



wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 03:34 AM EDT

PDB ID : 8TGV
EMDB ID : EMD-41245
Title : CryoEM structure of Fab HC84.26-HCV E2 complex
Authors : Shahid, S.; Liqun, J.; Liu, Y.; Hasan, S.S.; Mariuzza, R.A.
Deposited on : 2023-07-13
Resolution : 3.75 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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 : 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) : 2.39

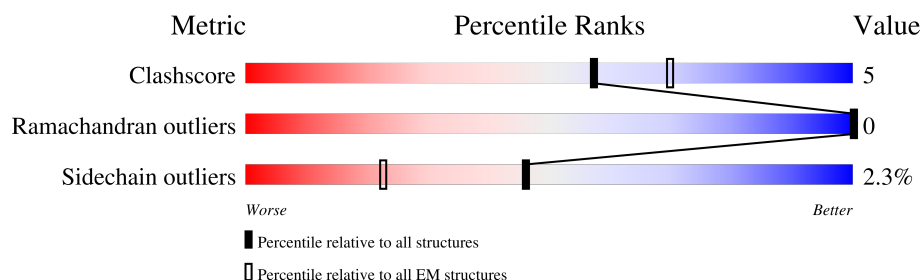
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.75 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	291	
1	D	291	
1	G	291	
2	B	255	
2	E	255	
2	I	255	
2	K	255	
3	C	234	

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Mol	Chain	Length	Quality of chain
3	F	234	<div><div></div><div>82%</div><div>9%</div><div>9%</div></div>
3	J	234	<div><div></div><div>84%</div><div>7%</div><div>9%</div></div>
3	L	234	<div><div></div><div>80%</div><div>7%</div><div>13%</div></div>
4	Z	3	<div><div></div><div>67%</div><div>33%</div></div>
5	H	2	<div><div></div><div>100%</div></div>
5	M	2	<div><div></div><div>50%</div><div>50%</div></div>
5	N	2	<div><div></div><div>50%</div><div>50%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31782 atoms, of which 15262 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 envelope glycoprotein E2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	218	Total	C	H	N	O	S	0	0
			2998	1016	1401	279	283	19		
1	D	174	Total	C	H	N	O	S	0	0
			2176	761	974	213	213	15		
1	G	170	Total	C	H	N	O	S	0	0
			2223	775	1012	212	206	18		

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	MET	-	initiating methionine	UNP X4ZFY7
A	364	GLU	-	expression tag	UNP X4ZFY7
A	365	THR	-	expression tag	UNP X4ZFY7
A	366	ASP	-	expression tag	UNP X4ZFY7
A	367	THR	-	expression tag	UNP X4ZFY7
A	368	LEU	-	expression tag	UNP X4ZFY7
A	369	LEU	-	expression tag	UNP X4ZFY7
A	370	LEU	-	expression tag	UNP X4ZFY7
A	371	TRP	-	expression tag	UNP X4ZFY7
A	372	VAL	-	expression tag	UNP X4ZFY7
A	373	LEU	-	expression tag	UNP X4ZFY7
A	374	LEU	-	expression tag	UNP X4ZFY7
A	375	LEU	-	expression tag	UNP X4ZFY7
A	376	TRP	-	expression tag	UNP X4ZFY7
A	377	VAL	-	expression tag	UNP X4ZFY7
A	378	PRO	-	expression tag	UNP X4ZFY7
A	379	GLY	-	expression tag	UNP X4ZFY7
A	380	SER	-	expression tag	UNP X4ZFY7
A	381	THR	-	expression tag	UNP X4ZFY7
A	382	GLY	-	expression tag	UNP X4ZFY7
A	383	ASP	-	expression tag	UNP X4ZFY7
A	646	ILE	-	expression tag	UNP X4ZFY7
A	647	GLY	-	expression tag	UNP X4ZFY7
A	648	HIS	-	expression tag	UNP X4ZFY7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	649	HIS	-	expression tag	UNP X4ZFY7
A	650	HIS	-	expression tag	UNP X4ZFY7
A	651	HIS	-	expression tag	UNP X4ZFY7
A	652	HIS	-	expression tag	UNP X4ZFY7
A	653	HIS	-	expression tag	UNP X4ZFY7
D	363	MET	-	initiating methionine	UNP X4ZFY7
D	364	GLU	-	expression tag	UNP X4ZFY7
D	365	THR	-	expression tag	UNP X4ZFY7
D	366	ASP	-	expression tag	UNP X4ZFY7
D	367	THR	-	expression tag	UNP X4ZFY7
D	368	LEU	-	expression tag	UNP X4ZFY7
D	369	LEU	-	expression tag	UNP X4ZFY7
D	370	LEU	-	expression tag	UNP X4ZFY7
D	371	TRP	-	expression tag	UNP X4ZFY7
D	372	VAL	-	expression tag	UNP X4ZFY7
D	373	LEU	-	expression tag	UNP X4ZFY7
D	374	LEU	-	expression tag	UNP X4ZFY7
D	375	LEU	-	expression tag	UNP X4ZFY7
D	376	TRP	-	expression tag	UNP X4ZFY7
D	377	VAL	-	expression tag	UNP X4ZFY7
D	378	PRO	-	expression tag	UNP X4ZFY7
D	379	GLY	-	expression tag	UNP X4ZFY7
D	380	SER	-	expression tag	UNP X4ZFY7
D	381	THR	-	expression tag	UNP X4ZFY7
D	382	GLY	-	expression tag	UNP X4ZFY7
D	383	ASP	-	expression tag	UNP X4ZFY7
D	646	ILE	-	expression tag	UNP X4ZFY7
D	647	GLY	-	expression tag	UNP X4ZFY7
D	648	HIS	-	expression tag	UNP X4ZFY7
D	649	HIS	-	expression tag	UNP X4ZFY7
D	650	HIS	-	expression tag	UNP X4ZFY7
D	651	HIS	-	expression tag	UNP X4ZFY7
D	652	HIS	-	expression tag	UNP X4ZFY7
D	653	HIS	-	expression tag	UNP X4ZFY7
G	363	MET	-	initiating methionine	UNP X4ZFY7
G	364	GLU	-	expression tag	UNP X4ZFY7
G	365	THR	-	expression tag	UNP X4ZFY7
G	366	ASP	-	expression tag	UNP X4ZFY7
G	367	THR	-	expression tag	UNP X4ZFY7
G	368	LEU	-	expression tag	UNP X4ZFY7
G	369	LEU	-	expression tag	UNP X4ZFY7
G	370	LEU	-	expression tag	UNP X4ZFY7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	371	TRP	-	expression tag	UNP X4ZFY7
G	372	VAL	-	expression tag	UNP X4ZFY7
G	373	LEU	-	expression tag	UNP X4ZFY7
G	374	LEU	-	expression tag	UNP X4ZFY7
G	375	LEU	-	expression tag	UNP X4ZFY7
G	376	TRP	-	expression tag	UNP X4ZFY7
G	377	VAL	-	expression tag	UNP X4ZFY7
G	378	PRO	-	expression tag	UNP X4ZFY7
G	379	GLY	-	expression tag	UNP X4ZFY7
G	380	SER	-	expression tag	UNP X4ZFY7
G	381	THR	-	expression tag	UNP X4ZFY7
G	382	GLY	-	expression tag	UNP X4ZFY7
G	383	ASP	-	expression tag	UNP X4ZFY7
G	646	ILE	-	expression tag	UNP X4ZFY7
G	647	GLY	-	expression tag	UNP X4ZFY7
G	648	HIS	-	expression tag	UNP X4ZFY7
G	649	HIS	-	expression tag	UNP X4ZFY7
G	650	HIS	-	expression tag	UNP X4ZFY7
G	651	HIS	-	expression tag	UNP X4ZFY7
G	652	HIS	-	expression tag	UNP X4ZFY7
G	653	HIS	-	expression tag	UNP X4ZFY7

- Molecule 2 is a protein called HC84.26 Heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	212	Total	C	H	N	O	S	0	0
			3091	993	1516	263	311	8		
2	B	214	Total	C	H	N	O	S	0	0
			3040	985	1482	261	304	8		
2	I	213	Total	C	H	N	O	S	0	0
			3084	996	1511	260	309	8		
2	K	192	Total	C	H	N	O	S	0	0
			2709	884	1322	232	263	8		

- Molecule 3 is a protein called HC84.26 Light chain.

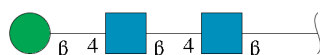
Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	213	Total	C	H	N	O	S	0	0
			3151	1002	1544	270	329	6		
3	C	213	Total	C	H	N	O	S	0	0
			3130	999	1530	269	326	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	J	213	Total	C	H	N	O	S	0	0
			3132	999	1530	269	328	6		
3	L	204	Total	C	H	N	O	S	0	0
			2789	918	1318	248	299	6		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

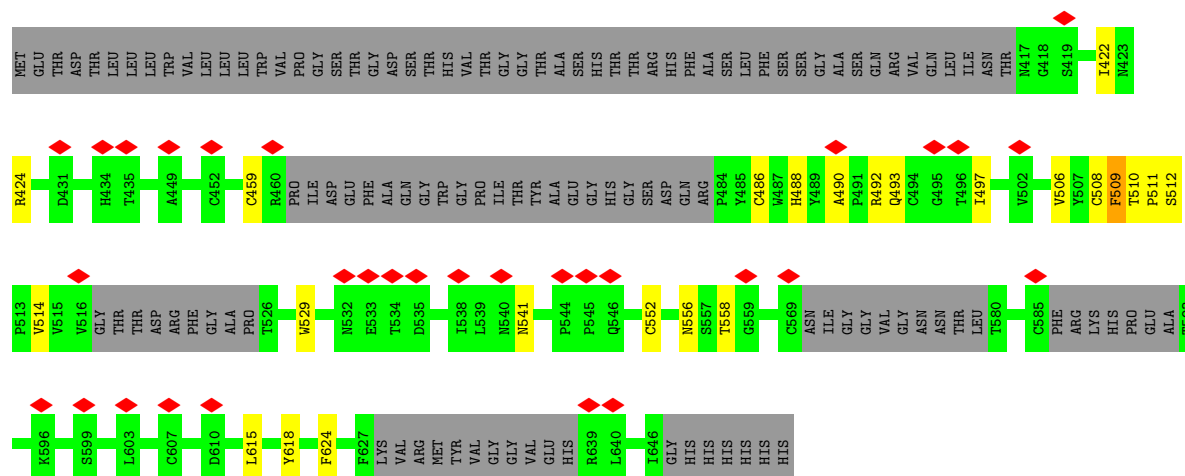


Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
5	M	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
5	N	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

