Full wwPDB EM Validation Report

Jan 7, 2025 – 10:29 PM EST

PDB ID	:	9DWE
EMDB ID	:	EMD-47241
Title	:	Cryo-EM structure of hemagglutinin H5 A/Texas/37/2024 in complex with LSTa and antibody CR9114
Authors	:	Fernandez-Quintero, M.L.; Han, J.; Rodriguez, A.J.; Ward, A.B.
Deposited on	:	2024-10-09
Resolution	:	2.80 Å(reported)
Based on initial models	:	4FQH, .

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 (i) 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 (i)) were used in the production of this report:

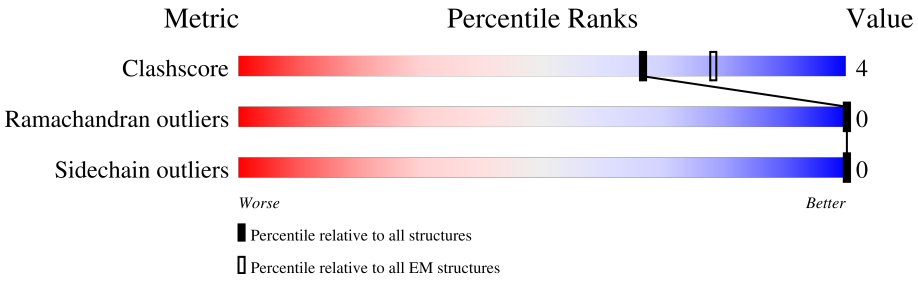
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.80 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 <=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	L	110	27% 97%
1	M	110	27% 97%
1	N	110	30% 96%
2	H	120	8% 97%
2	I	120	8% 97%
2	J	120	8% 96%
3	A	572	76% 12% 13%
3	B	572	78% 9% 13%

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Mol	Chain	Length	Quality of chain
3	C	572	
4	D	2	
4	E	2	
4	P	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SIA	E	2	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17400 atoms, of which 3 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 CR9114 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	110	Total	C	N	O	S	0	0
			807	499	140	166	2		
1	M	110	Total	C	N	O	S	0	0
			807	499	140	166	2		
1	N	110	Total	C	N	O	S	0	0
			807	499	140	166	2		

- Molecule 2 is a protein called CR9114 Fab Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	120	Total	C	N	O	S	0	0
			907	570	152	180	5		
2	I	120	Total	C	N	O	S	0	0
			907	570	152	180	5		
2	J	120	Total	C	N	O	S	0	0
			907	570	152	180	5		

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	499	Total	C	H	N	O	S	0	0
			3987	2507	3	692	762	23		
3	B	499	Total	C		N	O	S	0	0
			3984	2507		692	762	23		
3	C	499	Total	C		N	O	S	0	0
			3984	2507		692	762	23		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	MET	LEU	conflict	UNP A0A8E4ZAK5
A	122	GLN	LEU	conflict	UNP A0A8E4ZAK5
A	199	ILE	THR	conflict	UNP A0A8E4ZAK5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	214	ALA	VAL	conflict	UNP A0A8E4ZAK5
A	508	SER	-	expression tag	UNP A0A8E4ZAK5
A	509	GLY	-	expression tag	UNP A0A8E4ZAK5
A	510	TYR	-	expression tag	UNP A0A8E4ZAK5
A	511	ILE	-	expression tag	UNP A0A8E4ZAK5
A	512	PRO	-	expression tag	UNP A0A8E4ZAK5
A	513	GLU	-	expression tag	UNP A0A8E4ZAK5
A	514	ALA	-	expression tag	UNP A0A8E4ZAK5
A	515	PRO	-	expression tag	UNP A0A8E4ZAK5
A	516	ARG	-	expression tag	UNP A0A8E4ZAK5
A	517	ASP	-	expression tag	UNP A0A8E4ZAK5
A	518	GLY	-	expression tag	UNP A0A8E4ZAK5
A	519	GLN	-	expression tag	UNP A0A8E4ZAK5
A	520	ALA	-	expression tag	UNP A0A8E4ZAK5
A	521	TYR	-	expression tag	UNP A0A8E4ZAK5
A	522	VAL	-	expression tag	UNP A0A8E4ZAK5
A	523	ARG	-	expression tag	UNP A0A8E4ZAK5
A	524	LYS	-	expression tag	UNP A0A8E4ZAK5
A	525	ASP	-	expression tag	UNP A0A8E4ZAK5
A	526	GLY	-	expression tag	UNP A0A8E4ZAK5
A	527	GLU	-	expression tag	UNP A0A8E4ZAK5
A	528	TRP	-	expression tag	UNP A0A8E4ZAK5
A	529	VAL	-	expression tag	UNP A0A8E4ZAK5
A	530	LEU	-	expression tag	UNP A0A8E4ZAK5
A	531	LEU	-	expression tag	UNP A0A8E4ZAK5
A	532	SER	-	expression tag	UNP A0A8E4ZAK5
A	533	THR	-	expression tag	UNP A0A8E4ZAK5
A	534	PHE	-	expression tag	UNP A0A8E4ZAK5
A	535	LEU	-	expression tag	UNP A0A8E4ZAK5
A	536	GLY	-	expression tag	UNP A0A8E4ZAK5
A	537	SER	-	expression tag	UNP A0A8E4ZAK5
A	538	GLY	-	expression tag	UNP A0A8E4ZAK5
A	539	LEU	-	expression tag	UNP A0A8E4ZAK5
A	540	ASN	-	expression tag	UNP A0A8E4ZAK5
A	541	ASP	-	expression tag	UNP A0A8E4ZAK5
A	542	ILE	-	expression tag	UNP A0A8E4ZAK5
A	543	PHE	-	expression tag	UNP A0A8E4ZAK5
A	544	GLU	-	expression tag	UNP A0A8E4ZAK5
A	545	ALA	-	expression tag	UNP A0A8E4ZAK5
A	546	GLN	-	expression tag	UNP A0A8E4ZAK5
A	547	LYS	-	expression tag	UNP A0A8E4ZAK5
A	548	ILE	-	expression tag	UNP A0A8E4ZAK5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	549	GLU	-	expression tag	UNP A0A8E4ZAK5
A	550	TRP	-	expression tag	UNP A0A8E4ZAK5
A	551	HIS	-	expression tag	UNP A0A8E4ZAK5
A	552	GLU	-	expression tag	UNP A0A8E4ZAK5
A	553	GLY	-	expression tag	UNP A0A8E4ZAK5
A	554	HIS	-	expression tag	UNP A0A8E4ZAK5
A	555	HIS	-	expression tag	UNP A0A8E4ZAK5
A	556	HIS	-	expression tag	UNP A0A8E4ZAK5
A	557	HIS	-	expression tag	UNP A0A8E4ZAK5
A	558	HIS	-	expression tag	UNP A0A8E4ZAK5
A	559	HIS	-	expression tag	UNP A0A8E4ZAK5
B	111	MET	LEU	conflict	UNP A0A8E4ZAK5
B	122	GLN	LEU	conflict	UNP A0A8E4ZAK5
B	199	ILE	THR	conflict	UNP A0A8E4ZAK5
B	214	ALA	VAL	conflict	UNP A0A8E4ZAK5
B	508	SER	-	expression tag	UNP A0A8E4ZAK5
B	509	GLY	-	expression tag	UNP A0A8E4ZAK5
B	510	TYR	-	expression tag	UNP A0A8E4ZAK5
B	511	ILE	-	expression tag	UNP A0A8E4ZAK5
B	512	PRO	-	expression tag	UNP A0A8E4ZAK5
B	513	GLU	-	expression tag	UNP A0A8E4ZAK5
B	514	ALA	-	expression tag	UNP A0A8E4ZAK5
B	515	PRO	-	expression tag	UNP A0A8E4ZAK5
B	516	ARG	-	expression tag	UNP A0A8E4ZAK5
B	517	ASP	-	expression tag	UNP A0A8E4ZAK5
B	518	GLY	-	expression tag	UNP A0A8E4ZAK5
B	519	GLN	-	expression tag	UNP A0A8E4ZAK5
B	520	ALA	-	expression tag	UNP A0A8E4ZAK5
B	521	TYR	-	expression tag	UNP A0A8E4ZAK5
B	522	VAL	-	expression tag	UNP A0A8E4ZAK5
B	523	ARG	-	expression tag	UNP A0A8E4ZAK5
B	524	LYS	-	expression tag	UNP A0A8E4ZAK5
B	525	ASP	-	expression tag	UNP A0A8E4ZAK5
B	526	GLY	-	expression tag	UNP A0A8E4ZAK5
B	527	GLU	-	expression tag	UNP A0A8E4ZAK5
B	528	TRP	-	expression tag	UNP A0A8E4ZAK5
B	529	VAL	-	expression tag	UNP A0A8E4ZAK5
B	530	LEU	-	expression tag	UNP A0A8E4ZAK5
B	531	LEU	-	expression tag	UNP A0A8E4ZAK5
B	532	SER	-	expression tag	UNP A0A8E4ZAK5
B	533	THR	-	expression tag	UNP A0A8E4ZAK5
B	534	PHE	-	expression tag	UNP A0A8E4ZAK5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	535	LEU	-	expression tag	UNP A0A8E4ZAK5
B	536	GLY	-	expression tag	UNP A0A8E4ZAK5
B	537	SER	-	expression tag	UNP A0A8E4ZAK5
B	538	GLY	-	expression tag	UNP A0A8E4ZAK5
B	539	LEU	-	expression tag	UNP A0A8E4ZAK5
B	540	ASN	-	expression tag	UNP A0A8E4ZAK5
B	541	ASP	-	expression tag	UNP A0A8E4ZAK5
B	542	ILE	-	expression tag	UNP A0A8E4ZAK5
B	543	PHE	-	expression tag	UNP A0A8E4ZAK5
B	544	GLU	-	expression tag	UNP A0A8E4ZAK5
B	545	ALA	-	expression tag	UNP A0A8E4ZAK5
B	546	GLN	-	expression tag	UNP A0A8E4ZAK5
B	547	LYS	-	expression tag	UNP A0A8E4ZAK5
B	548	ILE	-	expression tag	UNP A0A8E4ZAK5
B	549	GLU	-	expression tag	UNP A0A8E4ZAK5
B	550	TRP	-	expression tag	UNP A0A8E4ZAK5
B	551	HIS	-	expression tag	UNP A0A8E4ZAK5
B	552	GLU	-	expression tag	UNP A0A8E4ZAK5
B	553	GLY	-	expression tag	UNP A0A8E4ZAK5
B	554	HIS	-	expression tag	UNP A0A8E4ZAK5
B	555	HIS	-	expression tag	UNP A0A8E4ZAK5
B	556	HIS	-	expression tag	UNP A0A8E4ZAK5
B	557	HIS	-	expression tag	UNP A0A8E4ZAK5
B	558	HIS	-	expression tag	UNP A0A8E4ZAK5
B	559	HIS	-	expression tag	UNP A0A8E4ZAK5
C	111	MET	LEU	conflict	UNP A0A8E4ZAK5
C	122	GLN	LEU	conflict	UNP A0A8E4ZAK5
C	199	ILE	THR	conflict	UNP A0A8E4ZAK5
C	214	ALA	VAL	conflict	UNP A0A8E4ZAK5
C	508	SER	-	expression tag	UNP A0A8E4ZAK5
C	509	GLY	-	expression tag	UNP A0A8E4ZAK5
C	510	TYR	-	expression tag	UNP A0A8E4ZAK5
C	511	ILE	-	expression tag	UNP A0A8E4ZAK5
C	512	PRO	-	expression tag	UNP A0A8E4ZAK5
C	513	GLU	-	expression tag	UNP A0A8E4ZAK5
C	514	ALA	-	expression tag	UNP A0A8E4ZAK5
C	515	PRO	-	expression tag	UNP A0A8E4ZAK5
C	516	ARG	-	expression tag	UNP A0A8E4ZAK5
C	517	ASP	-	expression tag	UNP A0A8E4ZAK5
C	518	GLY	-	expression tag	UNP A0A8E4ZAK5
C	519	GLN	-	expression tag	UNP A0A8E4ZAK5
C	520	ALA	-	expression tag	UNP A0A8E4ZAK5

