



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 11:42 AM EDT

PDB ID : 6XGC
EMDB ID : EMD-22180
Title : CryoEM structure of influenza hemagglutinin A/Michigan/45/2015 in complex with cyno antibody 1C4
Authors : Qiu, Y.; Zhou, Y.
Deposited on : 2020-06-17
Resolution : 4.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.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

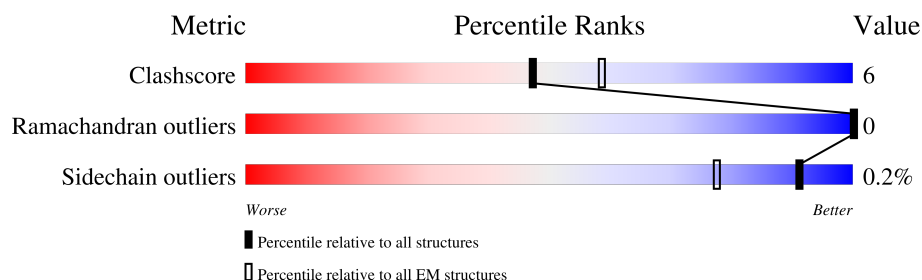
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	327	
1	C	327	
1	E	327	
2	B	220	
2	D	220	
2	F	220	
3	H	244	
3	I	244	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M	244	
4	J	216	
4	L	216	
4	N	216	
5	G	2	
5	K	2	
5	O	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17040 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		
1	C	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		
1	E	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	164	Total	C	N	O	S	0	0
			1339	838	230	265	6		
2	D	164	Total	C	N	O	S	0	0
			1339	838	230	265	6		
2	F	164	Total	C	N	O	S	0	0
			1339	838	230	265	6		

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A482NTT4
B	176	GLY	-	expression tag	UNP A0A482NTT4
B	177	ARG	-	expression tag	UNP A0A482NTT4
B	178	LEU	-	expression tag	UNP A0A482NTT4
B	179	VAL	-	expression tag	UNP A0A482NTT4
B	180	PRO	-	expression tag	UNP A0A482NTT4
B	181	ARG	-	expression tag	UNP A0A482NTT4
B	182	GLY	-	expression tag	UNP A0A482NTT4
B	183	SER	-	expression tag	UNP A0A482NTT4
B	184	PRO	-	expression tag	UNP A0A482NTT4
B	185	GLY	-	expression tag	UNP A0A482NTT4
B	186	SER	-	expression tag	UNP A0A482NTT4
B	187	GLY	-	expression tag	UNP A0A482NTT4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	TYR	-	expression tag	UNP A0A482NTT4
B	189	ILE	-	expression tag	UNP A0A482NTT4
B	190	PRO	-	expression tag	UNP A0A482NTT4
B	191	GLU	-	expression tag	UNP A0A482NTT4
B	192	ALA	-	expression tag	UNP A0A482NTT4
B	193	PRO	-	expression tag	UNP A0A482NTT4
B	194	ARG	-	expression tag	UNP A0A482NTT4
B	195	ASP	-	expression tag	UNP A0A482NTT4
B	196	GLY	-	expression tag	UNP A0A482NTT4
B	197	GLN	-	expression tag	UNP A0A482NTT4
B	198	ALA	-	expression tag	UNP A0A482NTT4
B	199	TYR	-	expression tag	UNP A0A482NTT4
B	200	VAL	-	expression tag	UNP A0A482NTT4
B	201	ARG	-	expression tag	UNP A0A482NTT4
B	202	LYS	-	expression tag	UNP A0A482NTT4
B	203	ASP	-	expression tag	UNP A0A482NTT4
B	204	GLY	-	expression tag	UNP A0A482NTT4
B	205	GLU	-	expression tag	UNP A0A482NTT4
B	206	TRP	-	expression tag	UNP A0A482NTT4
B	207	VAL	-	expression tag	UNP A0A482NTT4
B	208	LEU	-	expression tag	UNP A0A482NTT4
B	209	LEU	-	expression tag	UNP A0A482NTT4
B	210	SER	-	expression tag	UNP A0A482NTT4
B	211	THR	-	expression tag	UNP A0A482NTT4
B	212	PHE	-	expression tag	UNP A0A482NTT4
B	213	LEU	-	expression tag	UNP A0A482NTT4
B	214	GLY	-	expression tag	UNP A0A482NTT4
B	215	HIS	-	expression tag	UNP A0A482NTT4
B	216	HIS	-	expression tag	UNP A0A482NTT4
B	217	HIS	-	expression tag	UNP A0A482NTT4
B	218	HIS	-	expression tag	UNP A0A482NTT4
B	219	HIS	-	expression tag	UNP A0A482NTT4
B	220	HIS	-	expression tag	UNP A0A482NTT4
D	175	SER	-	expression tag	UNP A0A482NTT4
D	176	GLY	-	expression tag	UNP A0A482NTT4
D	177	ARG	-	expression tag	UNP A0A482NTT4
D	178	LEU	-	expression tag	UNP A0A482NTT4
D	179	VAL	-	expression tag	UNP A0A482NTT4
D	180	PRO	-	expression tag	UNP A0A482NTT4
D	181	ARG	-	expression tag	UNP A0A482NTT4
D	182	GLY	-	expression tag	UNP A0A482NTT4
D	183	SER	-	expression tag	UNP A0A482NTT4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	184	PRO	-	expression tag	UNP A0A482NTT4
D	185	GLY	-	expression tag	UNP A0A482NTT4
D	186	SER	-	expression tag	UNP A0A482NTT4
D	187	GLY	-	expression tag	UNP A0A482NTT4
D	188	TYR	-	expression tag	UNP A0A482NTT4
D	189	ILE	-	expression tag	UNP A0A482NTT4
D	190	PRO	-	expression tag	UNP A0A482NTT4
D	191	GLU	-	expression tag	UNP A0A482NTT4
D	192	ALA	-	expression tag	UNP A0A482NTT4
D	193	PRO	-	expression tag	UNP A0A482NTT4
D	194	ARG	-	expression tag	UNP A0A482NTT4
D	195	ASP	-	expression tag	UNP A0A482NTT4
D	196	GLY	-	expression tag	UNP A0A482NTT4
D	197	GLN	-	expression tag	UNP A0A482NTT4
D	198	ALA	-	expression tag	UNP A0A482NTT4
D	199	TYR	-	expression tag	UNP A0A482NTT4
D	200	VAL	-	expression tag	UNP A0A482NTT4
D	201	ARG	-	expression tag	UNP A0A482NTT4
D	202	LYS	-	expression tag	UNP A0A482NTT4
D	203	ASP	-	expression tag	UNP A0A482NTT4
D	204	GLY	-	expression tag	UNP A0A482NTT4
D	205	GLU	-	expression tag	UNP A0A482NTT4
D	206	TRP	-	expression tag	UNP A0A482NTT4
D	207	VAL	-	expression tag	UNP A0A482NTT4
D	208	LEU	-	expression tag	UNP A0A482NTT4
D	209	LEU	-	expression tag	UNP A0A482NTT4
D	210	SER	-	expression tag	UNP A0A482NTT4
D	211	THR	-	expression tag	UNP A0A482NTT4
D	212	PHE	-	expression tag	UNP A0A482NTT4
D	213	LEU	-	expression tag	UNP A0A482NTT4
D	214	GLY	-	expression tag	UNP A0A482NTT4
D	215	HIS	-	expression tag	UNP A0A482NTT4
D	216	HIS	-	expression tag	UNP A0A482NTT4
D	217	HIS	-	expression tag	UNP A0A482NTT4
D	218	HIS	-	expression tag	UNP A0A482NTT4
D	219	HIS	-	expression tag	UNP A0A482NTT4
D	220	HIS	-	expression tag	UNP A0A482NTT4
F	175	SER	-	expression tag	UNP A0A482NTT4
F	176	GLY	-	expression tag	UNP A0A482NTT4
F	177	ARG	-	expression tag	UNP A0A482NTT4
F	178	LEU	-	expression tag	UNP A0A482NTT4
F	179	VAL	-	expression tag	UNP A0A482NTT4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	180	PRO	-	expression tag	UNP A0A482NTT4
F	181	ARG	-	expression tag	UNP A0A482NTT4
F	182	GLY	-	expression tag	UNP A0A482NTT4
F	183	SER	-	expression tag	UNP A0A482NTT4
F	184	PRO	-	expression tag	UNP A0A482NTT4
F	185	GLY	-	expression tag	UNP A0A482NTT4
F	186	SER	-	expression tag	UNP A0A482NTT4
F	187	GLY	-	expression tag	UNP A0A482NTT4
F	188	TYR	-	expression tag	UNP A0A482NTT4
F	189	ILE	-	expression tag	UNP A0A482NTT4
F	190	PRO	-	expression tag	UNP A0A482NTT4
F	191	GLU	-	expression tag	UNP A0A482NTT4
F	192	ALA	-	expression tag	UNP A0A482NTT4
F	193	PRO	-	expression tag	UNP A0A482NTT4
F	194	ARG	-	expression tag	UNP A0A482NTT4
F	195	ASP	-	expression tag	UNP A0A482NTT4
F	196	GLY	-	expression tag	UNP A0A482NTT4
F	197	GLN	-	expression tag	UNP A0A482NTT4
F	198	ALA	-	expression tag	UNP A0A482NTT4
F	199	TYR	-	expression tag	UNP A0A482NTT4
F	200	VAL	-	expression tag	UNP A0A482NTT4
F	201	ARG	-	expression tag	UNP A0A482NTT4
F	202	LYS	-	expression tag	UNP A0A482NTT4
F	203	ASP	-	expression tag	UNP A0A482NTT4
F	204	GLY	-	expression tag	UNP A0A482NTT4
F	205	GLU	-	expression tag	UNP A0A482NTT4
F	206	TRP	-	expression tag	UNP A0A482NTT4
F	207	VAL	-	expression tag	UNP A0A482NTT4
F	208	LEU	-	expression tag	UNP A0A482NTT4
F	209	LEU	-	expression tag	UNP A0A482NTT4
F	210	SER	-	expression tag	UNP A0A482NTT4
F	211	THR	-	expression tag	UNP A0A482NTT4
F	212	PHE	-	expression tag	UNP A0A482NTT4
F	213	LEU	-	expression tag	UNP A0A482NTT4
F	214	GLY	-	expression tag	UNP A0A482NTT4
F	215	HIS	-	expression tag	UNP A0A482NTT4
F	216	HIS	-	expression tag	UNP A0A482NTT4
F	217	HIS	-	expression tag	UNP A0A482NTT4
F	218	HIS	-	expression tag	UNP A0A482NTT4
F	219	HIS	-	expression tag	UNP A0A482NTT4
F	220	HIS	-	expression tag	UNP A0A482NTT4

