



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 07:42 PM JST

PDB ID : 7WPC
EMDB ID : EMD-32682
Title : The second RBD of SARS-CoV-2 Omicron Variant in complexed with RBD-ACE2
Authors : Yin, W.; Xu, Y.; Xu, P.; Cao, X.; Wu, C.; Gu, C.; He, X.; Wang, X.; Huang, S.; Yuan, Q.; Wu, K.; Hu, W.; Huang, Z.; Liu, J.; Wang, Z.; Jia, F.; Xia, K.; Liu, P.; Wang, X.; Song, B.; Zheng, J.; Jiang, H.; Cheng, X.; Jiang, Y.; Deng, S.; Xu, E.
Deposited on : 2022-01-23
Resolution : 2.57 Å(reported)

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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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

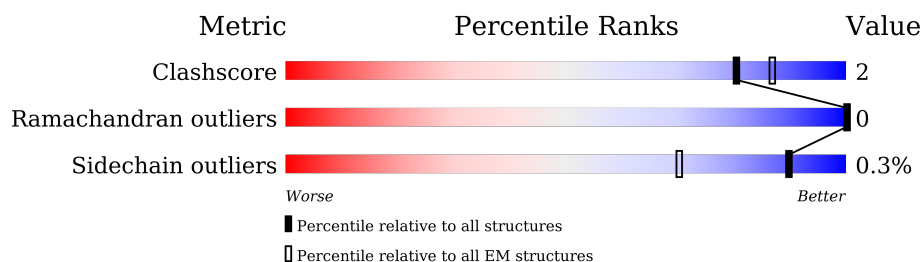
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



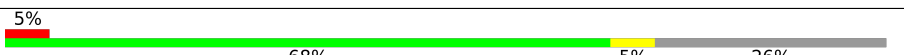
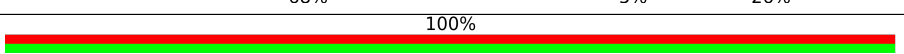
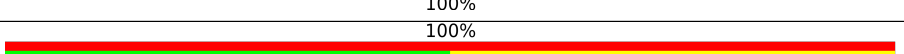
The reported resolution of this entry is 2.57 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1205	 16% 84%
1	B	1205	 6% 14% 84%
2	D	805	 5% 68% 5% 26%
3	C	2	 100%
3	E	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8057 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	197	Total	C	N	O	S	0	0
			1582	1021	267	286	8		
1	B	188	Total	C	N	O	S	0	0
			1518	977	257	277	7		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	variant	UNP P0DTC2
A	140	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	206	ILE	LEU	variant	UNP P0DTC2
A	209	GLU	-	insertion	UNP P0DTC2
A	210	PRO	-	insertion	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2
A	490	ARG	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	engineered mutation	UNP P0DTC2
A	680	SER	ARG	engineered mutation	UNP P0DTC2
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	variant	UNP P0DTC2
B	140	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	206	ILE	LEU	variant	UNP P0DTC2
B	209	GLU	-	insertion	UNP P0DTC2
B	210	PRO	-	insertion	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	336	ASP	GLY	variant	UNP P0DTC2
B	368	LEU	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	490	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	SER	GLY	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	544	LYS	THR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	679	GLY	ARG	engineered mutation	UNP P0DTC2
B	680	SER	ARG	engineered mutation	UNP P0DTC2
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	853	LYS	ASN	variant	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	978	PHE	LEU	variant	UNP P0DTC2
B	983	PRO	LYS	engineered mutation	UNP P0DTC2
B	984	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

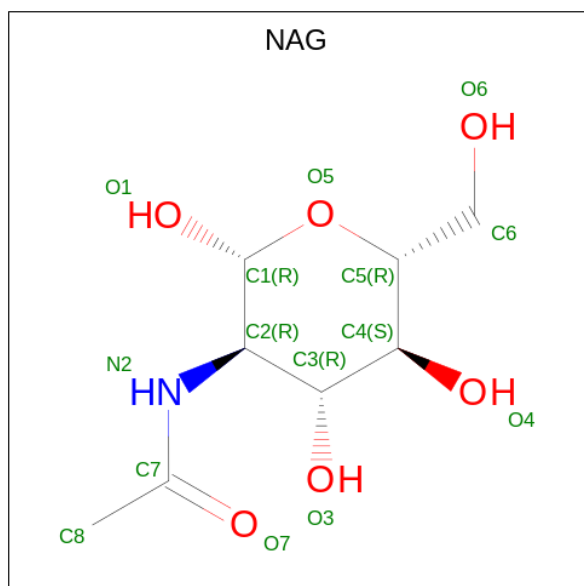
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Cl	0
			1	1	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

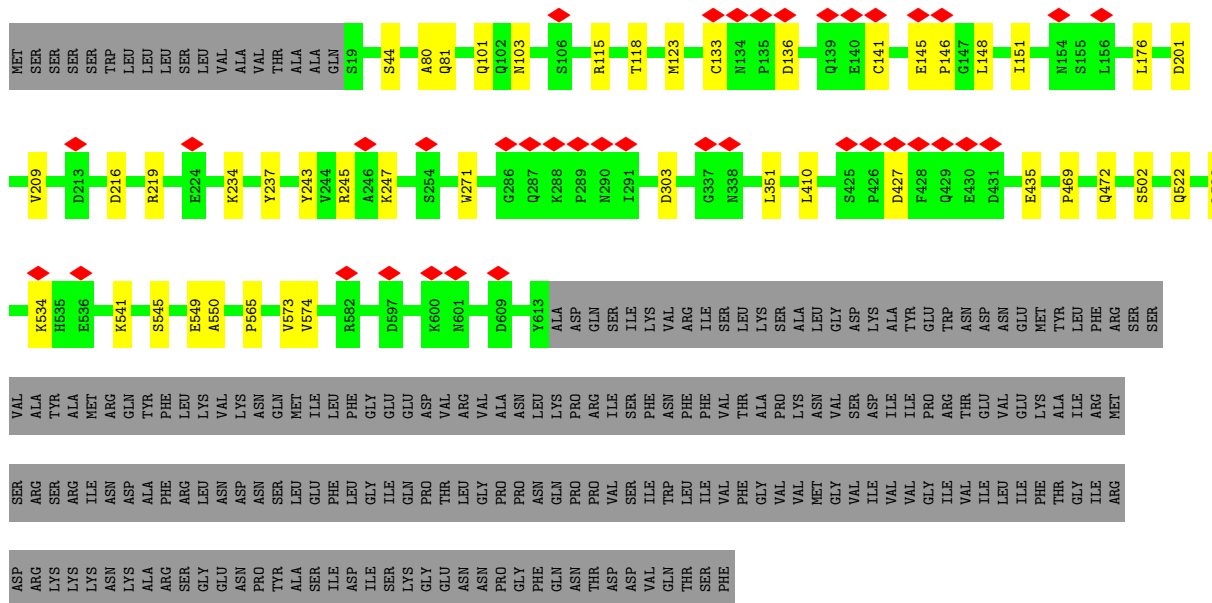
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