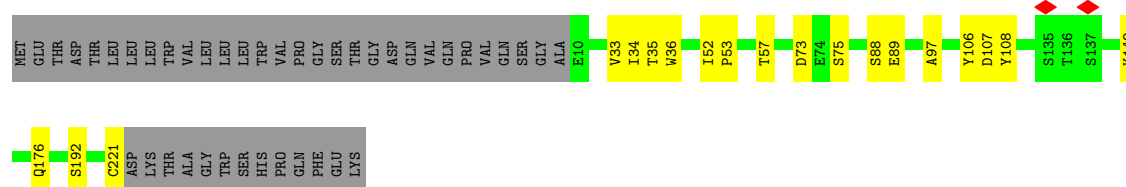
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



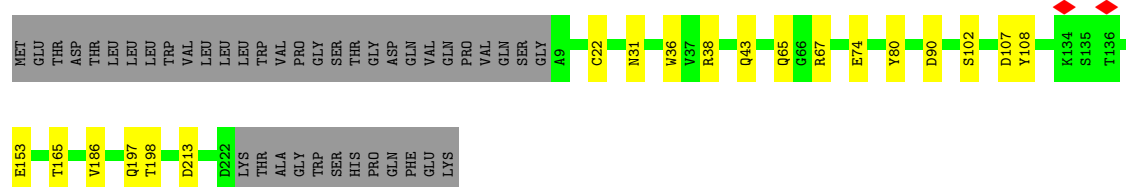
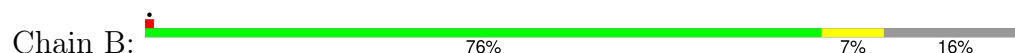
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
6	A	1	27	8	13	1	5	0



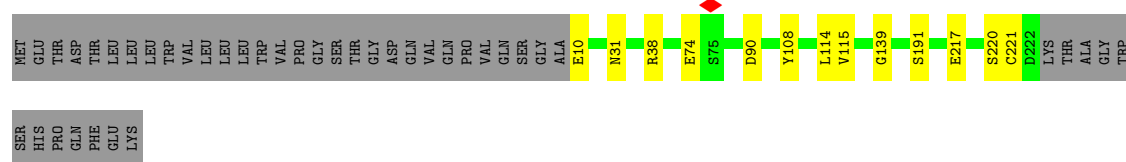
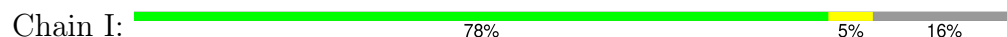
- Molecule 2: HC84.26 Heavy chain



- Molecule 2: HC84.26 Heavy chain

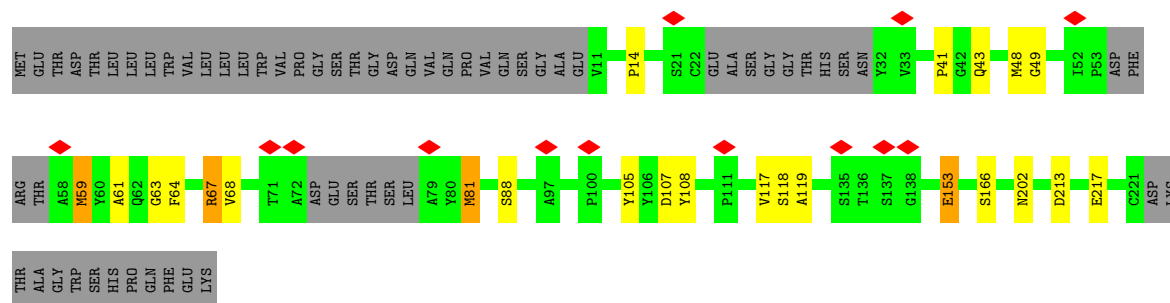


- Molecule 2: HC84.26 Heavy chain



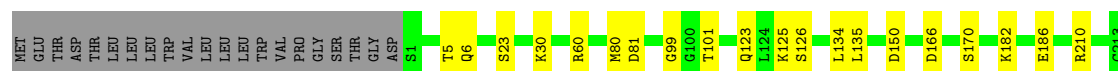
- Molecule 2: HC84.26 Heavy chain





- Molecule 3: HC84.26 Light chain

Chain F: 82% 9% 9%



- Molecule 3: HC84.26 Light chain

Chain C: 83% 8% 9%



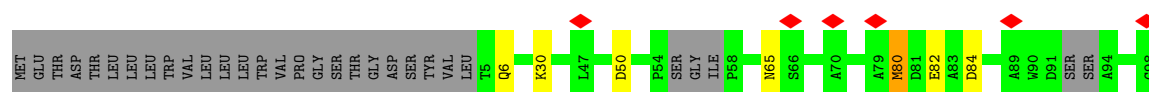
- Molecule 3: HC84.26 Light chain

Chain J: 84% 7% 9%



- Molecule 3: HC84.26 Light chain

Chain L: 80% 7% 13%



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

Chain Z: 67% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50%  50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50%  50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.758	Depositor
Minimum map value	-2.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	380.8, 380.8, 380.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4875, 1.4875, 1.4875	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/1652	0.49	0/2271
1	D	0.26	0/1242	0.48	0/1713
1	G	0.25	0/1253	0.47	0/1722
2	B	0.26	0/1599	0.49	0/2189
2	E	0.28	0/1616	0.49	0/2208
2	I	0.27	0/1614	0.48	0/2206
2	K	0.26	0/1422	0.48	0/1943
3	C	0.27	0/1635	0.47	0/2229
3	F	0.28	0/1642	0.46	0/2237
3	J	0.27	0/1637	0.47	0/2232
3	L	0.26	0/1503	0.45	0/2056
All	All	0.27	0/16815	0.48	0/23006

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1597	1401	1401	19	0
1	D	1202	974	974	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1211	1012	1012	16	0
2	B	1558	1482	1482	17	0
2	E	1575	1516	1516	12	0
2	I	1573	1511	1511	8	0
2	K	1387	1322	1322	15	0
3	C	1600	1530	1532	10	0
3	F	1607	1544	1546	11	0
3	J	1602	1530	1532	8	0
3	L	1471	1318	1318	11	0
4	Z	39	34	34	1	0
5	H	28	25	25	5	0
5	M	28	25	25	0	0
5	N	28	25	25	1	0
6	A	14	13	13	1	0
All	All	16520	15262	15268	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 146 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:F:123:GLN:O	3:F:126:SER:OG	1.99	0.80
1:D:416:THR:N	1:D:515:VAL:O	2.17	0.78
2:I:38:ARG:NH1	2:I:90:ASP:OD1	2.18	0.76
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.20	0.75
2:E:89:GLU:OE1	2:E:89:GLU:N	2.20	0.74

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	212/291 (73%)	194 (92%)	18 (8%)	0	100	100
1	D	162/291 (56%)	154 (95%)	8 (5%)	0	100	100
1	G	158/291 (54%)	147 (93%)	11 (7%)	0	100	100
2	B	212/255 (83%)	192 (91%)	20 (9%)	0	100	100
2	E	210/255 (82%)	196 (93%)	14 (7%)	0	100	100
2	I	211/255 (83%)	197 (93%)	14 (7%)	0	100	100
2	K	184/255 (72%)	175 (95%)	9 (5%)	0	100	100
3	C	211/234 (90%)	194 (92%)	17 (8%)	0	100	100
3	F	211/234 (90%)	198 (94%)	13 (6%)	0	100	100
3	J	211/234 (90%)	196 (93%)	15 (7%)	0	100	100
3	L	198/234 (85%)	181 (91%)	17 (9%)	0	100	100
All	All	2180/2829 (77%)	2024 (93%)	156 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	157/245 (64%)	152 (97%)	5 (3%)	34	58
1	D	105/245 (43%)	98 (93%)	7 (7%)	13	40
1	G	112/245 (46%)	108 (96%)	4 (4%)	30	55
2	B	167/214 (78%)	165 (99%)	2 (1%)	67	79
2	E	174/214 (81%)	171 (98%)	3 (2%)	56	73
2	I	172/214 (80%)	171 (99%)	1 (1%)	84	90
2	K	146/214 (68%)	140 (96%)	6 (4%)	26	52
3	C	179/203 (88%)	177 (99%)	2 (1%)	70	80
3	F	182/203 (90%)	178 (98%)	4 (2%)	47	66
3	J	180/203 (89%)	177 (98%)	3 (2%)	56	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	150/203 (74%)	148 (99%)	2 (1%)	65 77
All	All	1724/2403 (72%)	1685 (98%)	39 (2%)	46 65

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	91	ASP
2	K	153	GLU
3	J	136	ASN
2	K	67	ARG
3	L	80	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	6	GLN
3	J	123	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 ⓘ

