



Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 12:54 PM EDT

PDB ID : 9B8C / pdb_00009b8c
EMDB ID : EMD-44342
Title : RM018 Fab in complex with Apex GT 6.2 trimer and RM20A3 Fab
Authors : Pratap, P.P.; Ozorowski, G.; Ward, A.B.
Deposited on : 2024-03-29
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

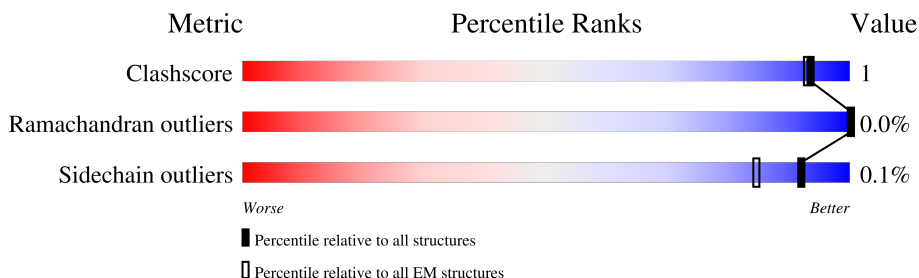
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	467	
1	C	467	
1	D	467	
2	B	153	
2	E	153	
2	F	153	
3	G	128	
3	J	128	

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Mol	Chain	Length	Quality of chain
3	N	128	
4	H	134	
5	I	125	
5	K	125	
5	M	125	
6	L	216	
7	O	8	
8	P	2	
8	Q	2	
8	R	2	
8	S	2	
8	U	2	
8	V	2	
8	W	2	
9	T	3	
9	X	3	

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	TYS	H	100(H)	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20899 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	421	Total	C	N	O	S	0	0
			3321	2091	585	619	26		
1	C	426	Total	C	N	O	S	0	0
			3358	2113	592	627	26		
1	D	422	Total	C	N	O	S	0	0
			3330	2096	587	621	26		

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	SER	PRO	conflict	UNP Q2N0S6
A	106	GLU	THR	conflict	UNP Q2N0S6
A	128	GLY	THR	conflict	UNP Q2N0S6
A	161	ALA	MET	conflict	UNP Q2N0S6
A	167	ASN	ASP	conflict	UNP Q2N0S6
A	169	ARG	LYS	conflict	UNP Q2N0S6
A	181	ILE	VAL	conflict	UNP Q2N0S6
A	183	PRO	GLN	conflict	UNP Q2N0S6
A	184	MET	ILE	conflict	UNP Q2N0S6
A	185	VAL	ASN	conflict	UNP Q2N0S6
A	186	ASP	GLU	conflict	UNP Q2N0S6
A	187	LEU	ASN	conflict	UNP Q2N0S6
A	188	TRP	GLN	conflict	UNP Q2N0S6
A	189	THR	GLY	conflict	UNP Q2N0S6
A	?	-	ARG	deletion	UNP Q2N0S6
A	?	-	SER	deletion	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	SER	deletion	UNP Q2N0S6
A	?	-	ASN	deletion	UNP Q2N0S6
A	?	-	LYS	deletion	UNP Q2N0S6
A	?	-	GLU	deletion	UNP Q2N0S6
A	195	SER	ASN	conflict	UNP Q2N0S6
A	240	GLN	PRO	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ASN	SER	conflict	UNP Q2N0S6
A	271	ILE	MET	conflict	UNP Q2N0S6
A	288	LEU	PHE	conflict	UNP Q2N0S6
A	291	SER	PRO	conflict	UNP Q2N0S6
A	304	VAL	ARG	conflict	UNP Q2N0S6
A	318	TYR	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	363	GLN	ASN	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
C	76	SER	PRO	conflict	UNP Q2N0S6
C	106	GLU	THR	conflict	UNP Q2N0S6
C	128	GLY	THR	conflict	UNP Q2N0S6
C	161	ALA	MET	conflict	UNP Q2N0S6
C	167	ASN	ASP	conflict	UNP Q2N0S6
C	169	ARG	LYS	conflict	UNP Q2N0S6
C	181	ILE	VAL	conflict	UNP Q2N0S6
C	183	PRO	GLN	conflict	UNP Q2N0S6
C	184	MET	ILE	conflict	UNP Q2N0S6
C	185	VAL	ASN	conflict	UNP Q2N0S6
C	186	ASP	GLU	conflict	UNP Q2N0S6
C	187	LEU	ASN	conflict	UNP Q2N0S6
C	188	TRP	GLN	conflict	UNP Q2N0S6
C	189	THR	GLY	conflict	UNP Q2N0S6
C	?	-	ARG	deletion	UNP Q2N0S6
C	?	-	SER	deletion	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	SER	deletion	UNP Q2N0S6
C	?	-	ASN	deletion	UNP Q2N0S6
C	?	-	LYS	deletion	UNP Q2N0S6
C	?	-	GLU	deletion	UNP Q2N0S6
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C	332	ASN	THR	conflict	UNP Q2N0S6
C	363	GLN	ASN	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	76	SER	PRO	conflict	UNP Q2N0S6
D	106	GLU	THR	conflict	UNP Q2N0S6
D	128	GLY	THR	conflict	UNP Q2N0S6
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D	183	PRO	GLN	conflict	UNP Q2N0S6
D	184	MET	ILE	conflict	UNP Q2N0S6
D	185	VAL	ASN	conflict	UNP Q2N0S6
D	186	ASP	GLU	conflict	UNP Q2N0S6
D	187	LEU	ASN	conflict	UNP Q2N0S6
D	188	TRP	GLN	conflict	UNP Q2N0S6
D	189	THR	GLY	conflict	UNP Q2N0S6
D	?	-	ARG	deletion	UNP Q2N0S6
D	?	-	SER	deletion	UNP Q2N0S6
D	?	-	ASN	deletion	UNP Q2N0S6
D	?	-	ASN	deletion	UNP Q2N0S6
D	?	-	SER	deletion	UNP Q2N0S6
D	?	-	ASN	deletion	UNP Q2N0S6
D	?	-	LYS	deletion	UNP Q2N0S6
D	?	-	GLU	deletion	UNP Q2N0S6
D	195	SER	ASN	conflict	UNP Q2N0S6
D	240	GLN	PRO	conflict	UNP Q2N0S6
D	241	ASN	SER	conflict	UNP Q2N0S6
D	271	ILE	MET	conflict	UNP Q2N0S6
D	288	LEU	PHE	conflict	UNP Q2N0S6
D	291	SER	PRO	conflict	UNP Q2N0S6
D	304	VAL	ARG	conflict	UNP Q2N0S6
D	318	TYR	ALA	conflict	UNP Q2N0S6
D	332	ASN	THR	conflict	UNP Q2N0S6
D	363	GLN	ASN	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	S	0	0
			934	587	162	179	6		
2	E	120	Total	C	N	O	S	0	0
			951	597	164	184	6		
2	F	121	Total	C	N	O	S	0	0
			957	600	165	186	6		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	519	SER	PHE	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	561	PRO	ALA	conflict	UNP Q2N0S6
B	568	ASP	LEU	conflict	UNP Q2N0S6
B	570	HIS	VAL	conflict	UNP Q2N0S6
B	585	HIS	ARG	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
E	519	SER	PHE	conflict	UNP Q2N0S6
E	559	PRO	ILE	conflict	UNP Q2N0S6
E	561	PRO	ALA	conflict	UNP Q2N0S6
E	568	ASP	LEU	conflict	UNP Q2N0S6
E	570	HIS	VAL	conflict	UNP Q2N0S6
E	585	HIS	ARG	conflict	UNP Q2N0S6
E	605	CYS	THR	conflict	UNP Q2N0S6
F	519	SER	PHE	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	561	PRO	ALA	conflict	UNP Q2N0S6
F	568	ASP	LEU	conflict	UNP Q2N0S6
F	570	HIS	VAL	conflict	UNP Q2N0S6
F	585	HIS	ARG	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called RM20A3 fragment antigen binding light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	108	Total	C	N	O	S	0	0
			803	499	135	166	3		
3	J	109	Total	C	N	O	S	0	0
			811	505	136	167	3		
3	N	109	Total	C	N	O	S	0	0
			811	505	136	167	3		

- Molecule 4 is a protein called RM018 fragment antigen binding heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	129	Total	C	N	O	S	0	0
			999	633	162	199	5		

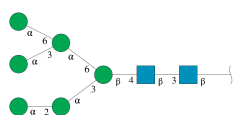
- Molecule 5 is a protein called RM20A3 fragment antigen binding heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	122	Total	C	N	O	S	0	0
			928	587	159	177	5		
5	K	123	Total	C	N	O	S	0	0
			934	590	160	179	5		
5	M	122	Total	C	N	O	S	0	0
			928	587	159	177	5		

- Molecule 6 is a protein called RM018 fragment antigen binding light chain.

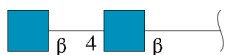
Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	106	Total	C	N	O	S	0	0
			794	490	132	169	3		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



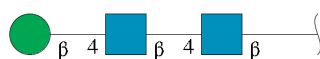
Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	2	Total	C	N	O	0	0
			28	16	2	10		
8	Q	2	Total	C	N	O	0	0
			28	16	2	10		
8	R	2	Total	C	N	O	0	0
			28	16	2	10		
8	S	2	Total	C	N	O	0	0
			28	16	2	10		

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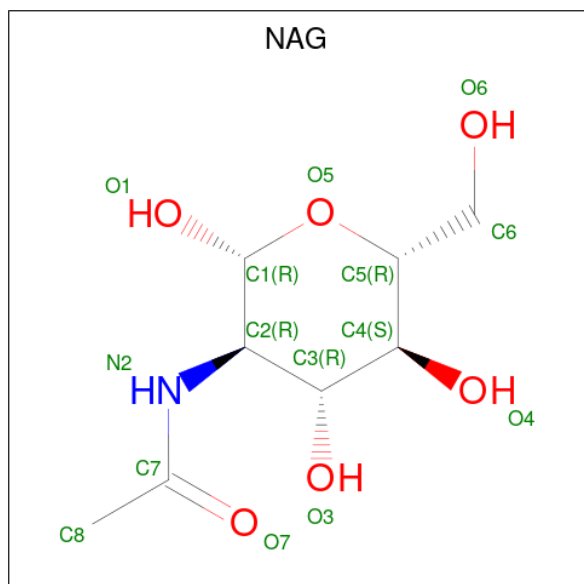
Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	2	Total	C	N	O	0	0
			28	16	2	10		
8	V	2	Total	C	N	O	0	0
			28	16	2	10		
8	W	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 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
9	T	3	Total	C	N	O	0	0
			39	22	2	15		
9	X	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

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

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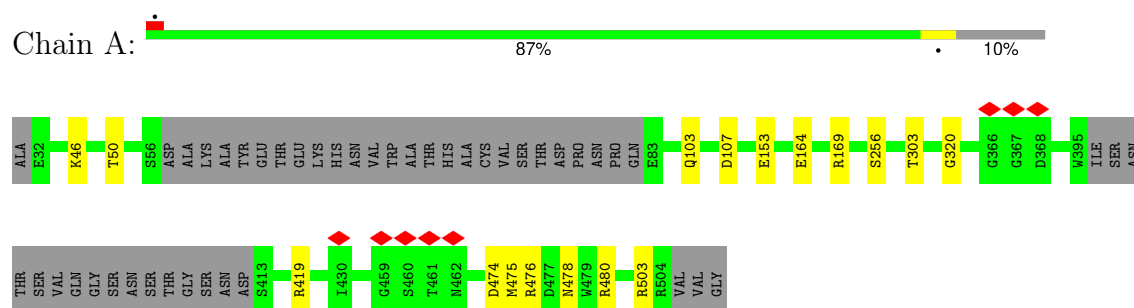
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Mol	Chain	Residues	Atoms				AltConf
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	

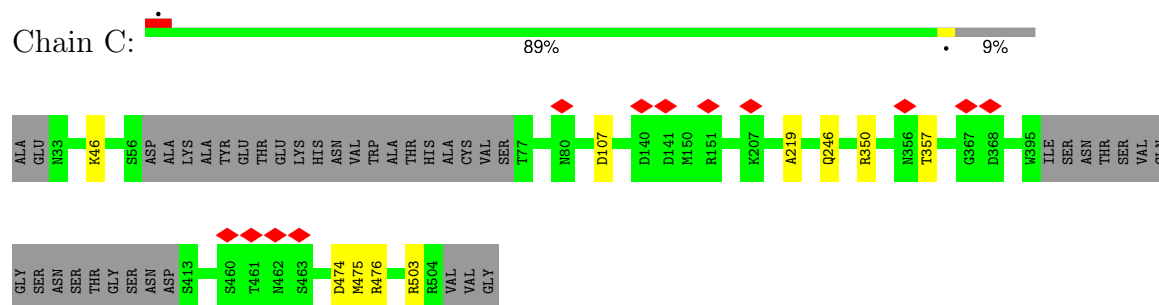
3 Residue-property plots [i](#)

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.