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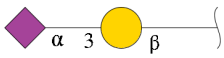
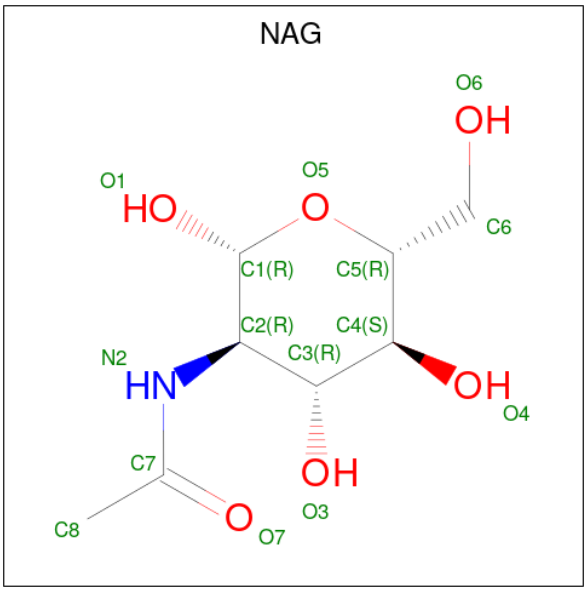
Chain	Residue	Modelled	Actual	Comment	Reference
C	521	TYR	-	expression tag	UNP A0A8E4ZAK5
C	522	VAL	-	expression tag	UNP A0A8E4ZAK5
C	523	ARG	-	expression tag	UNP A0A8E4ZAK5
C	524	LYS	-	expression tag	UNP A0A8E4ZAK5
C	525	ASP	-	expression tag	UNP A0A8E4ZAK5
C	526	GLY	-	expression tag	UNP A0A8E4ZAK5
C	527	GLU	-	expression tag	UNP A0A8E4ZAK5
C	528	TRP	-	expression tag	UNP A0A8E4ZAK5
C	529	VAL	-	expression tag	UNP A0A8E4ZAK5
C	530	LEU	-	expression tag	UNP A0A8E4ZAK5
C	531	LEU	-	expression tag	UNP A0A8E4ZAK5
C	532	SER	-	expression tag	UNP A0A8E4ZAK5
C	533	THR	-	expression tag	UNP A0A8E4ZAK5
C	534	PHE	-	expression tag	UNP A0A8E4ZAK5
C	535	LEU	-	expression tag	UNP A0A8E4ZAK5
C	536	GLY	-	expression tag	UNP A0A8E4ZAK5
C	537	SER	-	expression tag	UNP A0A8E4ZAK5
C	538	GLY	-	expression tag	UNP A0A8E4ZAK5
C	539	LEU	-	expression tag	UNP A0A8E4ZAK5
C	540	ASN	-	expression tag	UNP A0A8E4ZAK5
C	541	ASP	-	expression tag	UNP A0A8E4ZAK5
C	542	ILE	-	expression tag	UNP A0A8E4ZAK5
C	543	PHE	-	expression tag	UNP A0A8E4ZAK5
C	544	GLU	-	expression tag	UNP A0A8E4ZAK5
C	545	ALA	-	expression tag	UNP A0A8E4ZAK5
C	546	GLN	-	expression tag	UNP A0A8E4ZAK5
C	547	LYS	-	expression tag	UNP A0A8E4ZAK5
C	548	ILE	-	expression tag	UNP A0A8E4ZAK5
C	549	GLU	-	expression tag	UNP A0A8E4ZAK5
C	550	TRP	-	expression tag	UNP A0A8E4ZAK5
C	551	HIS	-	expression tag	UNP A0A8E4ZAK5
C	552	GLU	-	expression tag	UNP A0A8E4ZAK5
C	553	GLY	-	expression tag	UNP A0A8E4ZAK5
C	554	HIS	-	expression tag	UNP A0A8E4ZAK5
C	555	HIS	-	expression tag	UNP A0A8E4ZAK5
C	556	HIS	-	expression tag	UNP A0A8E4ZAK5
C	557	HIS	-	expression tag	UNP A0A8E4ZAK5
C	558	HIS	-	expression tag	UNP A0A8E4ZAK5
C	559	HIS	-	expression tag	UNP A0A8E4ZAK5

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
4	P	2	Total C N O 31 17 1 13	0	0
4	D	2	Total C N O 31 17 1 13	0	0
4	E	2	Total C N O 31 17 1 13	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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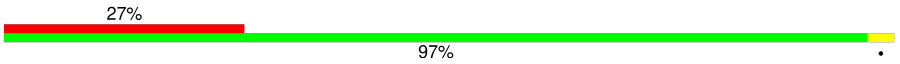
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5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

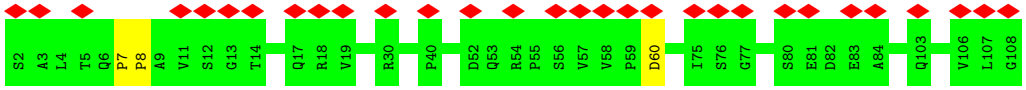
3 Residue-property plots (i)

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: CR9114 Fab light chain

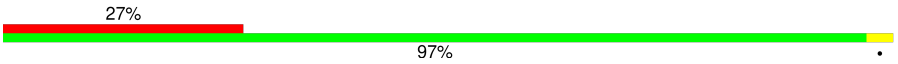
Chain L:

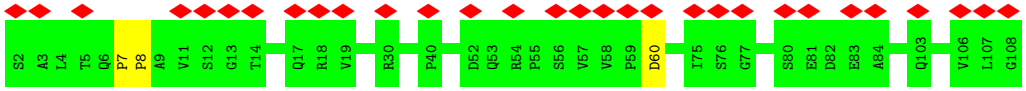




• Molecule 1: CR9114 Fab light chain

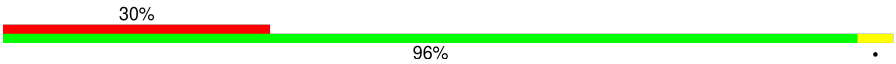
Chain M:

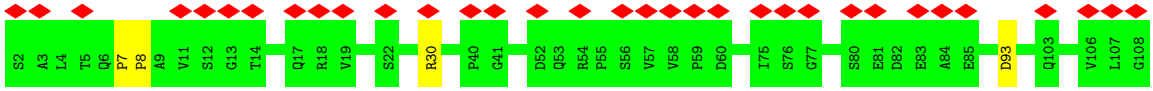




• Molecule 1: CR9114 Fab light chain

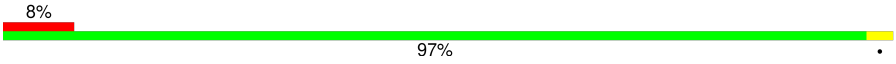
Chain N:

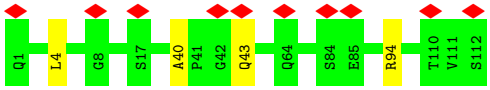




• Molecule 2: CR9114 Fab Fab heavy chain

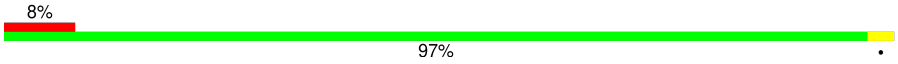
Chain H:

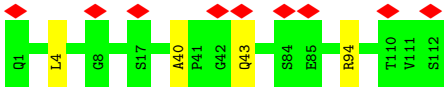




• Molecule 2: CR9114 Fab Fab heavy chain

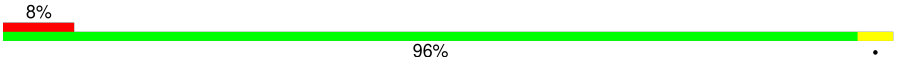
Chain I:

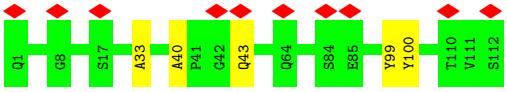




• Molecule 2: CR9114 Fab Fab heavy chain

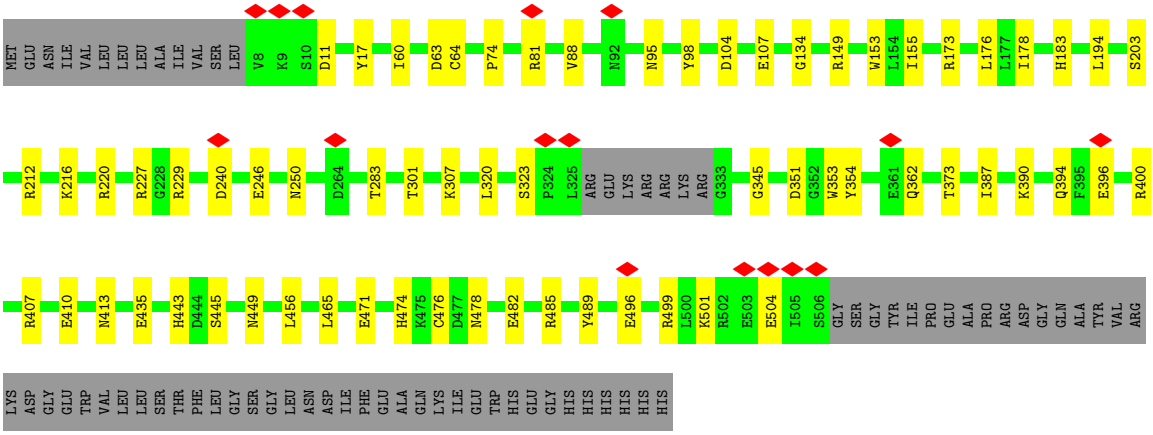
Chain J:





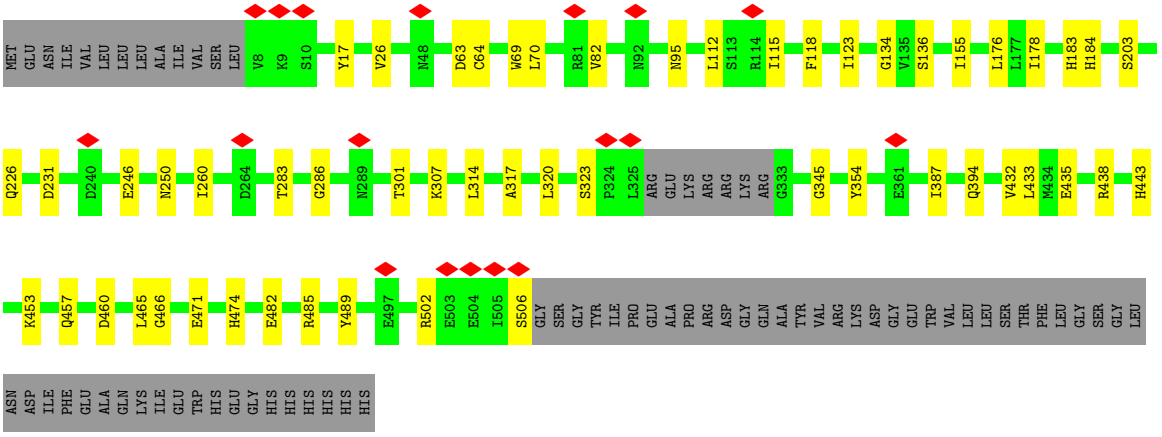
• Molecule 3: Hemagglutinin

Chain A:



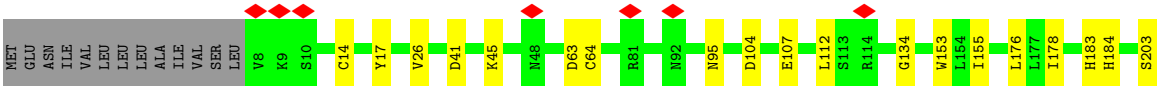
• Molecule 3: Hemagglutinin

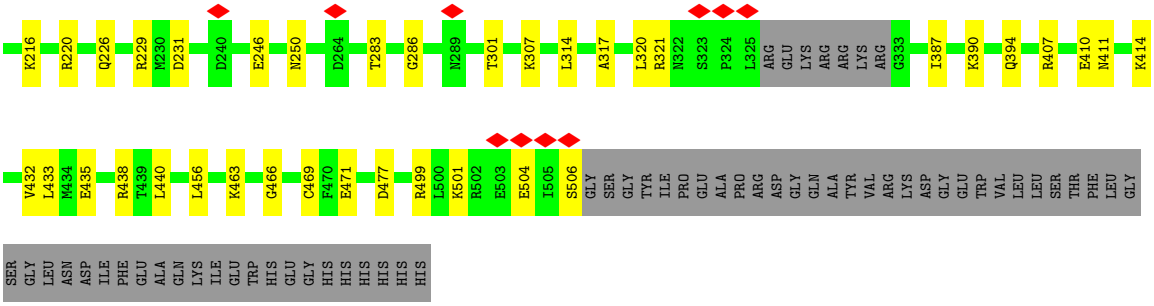
Chain B:



• Molecule 3: Hemagglutinin

Chain C:





• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain P:

• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain D:

• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain E:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	260000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	41.63	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.328	Depositor
Minimum map value	-1.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.173	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, 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	L	0.27	0/824	0.53	0/1121
1	M	0.27	0/824	0.54	0/1121
1	N	0.28	0/824	0.54	0/1121
2	H	0.29	0/928	0.51	0/1259
2	I	0.29	0/928	0.51	0/1259
2	J	0.29	0/928	0.51	0/1259
3	A	0.30	0/4075	0.53	0/5517
3	B	0.30	0/4075	0.55	0/5517
3	C	0.30	0/4075	0.53	0/5517
All	All	0.29	0/17481	0.53	0/23691

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	L	807	0	772	2	0
1	M	807	0	772	2	0
1	N	807	0	772	2	0
2	H	907	0	863	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	907	0	863	2	0
2	J	907	0	863	3	0
3	A	3984	3	3840	45	0
3	B	3984	0	3839	35	0
3	C	3984	0	3840	40	0
4	D	31	0	26	7	0
4	E	31	0	26	10	0
4	P	31	0	26	6	0
5	A	70	0	65	0	0
5	B	70	0	65	0	0
5	C	70	0	65	0	0
All	All	17397	3	16697	127	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 4.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:TRP:HH2	4:E:2:SIA:H8	1.49	0.78
3:C:463:LYS:HB3	3:C:471:GLU:HB3	1.78	0.64
3:A:203:SER:HB2	3:A:246:GLU:HB3	1.82	0.61
3:A:153:TRP:CH2	4:E:2:SIA:H8	2.35	0.61
3:C:203:SER:HB2	3:C:246:GLU:HB3	1.84	0.58
3:A:134:GLY:HA2	4:E:2:SIA:H113	1.87	0.56
3:A:445:SER:O	3:A:449:ASN:HB2	2.06	0.56
3:B:226:GLN:OE1	4:P:2:SIA:H92	2.05	0.56
3:B:134:GLY:HA2	4:P:2:SIA:H113	1.88	0.56
3:C:283:THR:HG22	3:C:301:THR:HG22	1.87	0.56
3:B:482:GLU:OE2	3:B:485:ARG:NH1	2.40	0.55
3:B:203:SER:HB2	3:B:246:GLU:HB3	1.87	0.55
3:A:283:THR:HG22	3:A:301:THR:HG22	1.89	0.55
3:B:283:THR:HG22	3:B:301:THR:HG22	1.88	0.54
3:B:465:LEU:HD21	3:B:471:GLU:HG2	1.89	0.53
3:A:351:ASP:HA	2:J:99:TYR:CE1	2.44	0.53
3:C:407:ARG:NH1	3:C:410:GLU:OE1	2.41	0.53
3:C:501:LYS:HA	3:C:504:GLU:HG2	1.91	0.53
3:A:155:ILE:CD1	4:E:2:SIA:H111	2.39	0.52
3:C:134:GLY:HA2	4:D:2:SIA:H113	1.90	0.52
3:B:460:ASP:O	3:B:502:ARG:NH2	2.42	0.52
3:A:98:TYR:HH	4:E:2:SIA:HO9	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:GLN:OE1	4:D:2:SIA:H92	2.10	0.52
3:B:17:TYR:HB2	3:B:320:LEU:HD11	1.91	0.51
3:B:506:SER:HA	3:C:499:ARG:HD2	1.92	0.51
3:A:496:GLU:OE1	3:A:499:ARG:NH2	2.43	0.51
3:C:220:ARG:HD2	3:C:229:ARG:HG2	1.93	0.50
3:A:173:ARG:NH2	3:A:240:ASP:OD2	2.43	0.49
3:A:400:ARG:NH1	3:A:413:ASN:OD1	2.45	0.49
3:C:17:TYR:HB2	3:C:320:LEU:HD11	1.95	0.49
3:A:456:LEU:HD22	3:C:466:GLY:HA2	1.95	0.49
3:B:323:SER:HB2	3:B:345:GLY:H	1.78	0.49
3:C:307:LYS:HD2	3:C:394:GLN:HB3	1.94	0.48
3:B:453:LYS:NZ	3:B:457:GLN:OE1	2.41	0.48
3:C:387:ILE:HD11	3:C:435:GLU:HG3	1.96	0.48
3:A:17:TYR:HB2	3:A:320:LEU:HD11	1.95	0.48
3:A:482:GLU:OE2	3:A:485:ARG:NH1	2.47	0.48
3:A:362:GLN:OE1	3:A:478:ASN:ND2	2.42	0.48
3:B:118:PHE:HE1	3:B:260:ILE:HG12	1.79	0.48
3:C:64:CYS:HA	3:C:95:ASN:HB2	1.96	0.47
3:A:194:LEU:HD21	4:E:2:SIA:O10	2.14	0.47
3:B:155:ILE:HD11	4:P:2:SIA:H111	1.96	0.47
3:C:155:ILE:HD11	4:D:2:SIA:H111	1.97	0.47
3:A:134:GLY:HA2	4:E:2:SIA:C11	2.44	0.47
3:A:307:LYS:NZ	3:A:396:GLU:OE2	2.47	0.47
3:A:307:LYS:HD2	3:A:394:GLN:HB3	1.97	0.47
3:A:499:ARG:NH1	3:C:506:SER:O	2.48	0.47
3:B:433:LEU:HD11	3:C:390:LYS:HE3	1.97	0.47
3:C:41:ASP:OD2	3:C:45:LYS:NZ	2.45	0.47
3:B:307:LYS:HD2	3:B:394:GLN:HB3	1.97	0.47
3:B:176:LEU:HD23	3:B:178:ILE:HD11	1.97	0.47
3:B:64:CYS:HA	3:B:95:ASN:HB2	1.97	0.47
3:A:220:ARG:HD2	3:A:229:ARG:HG2	1.97	0.46
3:A:387:ILE:HD11	3:A:435:GLU:HG3	1.96	0.46
4:E:2:SIA:C10	4:E:2:SIA:H7	2.45	0.46
3:B:438:ARG:HD3	3:C:438:ARG:HH22	1.81	0.46
3:B:466:GLY:HA2	3:C:456:LEU:HD22	1.97	0.46
3:C:104:ASP:HB3	3:C:107:GLU:HB2	1.98	0.46
3:C:176:LEU:HD23	3:C:178:ILE:HD11	1.97	0.46
2:I:40:ALA:HB3	2:I:43:GLN:HB2	1.98	0.46
3:B:387:ILE:HD11	3:B:435:GLU:HG3	1.97	0.46
3:A:98:TYR:OH	4:E:2:SIA:O9	2.28	0.46
3:A:354:TYR:OH	3:A:443:HIS:ND1	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:136:SER:HB2	4:P:2:SIA:O1A	2.16	0.45
3:A:155:ILE:HD11	4:E:2:SIA:H111	1.98	0.45
2:J:40:ALA:HB3	2:J:43:GLN:HB2	1.99	0.45
3:C:184:HIS:NE2	3:C:231:ASP:OD2	2.43	0.45
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.98	0.45
3:A:203:SER:OG	3:A:212:ARG:NH1	2.50	0.45
3:B:26:VAL:HG21	3:B:317:ALA:HB2	1.99	0.45
3:B:123:ILE:HG21	3:B:176:LEU:HD21	1.99	0.45
3:B:134:GLY:HA2	4:P:2:SIA:C11	2.47	0.45
4:P:1:GAL:H4	4:P:2:SIA:H92	1.99	0.45
3:C:153:TRP:HH2	4:D:2:SIA:H8	1.81	0.44
1:N:30:ARG:NH1	1:N:93:ASP:OD2	2.51	0.44
3:B:460:ASP:OD1	3:B:460:ASP:N	2.42	0.44
3:C:314:LEU:HG	3:C:432:VAL:HG21	1.99	0.44
3:B:184:HIS:NE2	3:B:231:ASP:OD2	2.43	0.44
3:B:354:TYR:OH	3:B:443:HIS:ND1	2.41	0.44
3:B:69:TRP:HE1	3:B:82:VAL:HG21	1.82	0.44
3:A:64:CYS:HA	3:A:95:ASN:HB2	2.00	0.44
3:A:104:ASP:HB3	3:A:107:GLU:HB2	1.99	0.44
3:C:321:ARG:HG3	3:C:440:LEU:HD22	2.00	0.44
3:C:134:GLY:HA2	4:D:2:SIA:C11	2.48	0.43
3:C:390:LYS:HD3	3:C:390:LYS:HA	1.81	0.43
3:A:176:LEU:HD23	3:A:178:ILE:HD11	1.99	0.43
3:A:183:HIS:O	3:A:250:ASN:ND2	2.43	0.43
3:B:314:LEU:HG	3:B:432:VAL:HG21	2.00	0.43
2:J:33:ALA:HB1	2:J:100:TYR:CE1	2.52	0.43
3:A:390:LYS:HE3	3:C:433:LEU:HD11	2.00	0.43
3:C:155:ILE:CD1	4:D:2:SIA:H111	2.48	0.43
3:B:283:THR:OG1	3:B:286:GLY:O	2.28	0.43
3:A:81:ARG:HD3	3:A:81:ARG:HA	1.86	0.43
3:A:474:HIS:NE2	3:A:489:TYR:OH	2.47	0.43
3:A:11:ASP:OD2	3:A:476:CYS:N	2.51	0.43
3:A:63:ASP:OD1	3:A:63:ASP:N	2.49	0.43
3:A:220:ARG:NH1	3:A:227:ARG:O	2.52	0.43
1:N:7:PRO:HA	1:N:8:PRO:HD3	1.92	0.42
3:A:60:ILE:HA	3:A:88:VAL:HB	2.01	0.42
3:A:216:LYS:O	3:A:220:ARG:NH2	2.52	0.42
3:A:407:ARG:NH2	3:A:410:GLU:OE1	2.53	0.42
3:B:63:ASP:OD1	3:B:63:ASP:N	2.51	0.42
3:C:216:LYS:O	3:C:220:ARG:NH2	2.53	0.42
3:A:323:SER:HB2	3:A:345:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:465:LEU:HD11	3:A:471:GLU:HB2	2.02	0.42
3:A:353:TRP:HB2	3:A:373:THR:HG23	2.02	0.41
2:I:4:LEU:HD11	2:I:94:ARG:HB2	2.01	0.41
3:C:26:VAL:HG21	3:C:317:ALA:HB2	2.02	0.41
3:C:183:HIS:O	3:C:250:ASN:ND2	2.44	0.41
3:B:112:LEU:HD23	3:B:115:ILE:HD12	2.02	0.41
3:C:477:ASP:OD1	3:C:477:ASP:N	2.49	0.41
3:A:74:PRO:HA	3:A:149:ARG:HE	1.85	0.41
3:B:183:HIS:O	3:B:250:ASN:ND2	2.44	0.41
3:C:226:GLN:NE2	4:D:2:SIA:O1A	2.54	0.41
3:C:283:THR:OG1	3:C:286:GLY:O	2.29	0.41
1:M:60:ASP:OD1	1:M:60:ASP:N	2.54	0.41
3:C:411:ASN:HA	3:C:414:LYS:HG2	2.02	0.41
3:C:14:CYS:HA	3:C:469:CYS:HA	2.03	0.41
3:C:63:ASP:OD1	3:C:63:ASP:N	2.50	0.41
3:C:112:LEU:HA	3:C:112:LEU:HD23	1.87	0.41
1:L:60:ASP:N	1:L:60:ASP:OD1	2.54	0.40
3:B:474:HIS:NE2	3:B:489:TYR:OH	2.49	0.40
3:A:501:LYS:HA	3:A:504:GLU:HG2	2.04	0.40
3:B:70:LEU:HD23	3:B:70:LEU:HA	1.93	0.40
1:L:7:PRO:HA	1:L:8:PRO:HD3	1.92	0.40
2:H:4:LEU:HD11	2:H:94:ARG:HB2	2.02	0.40
1:M:7:PRO:HA	1:M:8:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
1	M	108/110 (98%)	105 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
2	H	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
2	I	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
2	J	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
3	A	495/572 (86%)	481 (97%)	14 (3%)	0	100	100
3	B	495/572 (86%)	480 (97%)	15 (3%)	0	100	100
3	C	495/572 (86%)	480 (97%)	15 (3%)	0	100	100
All	All	2163/2406 (90%)	2103 (97%)	60 (3%)	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	L	88/88 (100%)	88 (100%)	0	100	100
1	M	88/88 (100%)	88 (100%)	0	100	100
1	N	88/88 (100%)	88 (100%)	0	100	100
2	H	97/97 (100%)	97 (100%)	0	100	100
2	I	97/97 (100%)	97 (100%)	0	100	100
2	J	97/97 (100%)	97 (100%)	0	100	100
3	A	438/500 (88%)	438 (100%)	0	100	100
3	B	438/500 (88%)	438 (100%)	0	100	100
3	C	438/500 (88%)	438 (100%)	0	100	100
All	All	1869/2055 (91%)	1869 (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. There are no such sidechains identified.