9 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
5	NAG	H	1	5,1	14,14,15	0.26	0	17,19,21	1.19	2 (11%)
5	NAG	H	2	5	14,14,15	0.41	0	17,19,21	0.85	1 (5%)
5	NAG	M	1	5,1	14,14,15	1.04	1 (7%)	17,19,21	1.06	1 (5%)
5	NAG	M	2	5	14,14,15	0.38	0	17,19,21	0.37	0
5	NAG	N	1	5,1	14,14,15	0.67	1 (7%)	17,19,21	1.12	1 (5%)
5	NAG	N	2	5	14,14,15	0.57	0	17,19,21	0.95	1 (5%)
4	NAG	Z	1	4,1	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
4	NAG	Z	2	4	14,14,15	0.50	0	17,19,21	0.49	0
4	BMA	Z	3	4	11,11,12	0.82	0	15,15,17	0.85	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
5	NAG	H	1	5,1	-	6/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	O5-C1	-3.54	1.37	1.43
5	N	1	NAG	O5-C1	2.32	1.47	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1	NAG	C1-O5-C5	4.36	118.03	112.19
4	Z	1	NAG	C1-O5-C5	3.60	117.01	112.19
5	N	2	NAG	C1-O5-C5	3.60	117.01	112.19
5	H	1	NAG	C2-N2-C7	3.13	127.10	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	C3-C4-C5	2.85	115.40	110.23

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

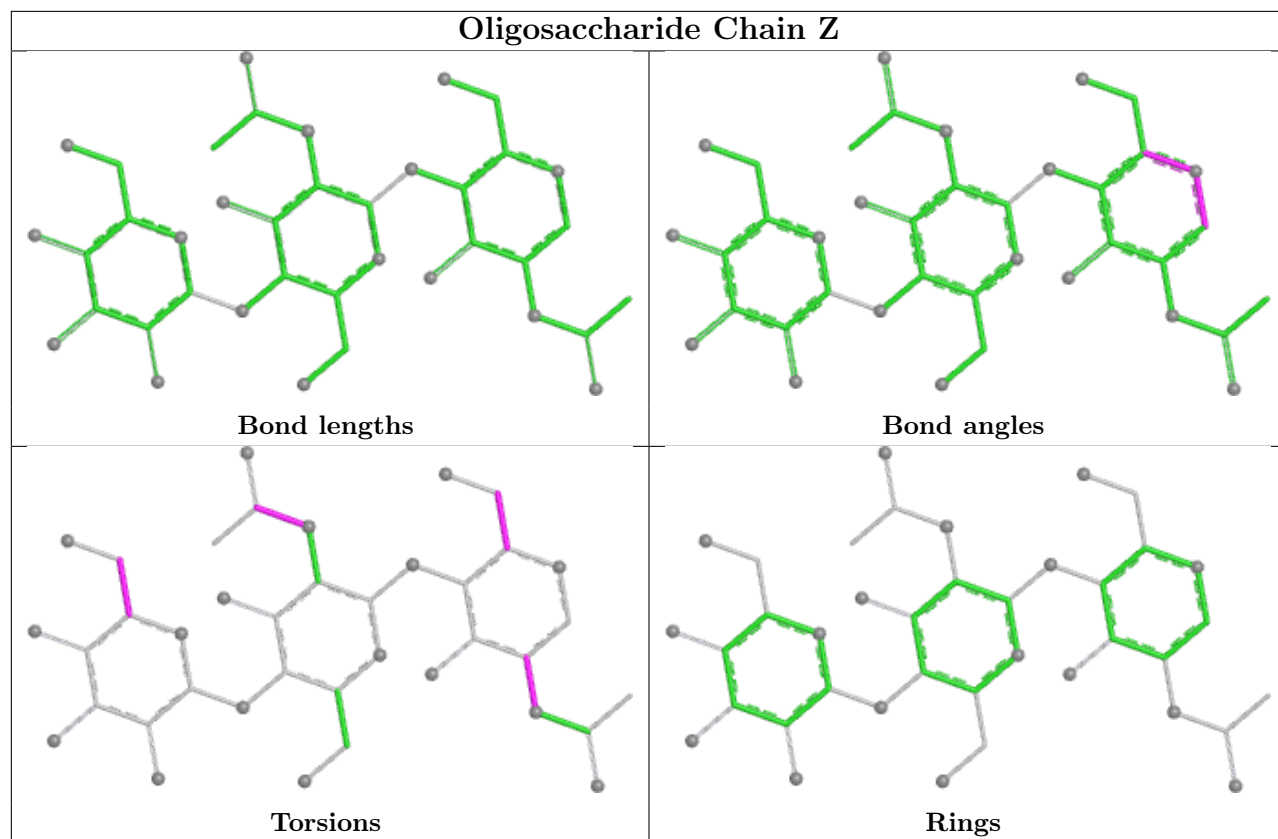
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C1-C2-N2-C7
5	H	1	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6

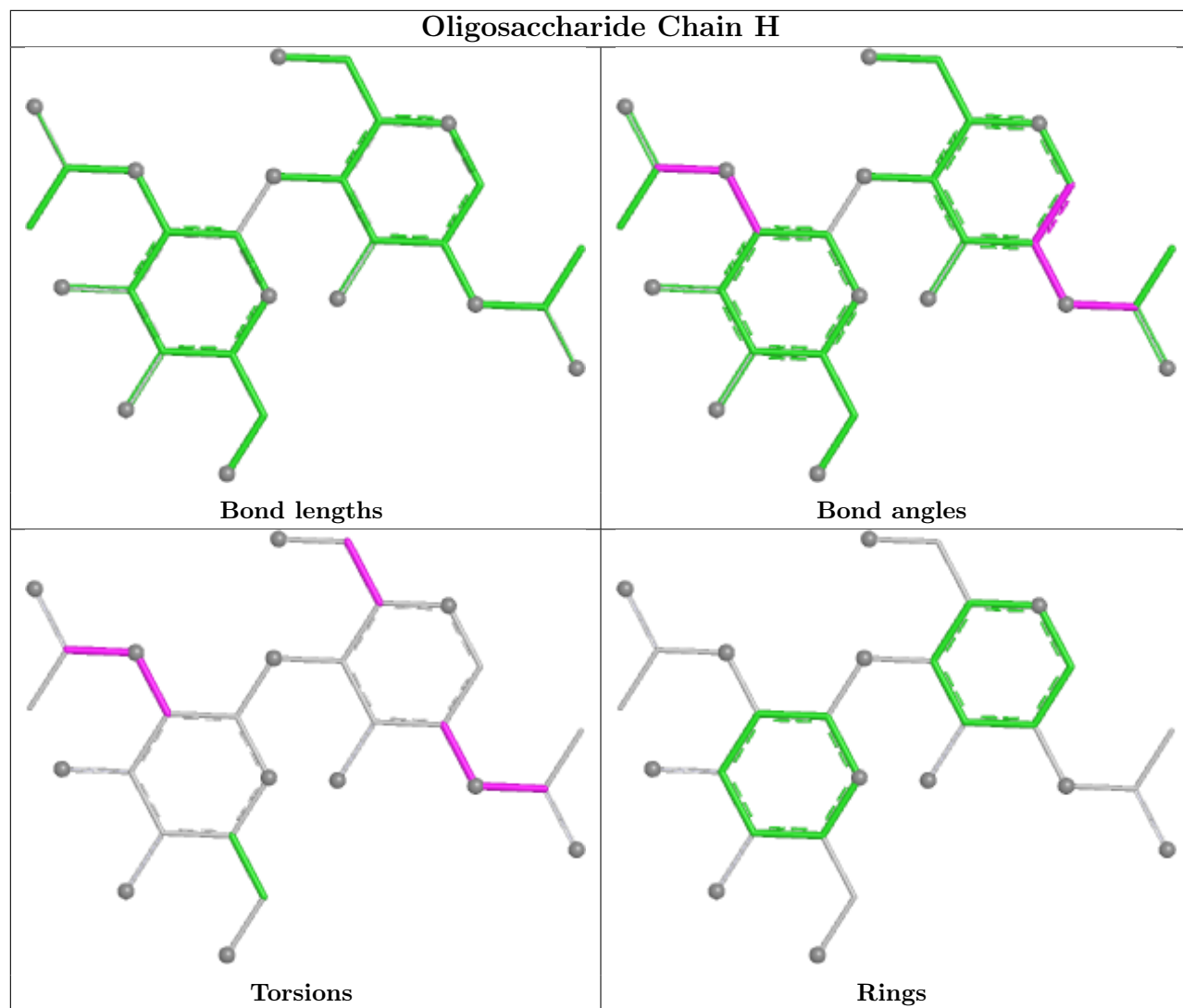
There are no ring outliers.