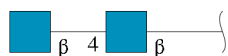
- Molecule 3 is a protein called 1C4 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	125	Total	C	N	O	S	0	0
			925	581	160	180	4		
3	H	125	Total	C	N	O	S	0	0
			925	581	160	180	4		
3	I	125	Total	C	N	O	S	0	0
			925	581	160	180	4		

- Molecule 4 is a protein called 1C4 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	107	Total	C	N	O	S	0	0
			790	487	138	163	2		
4	L	107	Total	C	N	O	S	0	0
			790	487	138	163	2		
4	J	107	Total	C	N	O	S	0	0
			790	487	138	163	2		

- 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	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

Continued on next page...

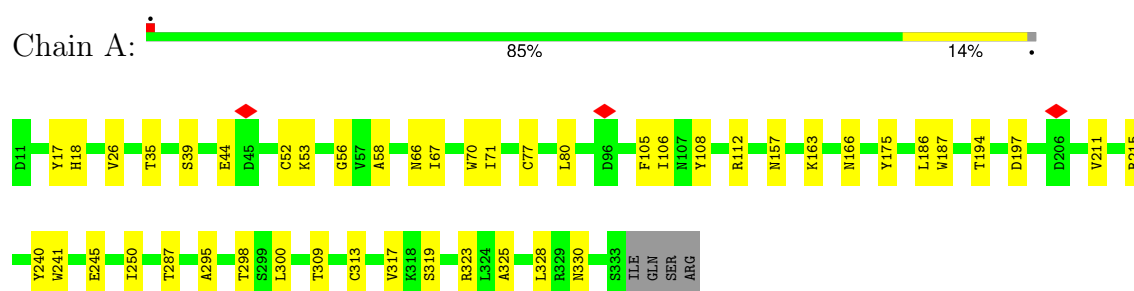
Continued from previous page...

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

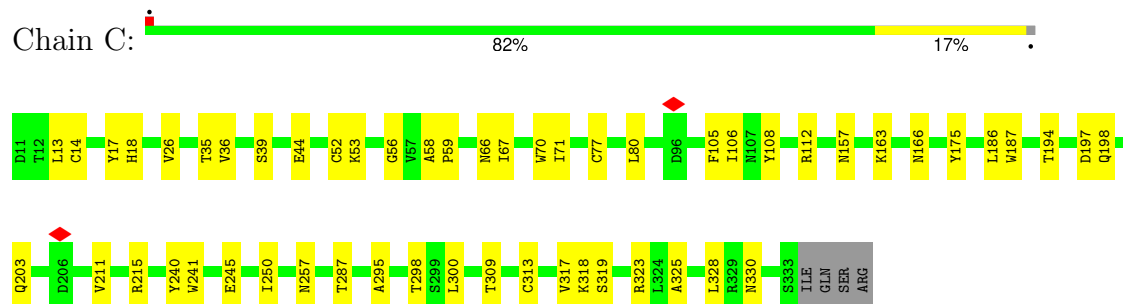
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

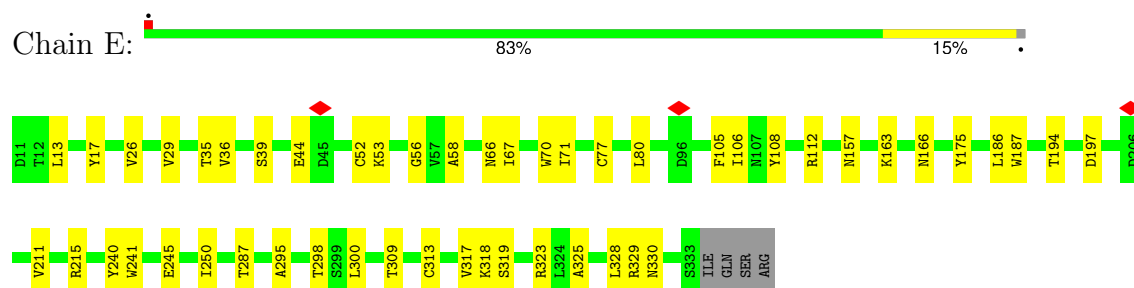
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

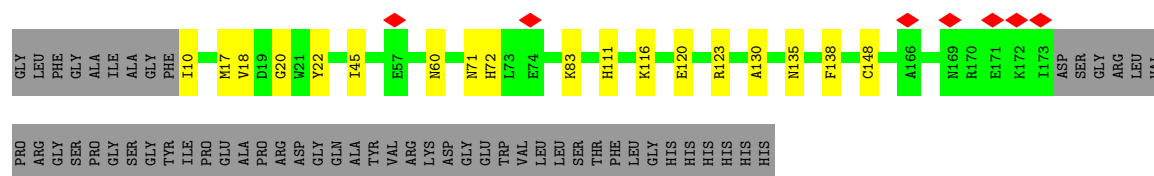


- Molecule 1: Hemagglutinin HA1 chain



- Molecule 2: Hemagglutinin HA2 chain





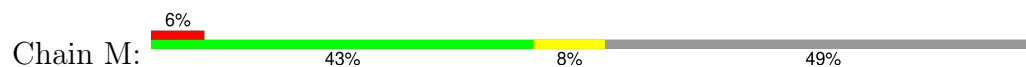
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 3: 1C4 Fab heavy chain