LEU	ASP	GLY	CYS	ALA	THR	ALA	PRO
ASP	LYS	VAL	VAL	ILE	GLN	GLN	PRO
LYS	THR	LEU	LEU	SER	ASN	LYS	ILE
PHE	VAL	GLY	GLN	SER	VAL	PHE	LYS
LYS	SER	SER	LEU	LEU	TVR	GLY	PHE
ASN	ASN	LYS	ASN	ASN	GLU	LEU	GLY
HIS	GLY	ARG	ARG	ASP	ASN	GLY	GLY
THR	HIS	VAL	VAL	ILE	GLN	VAL	PHE
SER	THR	ASP	ASP	PHE	LYS	LEU	ASN
PRO	PRO	PHE	PHE	SER	LEU	PRO	PHE
ASP	ASP	CYS	CYS	ARG	ILE	PRO	SER
VAL	VAL	GLY	GLY	LEU	ALA	LEU	GLN
ASP	THR	THR	GLY	ASP	ASN	LEU	ILE
LEU	LEU	GLN	GLY	PRO	GLN	THR	LEU
GLY	GLY	TYR	TYR	PRO	PHE	ASP	PRO
ASP	ASN	HIS	HIS	GLU	ASN	GLU	ASP
ILE	PHE	LEU	LEU	ALA	SER	MET	PRO
SER	THR	MET	MET	GLU	ALA	ILE	SER
GLY	GLU	SER	SER	VAL	ILE	ALA	LYS
ILE	ILE	PRO	PHE	GLN	GLY	GLN	PRO
ASN	ASN	GLN	ILE	ILE	LYS	TYR	SER
ALA	ALA	ILE	GLN	ASP	ILE	THR	LYS
SER	SER	ILE	SER	ARG	GLN	SER	ARG
VAL	THR	THR	ALA	LEU	ASP	ALA	SER
VAL	THR	ASP	PRO	ILE	SER	LEU	PHE
ASN	ASN	ASP	HIS	THR	LEU	LEU	ILE
ILE	ILE	ASN	ASN	GLY	SER	ALA	GLU
GLN	GLN	VAL	VAL	ARG	SER	GLY	ASP
LYS	PHE	VAL	VAL	LEU	THR	THR	LEU
GLU	VAL	PHE	PHE	GLN	ALA	ILE	LEU
ILE	SER	LEU	LEU	SER	THR	THR	PHE
ASP	GLY	GLY	HIS	LEU	ALA	SER	LYS
ARG	ASN	ASN	VAL	GLN	GLY	GLY	VAL
LEU	CYS	THR	THR	THR	GLY	TRP	VAL
ASN	ASN	ASP	TYR	TYR	LYS	THR	THR
GLU	VAL	VAL	VAL	VAL	LEU	LEU	LEU
VAL	VAL	PRO	PRO	THR	GLN	PHE	ALA
ALA	ILE	ALA	ALA	GLN	ASP	GLY	ALA
LYS	GLY	GLY	GLY	GLN	VAL	GLY	ALA
ASN	ILE	ILE	GLU	VAL	ASN	ALA	GLY
LEU	VAL	VAL	LYS	ILE	ASN	ALA	PHE
ASN	ASN	ASN	ASN	ARG	HIS	LEU	ILE
GLU	GLU	ASN	PHE	ALA	ASN	GLN	LYS
SER	SER	THR	THR	ALA	ALA	ILE	GLY
GLN	GLN	VAL	THR	SER	VAL	PRO	TVR
LEU	LEU	THR	THR	ILE	ALA	PHE	GLY
ILE	ILE	TVR	ALA	ILE	ALA	ALA	ASP
ASP	ASP	PRO	PRO	ARG	LEU	ASP	CYS
LEU	LEU	PRO	ALA	ALA	ASN	MET	LYS
GLN	GLN	ILE	ILE	SER	THR	GLN	LEU
GLY	GLN	CYS	CYS	ALA	LEU	MET	GLY
LEU	PRO	HIS	HIS	ASN	VAL	ALA	ASP
GLY	GLY	ASP	ASP	LEU	LYS	TYR	ILE
LYS	LYS	GLY	GLY	ALA	GLN	ARG	ALA
TYR	TYR	LEU	LYS	ALA	LEU	PHE	ALA
GLU	GLU	SER	ALA	THR	SER	ASN	ARG
GLN	GLN	PHE	HIS	LYS	SER	GLY	ASP
			PHE	THR	ILE	ILE	LEU
			LYS	MET	LYS	GLY	CYS
			THR	SER	PHE	THR	ILE
			PRO	SER	GLY	VAL	THR
			ARG	THR	GLY	VAL	CYS

- Molecule 2: Angiotensin-converting enzyme 2



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	242374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.389	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.541	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.824, 0.824, 0.824	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: CL, NAG, ZN

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	0.26	0/1629	0.45	0/2217
1	B	0.28	0/1558	0.48	0/2112
2	D	0.25	0/4994	0.44	0/6785
All	All	0.26	0/8181	0.45	0/11114

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1582	0	1517	4	0
1	B	1518	0	1452	11	0
2	D	4857	0	4631	24	0
3	C	28	0	25	0	0
3	E	28	0	25	0	0
4	D	1	0	0	0	0
5	D	1	0	0	0	0
6	D	42	0	39	1	0
All	All	8057	0	7689	39	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.