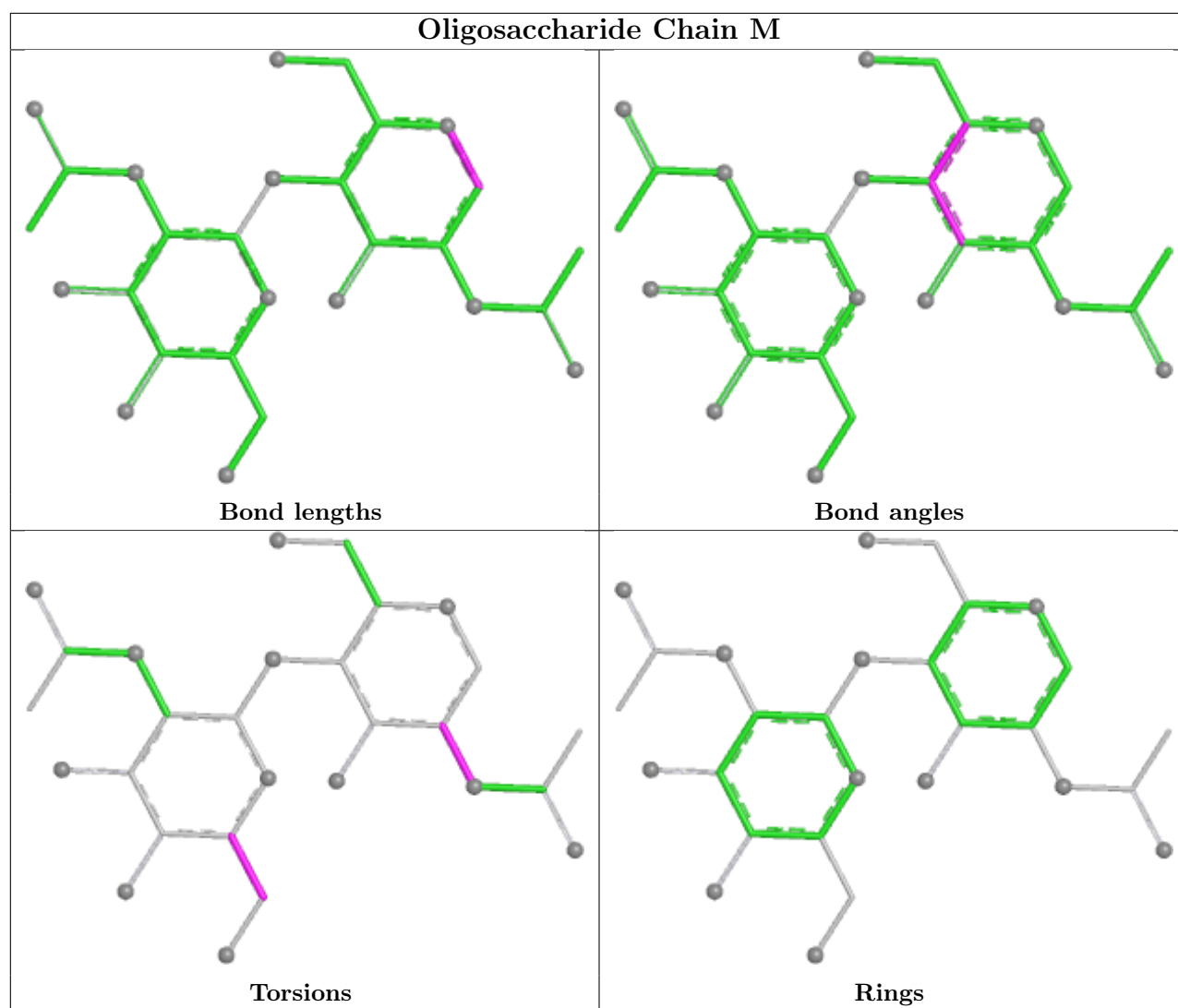
4 monomers are involved in 7 short contacts:

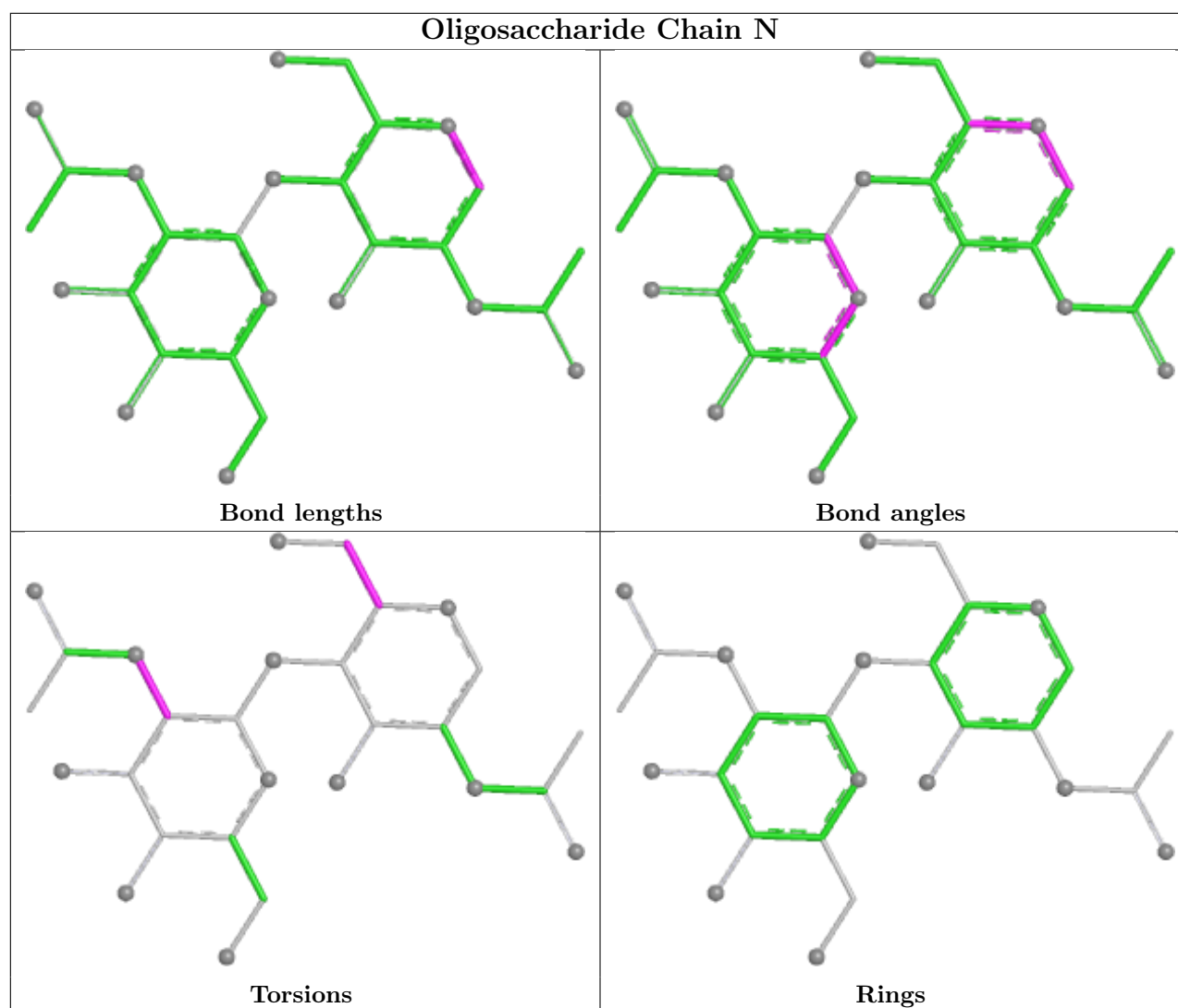
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	2	0
5	H	2	NAG	3	0
4	Z	1	NAG	1	0
5	N	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
6	NAG	A	701	1	14,14,15	0.25	0	17,19,21	0.39	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	A	701	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	701	NAG	O5-C5-C6-O6
6	A	701	NAG	C4-C5-C6-O6
6	A	701	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	A	701	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.

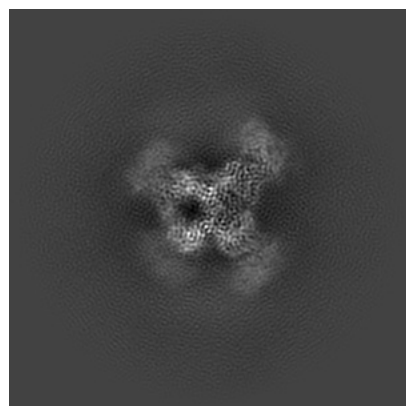
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41245. These allow visual inspection of the internal detail of the map and identification of artifacts.

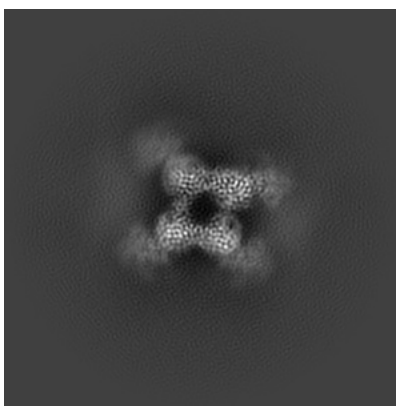
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

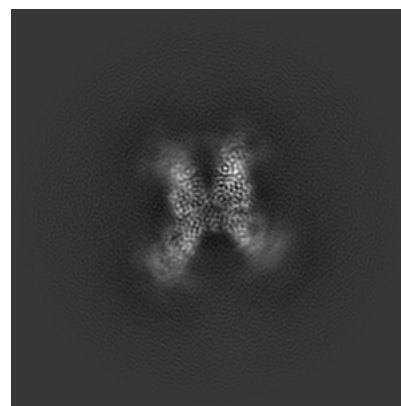
6.1.1 Primary map



X

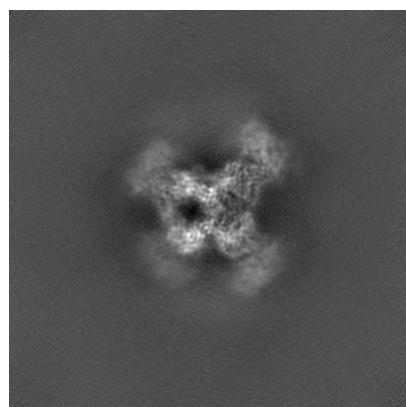


Y

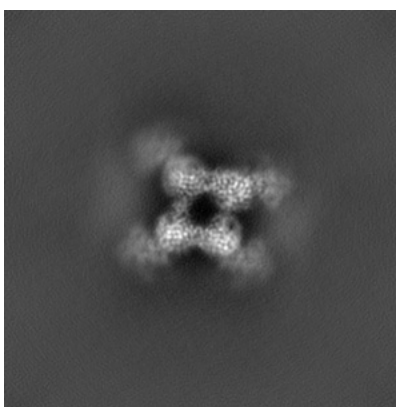


Z

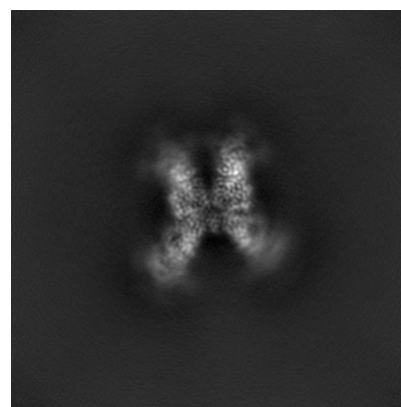
6.1.2 Raw map



X



Y

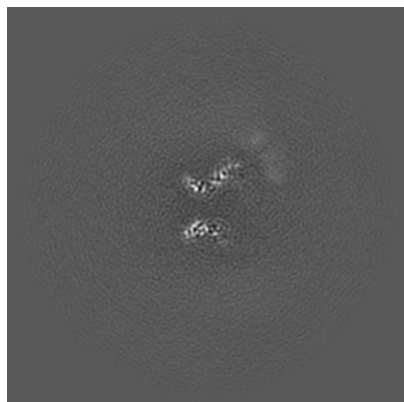


Z

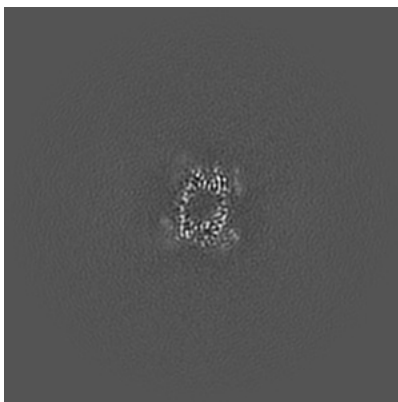
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