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

6 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	GAL	D	1	4	11,11,12	0.36	0	15,15,17	1.11	2 (13%)
4	SIA	D	2	4	20,20,21	0.79	1 (5%)	21,28,31	0.76	1 (4%)
4	GAL	E	1	4	11,11,12	0.57	0	15,15,17	1.70	2 (13%)
4	SIA	E	2	4	20,20,21	0.88	1 (5%)	21,28,31	0.84	1 (4%)
4	GAL	P	1	4	11,11,12	0.38	0	15,15,17	1.27	3 (20%)
4	SIA	P	2	4	20,20,21	0.80	1 (5%)	21,28,31	0.82	1 (4%)

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	GAL	D	1	4	-	2/2/19/22	0/1/1/1
4	SIA	D	2	4	-	4/18/34/38	0/1/1/1
4	GAL	E	1	4	-	2/2/19/22	0/1/1/1
4	SIA	E	2	4	-	10/18/34/38	0/1/1/1
4	GAL	P	1	4	-	2/2/19/22	0/1/1/1
4	SIA	P	2	4	-	0/18/34/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	SIA	O1B-C1	-3.25	1.20	1.30
4	P	2	SIA	O1B-C1	-3.06	1.20	1.30
4	D	2	SIA	O1B-C1	-3.06	1.20	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	GAL	C3-C4-C5	-3.38	104.10	110.23
4	E	1	GAL	C2-C3-C4	-3.24	105.17	110.86
4	D	1	GAL	C2-C3-C4	-2.79	105.96	110.86
4	P	1	GAL	C2-C3-C4	-2.72	106.09	110.86
4	P	1	GAL	C1-O5-C5	2.63	115.71	112.19
4	P	2	SIA	O1B-C1-C2	2.38	118.91	112.71
4	D	2	SIA	O1B-C1-C2	2.32	118.73	112.71
4	E	2	SIA	O1B-C1-C2	2.31	118.71	112.71
4	D	1	GAL	C1-O5-C5	2.22	115.16	112.19
4	P	1	GAL	C1-C2-C3	-2.20	106.44	109.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	SIA	O6-C6-C7-O7
4	E	2	SIA	C5-C6-C7-O7
4	E	2	SIA	O6-C6-C7-O7
4	E	2	SIA	O8-C8-C9-O9
4	D	1	GAL	C4-C5-C6-O6
4	D	1	GAL	O5-C5-C6-O6
4	P	1	GAL	O5-C5-C6-O6
4	E	2	SIA	C6-C7-C8-C9
4	E	1	GAL	O5-C5-C6-O6
4	E	1	GAL	C4-C5-C6-O6
4	E	2	SIA	C7-C8-C9-O9
4	E	2	SIA	O7-C7-C8-C9
4	P	1	GAL	C4-C5-C6-O6
4	E	2	SIA	O7-C7-C8-O8
4	E	2	SIA	C6-C7-C8-O8
4	E	2	SIA	O6-C6-C7-C8
4	D	2	SIA	C5-C6-C7-C8
4	E	2	SIA	C5-C6-C7-C8
4	D	2	SIA	C5-C6-C7-O7

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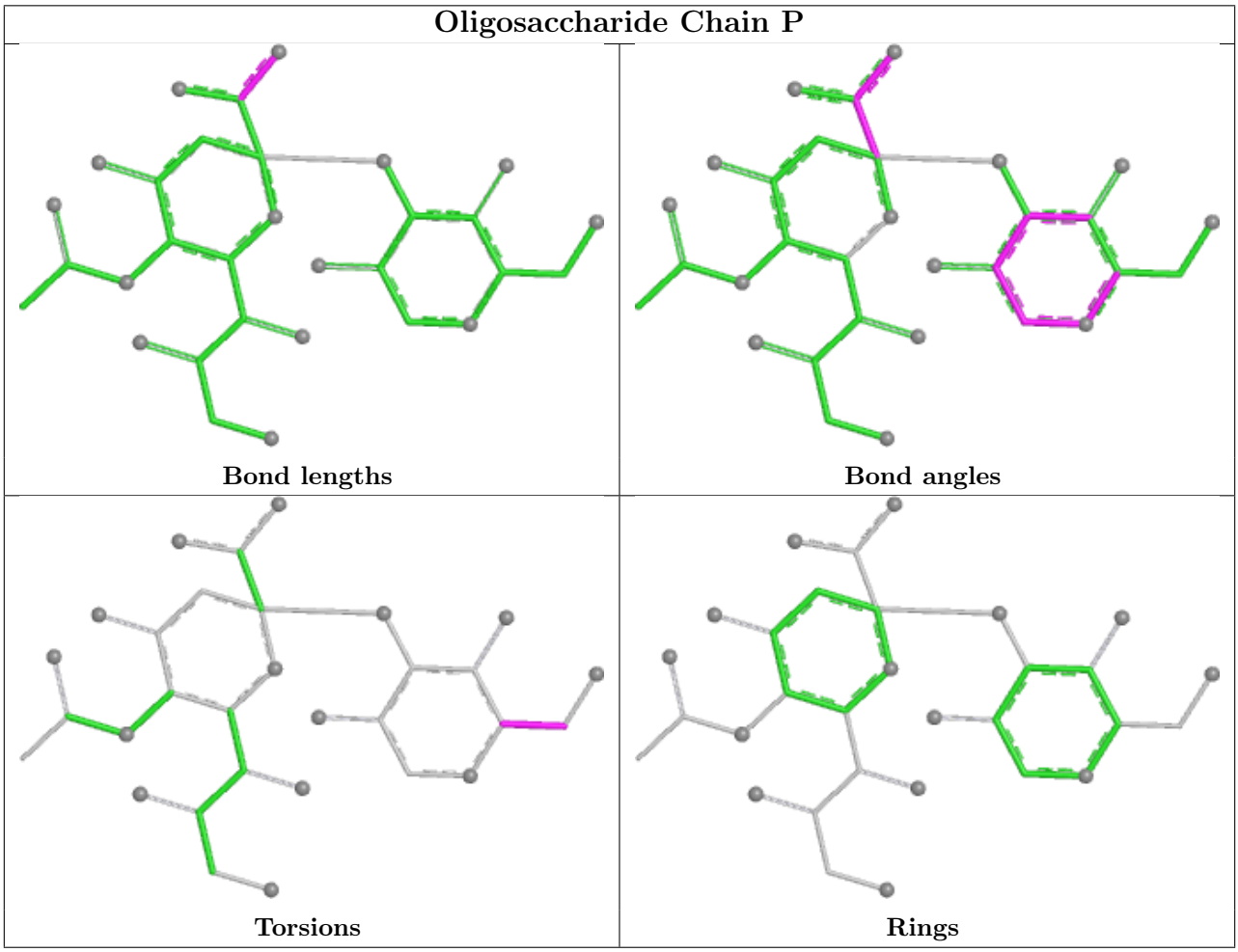
Mol	Chain	Res	Type	Atoms
4	D	2	SIA	O6-C6-C7-C8

There are no ring outliers.

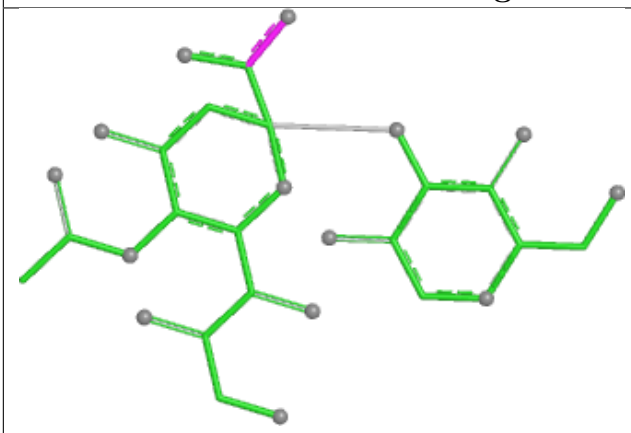
4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	SIA	10	0
4	D	2	SIA	7	0
4	P	2	SIA	6	0
4	P	1	GAL	1	0

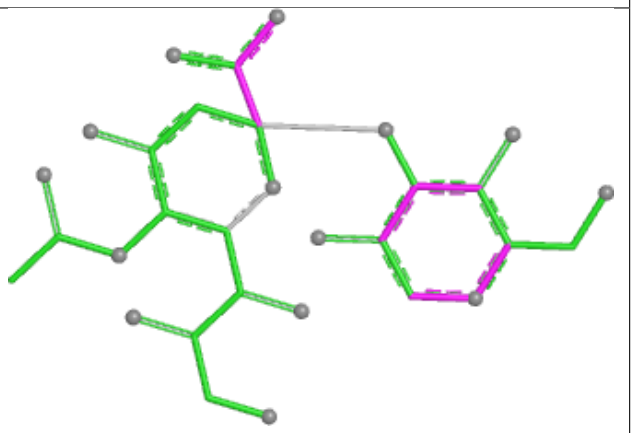
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



