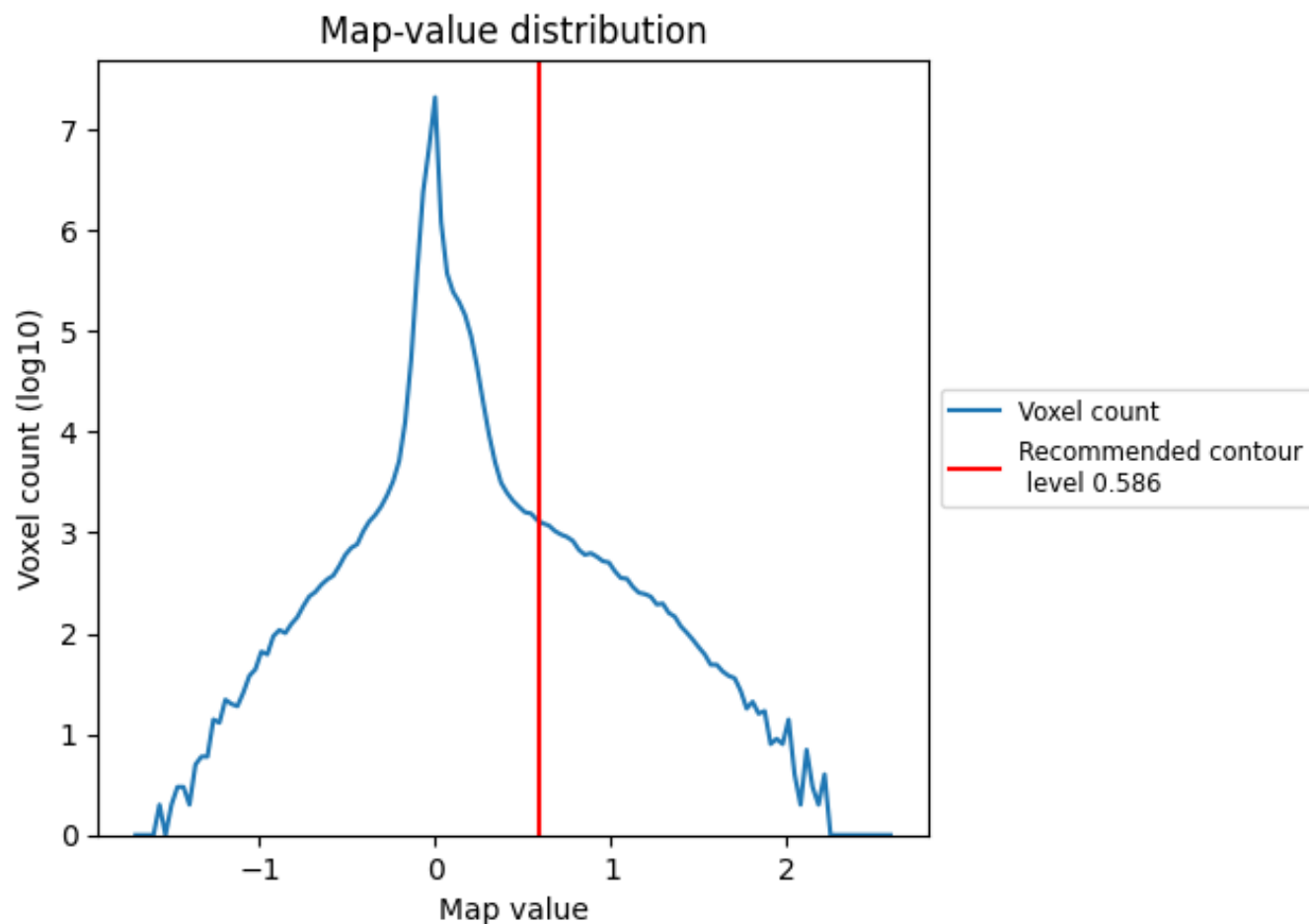
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