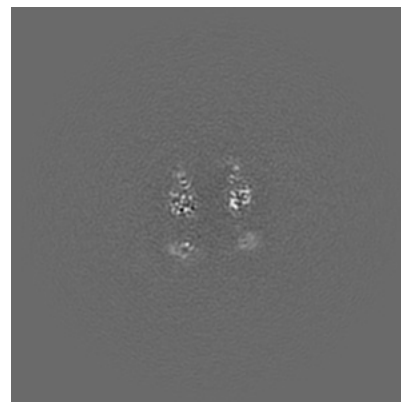
6.2.1 Primary map



X Index: 128

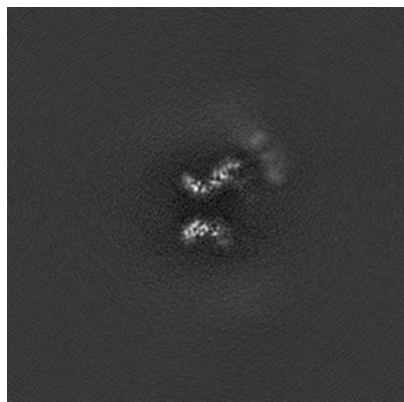


Y Index: 128

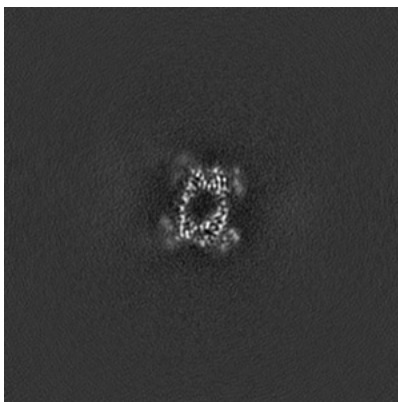


Z Index: 128

6.2.2 Raw map



X Index: 128



Y Index: 128

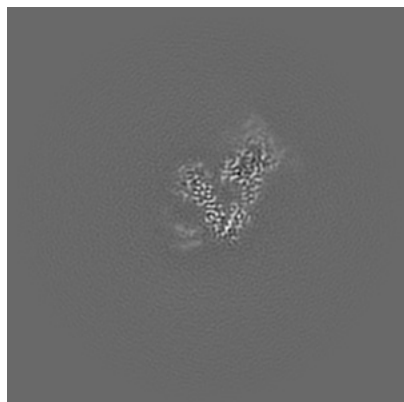


Z Index: 128

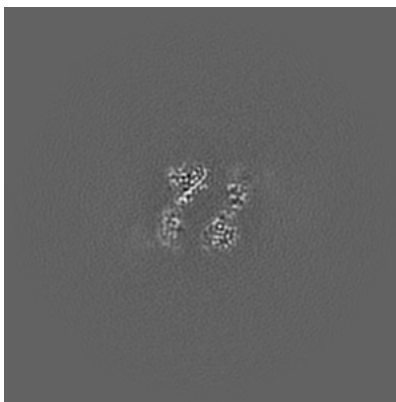
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

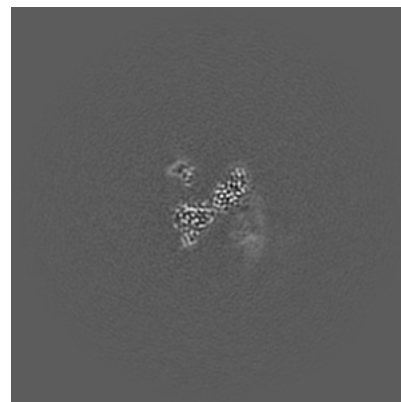
6.3.1 Primary map



X Index: 142

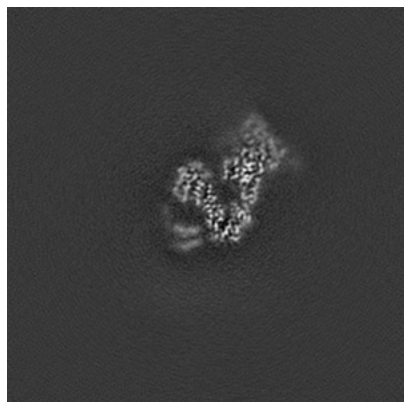


Y Index: 137

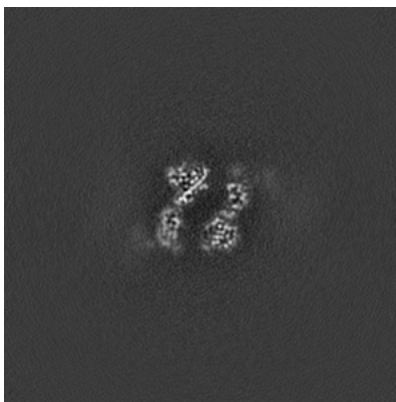


Z Index: 116

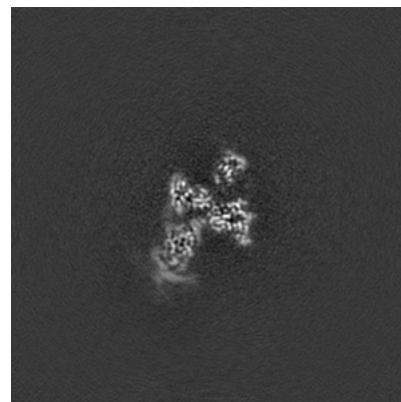
6.3.2 Raw map



X Index: 143



Y Index: 137

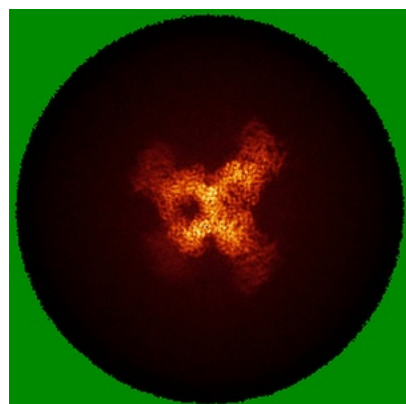


Z Index: 141

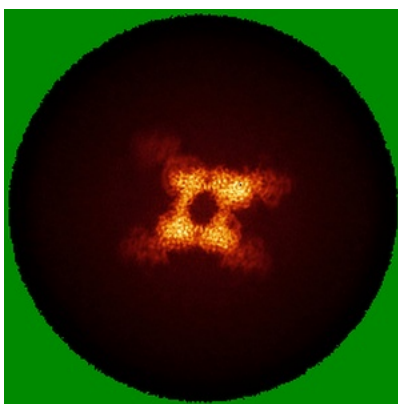
The images above show the largest variance slices of the map in three orthogonal directions.