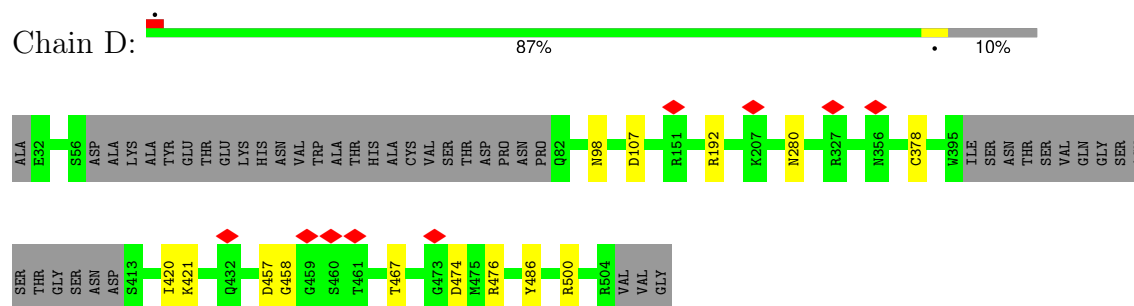
- Molecule 1: Envelope glycoprotein gp120



- Molecule 1: Envelope glycoprotein gp120

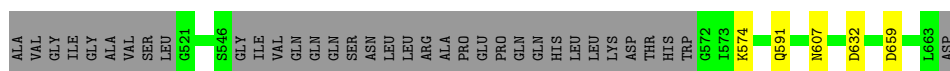


- Molecule 1: Envelope glycoprotein gp120



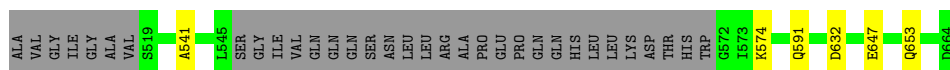
- Molecule 2: Transmembrane protein gp41





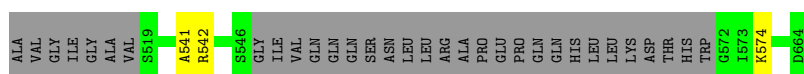
- Molecule 2: Transmembrane protein gp41

Chain E: 75% 22%



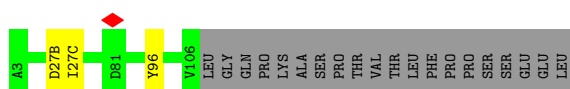
- Molecule 2: Transmembrane protein gp41

Chain F: 77% 21%



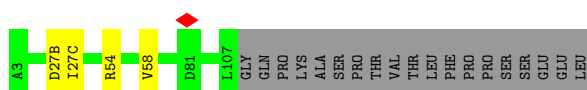
- Molecule 3: RM20A3 fragment antigen binding light chain

Chain G: 82% 16%



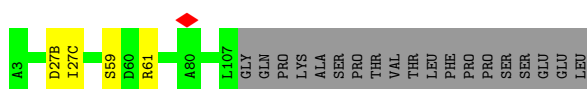
- Molecule 3: RM20A3 fragment antigen binding light chain

Chain J: 82% 15%



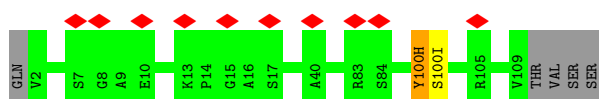
- Molecule 3: RM20A3 fragment antigen binding light chain

Chain N: 82% 15%



- Molecule 4: RM018 fragment antigen binding heavy chain

Chain H: 7% 95%



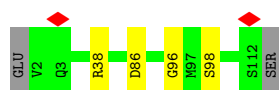
- Molecule 5: RM20A3 fragment antigen binding heavy chain

Chain I:  94%



- Molecule 5: RM20A3 fragment antigen binding heavy chain

Chain K:  95%



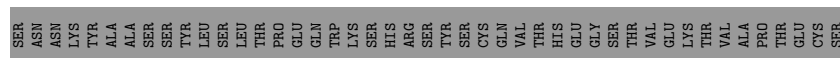
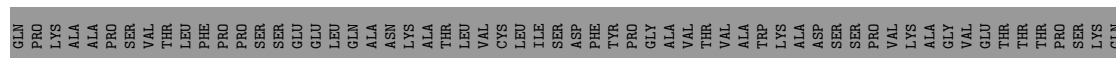
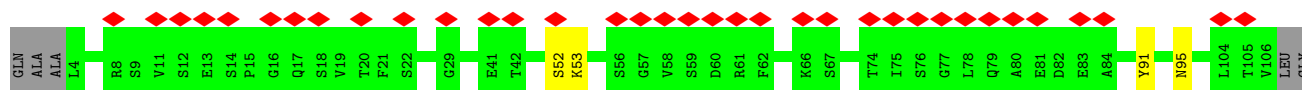
- Molecule 5: RM20A3 fragment antigen binding heavy chain

Chain M:  92%

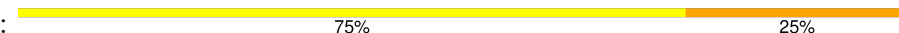


- Molecule 6: RM018 fragment antigen binding light chain

Chain L:  16% 47% 51%



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  75% 25%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  67% 33%



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  33% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108789	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.530	Depositor
Minimum map value	-0.807	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	522.0, 522.0, 522.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.305, 1.305, 1.305	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, BMA, TYS, MAN

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	0.23	0/3388	0.50	0/4597
1	C	0.22	0/3427	0.47	0/4653
1	D	0.23	0/3397	0.51	0/4609
2	B	0.23	0/950	0.44	0/1287
2	E	0.22	0/967	0.42	0/1309
2	F	0.20	0/973	0.39	0/1317
3	G	0.21	0/822	0.46	0/1118
3	J	0.22	0/830	0.45	0/1129
3	N	0.22	0/830	0.48	0/1129
4	H	0.25	0/1003	0.57	0/1363
5	I	0.21	0/948	0.46	0/1280
5	K	0.22	0/954	0.46	0/1288
5	M	0.20	0/948	0.48	0/1280
6	L	0.26	0/811	0.63	0/1101
All	All	0.23	0/20248	0.49	0/27460

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	3321	0	3276	17	0
1	C	3358	0	3311	7	0
1	D	3330	0	3284	8	0
2	B	934	0	907	5	0
2	E	951	0	922	6	0
2	F	957	0	927	3	0
3	G	803	0	756	2	0
3	J	811	0	767	2	0
3	N	811	0	767	2	0
4	H	999	0	968	6	0
5	I	928	0	901	2	0
5	K	934	0	906	3	0
5	M	928	0	901	4	0
6	L	794	0	742	1	0
7	O	94	0	79	1	0
8	P	28	0	25	0	0
8	Q	28	0	25	0	0
8	R	28	0	25	0	0
8	S	28	0	25	0	0
8	U	28	0	25	0	0
8	V	28	0	25	0	0
8	W	28	0	25	0	0
9	T	39	0	34	0	0
9	X	39	0	34	0	0
10	A	196	0	182	0	0
10	B	42	0	39	0	0
10	C	168	0	156	0	0
10	D	182	0	169	0	0
10	E	42	0	39	0	0
10	F	42	0	39	0	0
All	All	20899	0	20281	49	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 1.

All (49) 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:169:ARG:HH12	4:H:100(H):TYS:CE1	1.45	1.27
1:A:169:ARG:NH1	4:H:100(H):TYS:CE1	2.24	1.00
1:A:169:ARG:HH12	4:H:100(H):TYS:HE1	1.42	0.85
1:A:169:ARG:NH1	4:H:100(H):TYS:HE1	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1:NAG:O4	7:O:2:NAG:N2	2.19	0.74
1:C:46:LYS:NZ	2:E:632:ASP:OD2	2.20	0.74
1:A:107:ASP:OD1	2:B:574:LYS:NZ	2.29	0.66
5:I:29:PHE:O	5:I:71:ARG:NH2	2.28	0.66
1:A:46:LYS:NZ	2:B:632:ASP:OD2	2.29	0.66
3:J:54:ARG:NH1	3:J:58:VAL:O	2.31	0.64
2:B:591:GLN:NE2	2:E:541:ALA:O	2.31	0.64
1:C:107:ASP:OD1	2:E:574:LYS:NZ	2.34	0.60
5:M:23:ARG:NH1	5:M:77:THR:OG1	2.39	0.56
1:A:474:ASP:OD1	1:A:475:MET:N	2.39	0.55
1:A:256:SER:O	1:A:478:ASN:ND2	2.38	0.55
3:N:27(B):ASP:OD1	3:N:27(C):ILE:N	2.38	0.55
1:C:474:ASP:OD2	1:C:476:ARG:NH1	2.40	0.54
1:C:474:ASP:OD1	1:C:475:MET:N	2.40	0.54
1:C:219:ALA:O	1:C:246:GLN:NE2	2.42	0.53
1:A:474:ASP:OD2	1:A:476:ARG:NH1	2.40	0.53
5:K:38:ARG:NH1	5:K:86:ASP:OD1	2.43	0.52
1:C:503:ARG:NH2	2:E:653:GLN:OE1	2.42	0.52
1:D:107:ASP:OD1	2:F:574:LYS:NZ	2.43	0.52
2:E:591:GLN:NE2	2:F:541:ALA:O	2.43	0.52
1:D:98:ASN:ND2	1:D:486:TYR:O	2.44	0.51
1:A:169:ARG:HH12	4:H:100(H):TYS:CD1	2.14	0.50
3:G:27(B):ASP:OD1	3:G:27(C):ILE:N	2.41	0.50
1:D:457:ASP:N	1:D:467:THR:O	2.44	0.50
1:C:350:ARG:NH1	1:C:357:THR:O	2.44	0.49
1:A:169:ARG:NH1	4:H:100(H):TYS:CD1	2.75	0.48
1:D:420:ILE:HG22	1:D:421:LYS:H	1.79	0.47
5:M:62:SER:O	5:M:66:ARG:NH1	2.47	0.47
1:A:503:ARG:O	2:B:607:ASN:ND2	2.45	0.46
6:L:91:TYR:OH	6:L:95:ASN:ND2	2.45	0.46
3:G:96:TYR:OH	5:K:96:GLY:O	2.33	0.45
1:A:164:GLU:OE2	1:D:192:ARG:NH1	2.46	0.45
3:J:27(B):ASP:OD1	3:J:27(C):ILE:N	2.39	0.45
2:E:647:GLU:OE2	2:F:542:ARG:NH1	2.50	0.45
1:D:500:ARG:NH2	5:K:98:SER:OG	2.50	0.44
3:N:59:SER:OG	3:N:61:ARG:NH1	2.51	0.44
1:D:280:ASN:ND2	1:D:458:GLY:O	2.52	0.42
1:D:474:ASP:OD2	1:D:476:ARG:NE	2.52	0.42
2:B:659:ASP:OD2	5:M:53:ARG:NH2	2.50	0.42
1:A:153:GLU:OE2	1:A:419:ARG:NH1	2.48	0.42
1:A:476:ARG:O	1:A:480:ARG:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:O	1:A:320:GLY:N	2.50	0.41
5:I:38:ARG:NH1	5:I:86:ASP:OD1	2.53	0.41
5:M:52:ASN:O	5:M:71:ARG:NH1	2.54	0.41
1:A:50:THR:O	1:A:103:GLN:NE2	2.48	0.40

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	415/467 (89%)	398 (96%)	17 (4%)	0	100	100
1	C	420/467 (90%)	413 (98%)	7 (2%)	0	100	100
1	D	416/467 (89%)	397 (95%)	19 (5%)	0	100	100
2	B	114/153 (74%)	113 (99%)	1 (1%)	0	100	100
2	E	116/153 (76%)	114 (98%)	2 (2%)	0	100	100
2	F	117/153 (76%)	117 (100%)	0	0	100	100
3	G	106/128 (83%)	103 (97%)	3 (3%)	0	100	100
3	J	107/128 (84%)	102 (95%)	5 (5%)	0	100	100
3	N	107/128 (84%)	103 (96%)	4 (4%)	0	100	100
4	H	126/134 (94%)	111 (88%)	14 (11%)	1 (1%)	16	46
5	I	120/125 (96%)	115 (96%)	5 (4%)	0	100	100
5	K	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
5	M	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
6	L	104/216 (48%)	94 (90%)	10 (10%)	0	100	100
All	All	2509/2969 (84%)	2414 (96%)	94 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	100(I)	SER