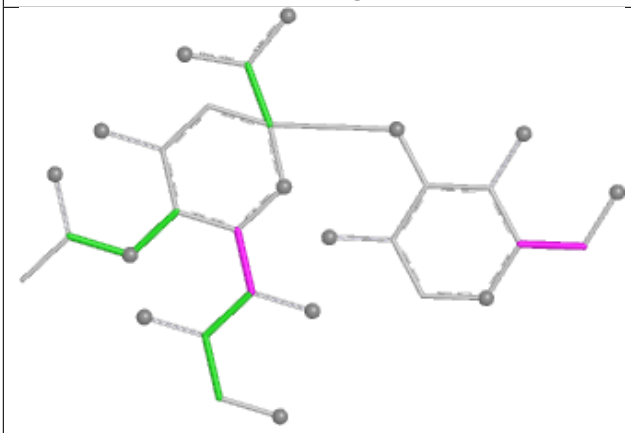
Oligosaccharide Chain D



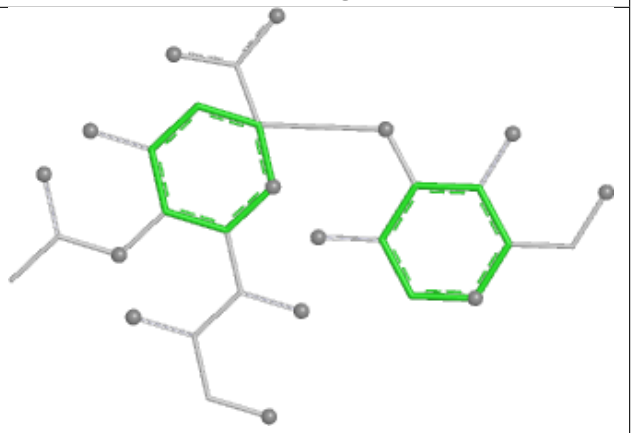
Bond lengths



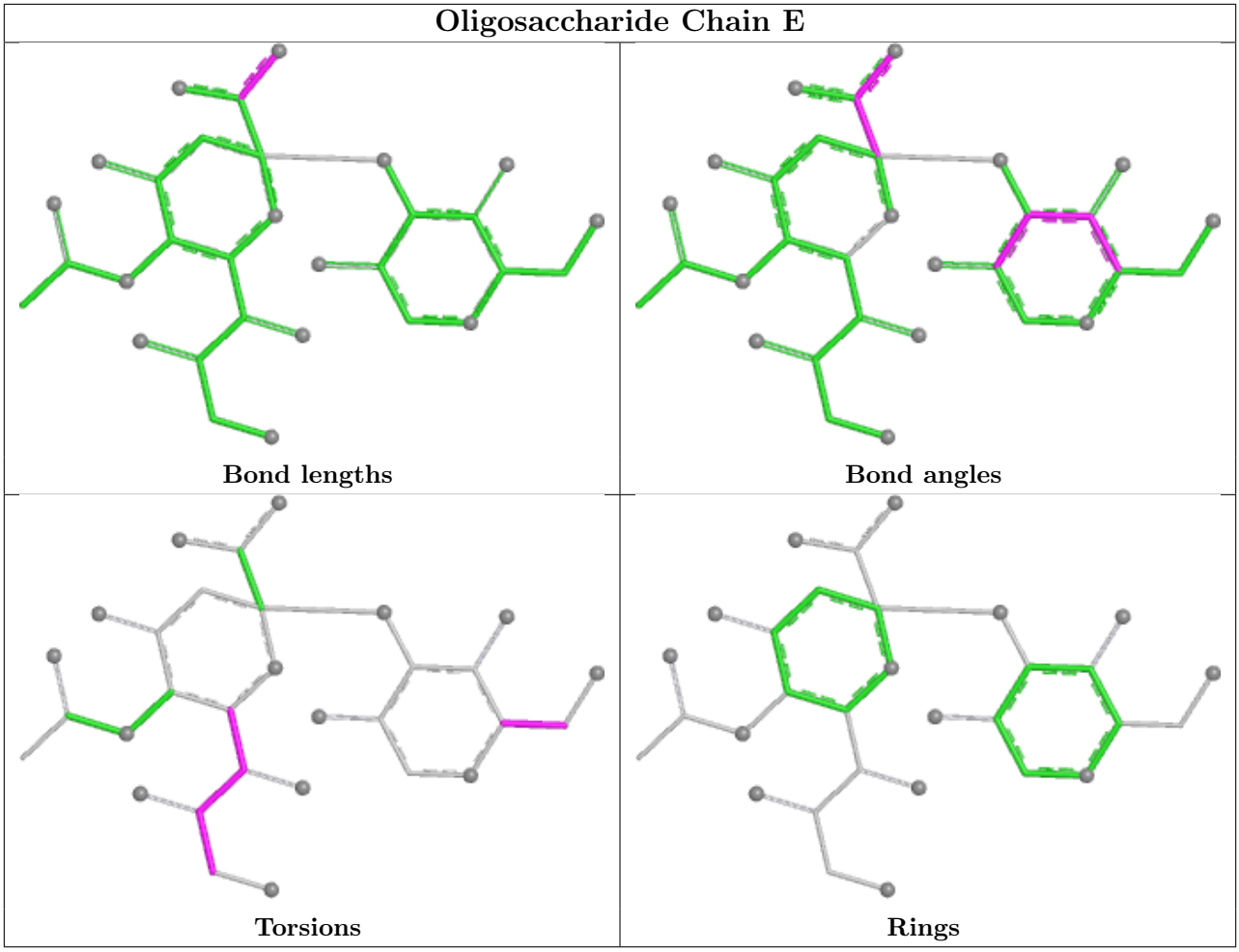
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

15 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	A	601	3	14,14,15	0.72	0	17,19,21	0.87	0
5	NAG	A	604	3	14,14,15	0.71	0	17,19,21	1.11	1 (5%)
5	NAG	C	605	3	14,14,15	0.82	1 (7%)	17,19,21	1.97	3 (17%)
5	NAG	B	601	3	14,14,15	0.77	0	17,19,21	1.05	1 (5%)
5	NAG	A	605	3	14,14,15	0.85	1 (7%)	17,19,21	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	604	3	14,14,15	0.75	0	17,19,21	0.79	0
5	NAG	C	604	3	14,14,15	0.76	0	17,19,21	0.85	0
5	NAG	B	603	3	14,14,15	0.73	0	17,19,21	1.38	2 (11%)
5	NAG	C	603	3	14,14,15	0.73	0	17,19,21	1.10	1 (5%)
5	NAG	A	602	3	14,14,15	0.70	0	17,19,21	1.03	1 (5%)
5	NAG	A	603	3	14,14,15	0.71	0	17,19,21	1.31	2 (11%)
5	NAG	C	601	3	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
5	NAG	C	602	3	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
5	NAG	B	605	3	14,14,15	0.77	0	17,19,21	1.55	2 (11%)
5	NAG	B	602	3	14,14,15	0.89	1 (7%)	17,19,21	1.19	3 (17%)

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	A	601	3	-	0/6/23/26	0/1/1/1
5	NAG	A	604	3	-	0/6/23/26	0/1/1/1
5	NAG	C	605	3	-	0/6/23/26	0/1/1/1
5	NAG	B	601	3	-	0/6/23/26	0/1/1/1
5	NAG	A	605	3	-	0/6/23/26	0/1/1/1
5	NAG	B	604	3	-	1/6/23/26	0/1/1/1
5	NAG	C	604	3	-	1/6/23/26	0/1/1/1
5	NAG	B	603	3	-	4/6/23/26	0/1/1/1
5	NAG	C	603	3	-	0/6/23/26	0/1/1/1
5	NAG	A	602	3	-	0/6/23/26	0/1/1/1
5	NAG	A	603	3	-	2/6/23/26	0/1/1/1
5	NAG	C	601	3	-	1/6/23/26	0/1/1/1
5	NAG	C	602	3	-	0/6/23/26	0/1/1/1
5	NAG	B	605	3	-	1/6/23/26	0/1/1/1
5	NAG	B	602	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	NAG	C1-C2	2.24	1.55	1.52
5	B	602	NAG	C1-C2	2.18	1.55	1.52
5	C	605	NAG	C1-C2	2.09	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	605	NAG	C1-O5-C5	6.29	120.61	112.19
5	B	605	NAG	C2-N2-C7	4.50	128.94	122.90
5	B	603	NAG	C1-O5-C5	3.50	116.88	112.19
5	A	604	NAG	C1-O5-C5	3.31	116.62	112.19
5	A	603	NAG	C1-O5-C5	3.21	116.48	112.19
5	C	603	NAG	C1-O5-C5	3.20	116.47	112.19
5	B	603	NAG	C2-N2-C7	3.17	127.15	122.90
5	A	603	NAG	C2-N2-C7	3.03	126.97	122.90
5	B	605	NAG	C4-C3-C2	2.89	115.25	111.02
5	B	601	NAG	C1-O5-C5	2.87	116.03	112.19
5	C	605	NAG	C2-N2-C7	2.59	126.37	122.90
5	A	602	NAG	C1-O5-C5	2.43	115.45	112.19
5	C	602	NAG	C1-O5-C5	2.40	115.40	112.19
5	C	605	NAG	C4-C3-C2	2.31	114.40	111.02
5	B	602	NAG	C4-C3-C2	2.26	114.33	111.02
5	C	601	NAG	C1-O5-C5	2.12	115.03	112.19
5	B	602	NAG	C1-O5-C5	2.07	114.96	112.19
5	B	602	NAG	O5-C1-C2	-2.05	108.12	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	603	NAG	O5-C5-C6-O6
5	B	603	NAG	C4-C5-C6-O6
5	A	603	NAG	C8-C7-N2-C2
5	A	603	NAG	O7-C7-N2-C2
5	B	603	NAG	C8-C7-N2-C2
5	B	603	NAG	O7-C7-N2-C2
5	C	601	NAG	O5-C5-C6-O6
5	B	605	NAG	O5-C5-C6-O6
5	B	604	NAG	O5-C5-C6-O6
5	C	604	NAG	O5-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.

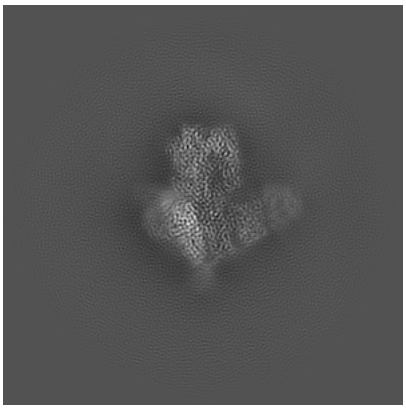
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47241. These allow visual inspection of the internal detail of the map and identification of artifacts.

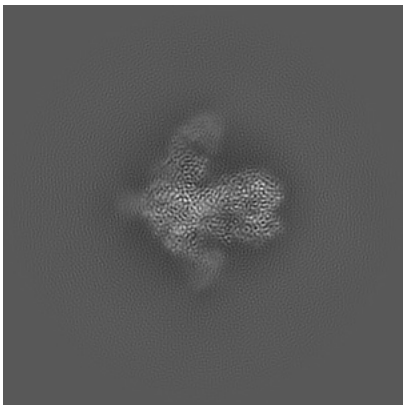
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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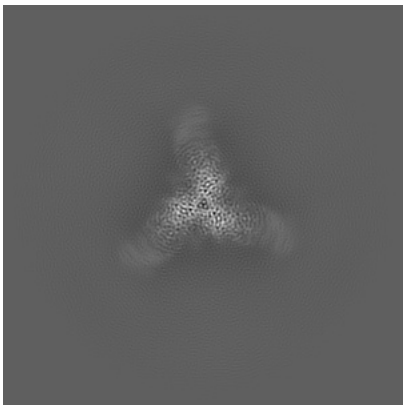
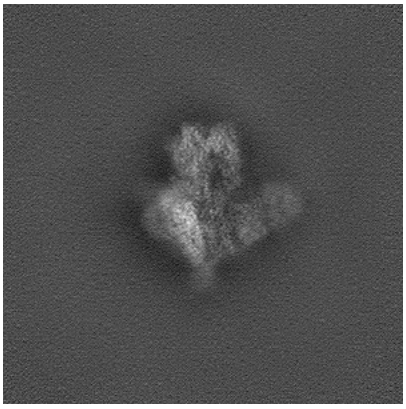


Z

6.1.2 Raw map



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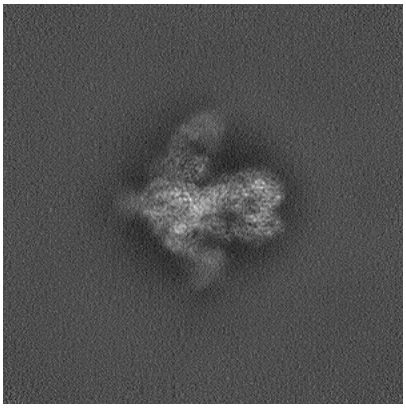