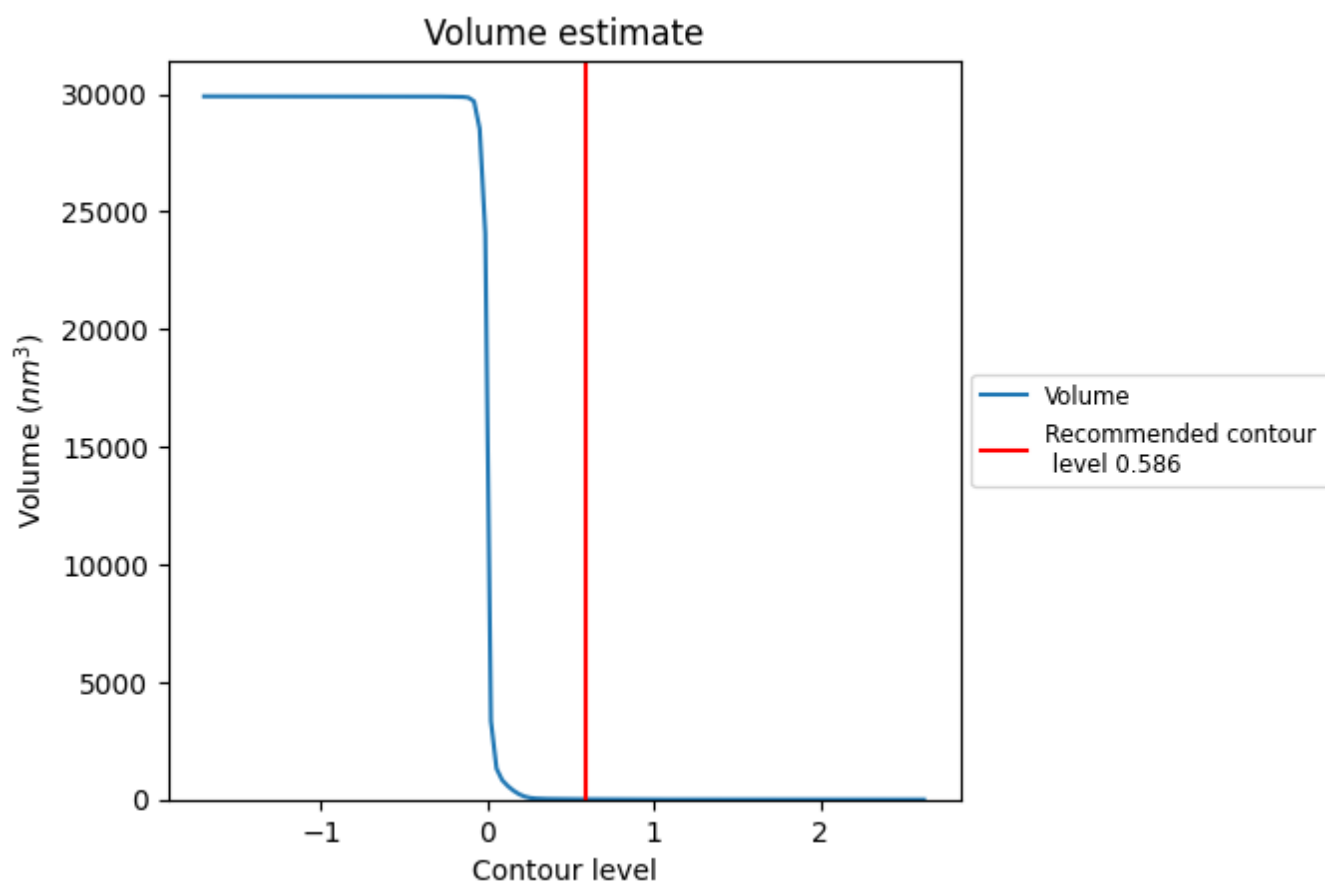
This section contains the results of statistical analysis of the map.

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.