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	376/414 (91%)	376 (100%)	0	100	100
1	C	381/414 (92%)	381 (100%)	0	100	100
1	D	377/414 (91%)	376 (100%)	1 (0%)	91	94
2	B	101/130 (78%)	101 (100%)	0	100	100
2	E	103/130 (79%)	103 (100%)	0	100	100
2	F	104/130 (80%)	104 (100%)	0	100	100
3	G	88/106 (83%)	88 (100%)	0	100	100
3	J	89/106 (84%)	89 (100%)	0	100	100
3	N	89/106 (84%)	89 (100%)	0	100	100
4	H	106/111 (96%)	106 (100%)	0	100	100
5	I	99/102 (97%)	99 (100%)	0	100	100
5	K	100/102 (98%)	100 (100%)	0	100	100
5	M	99/102 (97%)	99 (100%)	0	100	100
6	L	90/183 (49%)	88 (98%)	2 (2%)	47	69
All	All	2202/2550 (86%)	2199 (100%)	3 (0%)	92	96

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

Mol	Chain	Res	Type
1	D	378	CYS
6	L	52	SER
6	L	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
2	B	591	GLN
1	C	425	ASN
1	D	114	GLN
1	D	314	GLN
3	G	38	GLN
5	I	39	GLN
3	J	38	GLN
5	K	39	GLN
5	K	82(A)	HIS
6	L	31	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
4	TYS	H	100(H)	4	15,16,17	1.57	2 (13%)	15,22,24	1.41	2 (13%)

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	TYS	H	100(H)	4	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	100(H)	TYS	OH-S	4.91	1.68	1.58
4	H	100(H)	TYS	OH-CZ	-3.22	1.37	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	100(H)	TYS	OH-S-O1	-2.71	99.30	107.56
4	H	100(H)	TYS	CB-CG-CD2	2.48	125.53	120.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	100(H)	TYS	6	0

5.5 Carbohydrates [i](#)

28 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	$\# Z > 2$
7	NAG	O	1	1,7	14,14,15	0.73	0	17,19,21	1.48	2 (11%)
7	NAG	O	2	7	14,14,15	0.93	0	17,19,21	1.20	1 (5%)
7	BMA	O	3	7	11,11,12	0.91	0	15,15,17	1.02	1 (6%)
7	MAN	O	4	7	11,11,12	0.72	0	15,15,17	1.19	2 (13%)
7	MAN	O	5	7	11,11,12	0.68	0	15,15,17	1.23	1 (6%)
7	MAN	O	6	7	11,11,12	0.75	0	15,15,17	1.06	1 (6%)
7	MAN	O	7	7	11,11,12	0.72	0	15,15,17	1.14	1 (6%)
7	MAN	O	8	7	11,11,12	0.73	0	15,15,17	1.05	1 (6%)
8	NAG	P	1	8,1	14,14,15	0.70	0	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	P	2	8	14,14,15	0.67	0	17,19,21	0.84	0
8	NAG	Q	1	8,1	14,14,15	0.68	0	17,19,21	0.80	0
8	NAG	Q	2	8	14,14,15	0.74	0	17,19,21	0.73	0
8	NAG	R	1	8,1	14,14,15	0.67	0	17,19,21	1.14	2 (11%)
8	NAG	R	2	8	14,14,15	0.67	0	17,19,21	0.96	1 (5%)
8	NAG	S	1	8,1	14,14,15	0.69	0	17,19,21	0.91	1 (5%)
8	NAG	S	2	8	14,14,15	0.68	0	17,19,21	0.85	1 (5%)
9	NAG	T	1	9,1	14,14,15	0.73	0	17,19,21	0.86	0
9	NAG	T	2	9	14,14,15	0.81	0	17,19,21	0.75	0
9	BMA	T	3	9	11,11,12	0.74	0	15,15,17	0.99	1 (6%)
8	NAG	U	1	8,1	14,14,15	0.71	0	17,19,21	0.78	0
8	NAG	U	2	8	14,14,15	0.70	0	17,19,21	0.64	0
8	NAG	V	1	8,1	14,14,15	0.76	0	17,19,21	0.77	1 (5%)
8	NAG	V	2	8	14,14,15	0.68	0	17,19,21	0.87	1 (5%)
8	NAG	W	1	8,1	14,14,15	0.73	0	17,19,21	0.89	1 (5%)
8	NAG	W	2	8	14,14,15	0.66	0	17,19,21	0.86	1 (5%)
9	NAG	X	1	9,1	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
9	NAG	X	2	9	14,14,15	0.76	0	17,19,21	0.78	0
9	BMA	X	3	9	11,11,12	0.79	0	15,15,17	1.00	1 (6%)

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
7	NAG	O	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
7	MAN	O	4	7	-	1/2/19/22	0/1/1/1
7	MAN	O	5	7	-	0/2/19/22	1/1/1/1
7	MAN	O	6	7	-	2/2/19/22	0/1/1/1
7	MAN	O	7	7	-	0/2/19/22	0/1/1/1
7	MAN	O	8	7	-	2/2/19/22	0/1/1/1
8	NAG	P	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	P	2	8	-	1/6/23/26	0/1/1/1
8	NAG	Q	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	NAG	R	1	8,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	R	2	8	-	0/6/23/26	0/1/1/1
8	NAG	S	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	S	2	8	-	1/6/23/26	0/1/1/1
9	NAG	T	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	T	2	9	-	0/6/23/26	0/1/1/1
9	BMA	T	3	9	-	1/2/19/22	0/1/1/1
8	NAG	U	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	1/6/23/26	0/1/1/1
8	NAG	V	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	V	2	8	-	0/6/23/26	0/1/1/1
8	NAG	W	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
9	NAG	X	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	5	MAN	C1-O5-C5	3.73	117.19	112.19
7	O	1	NAG	O3-C3-C4	3.69	119.08	110.38
7	O	1	NAG	C4-C3-C2	-3.09	106.49	111.02
7	O	7	MAN	C1-O5-C5	3.07	116.30	112.19
9	X	3	BMA	C1-O5-C5	2.91	116.09	112.19
7	O	6	MAN	C1-O5-C5	2.83	115.98	112.19
9	T	3	BMA	C1-O5-C5	2.81	115.96	112.19
7	O	8	MAN	C1-O5-C5	2.80	115.94	112.19
8	R	1	NAG	C1-O5-C5	2.72	115.84	112.19
7	O	3	BMA	C1-O5-C5	2.67	115.76	112.19
7	O	4	MAN	C1-O5-C5	2.65	115.73	112.19
7	O	2	NAG	C1-O5-C5	2.62	115.69	112.19
9	X	1	NAG	C1-O5-C5	2.58	115.64	112.19
8	V	2	NAG	C1-O5-C5	2.43	115.45	112.19
7	O	4	MAN	O2-C2-C3	2.25	114.82	110.15
8	S	2	NAG	C1-O5-C5	2.15	115.07	112.19
8	S	1	NAG	C1-O5-C5	2.14	115.05	112.19
8	R	2	NAG	C1-O5-C5	2.10	115.00	112.19
8	V	1	NAG	C1-O5-C5	2.05	114.94	112.19
8	R	1	NAG	C2-N2-C7	2.04	125.63	122.90
8	W	2	NAG	C1-O5-C5	2.03	114.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	1	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	O	6	MAN	O5-C5-C6-O6
8	W	1	NAG	O5-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
7	O	6	MAN	C4-C5-C6-O6
8	W	1	NAG	C4-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
7	O	8	MAN	O5-C5-C6-O6
8	P	2	NAG	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
8	Q	2	NAG	O5-C5-C6-O6
7	O	4	MAN	O5-C5-C6-O6
9	X	3	BMA	O5-C5-C6-O6
9	T	3	BMA	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
9	X	2	NAG	C4-C5-C6-O6
8	S	2	NAG	O5-C5-C6-O6
8	P	1	NAG	C4-C5-C6-O6
8	P	1	NAG	O5-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
7	O	8	MAN	C4-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
8	R	1	NAG	C4-C5-C6-O6

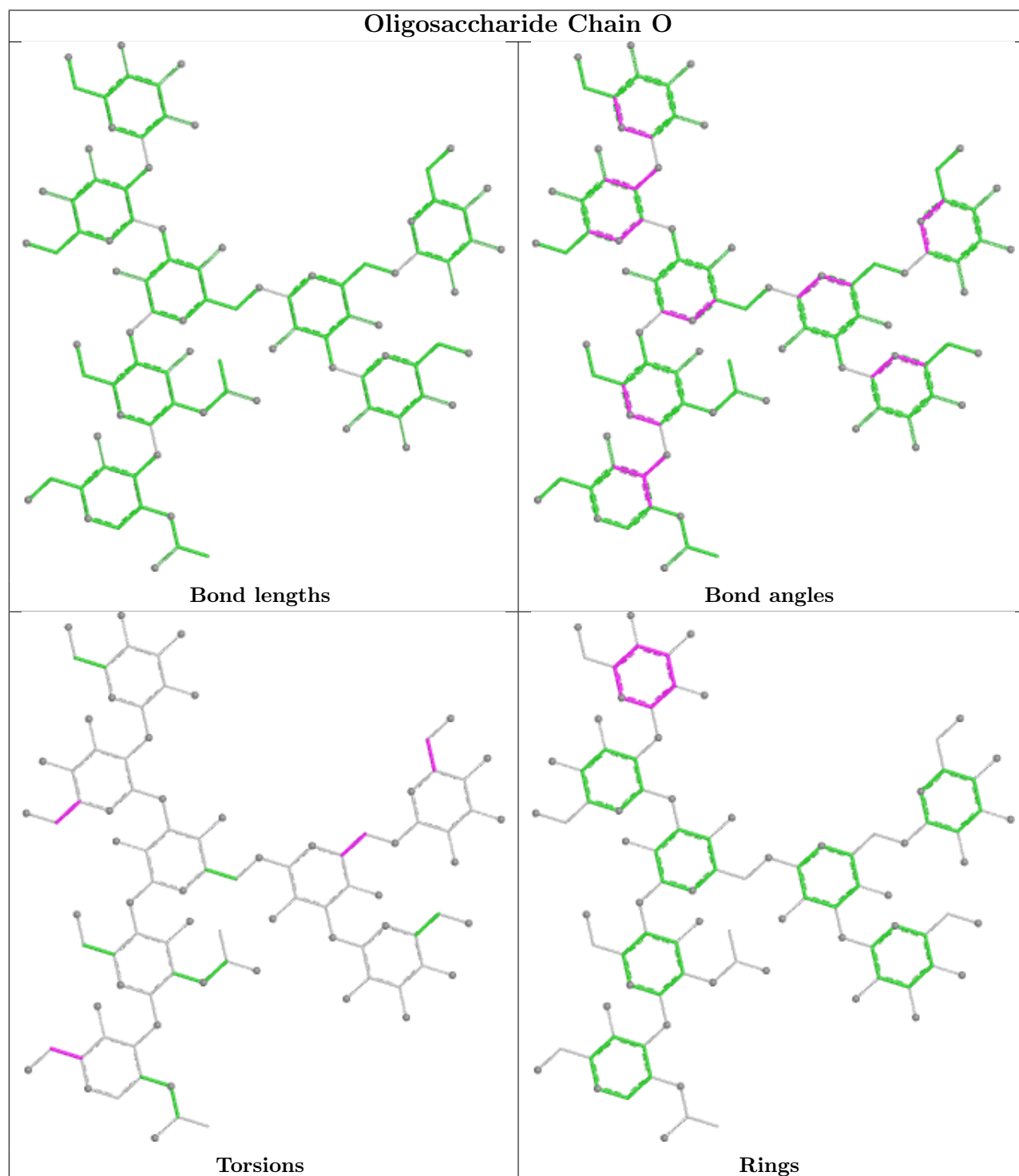
All (1) ring outliers are listed below:

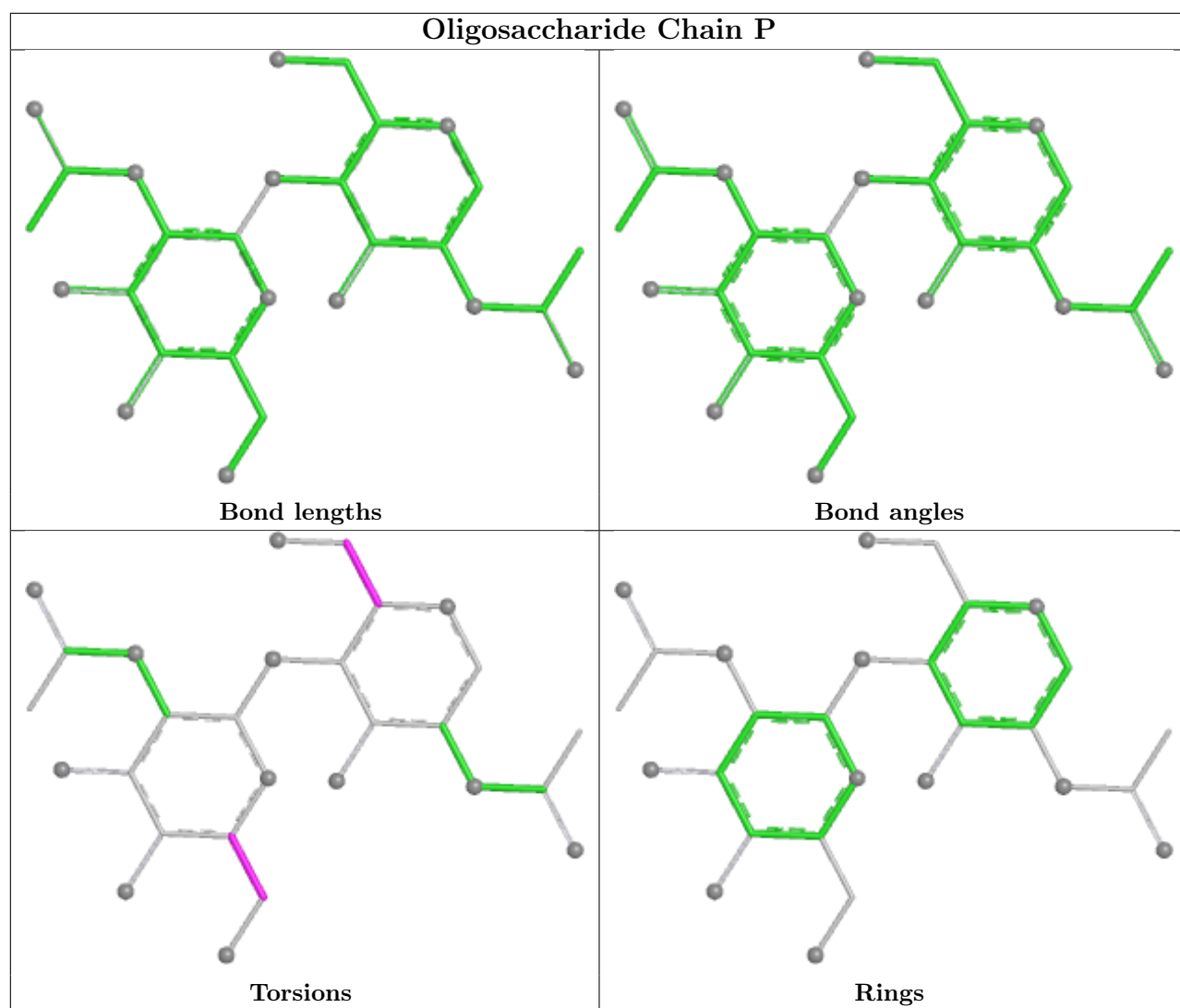
Mol	Chain	Res	Type	Atoms
7	O	5	MAN	C1-C2-C3-C4-C5-O5

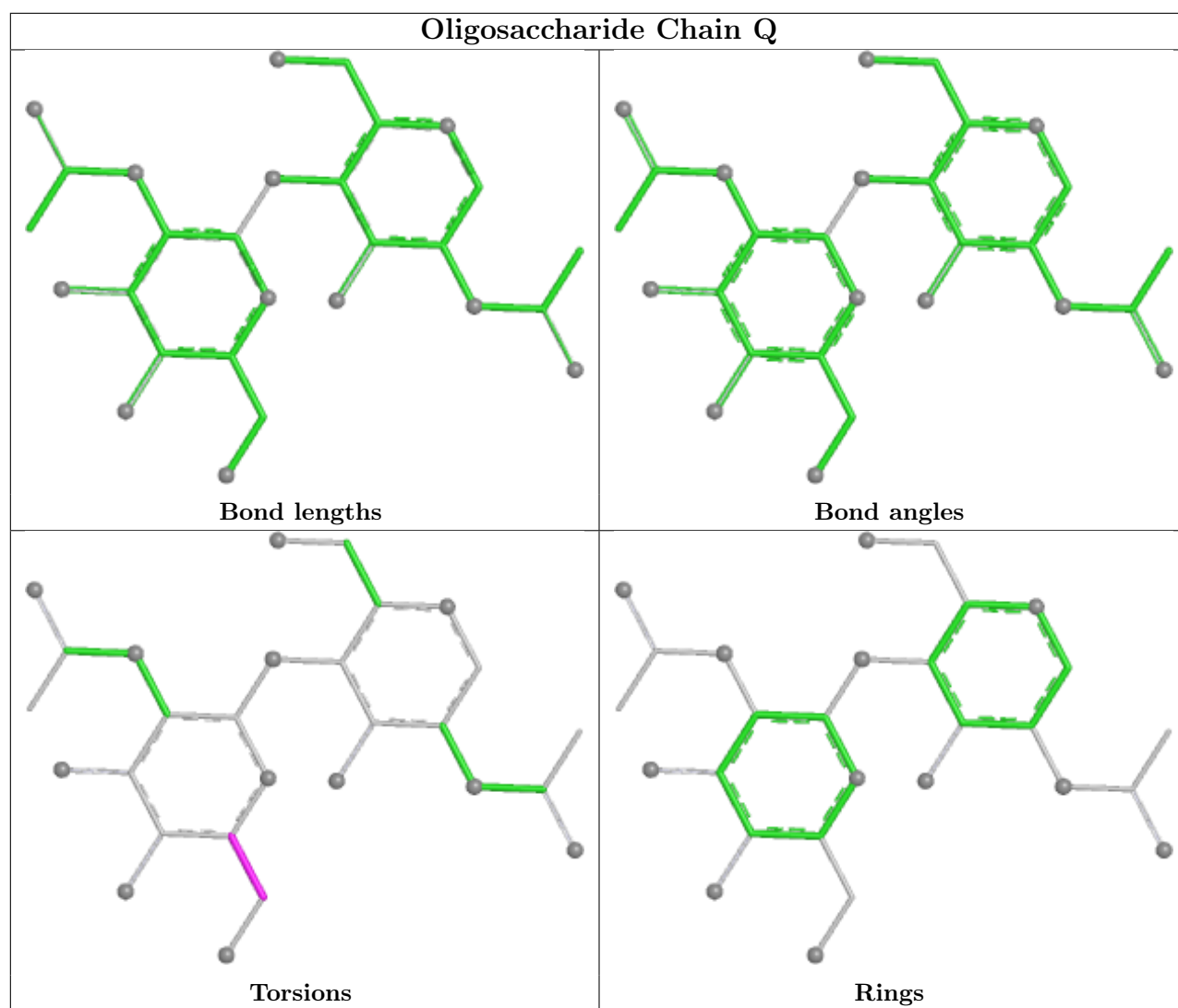
2 monomers are involved in 1 short contact:

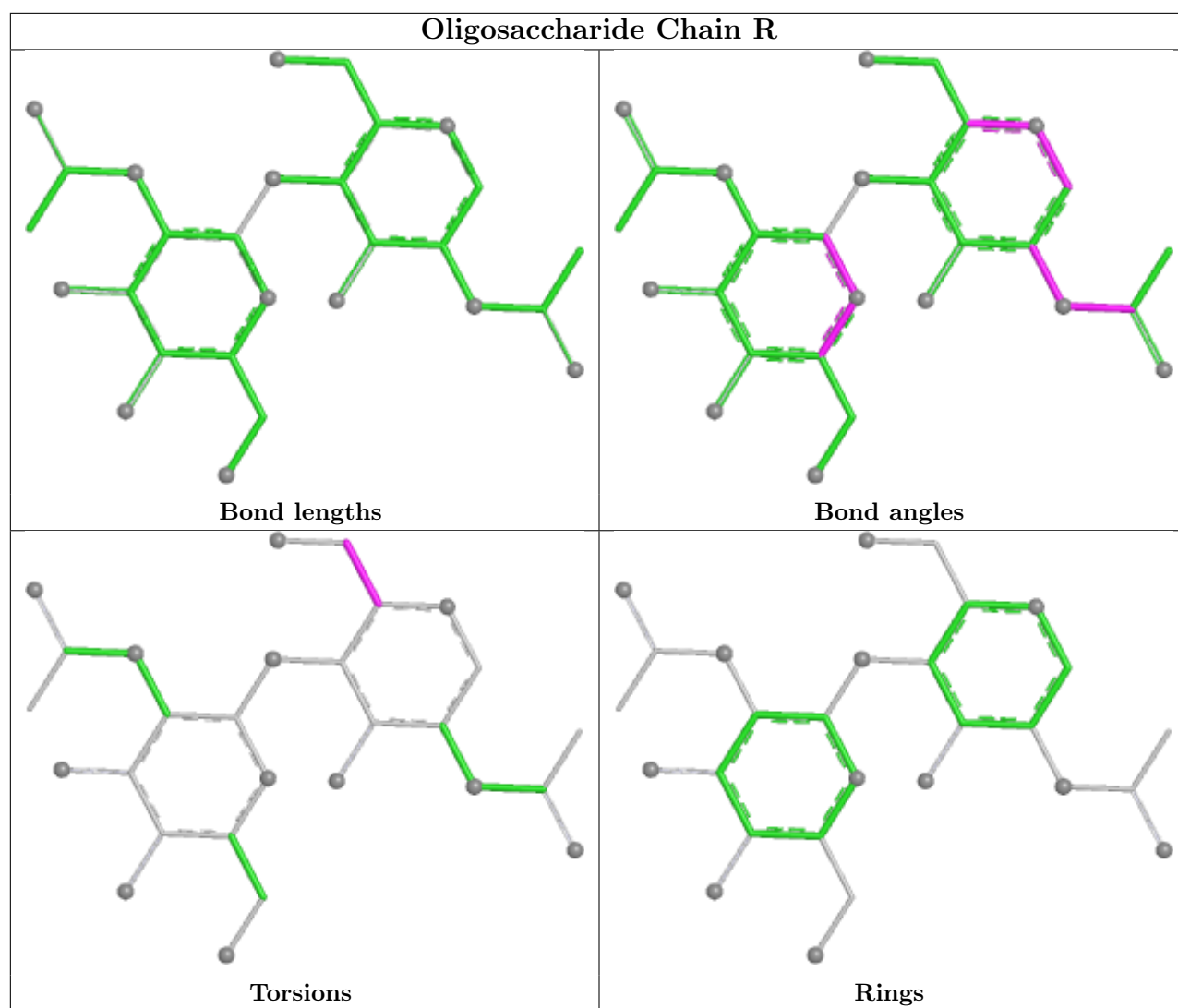
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	O	2	NAG	1	0
7	O	1	NAG	1	0

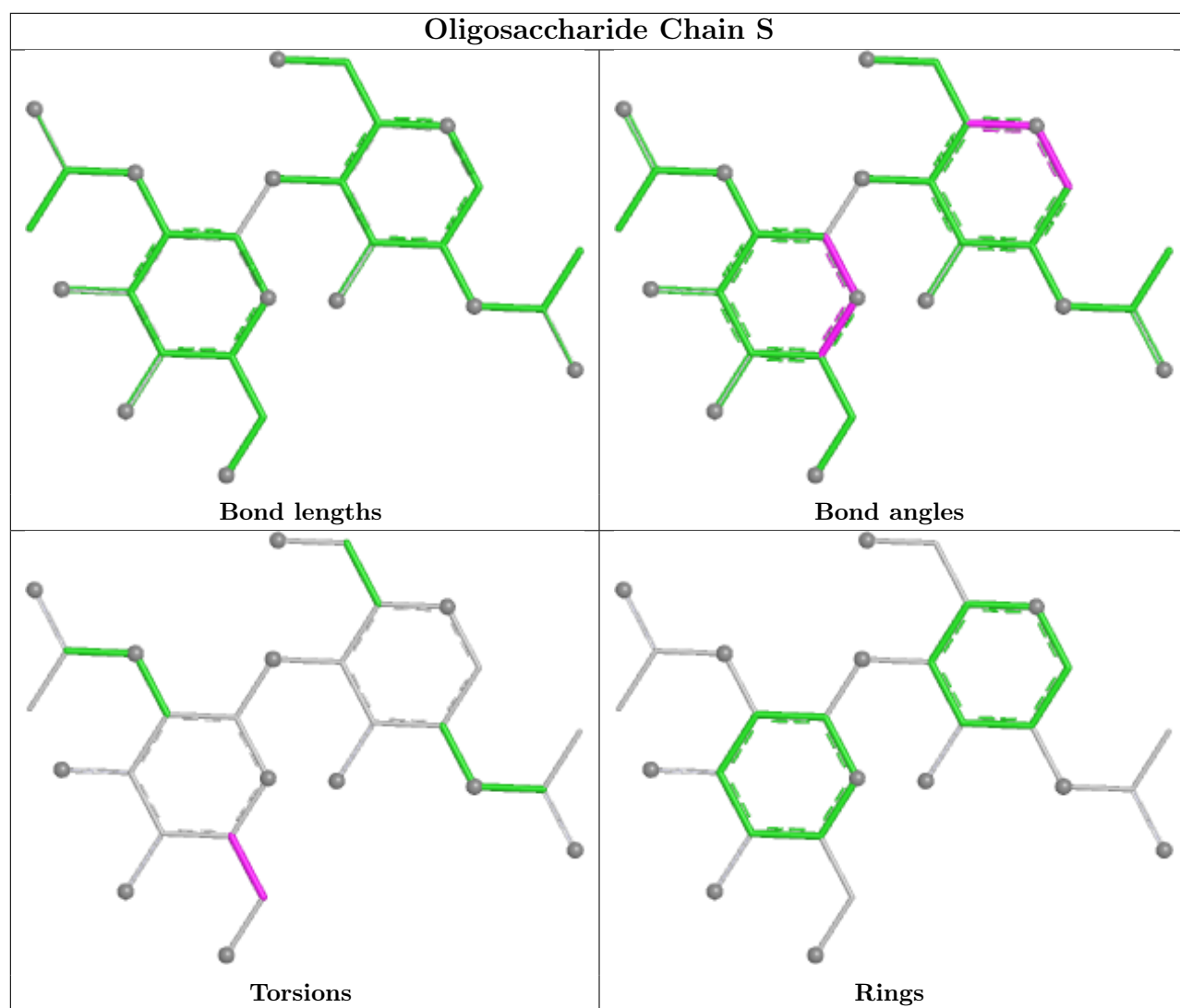
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