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

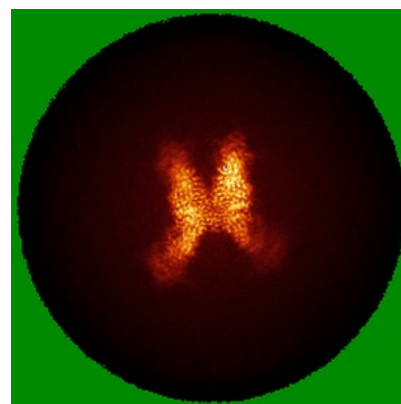
6.4.1 Primary map



X

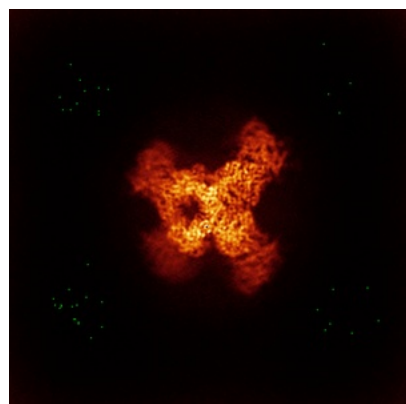


Y

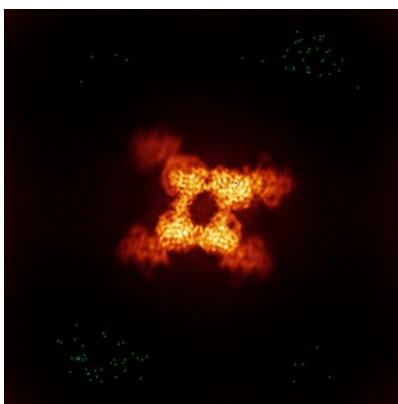


Z

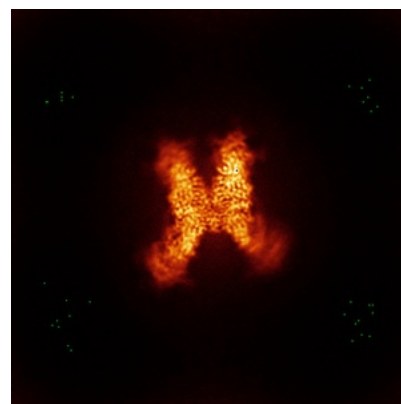
6.4.2 Raw map



X



Y

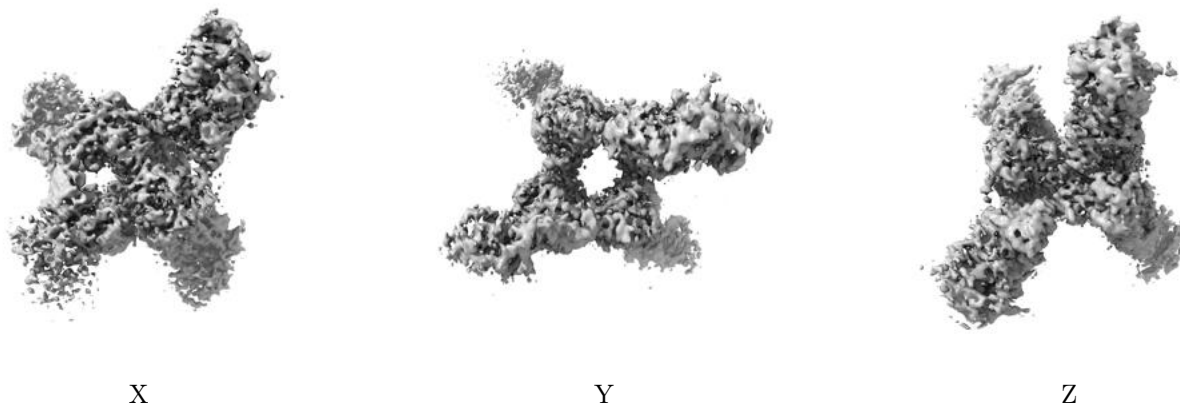


Z

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.

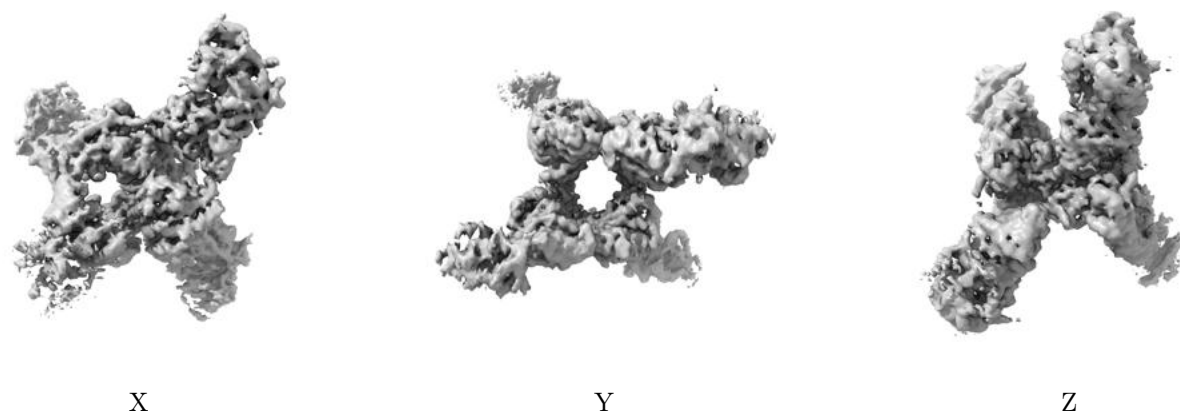
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. 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.

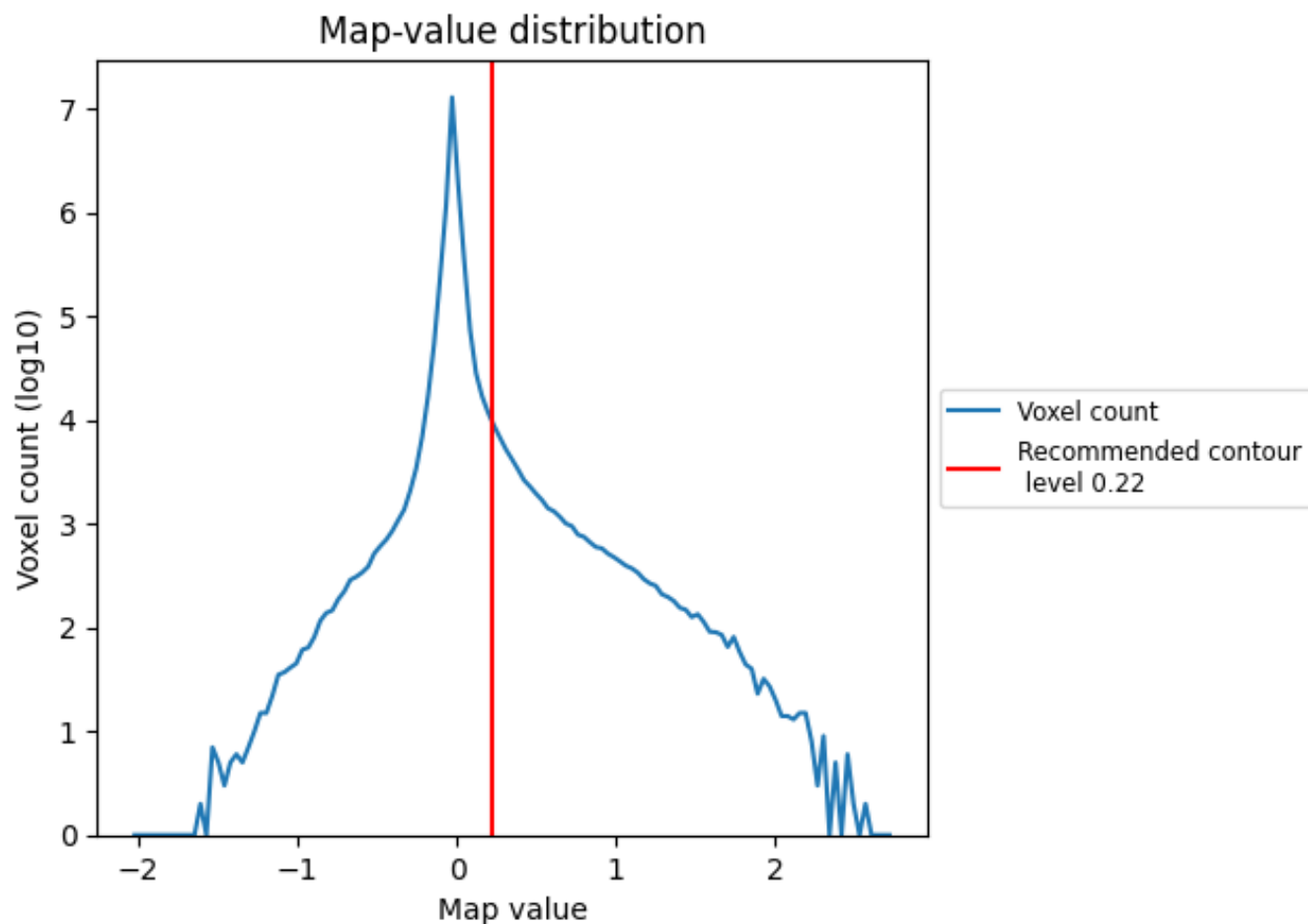
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

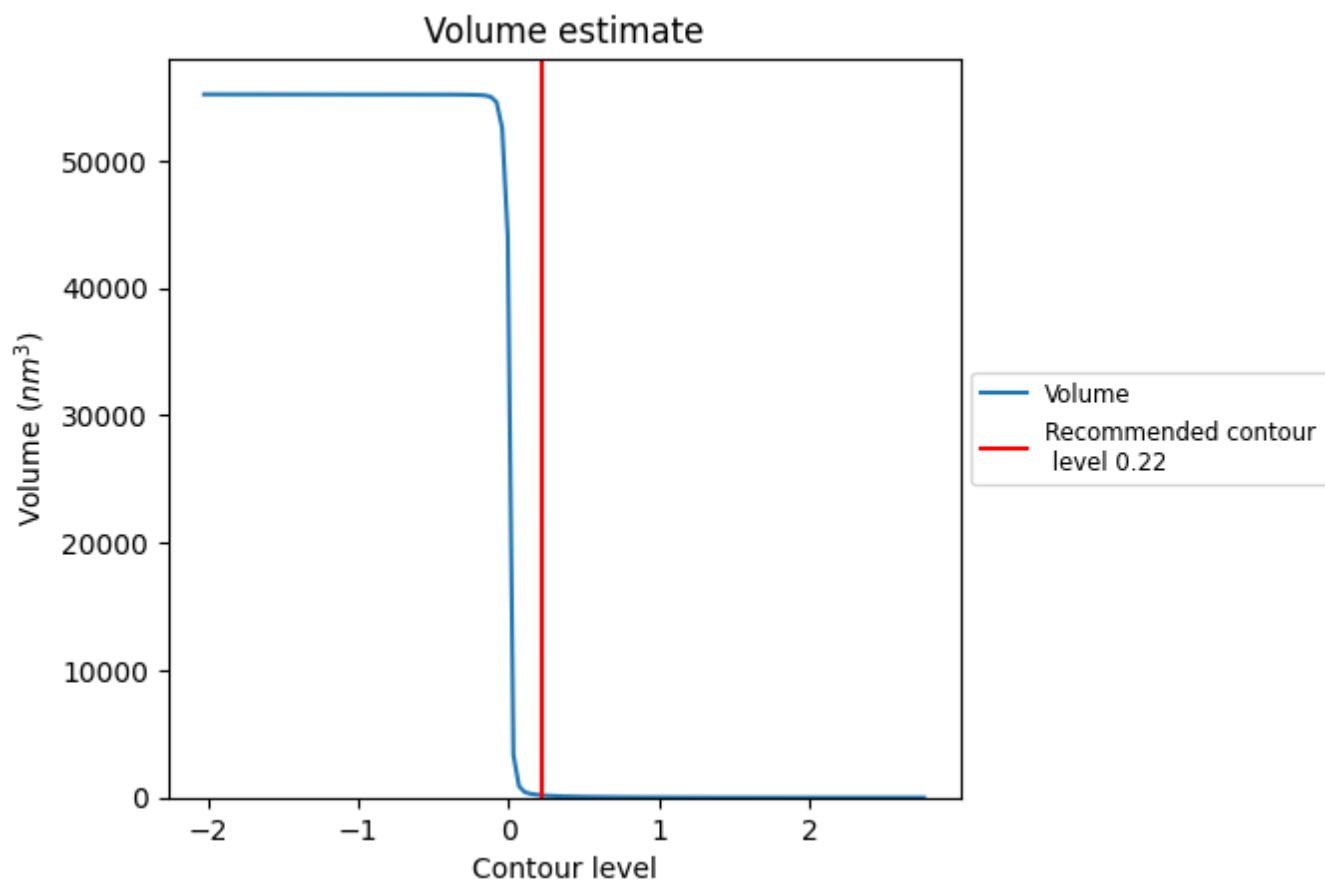
This section contains the results of statistical analysis of the map.