• Molecule 3: 1C4 Fab heavy chain




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

Chain G:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain O:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	449762	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	317.7, 317.7, 317.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/2591	0.42	0/3525
1	C	0.24	0/2591	0.42	0/3525
1	E	0.24	0/2591	0.42	0/3525
2	B	0.24	0/1365	0.36	0/1838
2	D	0.24	0/1365	0.36	0/1838
2	F	0.24	0/1365	0.36	0/1838
3	H	0.24	0/944	0.43	0/1278
3	I	0.24	0/944	0.43	0/1278
3	M	0.24	0/944	0.43	0/1278
4	J	0.24	0/808	0.42	0/1098
4	L	0.24	0/808	0.42	0/1098
4	N	0.24	0/808	0.42	0/1098
All	All	0.24	0/17124	0.41	0/23217

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2528	0	2459	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2528	0	2459	36	0
1	E	2528	0	2459	35	0
2	B	1339	0	1272	13	0
2	D	1339	0	1272	16	0
2	F	1339	0	1272	14	0
3	H	925	0	900	11	0
3	I	925	0	900	10	0
3	M	925	0	900	14	0
4	J	790	0	746	10	0
4	L	790	0	746	12	0
4	N	790	0	746	11	0
5	G	28	0	25	2	0
5	K	28	0	25	1	0
5	O	28	0	25	2	0
6	A	56	0	52	1	0
6	B	14	0	13	0	0
6	C	56	0	52	1	0
6	D	14	0	13	0	0
6	E	56	0	52	1	0
6	F	14	0	13	0	0
All	All	17040	0	16401	195	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 6.

The worst 5 of 195 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HG3	1:A:298:THR:HG21	1.71	0.72
1:E:44:GLU:HG3	1:E:298:THR:HG21	1.71	0.71
4:L:98:VAL:HG12	4:L:99:TRP:N	2.07	0.70
1:C:44:GLU:HG3	1:C:298:THR:HG21	1.71	0.70
4:N:98:VAL:HG12	4:N:99:TRP:N	2.07	0.69

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	321/327 (98%)	314 (98%)	7 (2%)	0	100	100
1	C	321/327 (98%)	314 (98%)	7 (2%)	0	100	100
1	E	321/327 (98%)	314 (98%)	7 (2%)	0	100	100
2	B	162/220 (74%)	157 (97%)	5 (3%)	0	100	100
2	D	162/220 (74%)	157 (97%)	5 (3%)	0	100	100
2	F	162/220 (74%)	157 (97%)	5 (3%)	0	100	100
3	H	123/244 (50%)	121 (98%)	2 (2%)	0	100	100
3	I	123/244 (50%)	121 (98%)	2 (2%)	0	100	100
3	M	123/244 (50%)	121 (98%)	2 (2%)	0	100	100
4	J	105/216 (49%)	103 (98%)	2 (2%)	0	100	100
4	L	105/216 (49%)	103 (98%)	2 (2%)	0	100	100
4	N	105/216 (49%)	103 (98%)	2 (2%)	0	100	100
All	All	2133/3021 (71%)	2085 (98%)	48 (2%)	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	284/288 (99%)	284 (100%)	0	100	100
1	C	284/288 (99%)	284 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	284/288 (99%)	284 (100%)	0	100	100
2	B	145/187 (78%)	144 (99%)	1 (1%)	81	86
2	D	145/187 (78%)	144 (99%)	1 (1%)	81	86
2	F	145/187 (78%)	144 (99%)	1 (1%)	81	86
3	H	96/201 (48%)	96 (100%)	0	100	100
3	I	96/201 (48%)	96 (100%)	0	100	100
3	M	96/201 (48%)	96 (100%)	0	100	100
4	J	89/183 (49%)	89 (100%)	0	100	100
4	L	89/183 (49%)	89 (100%)	0	100	100
4	N	89/183 (49%)	89 (100%)	0	100	100
All	All	1842/2577 (72%)	1839 (100%)	3 (0%)	91	94

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

Mol	Chain	Res	Type
2	B	148	CYS
2	D	148	CYS
2	F	148	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
5	NAG	G	1	1,5	14,14,15	0.23	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.46	0	17,19,21	0.58	0
5	NAG	K	1	1,5	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	K	2	5	14,14,15	0.47	0	17,19,21	0.57	0
5	NAG	O	1	1,5	14,14,15	0.23	0	17,19,21	0.48	0
5	NAG	O	2	5	14,14,15	0.46	0	17,19,21	0.58	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	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

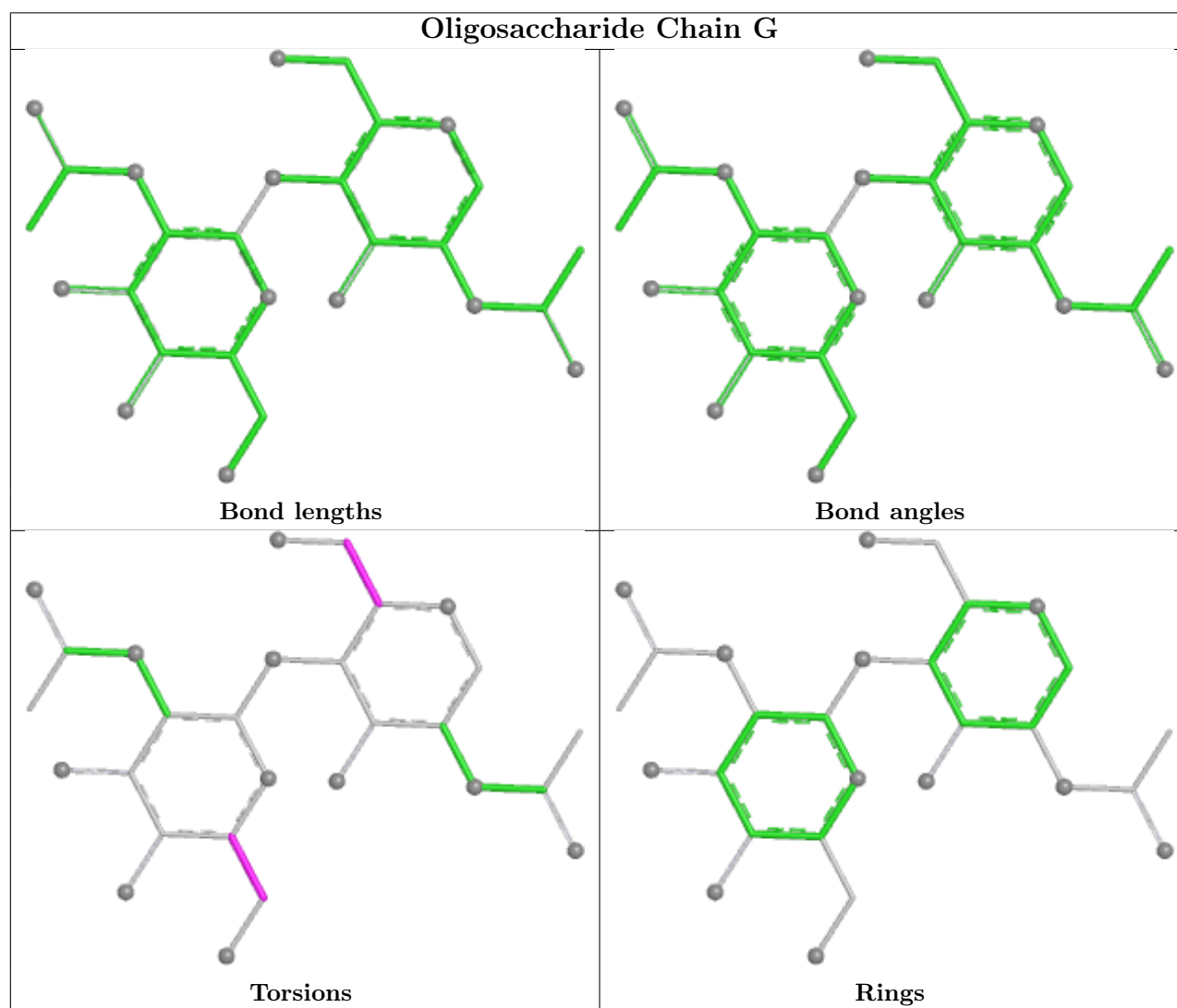
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6