The worst 5 of 39 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:D:145:GLU:HG2	2:D:146:PRO:HD3	1.84	0.59
1:B:343:ARG:HH22	1:B:438:LEU:HB3	1.70	0.57
2:D:545:SER:HB3	6:D:905:NAG:H83	1.90	0.53
1:A:487:PHE:HB3	1:A:490:ARG:HH22	1.74	0.53
2:D:81:GLN:NE2	2:D:103:ASN:OD1	2.43	0.51

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	195/1205 (16%)	187 (96%)	8 (4%)	0	100	100
1	B	180/1205 (15%)	166 (92%)	14 (8%)	0	100	100
2	D	593/805 (74%)	574 (97%)	19 (3%)	0	100	100
All	All	968/3215 (30%)	927 (96%)	41 (4%)	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	172/1053 (16%)	171 (99%)	1 (1%)	84	93
1	B	165/1053 (16%)	164 (99%)	1 (1%)	84	93
2	D	526/711 (74%)	525 (100%)	1 (0%)	92	98
All	All	863/2817 (31%)	860 (100%)	3 (0%)	90	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	ARG
1	B	515	LEU
2	D	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	154	ASN
2	D	194	ASN
2	D	599	ASN
2	D	522	GLN
2	D	531	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 ⓘ

4 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	3,1	14,14,15	0.49	0	17,19,21	0.49	0
3	NAG	C	2	3	14,14,15	0.43	0	17,19,21	0.50	0
3	NAG	E	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	1.59	1 (5%)
3	NAG	E	2	3	14,14,15	0.42	0	17,19,21	0.50	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
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	2.35	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	6.03	120.36	112.19

There are no chirality outliers.

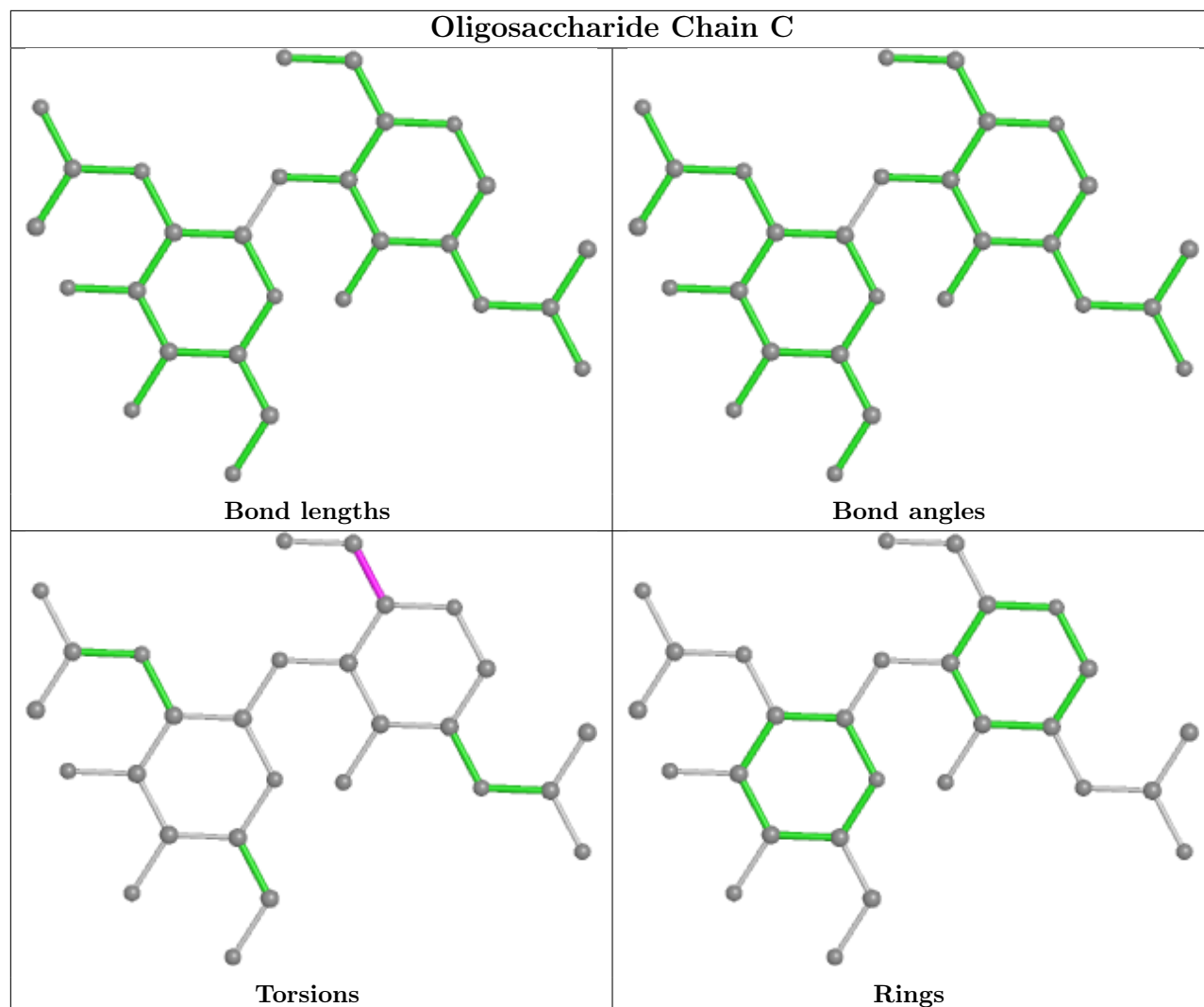
5 of 6 torsion outliers are listed below:

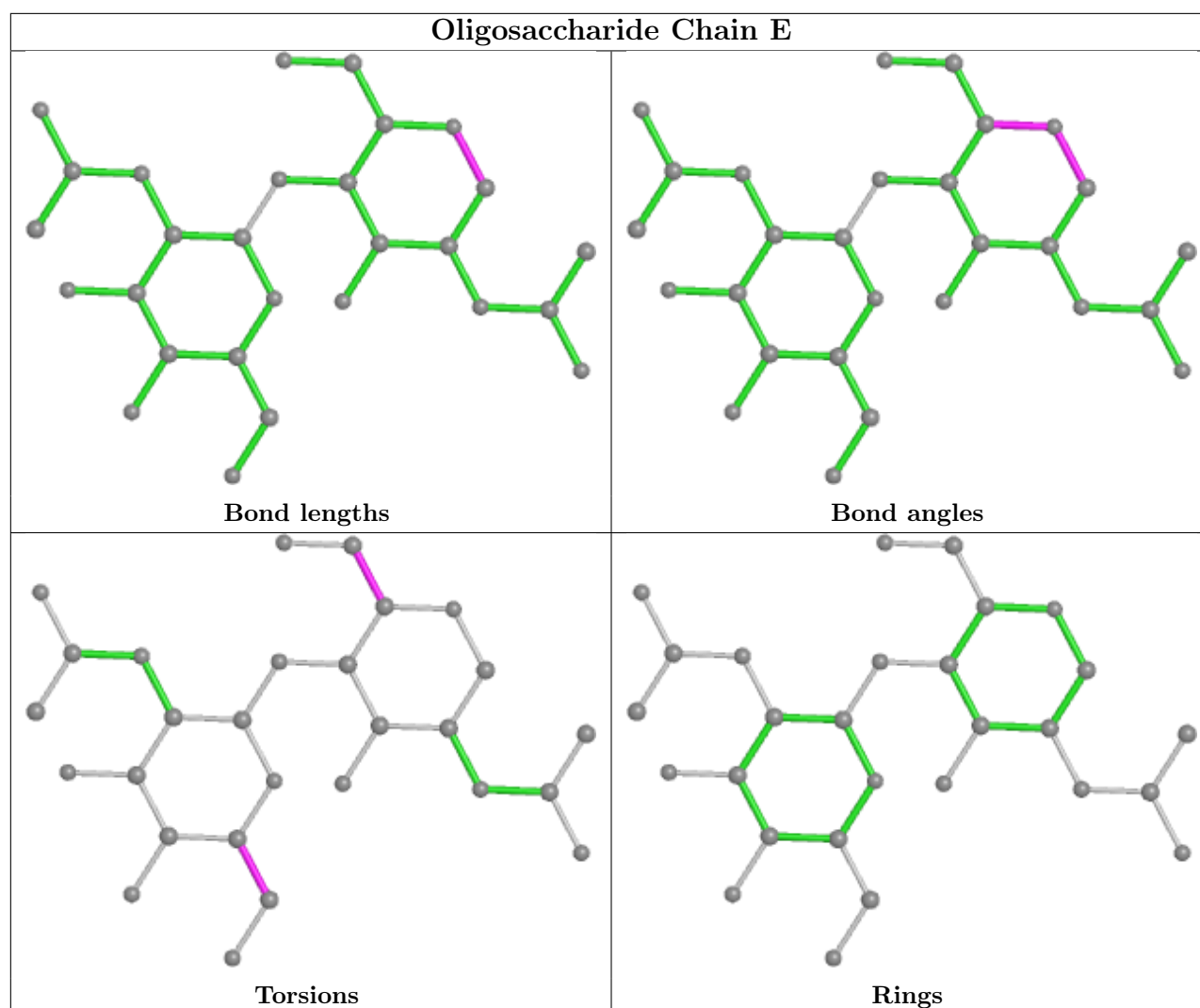
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
6	NAG	D	905	2	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
6	NAG	D	903	2	14,14,15	0.35	0	17,19,21	0.49	0
6	NAG	D	904	2	14,14,15	0.36	0	17,19,21	0.49	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
6	NAG	D	905	2	-	1/6/23/26	0/1/1/1
6	NAG	D	903	2	-	0/6/23/26	0/1/1/1
6	NAG	D	904	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	905	NAG	C2-N2-C7	3.01	127.20	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	904	NAG	C4-C5-C6-O6
6	D	904	NAG	O5-C5-C6-O6
6	D	905	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	905	NAG	1	0

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-32682. These allow visual inspection of the internal detail of the map and identification of artifacts.

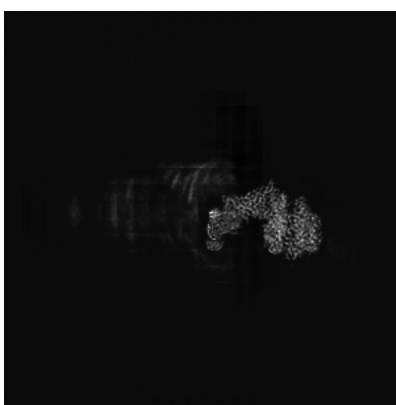
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

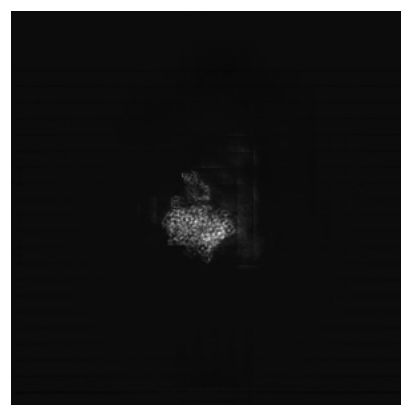
6.1.1 Primary map



X



Y

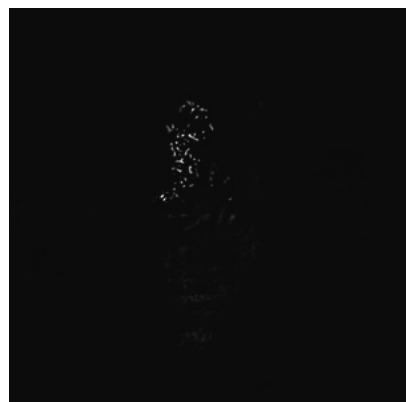


Z

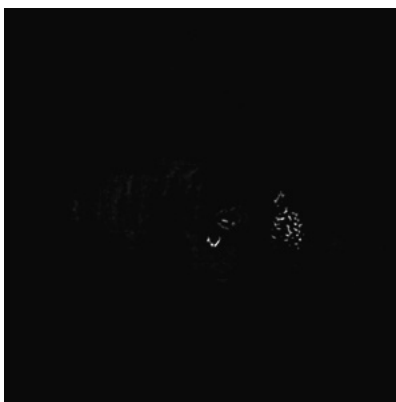
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240