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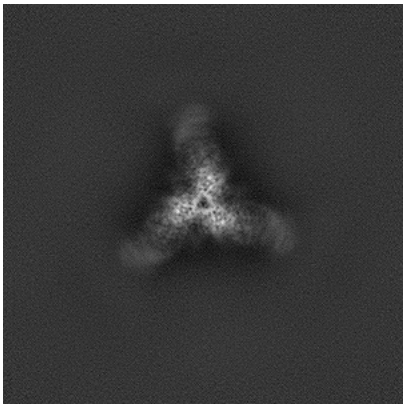
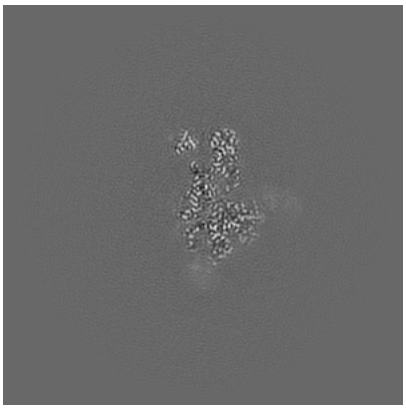


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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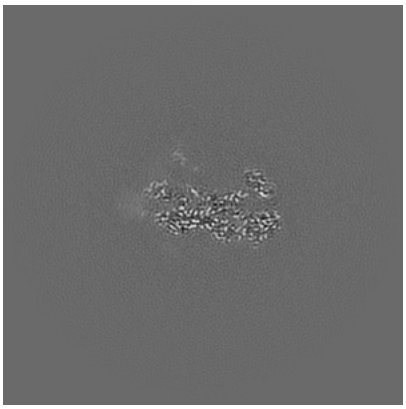
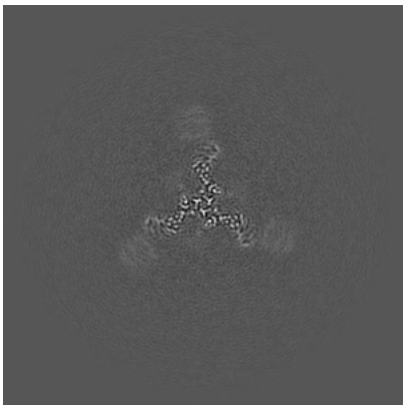
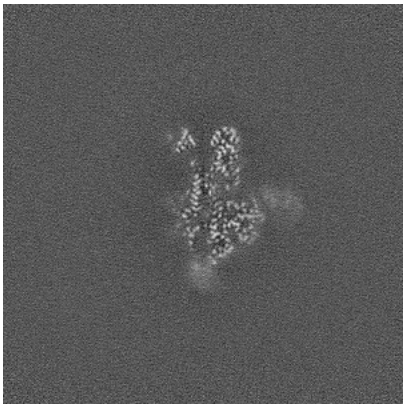


Y Index: 256



Z Index: 256

6.2.2 Raw map



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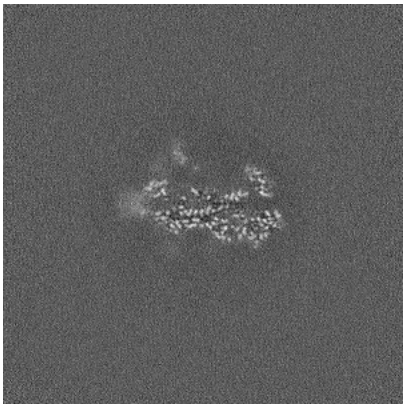

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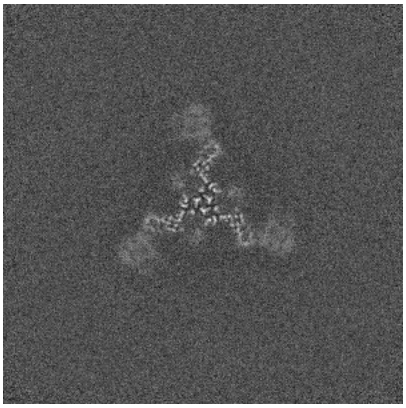
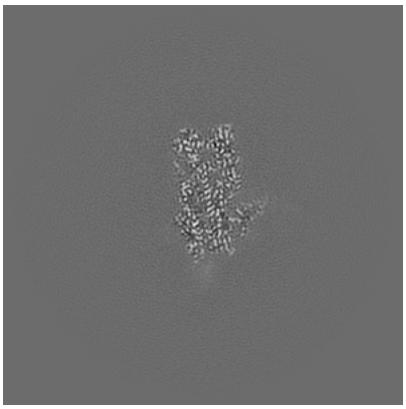


Z Index: 256

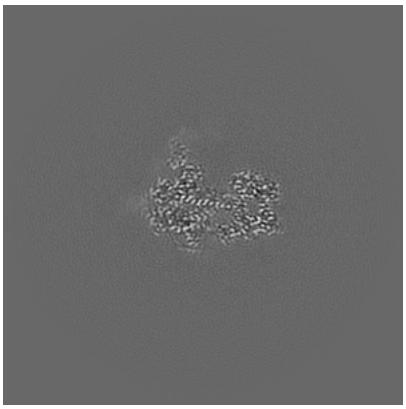
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 266



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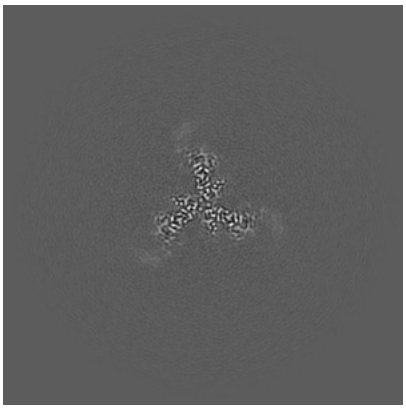
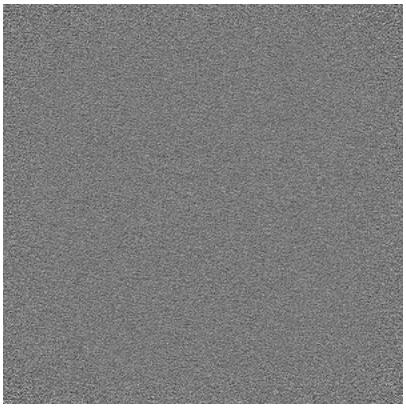
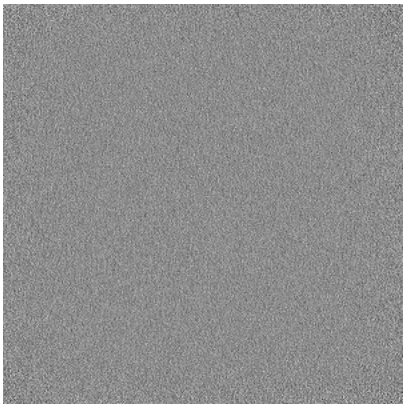


Z Index: 233

6.3.2 Raw map



X Index: 0



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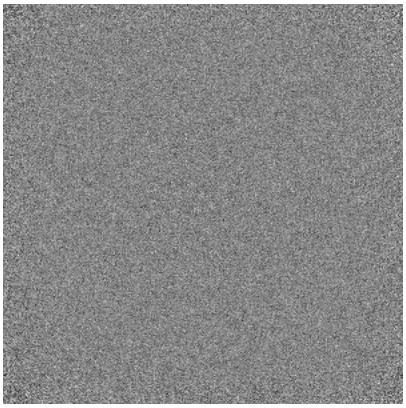
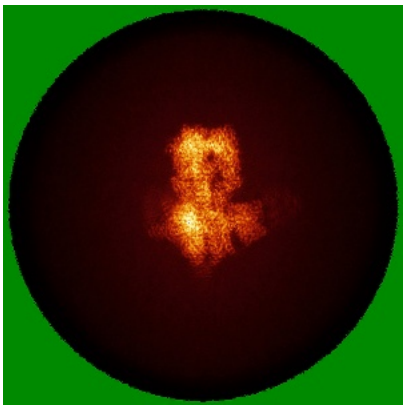


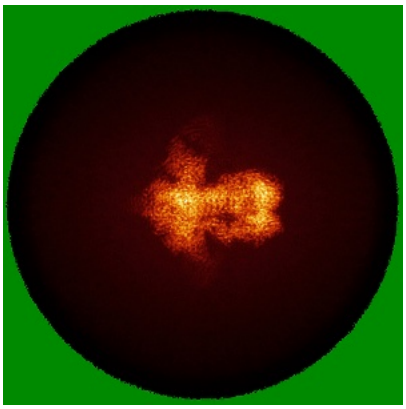
Z Index: 511

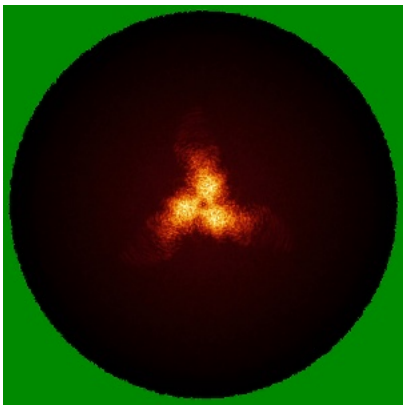
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

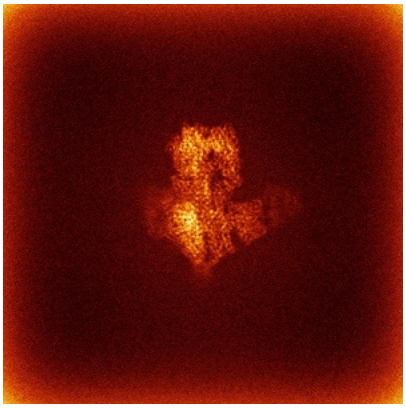
6.4.1 Primary map

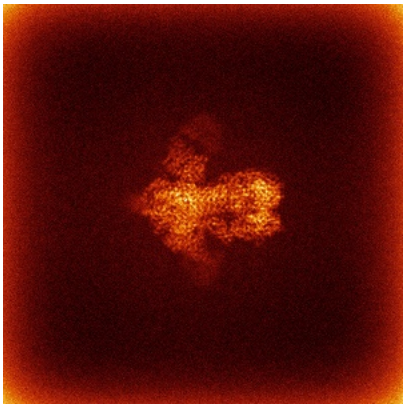

X

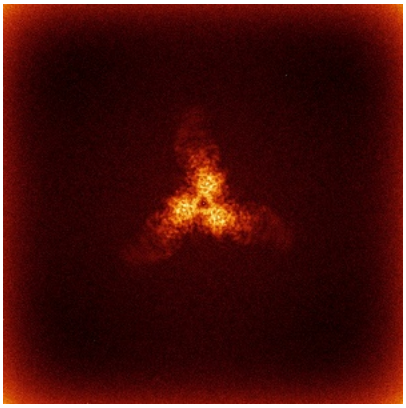

Y


Z

6.4.2 Raw map


X

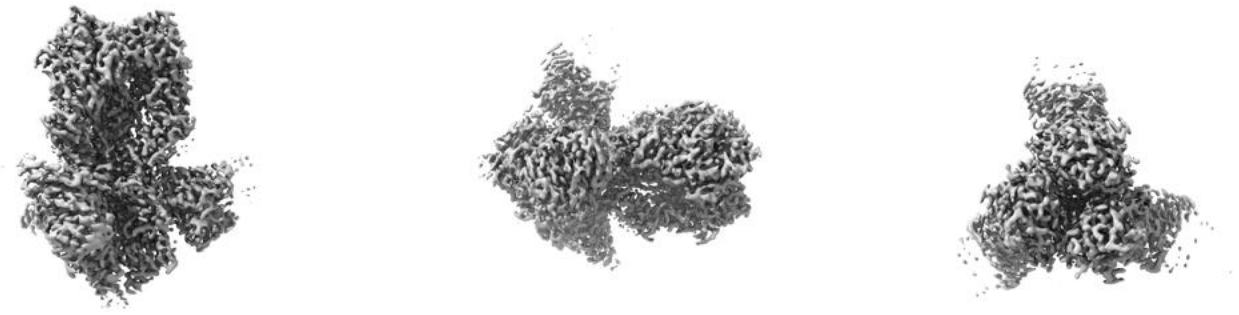

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.173. 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

X Y Z

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.