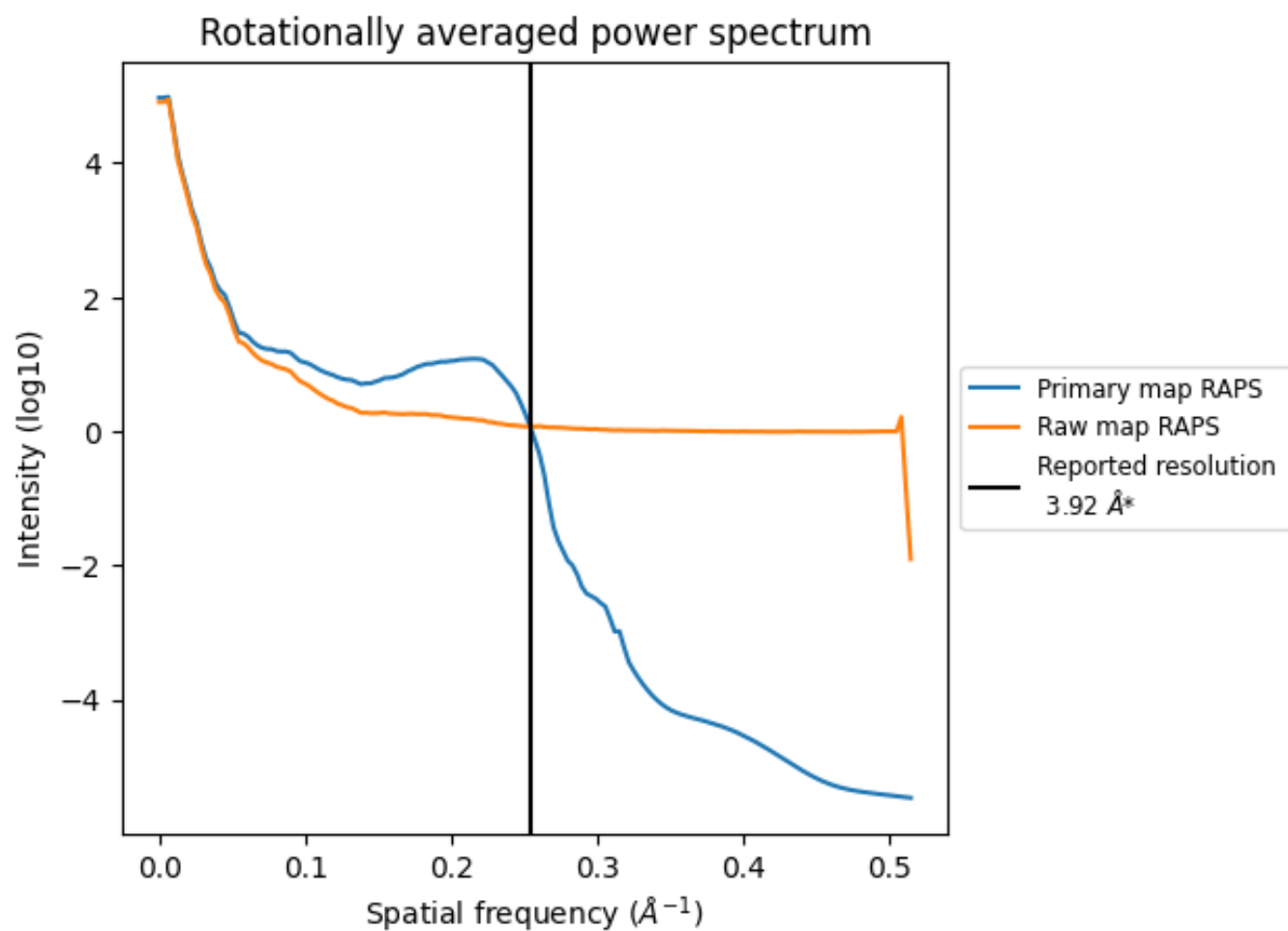
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13 nm³; this corresponds to an approximate mass of 12 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 ⓘ