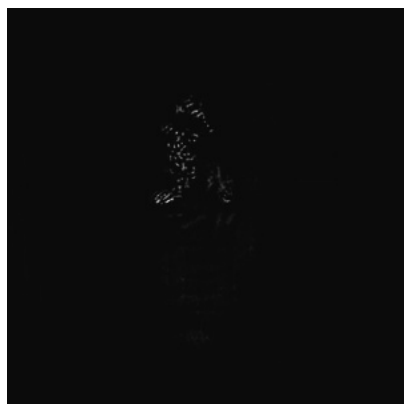


Z Index: 240

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: 237



Y Index: 223

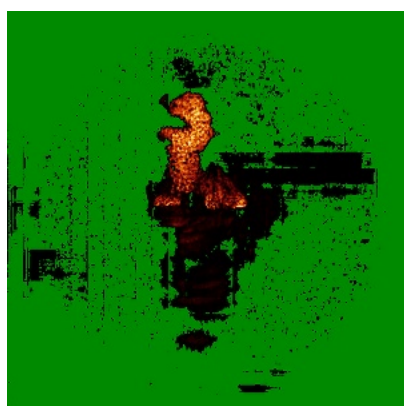


Z Index: 330

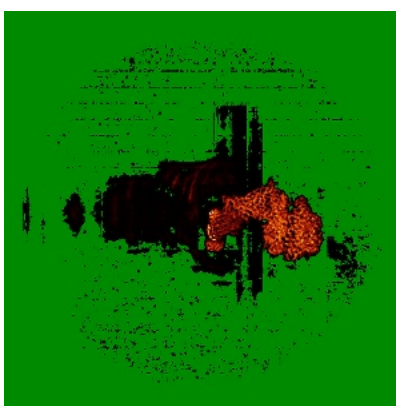
The images above show the largest variance slices of the map in three orthogonal directions.

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

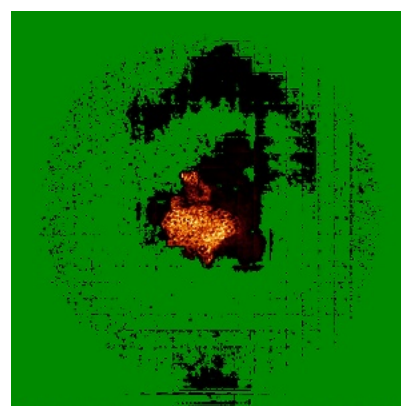
6.4.1 Primary map



X



Y

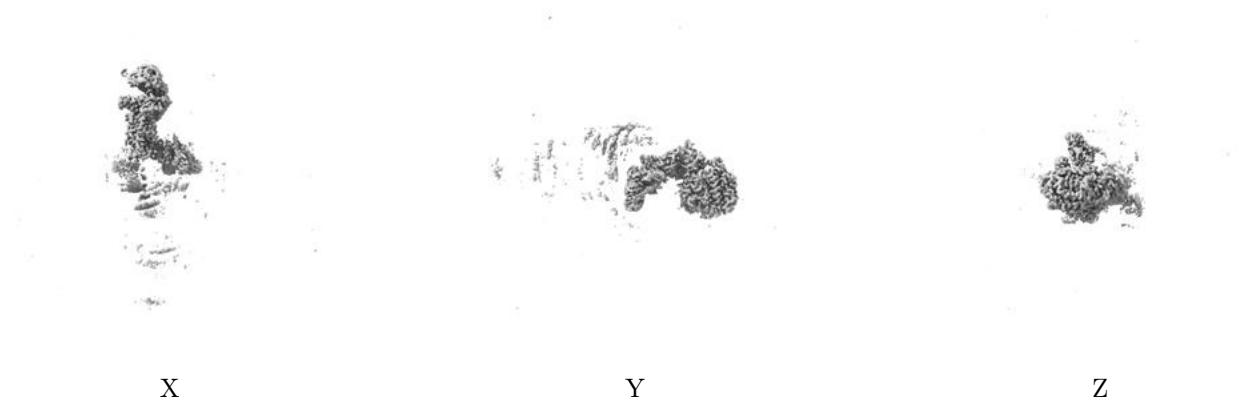


Z

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

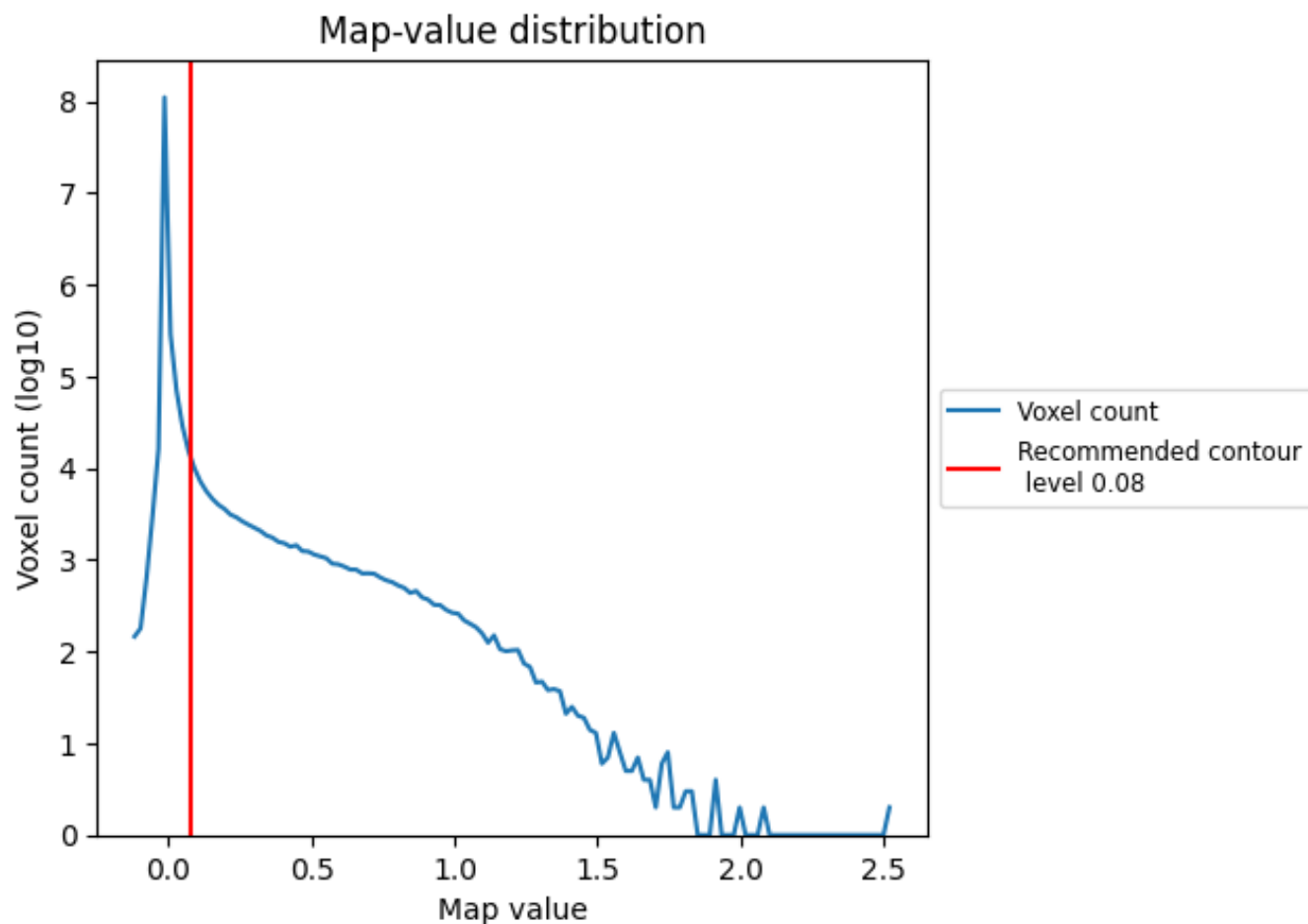
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