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.

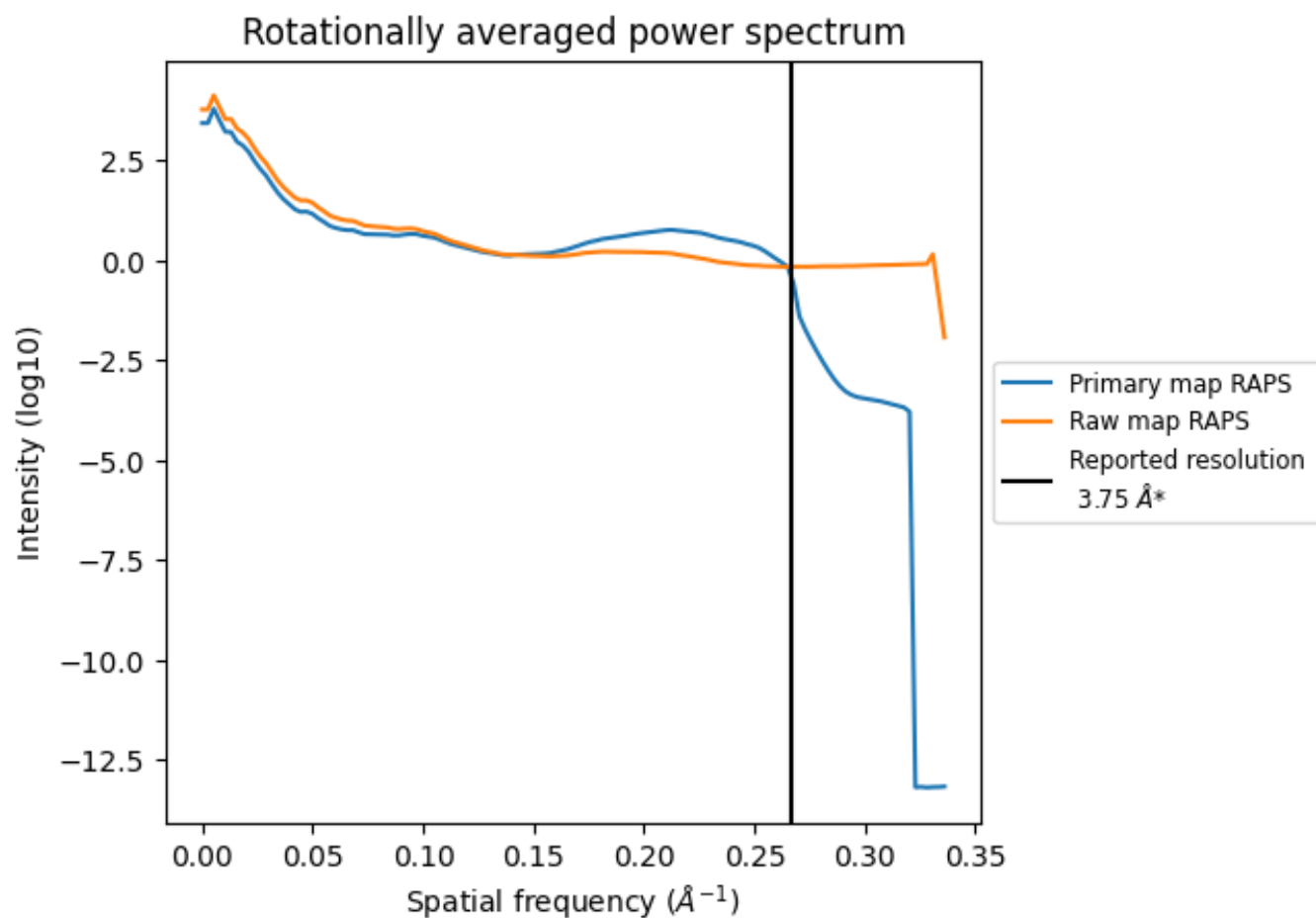
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183 nm³; this corresponds to an approximate mass of 165 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 ⓘ

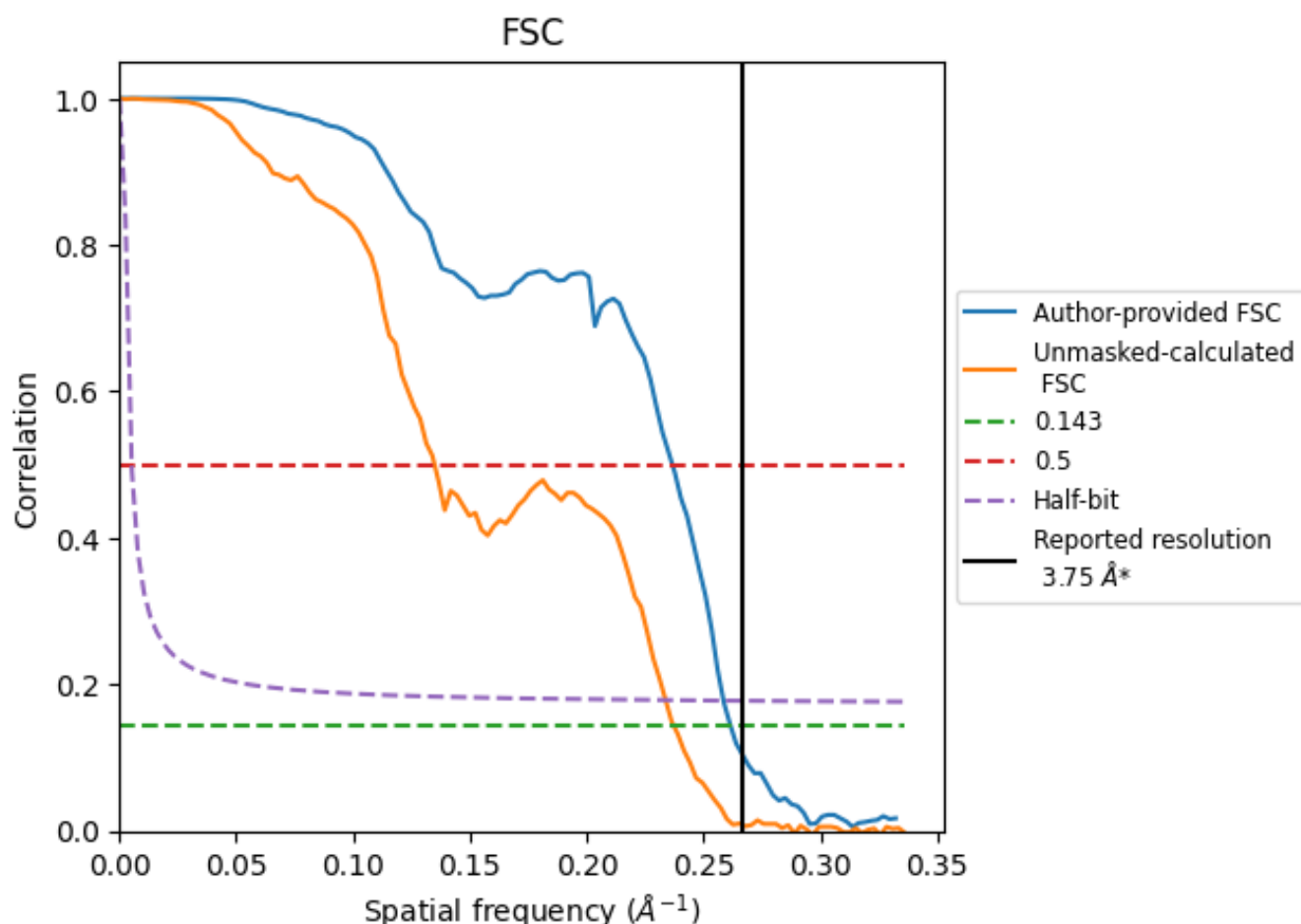


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 0.267 \AA^{-1}

8.2 Resolution estimates [i](#)

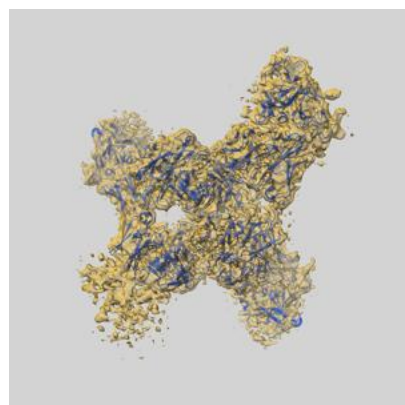
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.82	4.23	3.87
Unmasked-calculated*	4.21	7.42	4.28