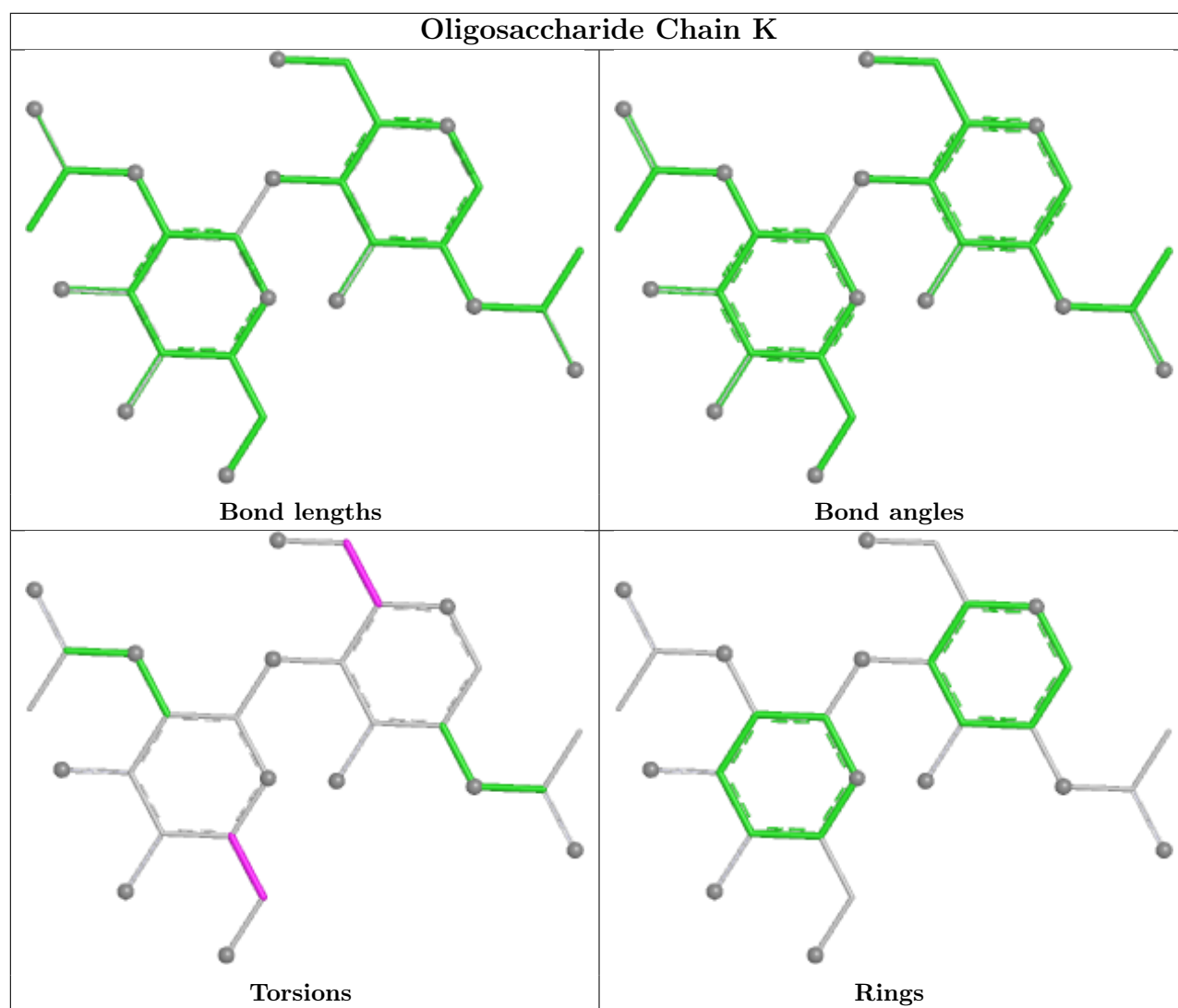
There are no ring outliers.

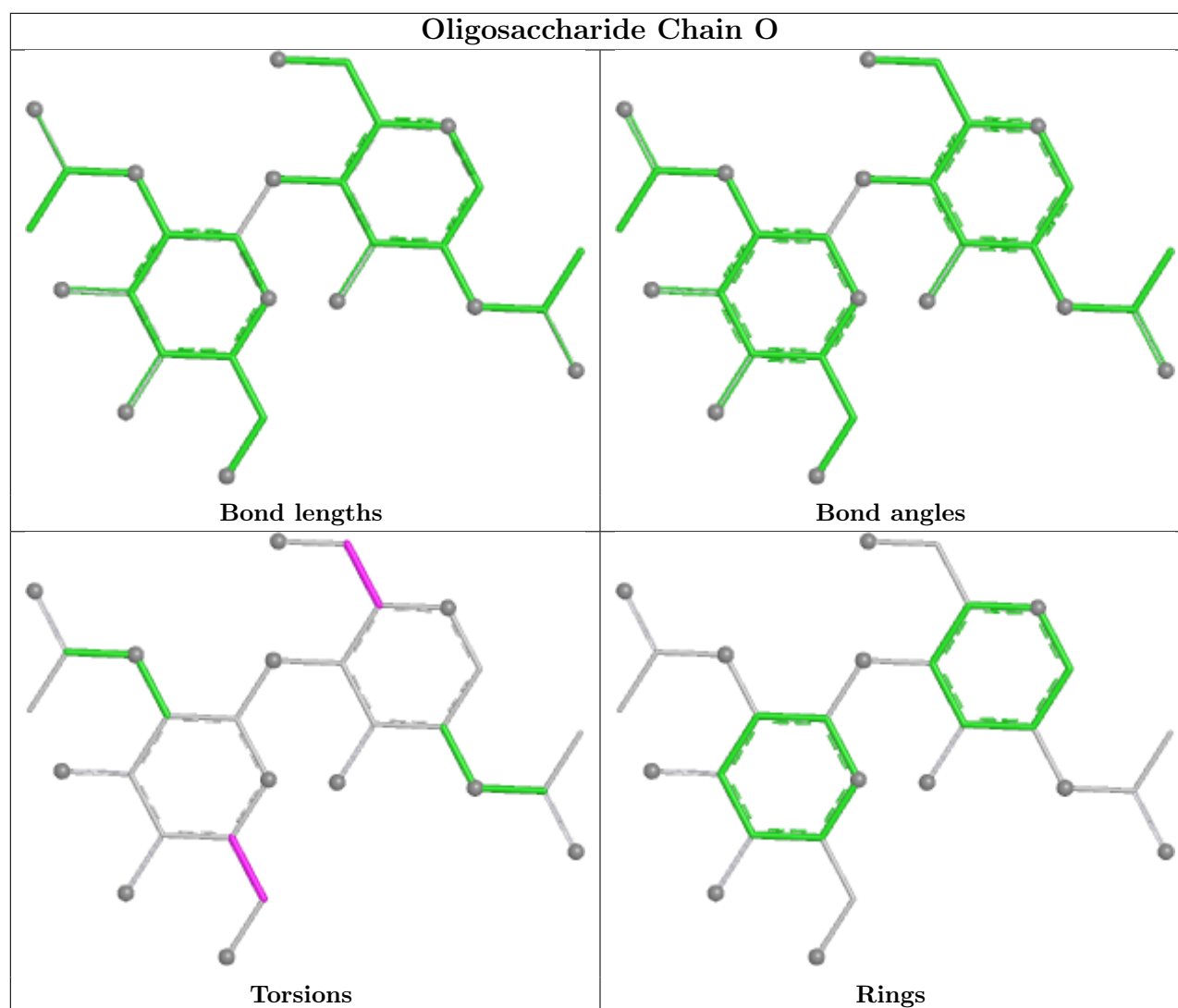
6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	2	0
5	G	1	NAG	2	0
5	K	2	NAG	1	0
5	O	1	NAG	2	0
5	O	2	NAG	2	0
5	K	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](#)