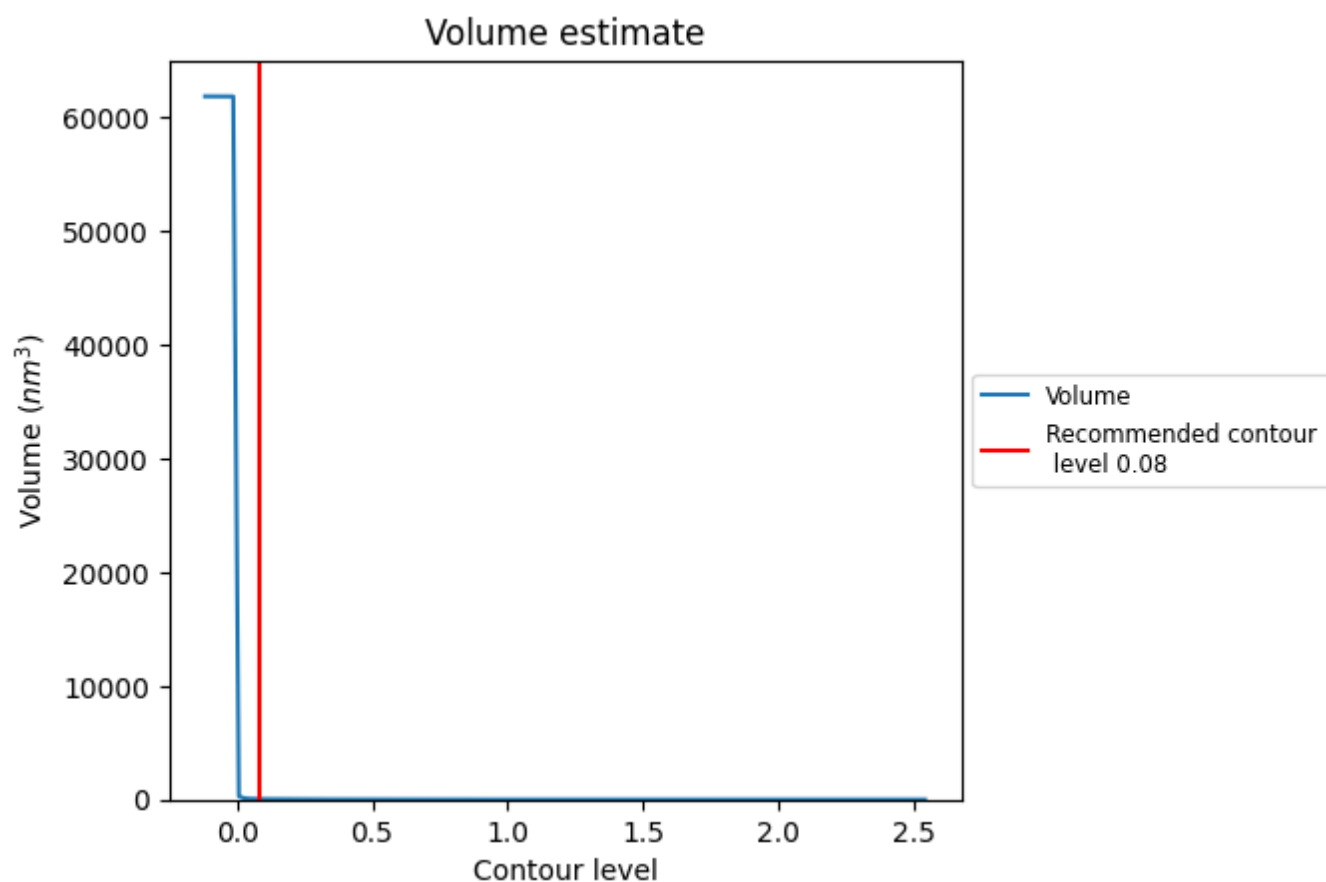
This section contains the results of statistical analysis of the map.

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.