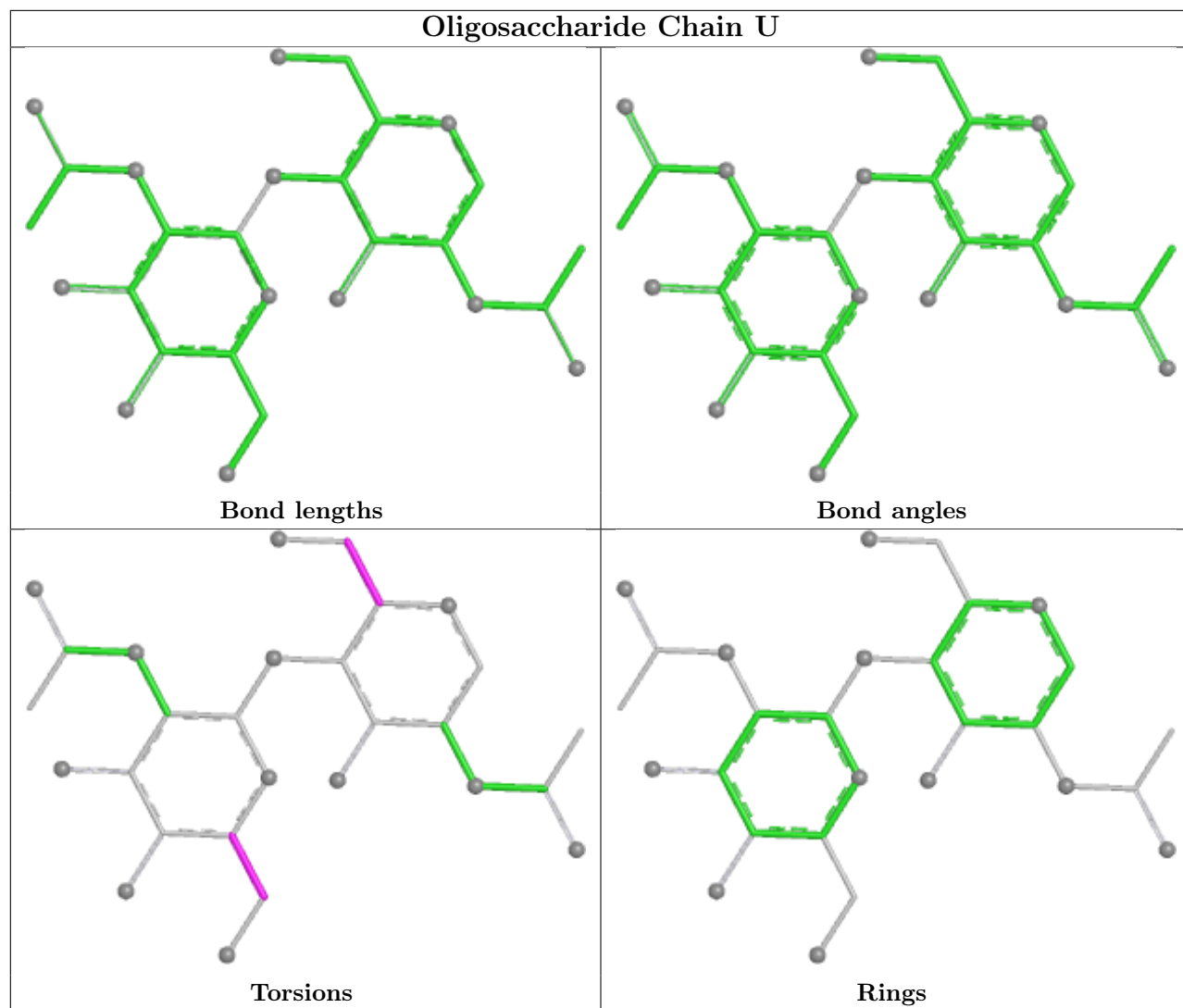


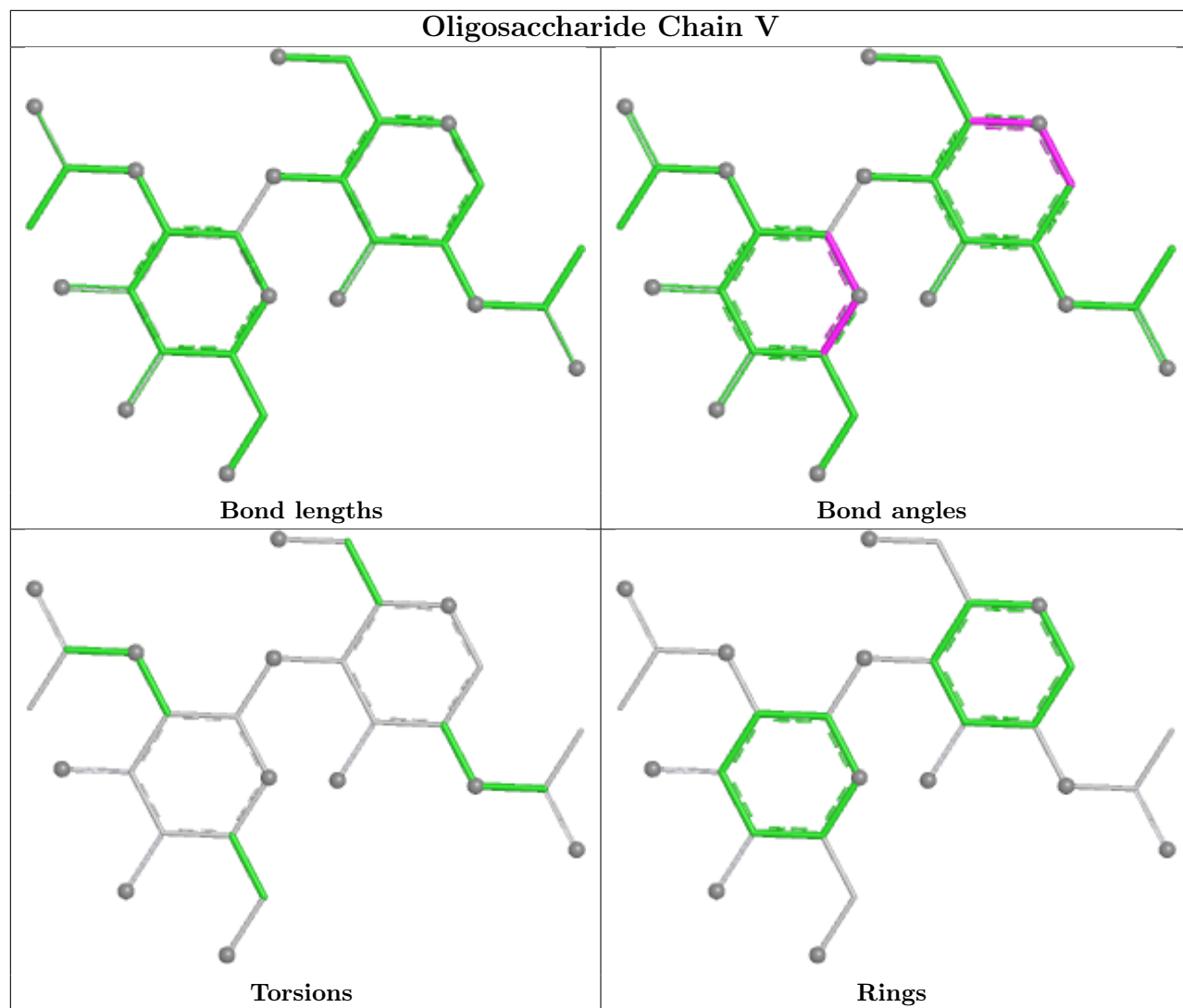


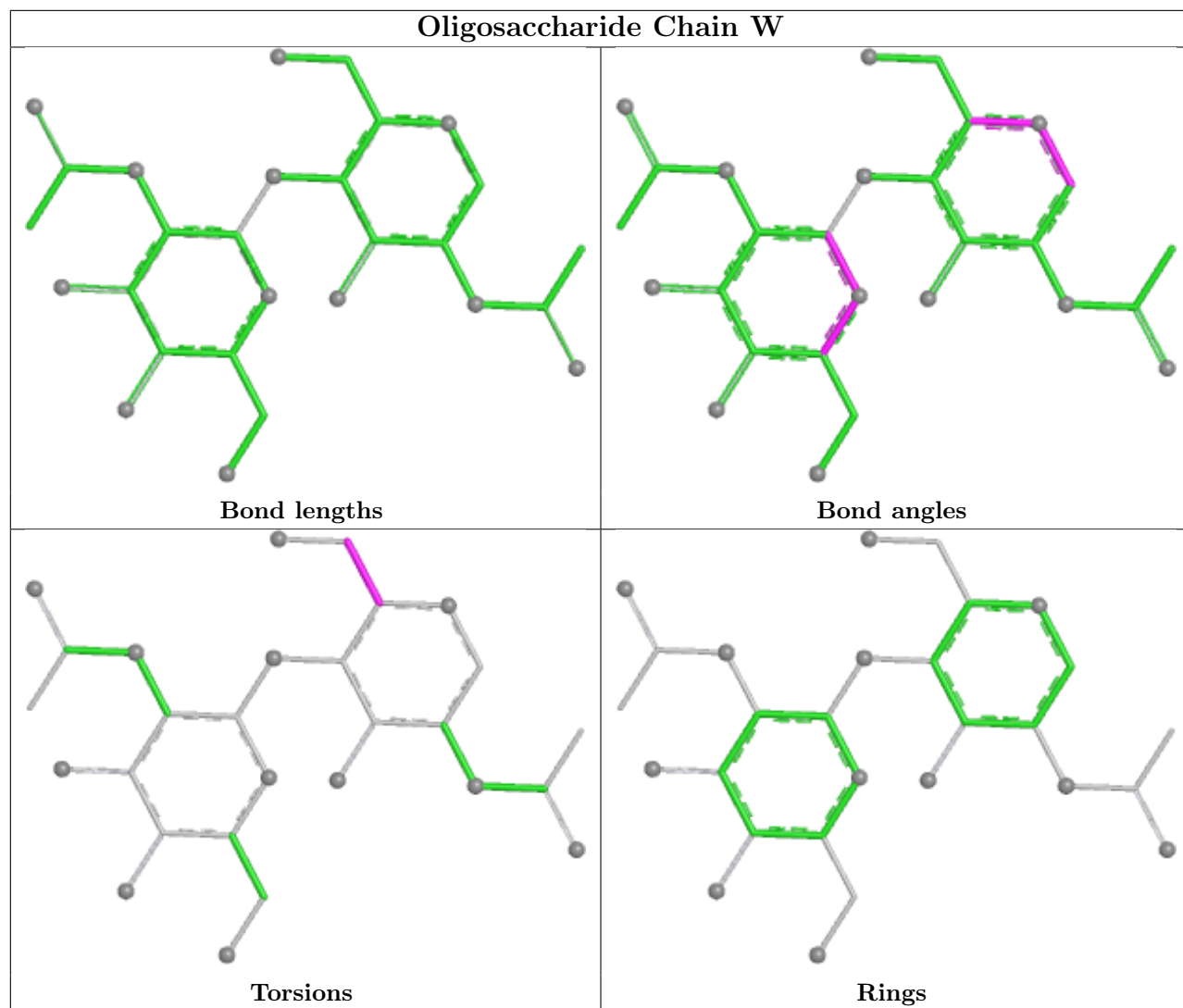


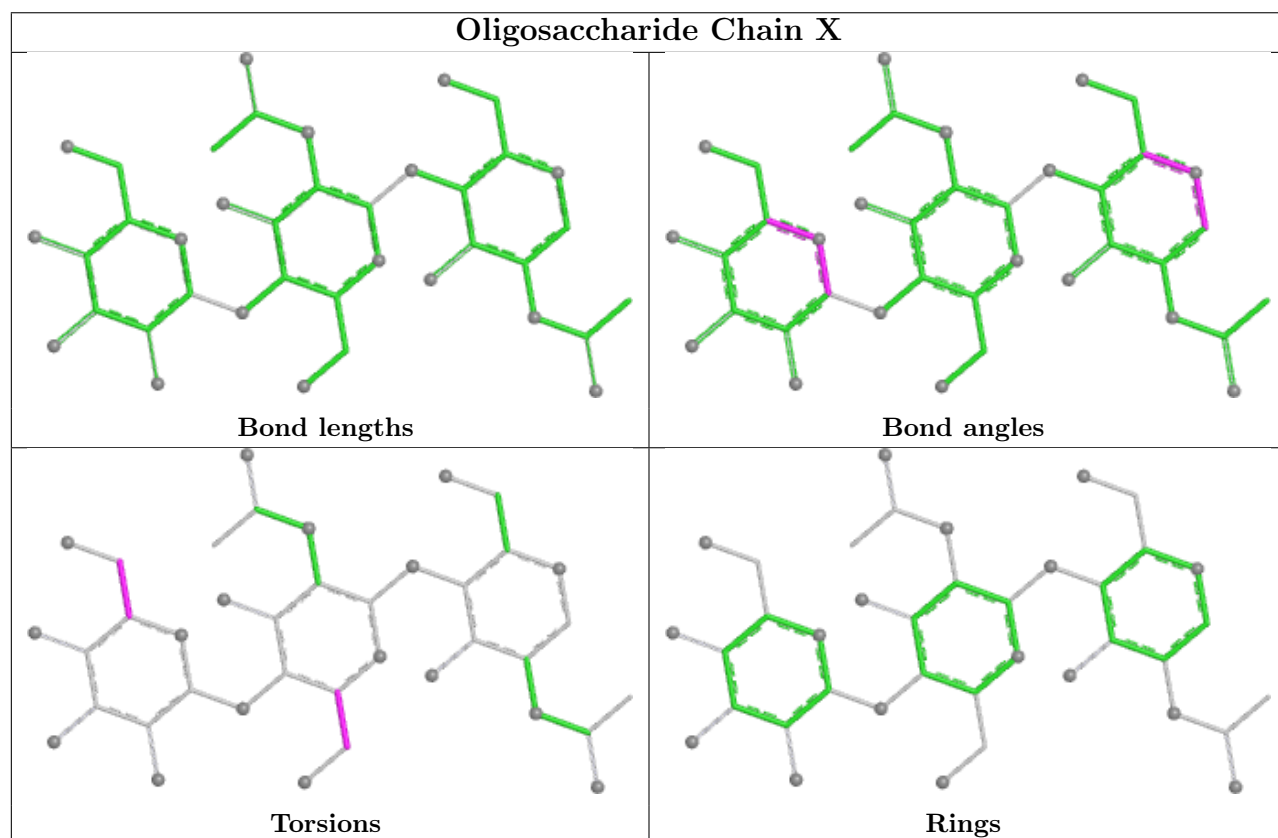
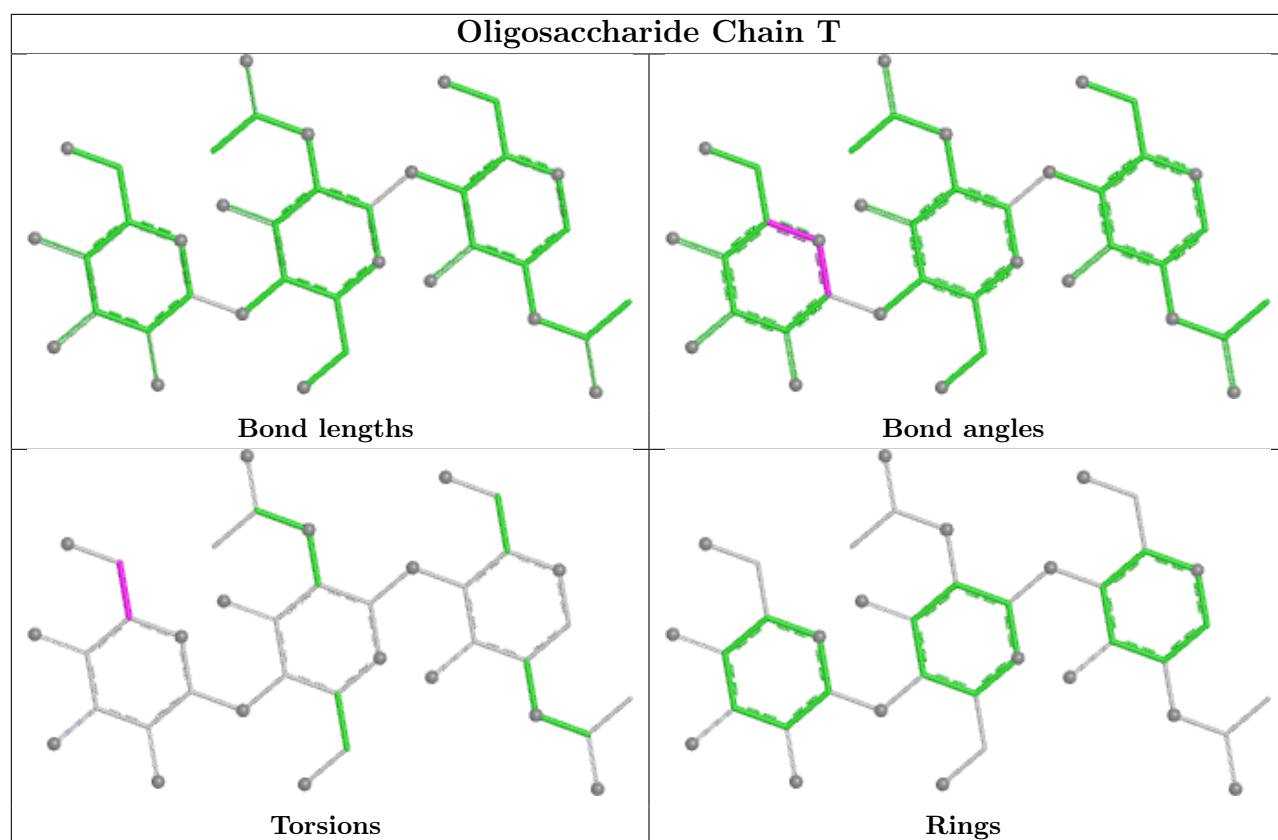