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	$\# Z > 2$
6	NAG	E	403	1	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	D	301	2	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	C	403	1	14,14,15	0.23	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	406	1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	E	406	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	B	301	2	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	C	404	1	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	F	301	2	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	A	406	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	A	403	1	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	A	405	1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	A	404	1	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	E	405	1	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	C	405	1	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	E	404	1	14,14,15	0.20	0	17,19,21	0.44	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	E	403	1	-	2/6/23/26	0/1/1/1
6	NAG	D	301	2	-	2/6/23/26	0/1/1/1
6	NAG	C	403	1	-	2/6/23/26	0/1/1/1
6	NAG	C	406	1	-	2/6/23/26	0/1/1/1
6	NAG	E	406	1	-	2/6/23/26	0/1/1/1
6	NAG	B	301	2	-	2/6/23/26	0/1/1/1
6	NAG	C	404	1	-	0/6/23/26	0/1/1/1
6	NAG	F	301	2	-	2/6/23/26	0/1/1/1
6	NAG	A	406	1	-	2/6/23/26	0/1/1/1
6	NAG	A	403	1	-	2/6/23/26	0/1/1/1
6	NAG	A	405	1	-	2/6/23/26	0/1/1/1
6	NAG	A	404	1	-	0/6/23/26	0/1/1/1
6	NAG	E	405	1	-	2/6/23/26	0/1/1/1
6	NAG	C	405	1	-	2/6/23/26	0/1/1/1
6	NAG	E	404	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	405	NAG	C4-C5-C6-O6
6	C	405	NAG	C4-C5-C6-O6
6	E	405	NAG	C4-C5-C6-O6
6	B	301	NAG	O5-C5-C6-O6
6	D	301	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	403	NAG	1	0
6	C	403	NAG	1	0
6	A	403	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.

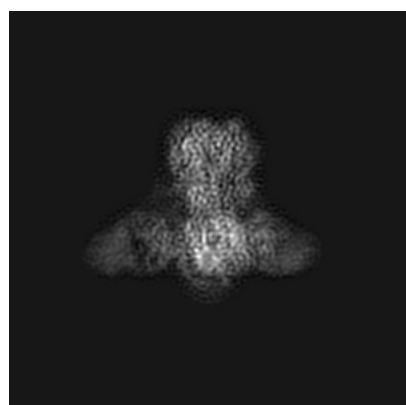
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22180. These allow visual inspection of the internal detail of the map and identification of artifacts.

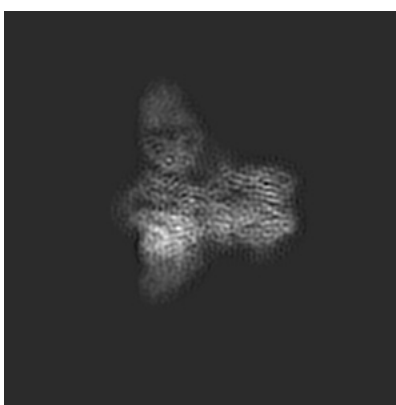
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

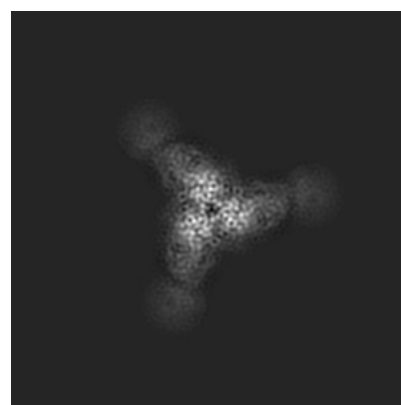
6.1.1 Primary map



X



Y



Z

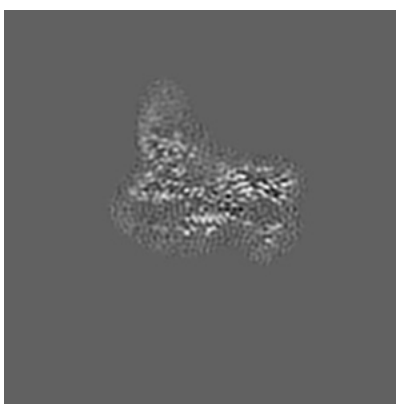
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

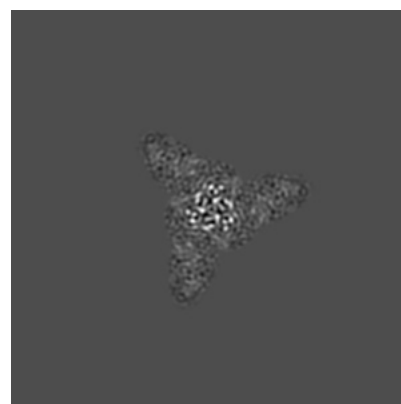
6.2.1 Primary map



X Index: 150



Y Index: 150

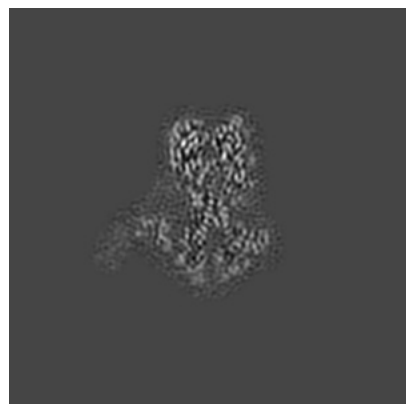


Z Index: 150

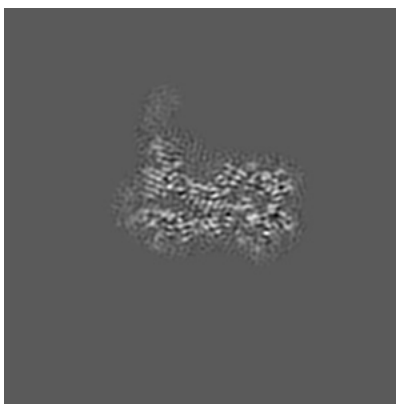
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

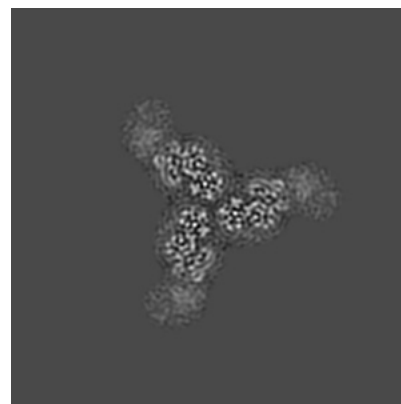
6.3.1 Primary map



X Index: 141



Y Index: 142

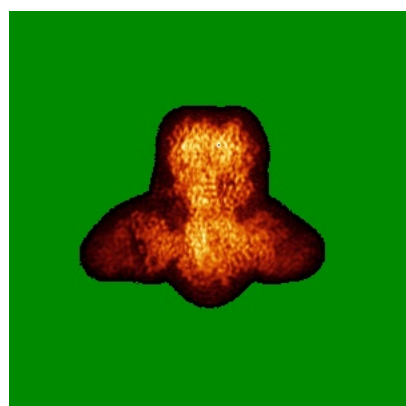


Z Index: 130

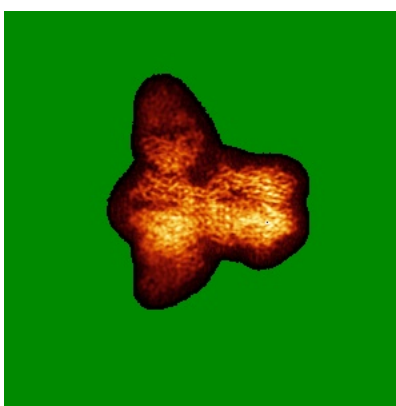
The images above show the largest variance slices of the map in three orthogonal directions.