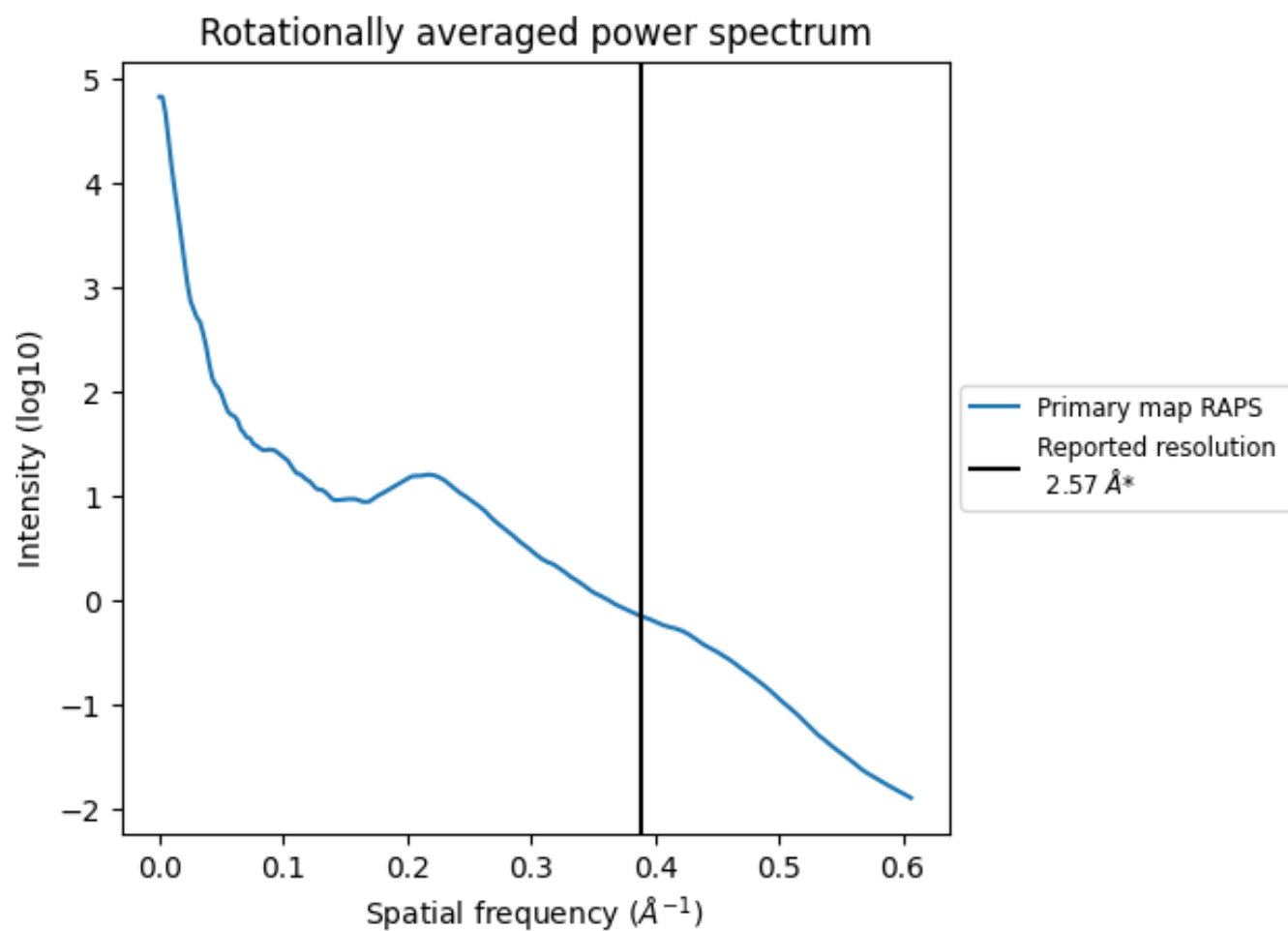
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50 nm³; this corresponds to an approximate mass of 45 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 0.389 Å⁻¹

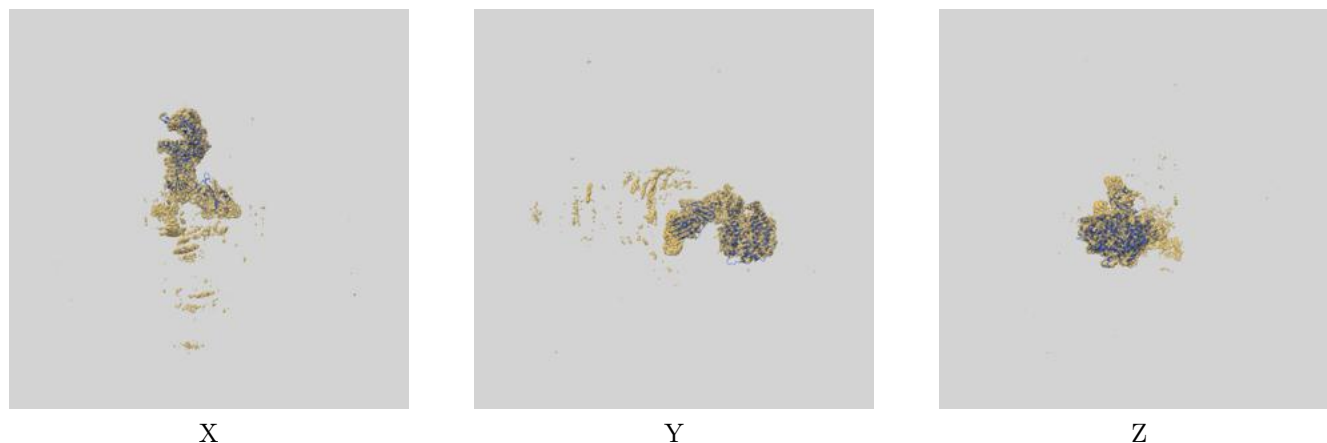
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

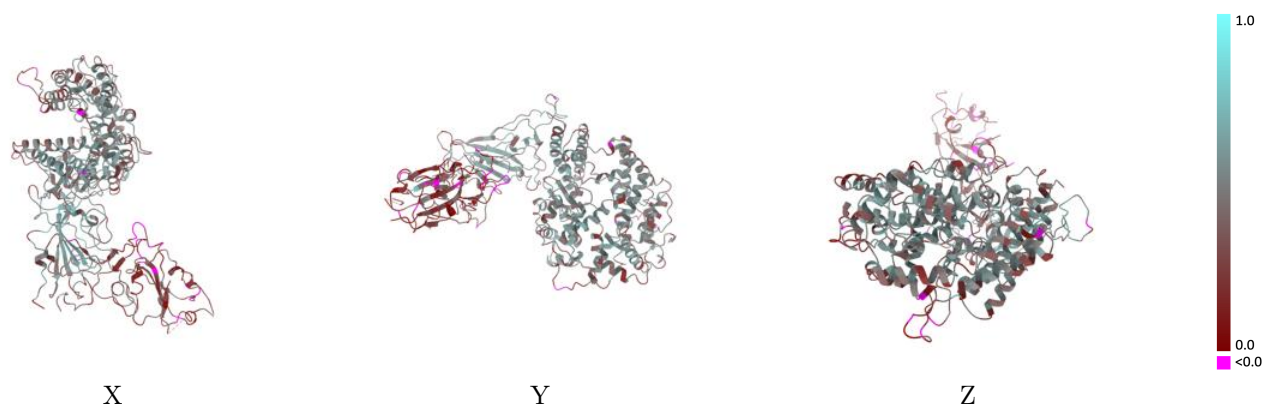
This section contains information regarding the fit between EMDB map EMD-32682 and PDB model 7WPC. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