5.6 Ligand geometry

48 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	$\# Z > 2$
10	NAG	A	612	1	14,14,15	0.67	0	17,19,21	0.97	1 (5%)
10	NAG	D	610	1	14,14,15	0.66	0	17,19,21	0.90	1 (5%)
10	NAG	D	602	1	14,14,15	0.69	0	17,19,21	0.83	0
10	NAG	D	605	1	14,14,15	0.67	0	17,19,21	0.83	0
10	NAG	A	601	1	14,14,15	0.67	0	17,19,21	0.87	0
10	NAG	C	608	1	14,14,15	0.68	0	17,19,21	0.91	1 (5%)
10	NAG	E	701	2	14,14,15	0.66	0	17,19,21	0.82	0
10	NAG	A	603	1	14,14,15	0.67	0	17,19,21	0.91	1 (5%)
10	NAG	F	701	2	14,14,15	0.68	0	17,19,21	0.84	1 (5%)
10	NAG	D	601	1	14,14,15	0.66	0	17,19,21	0.79	0
10	NAG	A	614	1	14,14,15	0.66	0	17,19,21	0.81	0
10	NAG	D	613	1	14,14,15	0.68	0	17,19,21	0.85	1 (5%)
10	NAG	D	608	1	14,14,15	0.69	0	17,19,21	0.84	0
10	NAG	A	608	1	14,14,15	0.68	0	17,19,21	0.86	0
10	NAG	C	612	1	14,14,15	0.66	0	17,19,21	0.91	2 (11%)
10	NAG	A	609	1	14,14,15	0.65	0	17,19,21	0.82	0
10	NAG	D	604	1	14,14,15	0.69	0	17,19,21	0.71	0
10	NAG	A	611	1	14,14,15	0.69	0	17,19,21	0.80	1 (5%)
10	NAG	A	604	1	14,14,15	0.68	0	17,19,21	0.77	0
10	NAG	E	702	2	14,14,15	0.69	0	17,19,21	0.80	0
10	NAG	C	607	1	14,14,15	0.67	0	17,19,21	0.83	0
10	NAG	C	611	1	14,14,15	0.69	0	17,19,21	0.83	0
10	NAG	C	605	1	14,14,15	0.67	0	17,19,21	0.70	0
10	NAG	D	603	1	14,14,15	0.67	0	17,19,21	0.84	0
10	NAG	D	606	1	14,14,15	0.66	0	17,19,21	0.86	0
10	NAG	A	607	1	14,14,15	0.68	0	17,19,21	0.79	0
10	NAG	C	609	1	14,14,15	0.68	0	17,19,21	0.79	1 (5%)
10	NAG	A	602	1	14,14,15	0.68	0	17,19,21	0.86	0
10	NAG	A	610	1	14,14,15	0.67	0	17,19,21	0.79	0
10	NAG	F	702	2	14,14,15	0.67	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	A	605	1	14,14,15	0.67	0	17,19,21	0.73	0
10	NAG	E	703	2	14,14,15	0.70	0	17,19,21	0.93	1 (5%)
10	NAG	C	610	1	14,14,15	0.66	0	17,19,21	0.91	0
10	NAG	D	607	1	14,14,15	0.67	0	17,19,21	0.98	2 (11%)
10	NAG	D	611	1	14,14,15	0.67	0	17,19,21	0.80	0
10	NAG	D	612	1	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
10	NAG	B	702	2	14,14,15	0.68	0	17,19,21	0.93	1 (5%)
10	NAG	B	703	2	14,14,15	0.66	0	17,19,21	1.04	2 (11%)
10	NAG	A	613	1	14,14,15	0.65	0	17,19,21	0.79	0
10	NAG	C	603	1	14,14,15	0.73	0	17,19,21	1.05	2 (11%)
10	NAG	C	606	1	14,14,15	0.68	0	17,19,21	0.84	1 (5%)
10	NAG	C	602	1	14,14,15	0.70	0	17,19,21	0.84	0
10	NAG	C	601	1	14,14,15	0.68	0	17,19,21	0.84	0
10	NAG	B	701	2	14,14,15	0.67	0	17,19,21	0.92	1 (5%)
10	NAG	A	606	1	14,14,15	0.67	0	17,19,21	0.80	0
10	NAG	D	609	1	14,14,15	0.68	0	17,19,21	0.88	0
10	NAG	F	703	2	14,14,15	0.68	0	17,19,21	0.76	0
10	NAG	C	604	1	14,14,15	0.69	0	17,19,21	1.09	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	612	1	-	2/6/23/26	0/1/1/1
10	NAG	D	610	1	-	2/6/23/26	0/1/1/1
10	NAG	D	602	1	-	2/6/23/26	0/1/1/1
10	NAG	D	605	1	-	1/6/23/26	0/1/1/1
10	NAG	A	601	1	-	1/6/23/26	0/1/1/1
10	NAG	C	608	1	-	1/6/23/26	0/1/1/1
10	NAG	E	701	2	-	2/6/23/26	0/1/1/1
10	NAG	A	603	1	-	2/6/23/26	0/1/1/1
10	NAG	F	701	2	-	0/6/23/26	0/1/1/1
10	NAG	D	601	1	-	1/6/23/26	0/1/1/1
10	NAG	A	614	1	-	2/6/23/26	0/1/1/1
10	NAG	D	613	1	-	2/6/23/26	0/1/1/1
10	NAG	D	608	1	-	1/6/23/26	0/1/1/1
10	NAG	A	608	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	C	612	1	-	2/6/23/26	0/1/1/1
10	NAG	A	609	1	-	1/6/23/26	0/1/1/1
10	NAG	D	604	1	-	2/6/23/26	0/1/1/1
10	NAG	A	611	1	-	2/6/23/26	0/1/1/1
10	NAG	A	604	1	-	3/6/23/26	0/1/1/1
10	NAG	E	702	2	-	2/6/23/26	0/1/1/1
10	NAG	C	607	1	-	1/6/23/26	0/1/1/1
10	NAG	C	611	1	-	2/6/23/26	0/1/1/1
10	NAG	C	605	1	-	1/6/23/26	0/1/1/1
10	NAG	D	603	1	-	2/6/23/26	0/1/1/1
10	NAG	D	606	1	-	2/6/23/26	0/1/1/1
10	NAG	A	607	1	-	1/6/23/26	0/1/1/1
10	NAG	C	609	1	-	2/6/23/26	0/1/1/1
10	NAG	A	602	1	-	1/6/23/26	0/1/1/1
10	NAG	A	610	1	-	1/6/23/26	0/1/1/1
10	NAG	F	702	2	-	2/6/23/26	0/1/1/1
10	NAG	A	605	1	-	1/6/23/26	0/1/1/1
10	NAG	E	703	2	-	1/6/23/26	0/1/1/1
10	NAG	C	610	1	-	2/6/23/26	0/1/1/1
10	NAG	D	607	1	-	1/6/23/26	0/1/1/1
10	NAG	D	611	1	-	1/6/23/26	0/1/1/1
10	NAG	D	612	1	-	2/6/23/26	0/1/1/1
10	NAG	B	702	2	-	2/6/23/26	0/1/1/1
10	NAG	B	703	2	-	2/6/23/26	0/1/1/1
10	NAG	A	613	1	-	2/6/23/26	0/1/1/1
10	NAG	C	603	1	-	2/6/23/26	0/1/1/1
10	NAG	C	606	1	-	2/6/23/26	0/1/1/1