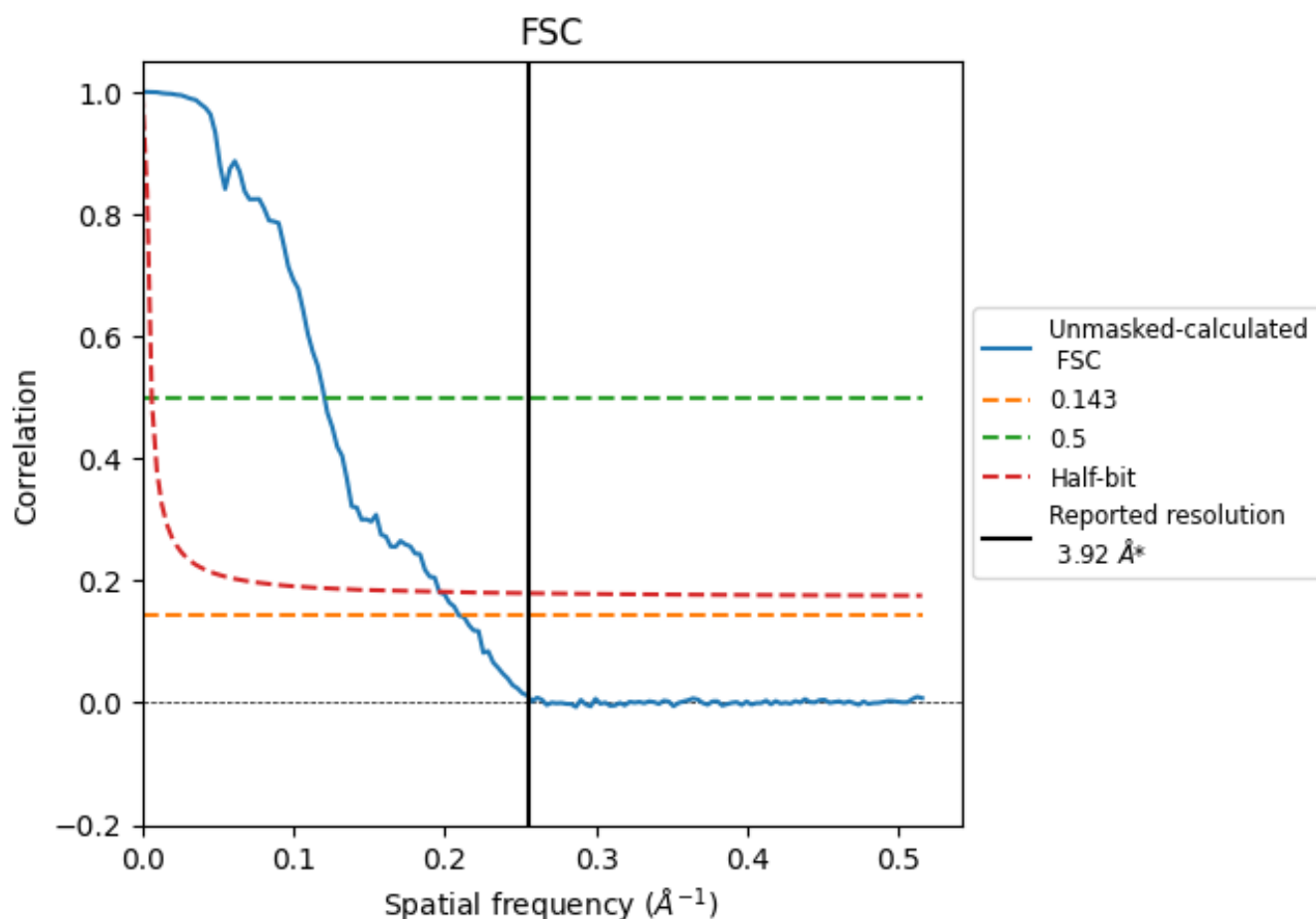


*Reported resolution corresponds to spatial frequency of 0.255 Å⁻¹

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 0.255 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

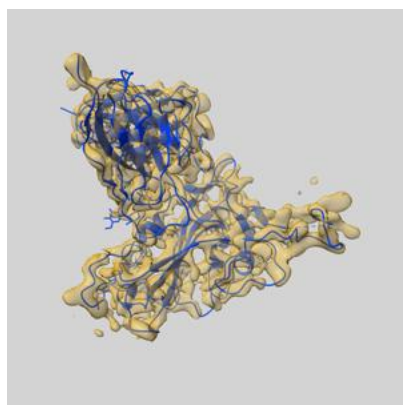
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.92	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.78	8.31	5.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 8.31 differs from the reported value 3.92 by more than 10 %

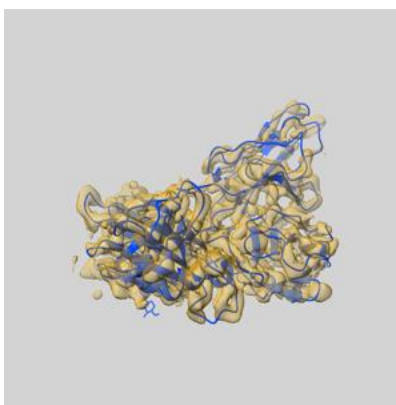
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36122 and PDB model 8JAM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