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

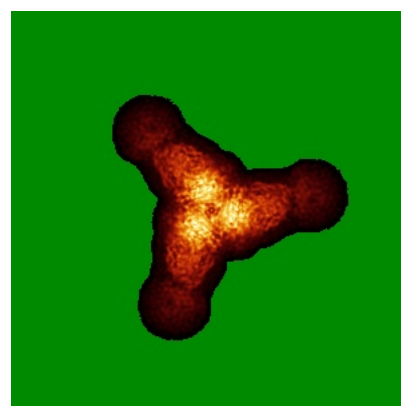
6.4.1 Primary map



X



Y

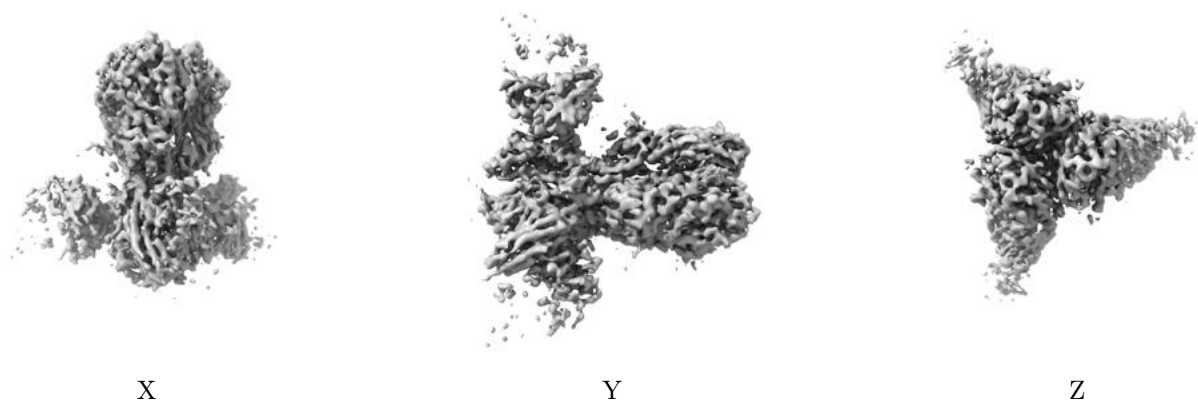


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

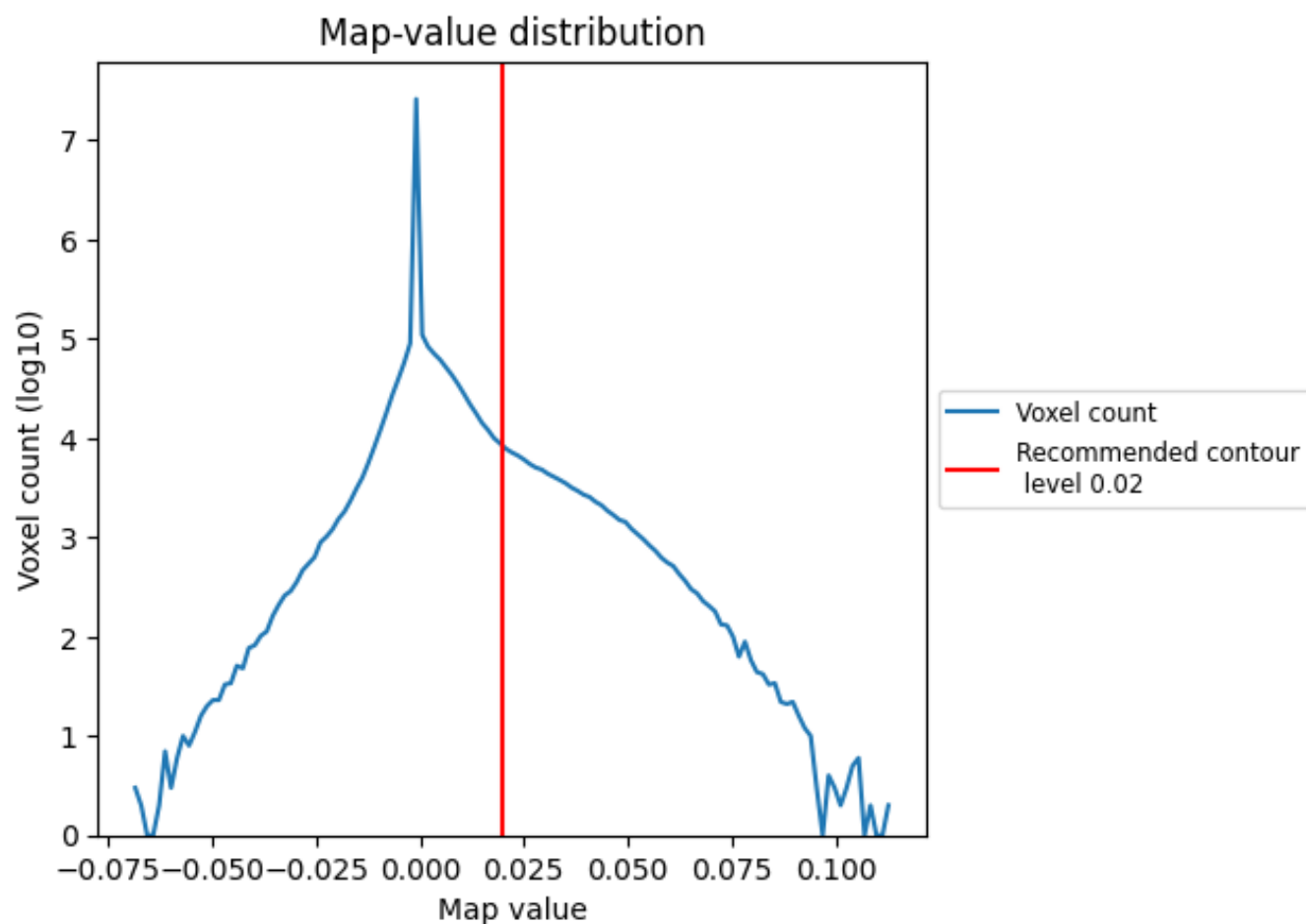
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

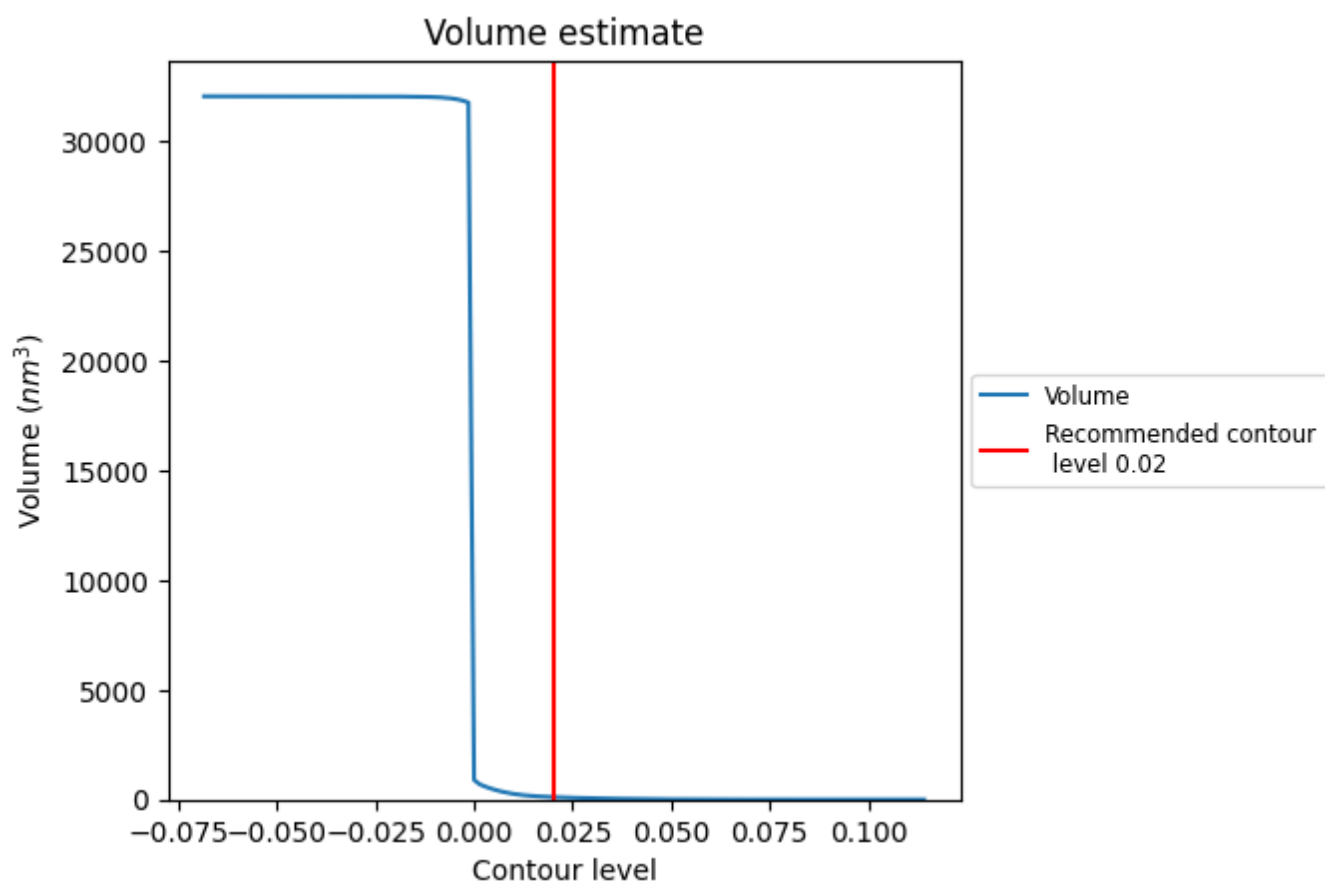
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