10	NAG	C	602	1	-	2/6/23/26	0/1/1/1
10	NAG	C	601	1	-	1/6/23/26	0/1/1/1
10	NAG	B	701	2	-	2/6/23/26	0/1/1/1
10	NAG	A	606	1	-	1/6/23/26	0/1/1/1
10	NAG	D	609	1	-	2/6/23/26	0/1/1/1
10	NAG	F	703	2	-	2/6/23/26	0/1/1/1
10	NAG	C	604	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	604	NAG	C1-O5-C5	3.03	116.25	112.19
10	B	703	NAG	C2-N2-C7	2.67	126.47	122.90
10	E	703	NAG	C2-N2-C7	2.59	126.37	122.90
10	C	603	NAG	O5-C1-C2	2.55	115.24	111.29
10	B	703	NAG	C1-O5-C5	2.54	115.59	112.19
10	D	607	NAG	C1-O5-C5	2.50	115.53	112.19
10	C	603	NAG	C1-O5-C5	2.47	115.50	112.19
10	A	612	NAG	C1-O5-C5	2.34	115.32	112.19
10	C	608	NAG	C1-O5-C5	2.29	115.25	112.19
10	D	610	NAG	C1-O5-C5	2.28	115.24	112.19
10	C	609	NAG	C1-O5-C5	2.22	115.17	112.19
10	C	612	NAG	C2-N2-C7	2.17	125.81	122.90
10	C	612	NAG	C1-O5-C5	2.16	115.09	112.19
10	D	607	NAG	C2-N2-C7	2.16	125.80	122.90
10	B	701	NAG	C1-O5-C5	2.16	115.08	112.19
10	B	702	NAG	C1-O5-C5	2.13	115.05	112.19
10	D	612	NAG	C1-O5-C5	2.13	115.04	112.19
10	D	613	NAG	C1-O5-C5	2.11	115.01	112.19
10	C	606	NAG	C1-O5-C5	2.11	115.01	112.19
10	A	611	NAG	C1-O5-C5	2.08	114.98	112.19
10	A	603	NAG	C1-O5-C5	2.02	114.89	112.19
10	F	701	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	701	NAG	C4-C5-C6-O6
10	C	602	NAG	C4-C5-C6-O6
10	A	603	NAG	O5-C5-C6-O6
10	C	604	NAG	O5-C5-C6-O6
10	D	603	NAG	O5-C5-C6-O6
10	D	610	NAG	O5-C5-C6-O6
10	C	612	NAG	C4-C5-C6-O6
10	A	611	NAG	O5-C5-C6-O6
10	B	701	NAG	O5-C5-C6-O6
10	D	602	NAG	O5-C5-C6-O6
10	C	609	NAG	C4-C5-C6-O6
10	B	702	NAG	O5-C5-C6-O6
10	B	703	NAG	O5-C5-C6-O6
10	D	613	NAG	O5-C5-C6-O6
10	E	702	NAG	O5-C5-C6-O6
10	F	702	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	D	606	NAG	O5-C5-C6-O6
10	C	606	NAG	O5-C5-C6-O6
10	D	609	NAG	O5-C5-C6-O6
10	D	612	NAG	O5-C5-C6-O6
10	C	609	NAG	O5-C5-C6-O6
10	A	614	NAG	O5-C5-C6-O6
10	E	701	NAG	O5-C5-C6-O6
10	A	611	NAG	C4-C5-C6-O6
10	D	612	NAG	C4-C5-C6-O6
10	A	612	NAG	O5-C5-C6-O6
10	B	701	NAG	C4-C5-C6-O6
10	E	702	NAG	C4-C5-C6-O6
10	C	602	NAG	O5-C5-C6-O6
10	C	612	NAG	O5-C5-C6-O6
10	A	603	NAG	C4-C5-C6-O6
10	D	602	NAG	C4-C5-C6-O6
10	D	603	NAG	C4-C5-C6-O6
10	F	702	NAG	C4-C5-C6-O6
10	D	613	NAG	C4-C5-C6-O6
10	A	604	NAG	O5-C5-C6-O6
10	C	603	NAG	O5-C5-C6-O6
10	A	612	NAG	C4-C5-C6-O6
10	F	703	NAG	O5-C5-C6-O6
10	D	610	NAG	C4-C5-C6-O6
10	C	603	NAG	C4-C5-C6-O6
10	C	610	NAG	O5-C5-C6-O6
10	B	703	NAG	C4-C5-C6-O6
10	C	604	NAG	C4-C5-C6-O6
10	D	604	NAG	C4-C5-C6-O6
10	D	605	NAG	O5-C5-C6-O6
10	C	607	NAG	O5-C5-C6-O6
10	B	702	NAG	C4-C5-C6-O6
10	D	604	NAG	O5-C5-C6-O6
10	C	611	NAG	O5-C5-C6-O6
10	A	606	NAG	O5-C5-C6-O6
10	A	601	NAG	O5-C5-C6-O6
10	A	609	NAG	O5-C5-C6-O6
10	D	607	NAG	O5-C5-C6-O6
10	D	608	NAG	O5-C5-C6-O6
10	C	601	NAG	O5-C5-C6-O6
10	D	601	NAG	O5-C5-C6-O6
10	A	614	NAG	C4-C5-C6-O6

Continued on next page...

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Mol	Chain	Res	Type	Atoms
10	D	611	NAG	O5-C5-C6-O6
10	E	703	NAG	O5-C5-C6-O6
10	C	608	NAG	O5-C5-C6-O6
10	A	607	NAG	O5-C5-C6-O6
10	C	605	NAG	O5-C5-C6-O6
10	A	602	NAG	O5-C5-C6-O6
10	A	613	NAG	O5-C5-C6-O6
10	A	610	NAG	O5-C5-C6-O6
10	A	605	NAG	O5-C5-C6-O6
10	A	608	NAG	O5-C5-C6-O6
10	D	606	NAG	C4-C5-C6-O6
10	C	606	NAG	C4-C5-C6-O6
10	D	609	NAG	C4-C5-C6-O6
10	A	604	NAG	C4-C5-C6-O6
10	C	611	NAG	C4-C5-C6-O6
10	F	703	NAG	C4-C5-C6-O6
10	C	610	NAG	C4-C5-C6-O6
10	A	604	NAG	C1-C2-N2-C7
10	A	613	NAG	C1-C2-N2-C7

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.

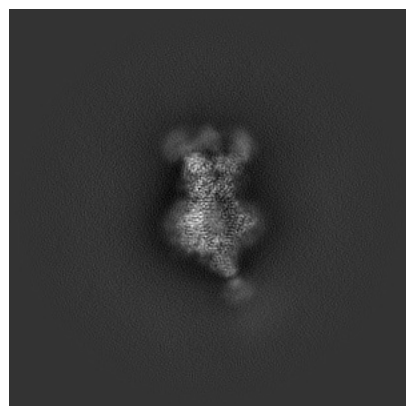
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44342. These allow visual inspection of the internal detail of the map and identification of artifacts.

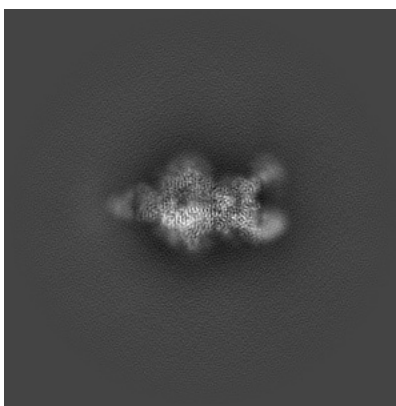
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

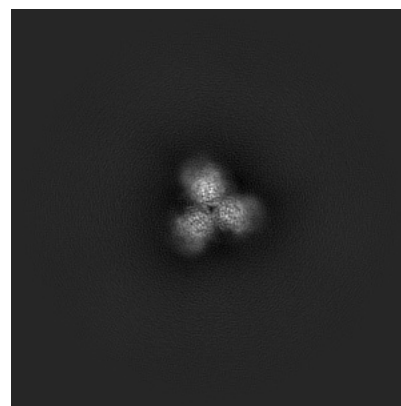
6.1.1 Primary map



X

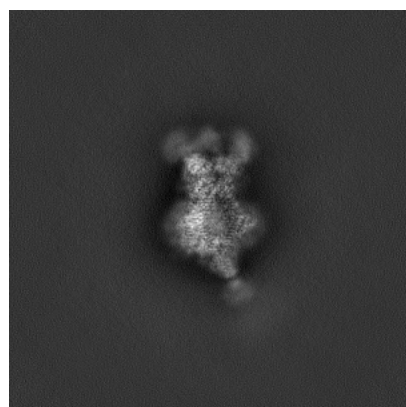


Y

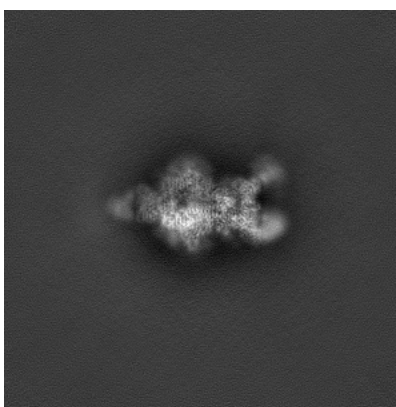


Z

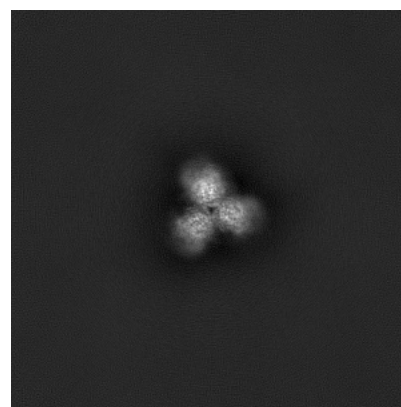
6.1.2 Raw map



X



Y

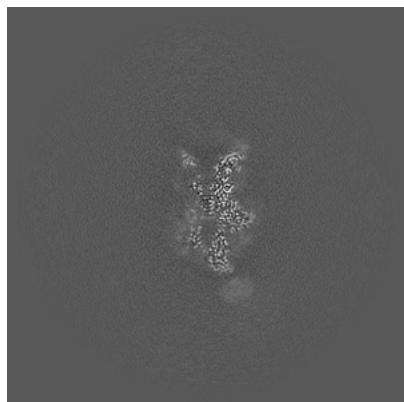


Z

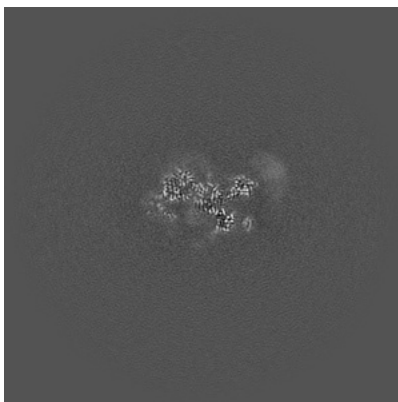
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