*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 4.21 differs from the reported value 3.75 by more than 10 %

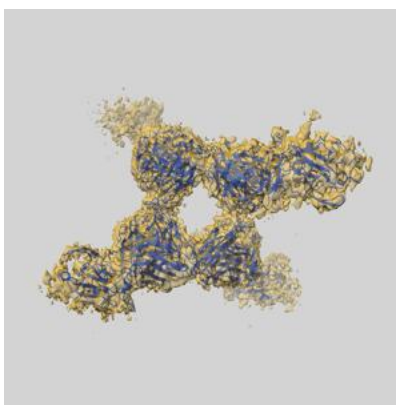
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41245 and PDB model 8TGV. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

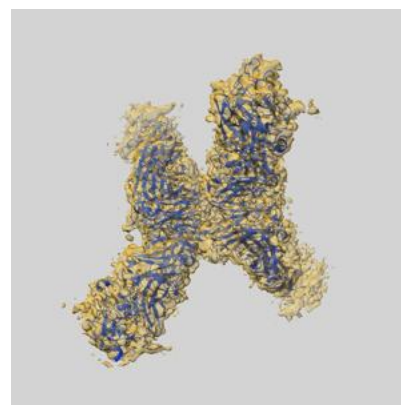
9.1 Map-model overlay [i](#)



X



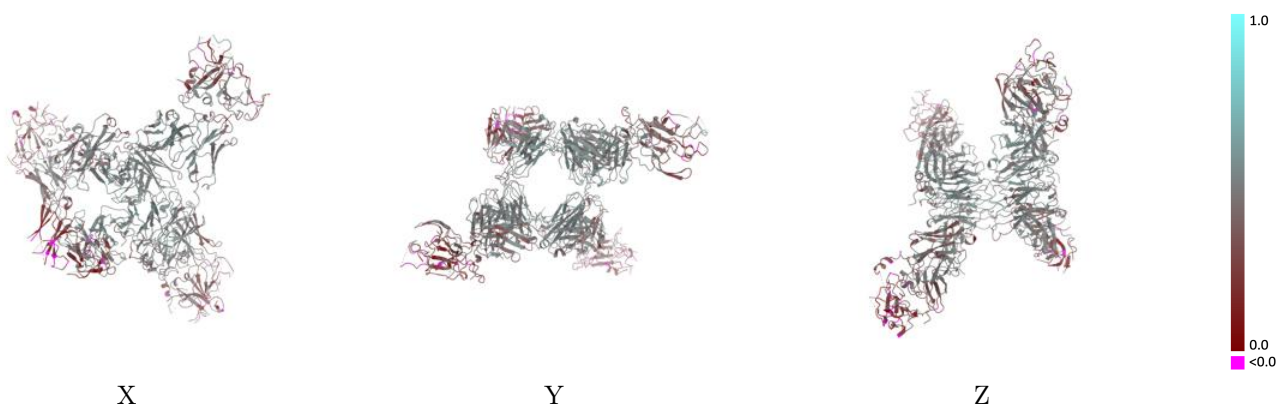
Y



Z

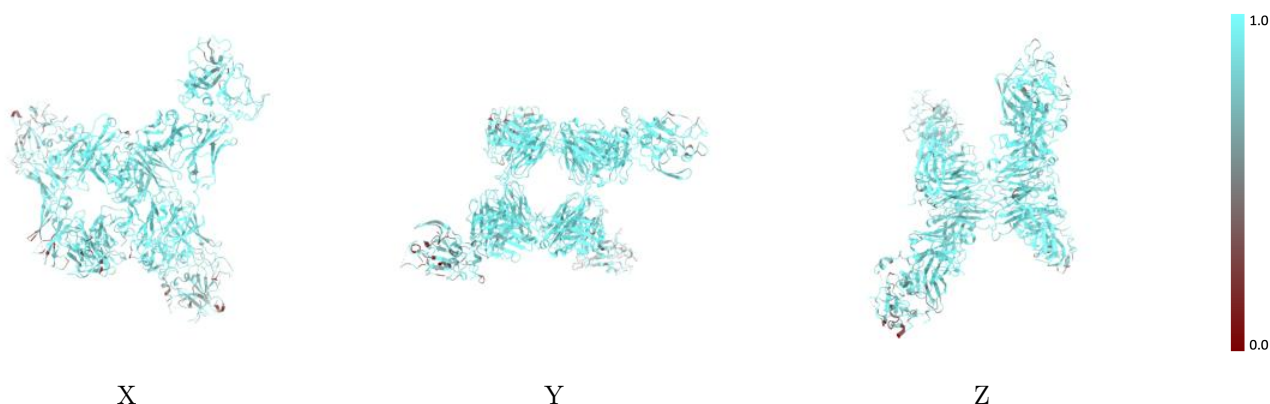
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



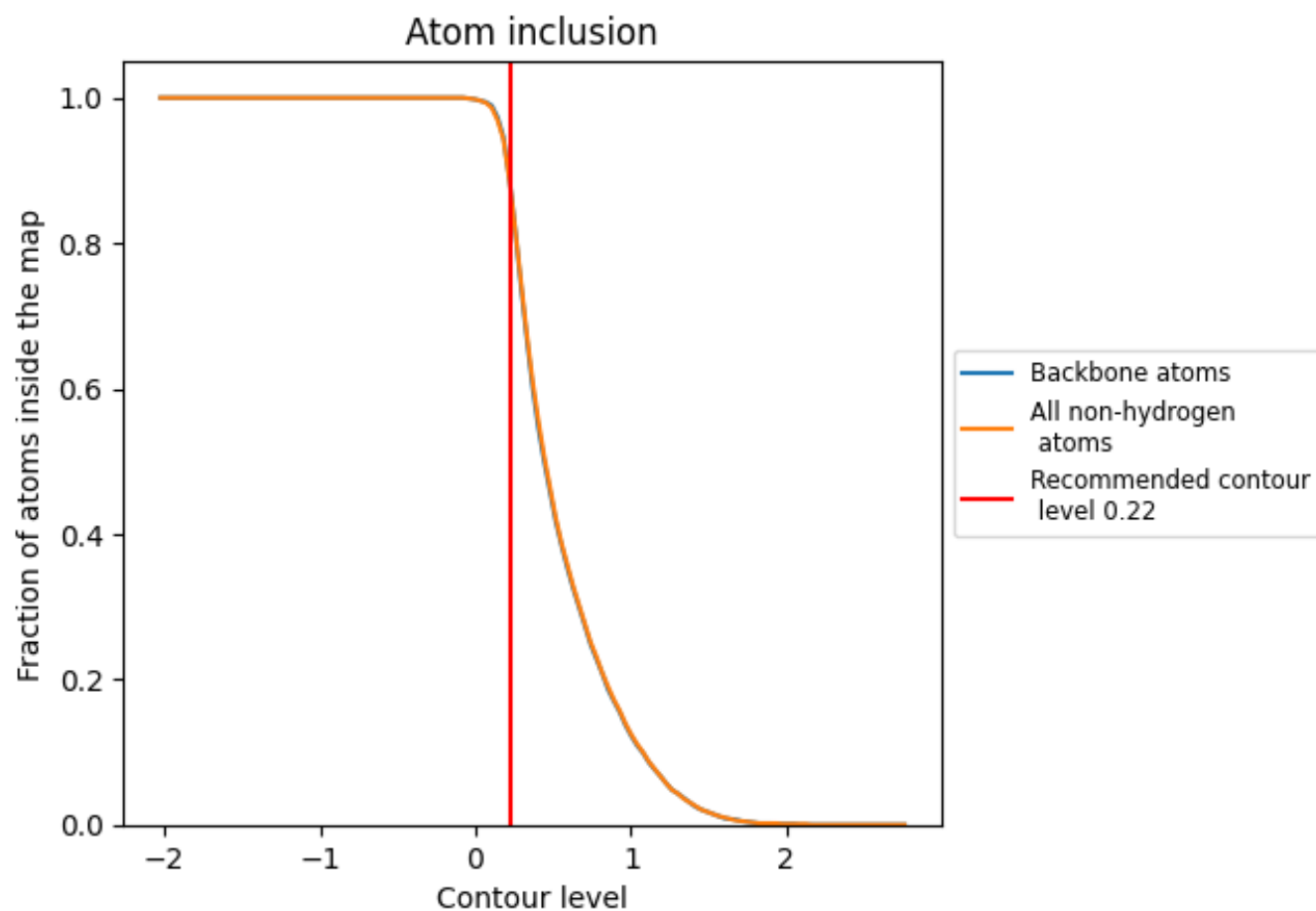
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8850	<div></div> 0.4250
A	<div></div> 0.8680	<div></div> 0.3780
B	<div></div> 0.9200	<div></div> 0.4550
C	<div></div> 0.9420	<div></div> 0.4930
D	<div></div> 0.7300	<div></div> 0.3010
E	<div></div> 0.9360	<div></div> 0.4910
F	<div></div> 0.9530	<div></div> 0.5130
G	<div></div> 0.7440	<div></div> 0.2910
H	<div></div> 0.7140	<div></div> 0.3370
I	<div></div> 0.9280	<div></div> 0.4550
J	<div></div> 0.9300	<div></div> 0.4580
K	<div></div> 0.8630	<div></div> 0.3630
L	<div></div> 0.8850	<div></div> 0.4110
M	<div></div> 0.7140	<div></div> 0.2650
N	<div></div> 0.8930	<div></div> 0.3460
Z	<div></div> 0.8970	<div></div> 0.4260

1.0

0.0

<0.0