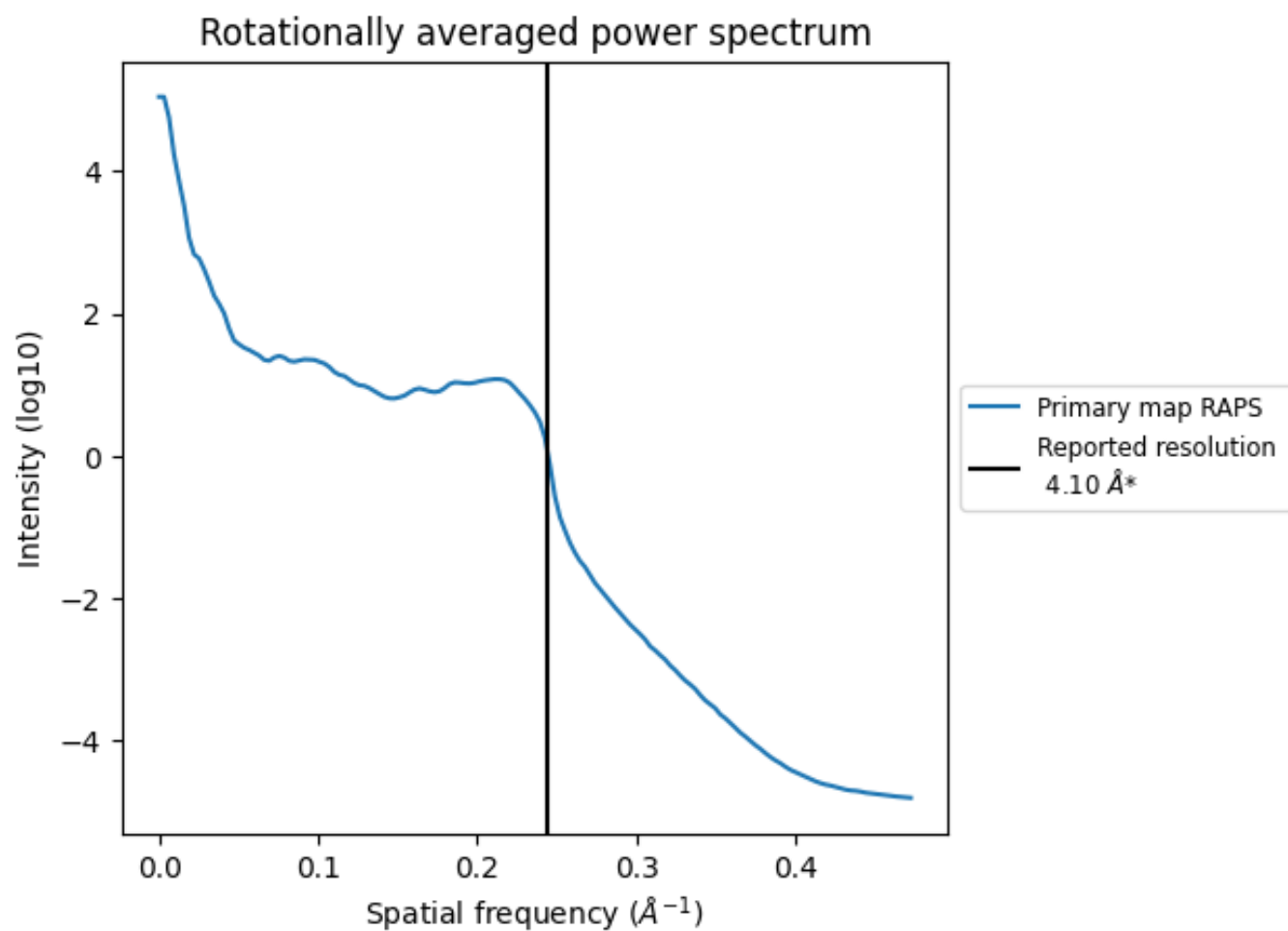
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm^3 ; this corresponds to an approximate mass of 102 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 0.244 Å⁻¹

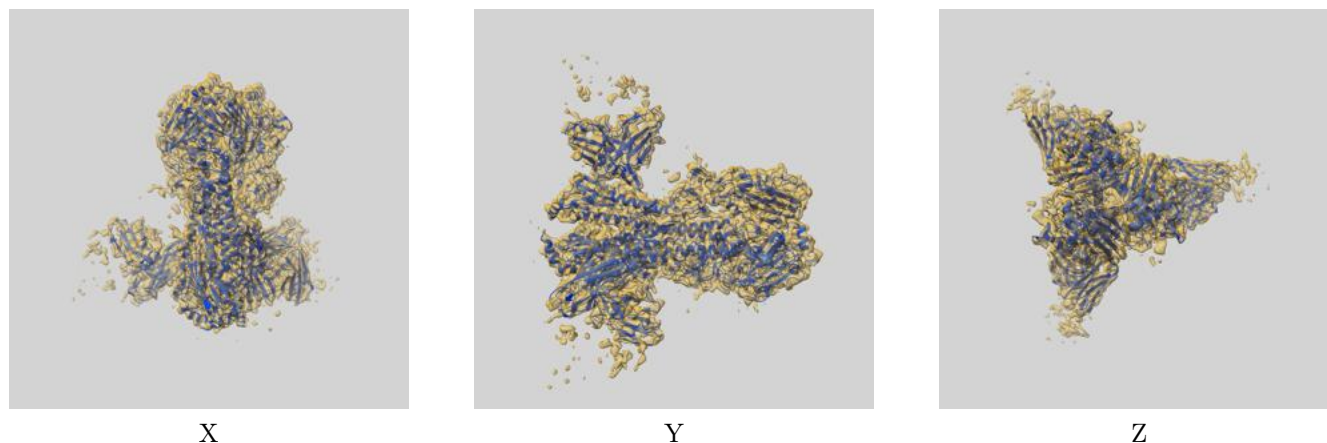
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