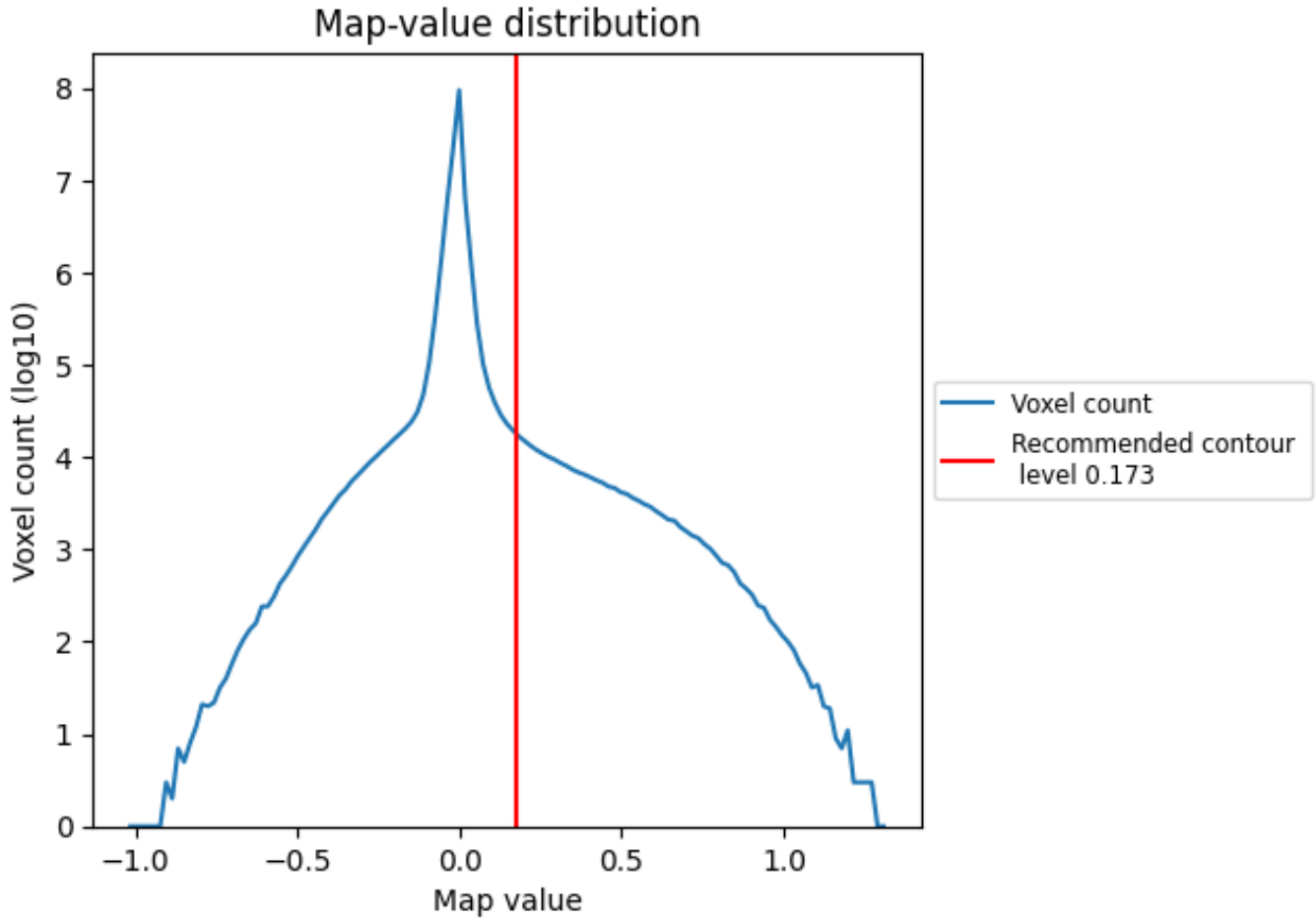
6.6 Mask visualisation (i)

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

7 Map analysis

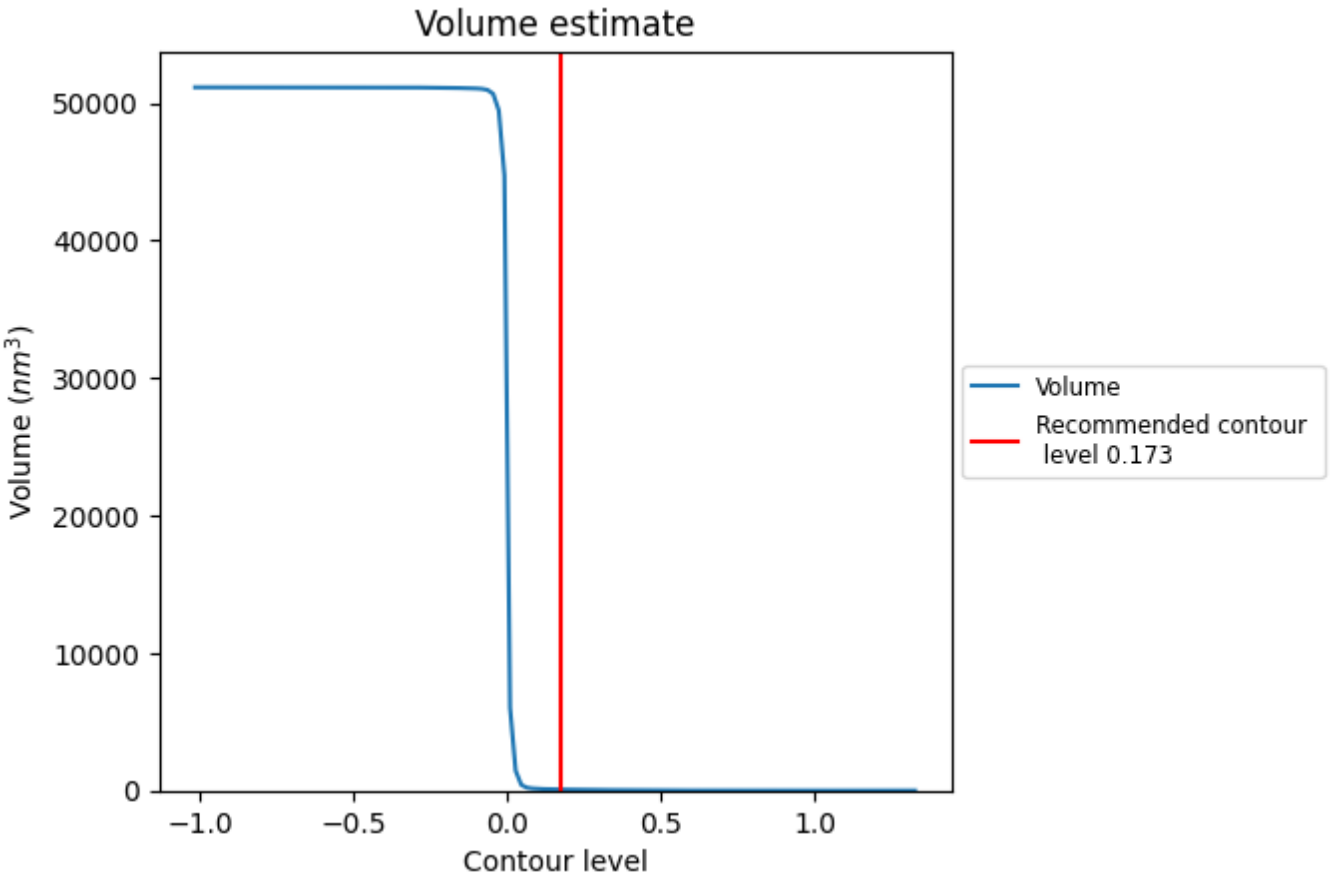
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

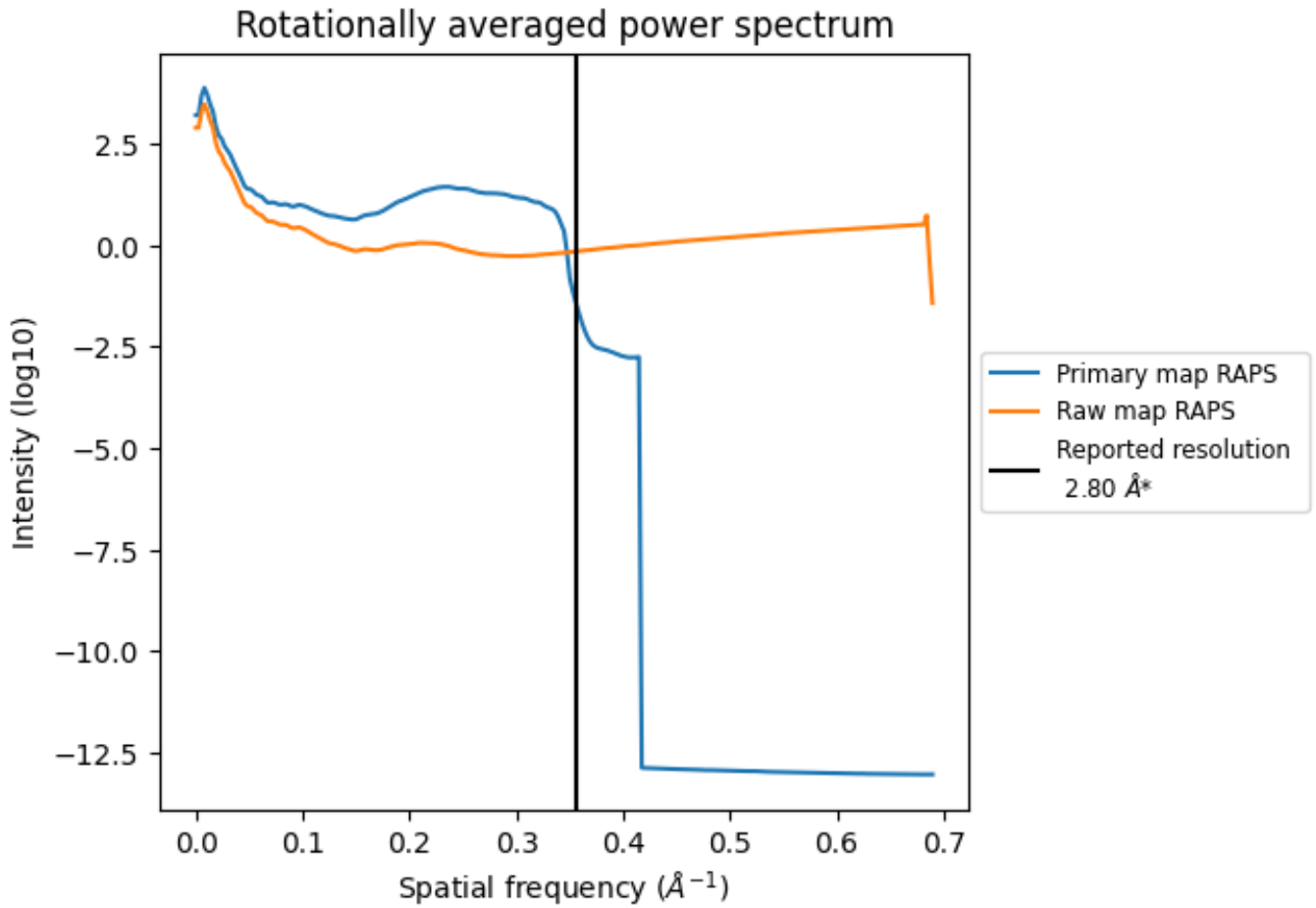
7.2 Volume estimate



The volume at the recommended contour level is 78 nm^3; this corresponds to an approximate mass of 71 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 (i)