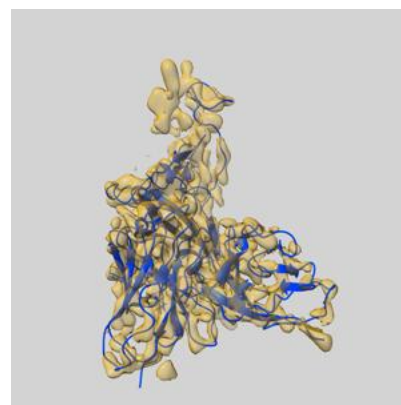
9.1 Map-model overlay [i](#)



X



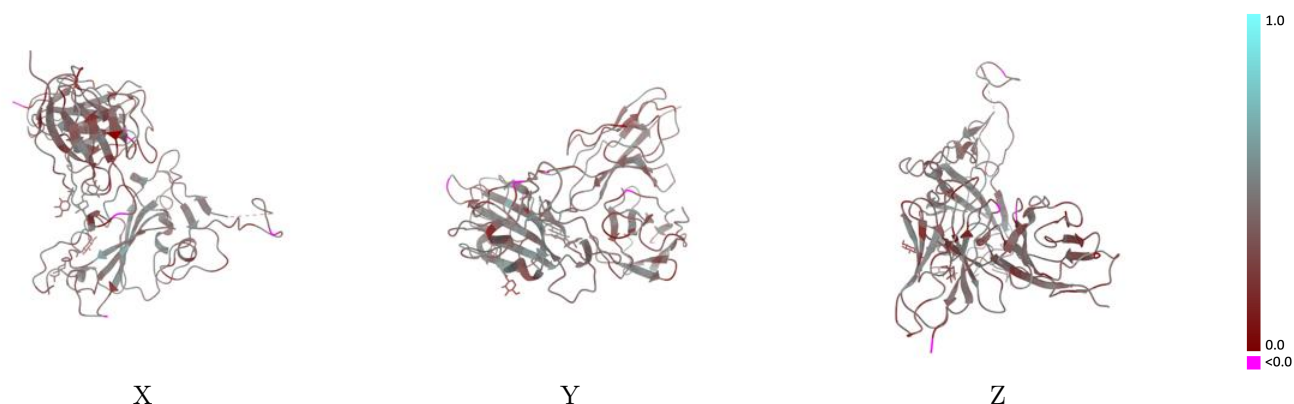
Y



Z

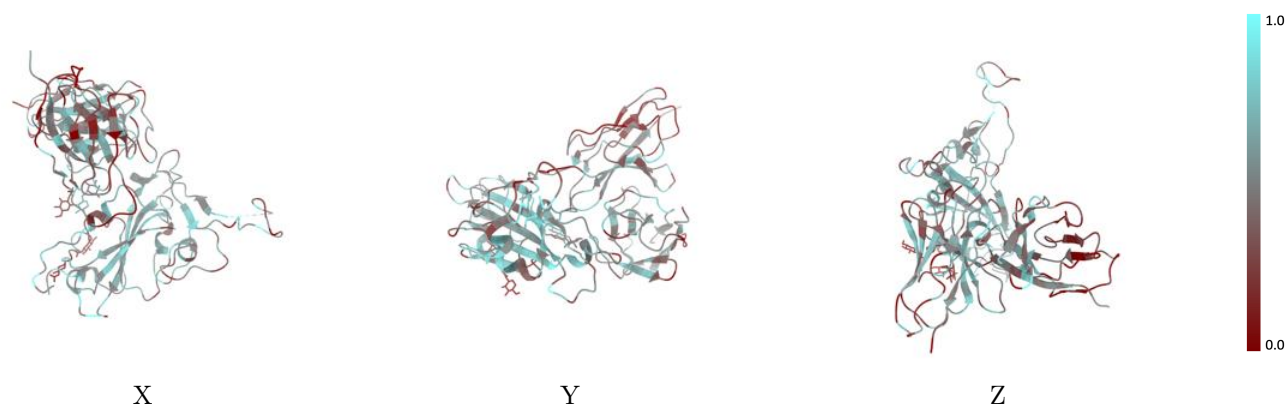
The images above show the 3D surface view of the map at the recommended contour level 0.586 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