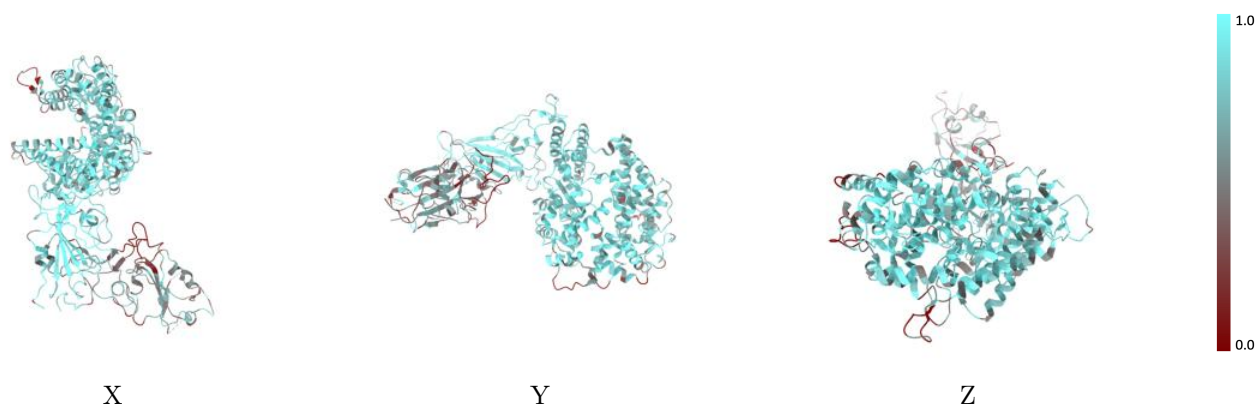
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



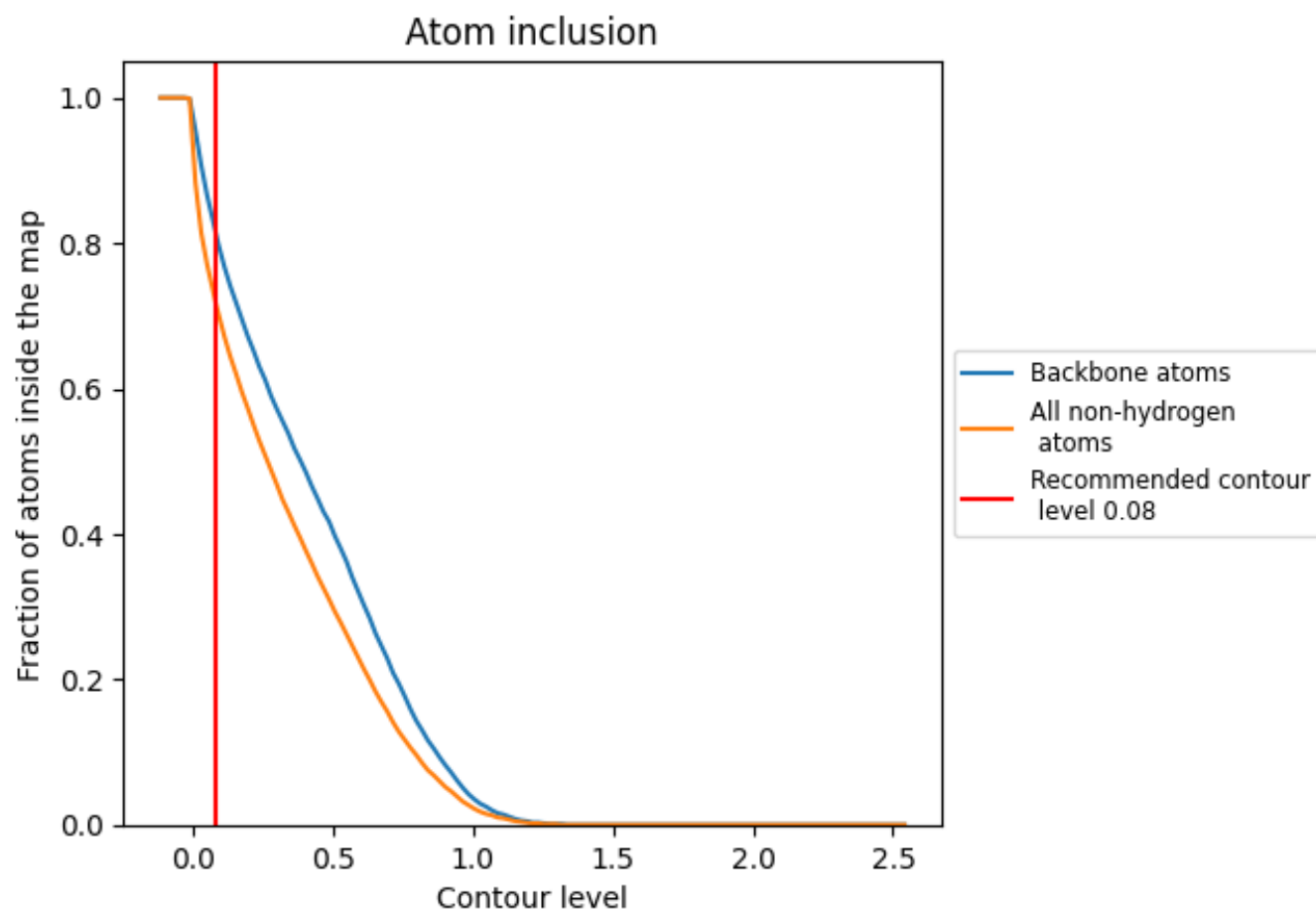
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7180	<div></div> 0.4050
A	<div></div> 0.8130	<div></div> 0.4650
B	<div></div> 0.4530	<div></div> 0.2180
C	<div></div> 0.2860	<div></div> 0.0950
D	<div></div> 0.7760	<div></div> 0.4470
E	<div></div> 0.0710	<div></div> 0.0110