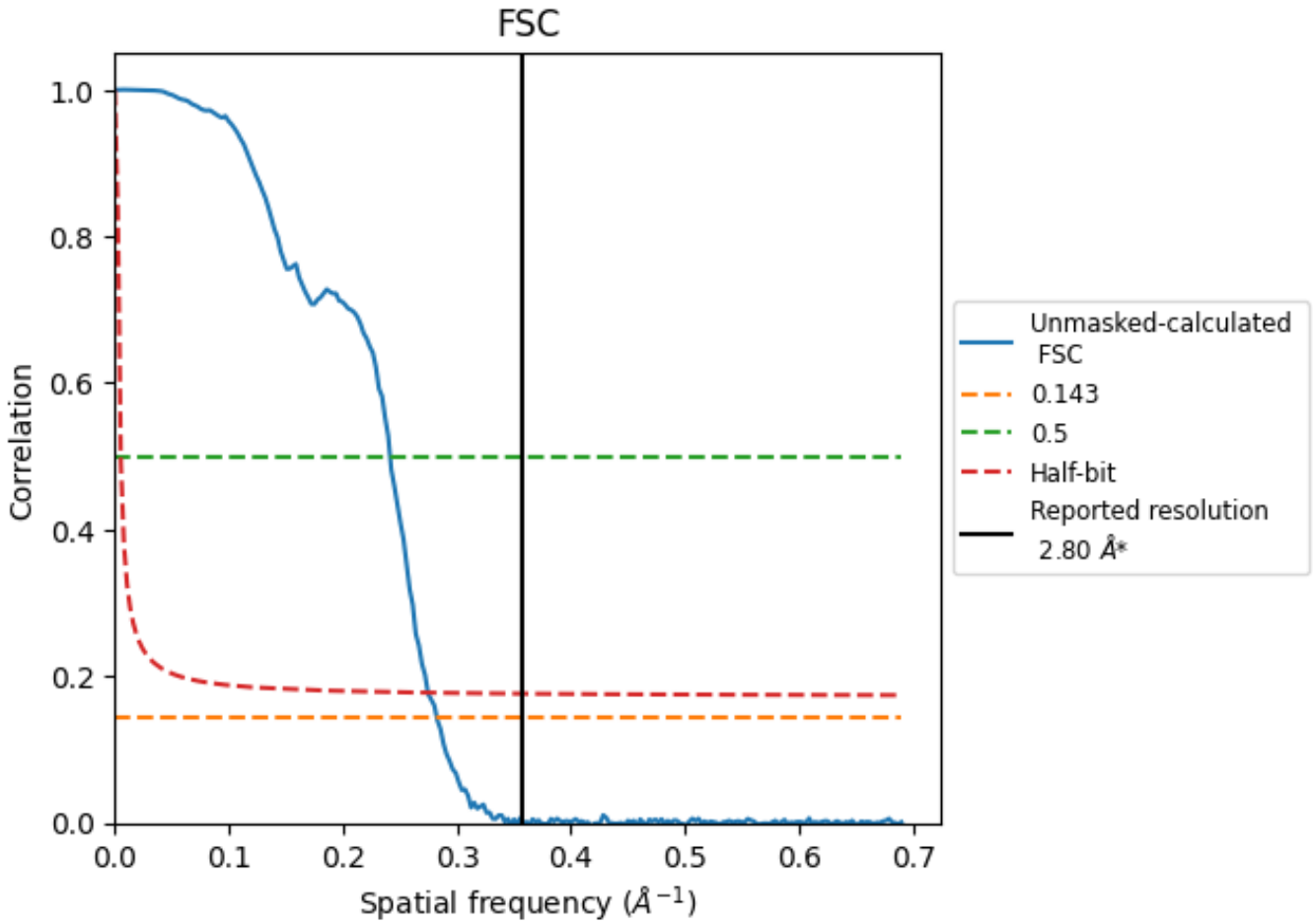


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

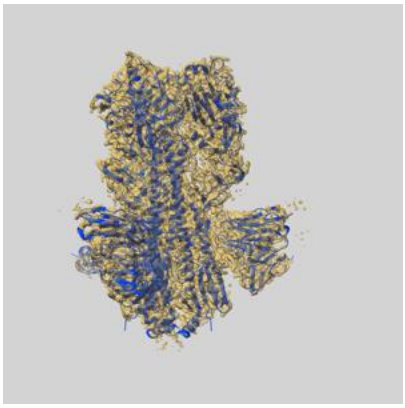
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.14	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 2.8 by more than 10 %

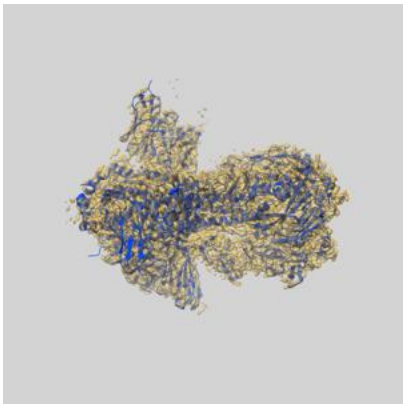
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47241 and PDB model 9DWE. Per-residue inclusion information can be found in section 3 on page 11.

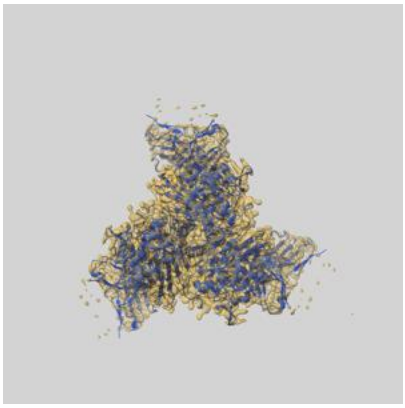
9.1 Map-model overlay



X



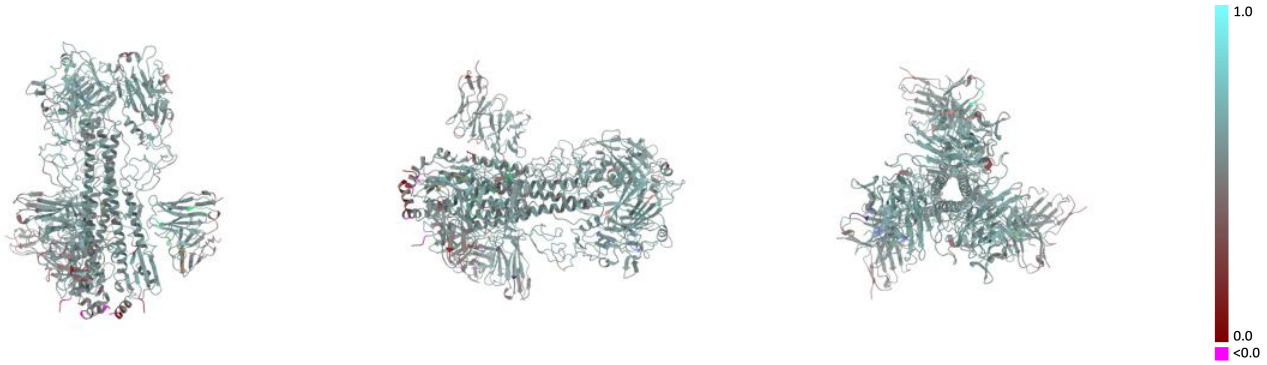
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.173 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.

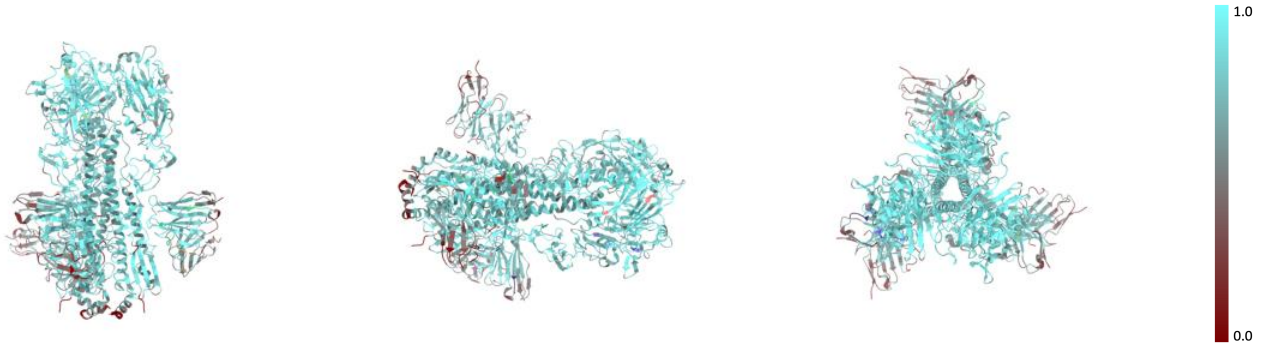
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

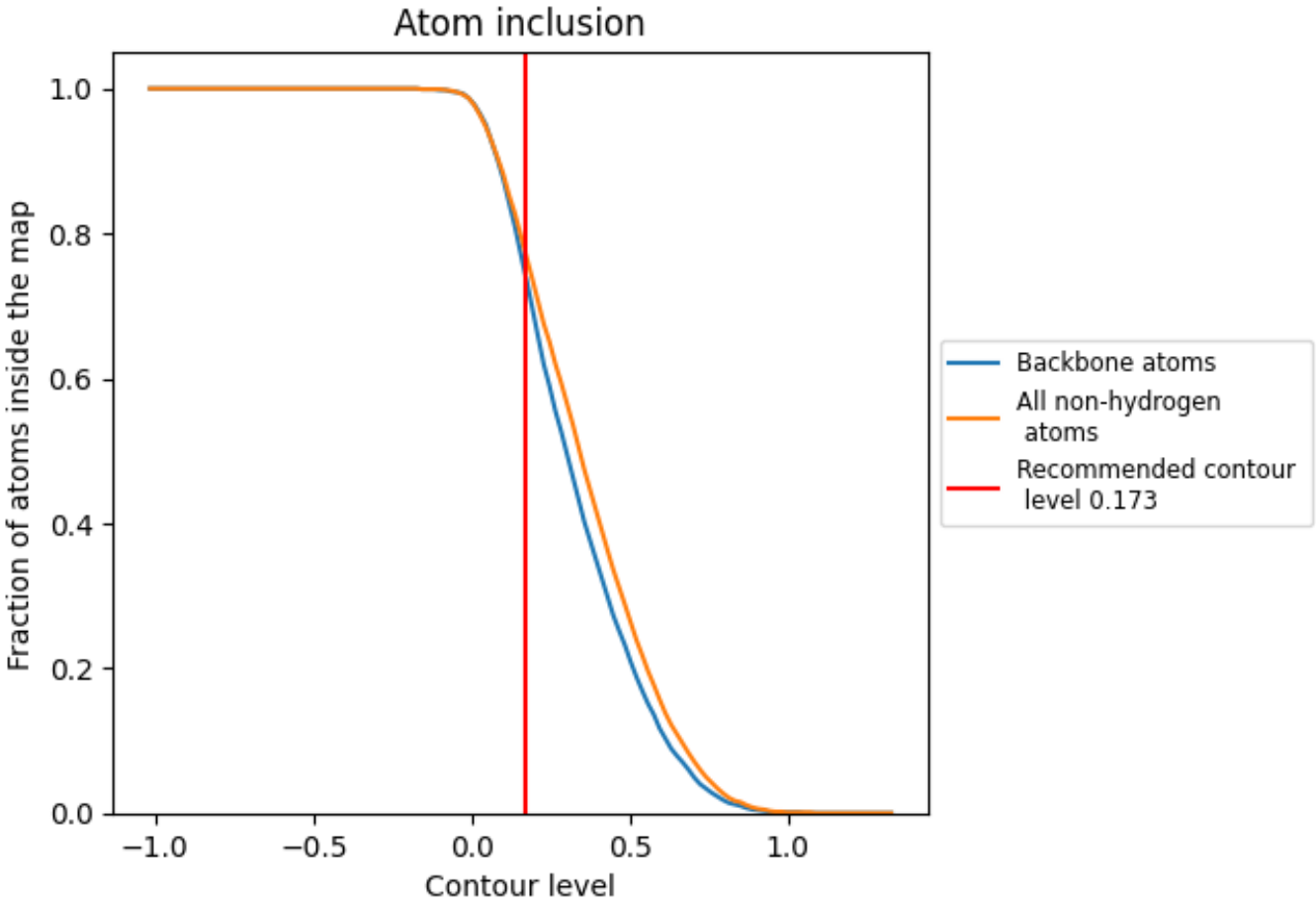
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.173).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 77% 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 (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7700	0.5590
A	0.8190	0.5740
B	0.8130	0.5660
C	0.8190	0.5690
D	0.7740	0.5470
E	0.8060	0.5450
H	0.7600	0.5690
I	0.7620	0.5710
J	0.7610	0.5670
L	0.5890	0.4930
M	0.5920	0.4950
N	0.5800	0.4930
P	0.7420	0.5260