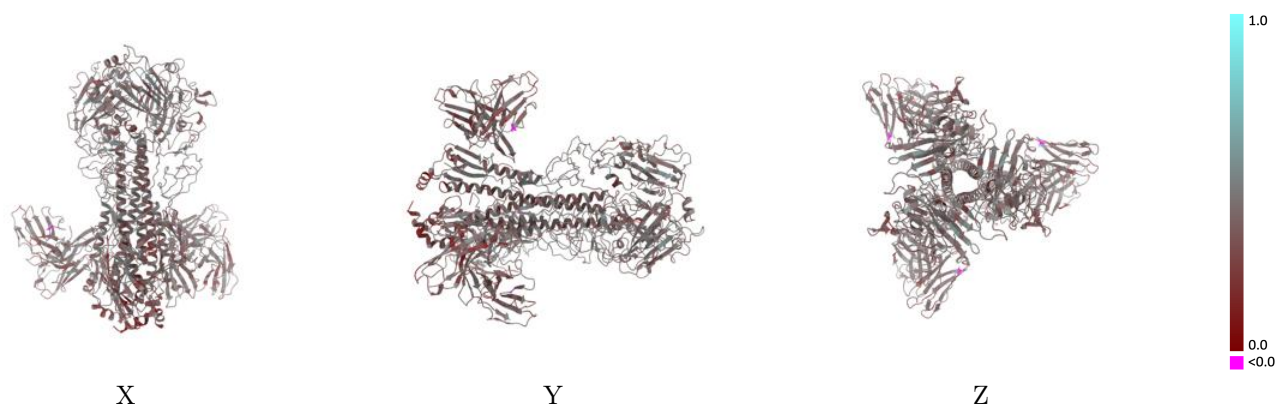
This section contains information regarding the fit between EMDB map EMD-22180 and PDB model 6XGC. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



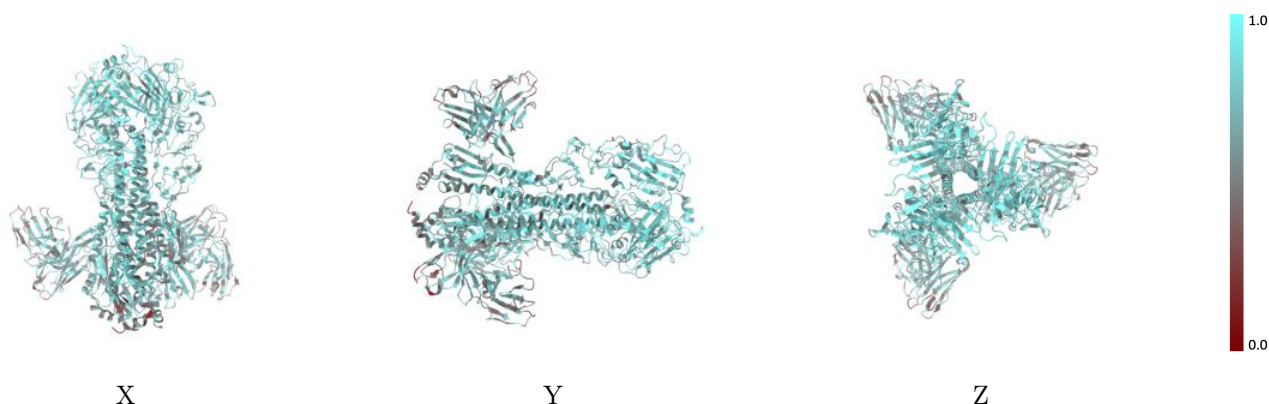
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



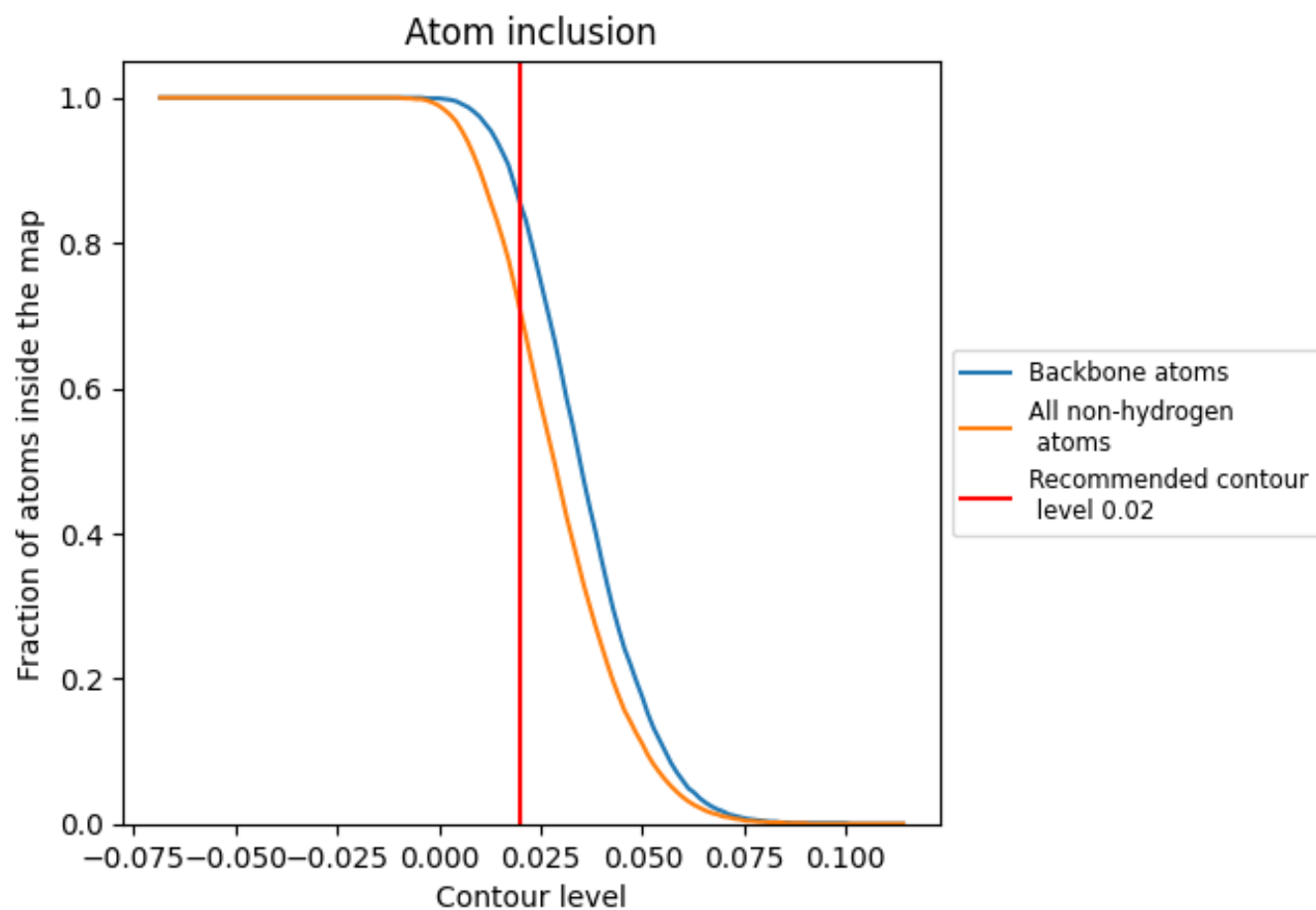
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7060	<div></div> 0.3920
A	<div></div> 0.7580	<div></div> 0.4180
B	<div></div> 0.7040	<div></div> 0.3790
C	<div></div> 0.7590	<div></div> 0.4150
D	<div></div> 0.7060	<div></div> 0.3770
E	<div></div> 0.7560	<div></div> 0.4160
F	<div></div> 0.7100	<div></div> 0.3750
G	<div></div> 0.6070	<div></div> 0.3280
H	<div></div> 0.6600	<div></div> 0.3760
I	<div></div> 0.6540	<div></div> 0.3730
J	<div></div> 0.5940	<div></div> 0.3580
K	<div></div> 0.6070	<div></div> 0.3190
L	<div></div> 0.5880	<div></div> 0.3590
M	<div></div> 0.6620	<div></div> 0.3760
N	<div></div> 0.5880	<div></div> 0.3620
O	<div></div> 0.6070	<div></div> 0.3300

1.0

0.0

<0.0