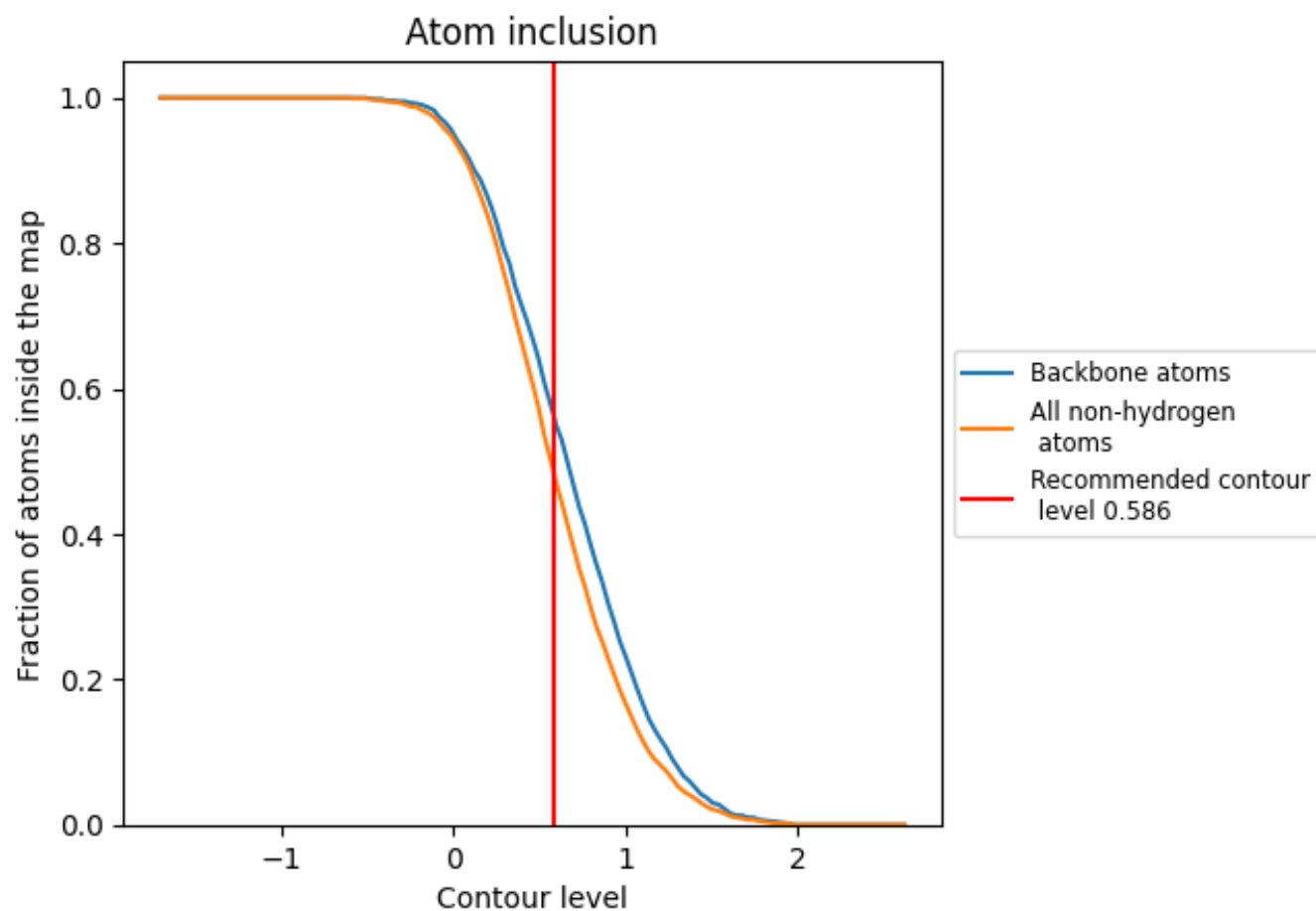
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.586).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 48% 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 (0.586) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4820	0.3740
A	0.4470	0.3620
B	0.5480	0.4050
H	0.3730	0.3400
L	0.4710	0.3490