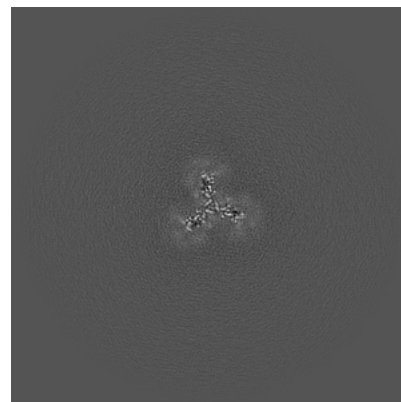
6.2.1 Primary map



X Index: 200

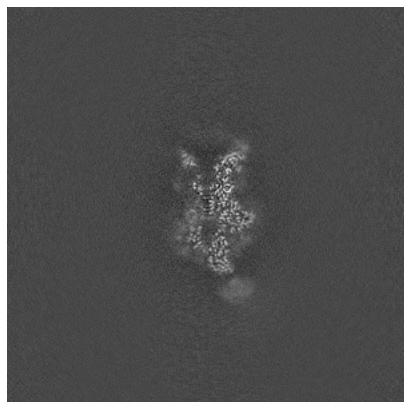


Y Index: 200

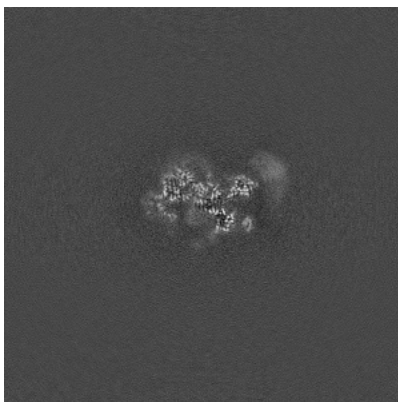


Z Index: 200

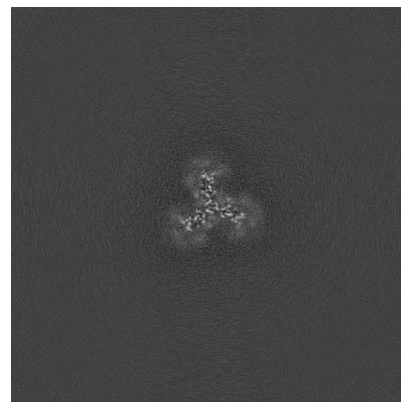
6.2.2 Raw map



X Index: 200



Y Index: 200

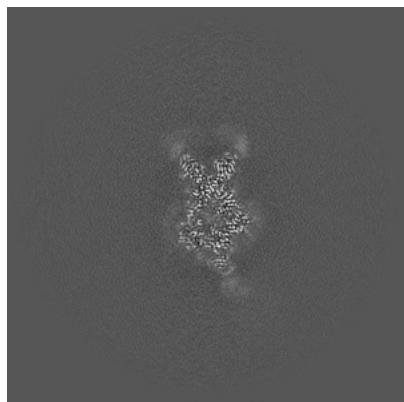


Z Index: 200

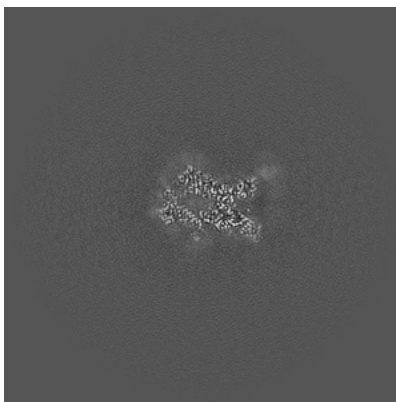
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

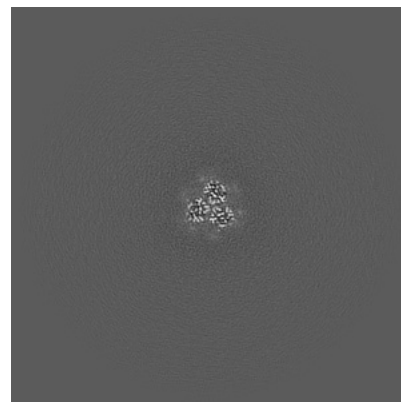
6.3.1 Primary map



X Index: 193

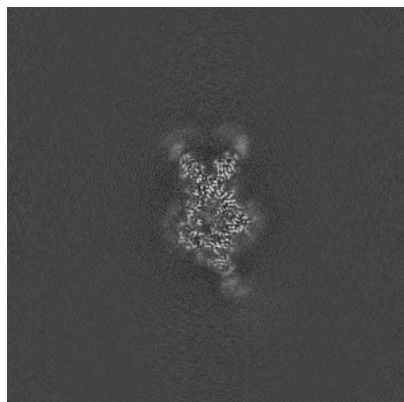


Y Index: 191

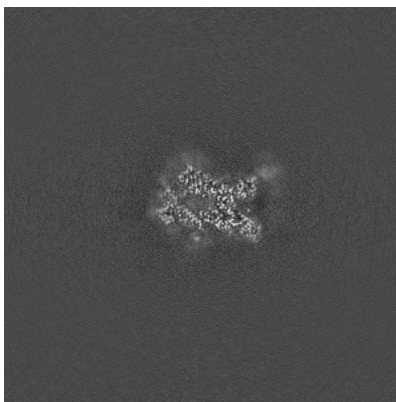


Z Index: 219

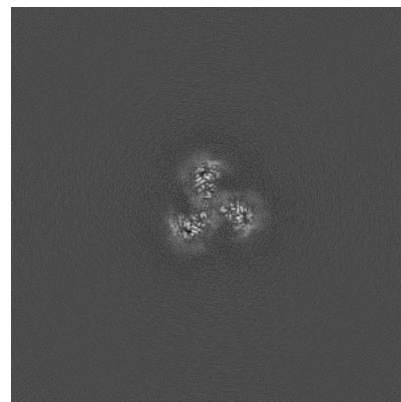
6.3.2 Raw map



X Index: 193



Y Index: 191

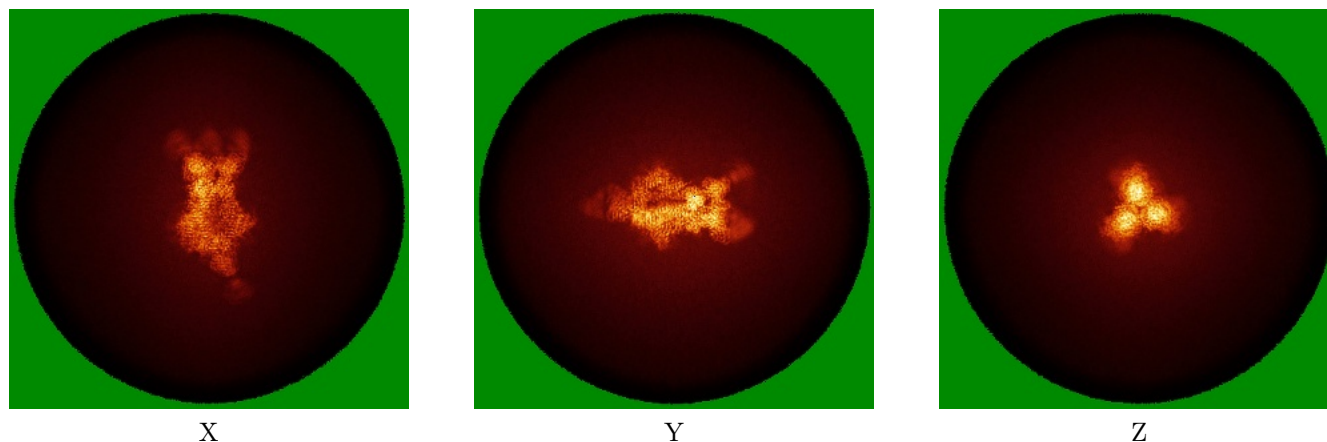


Z Index: 186

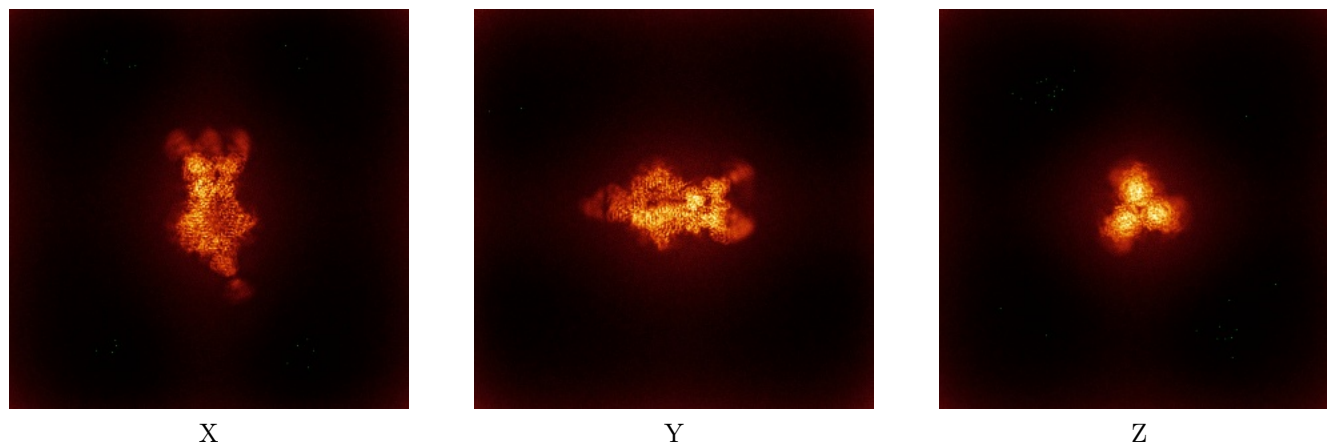
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



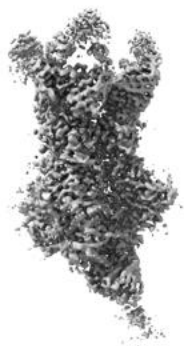
6.4.2 Raw map



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](#)

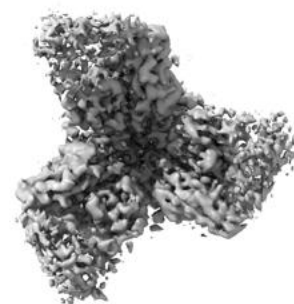
6.5.1 Primary map



X



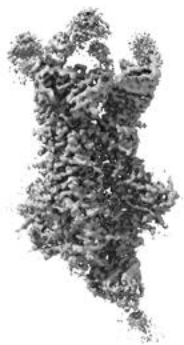
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

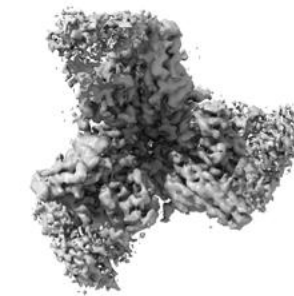
6.5.2 Raw map



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.

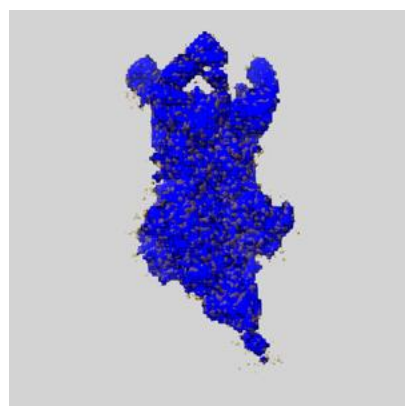
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

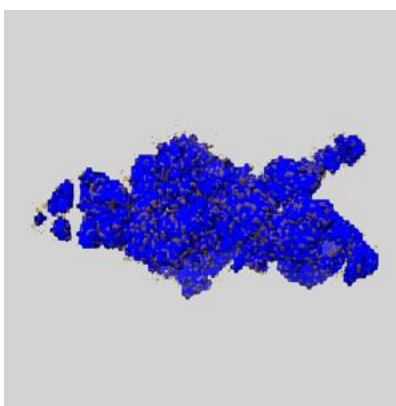
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

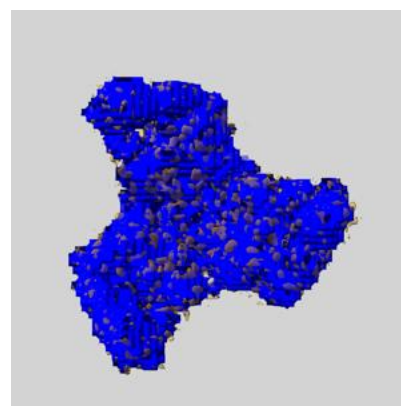
6.6.1 emd_44342_msk_1.map [i](#)



X



Y

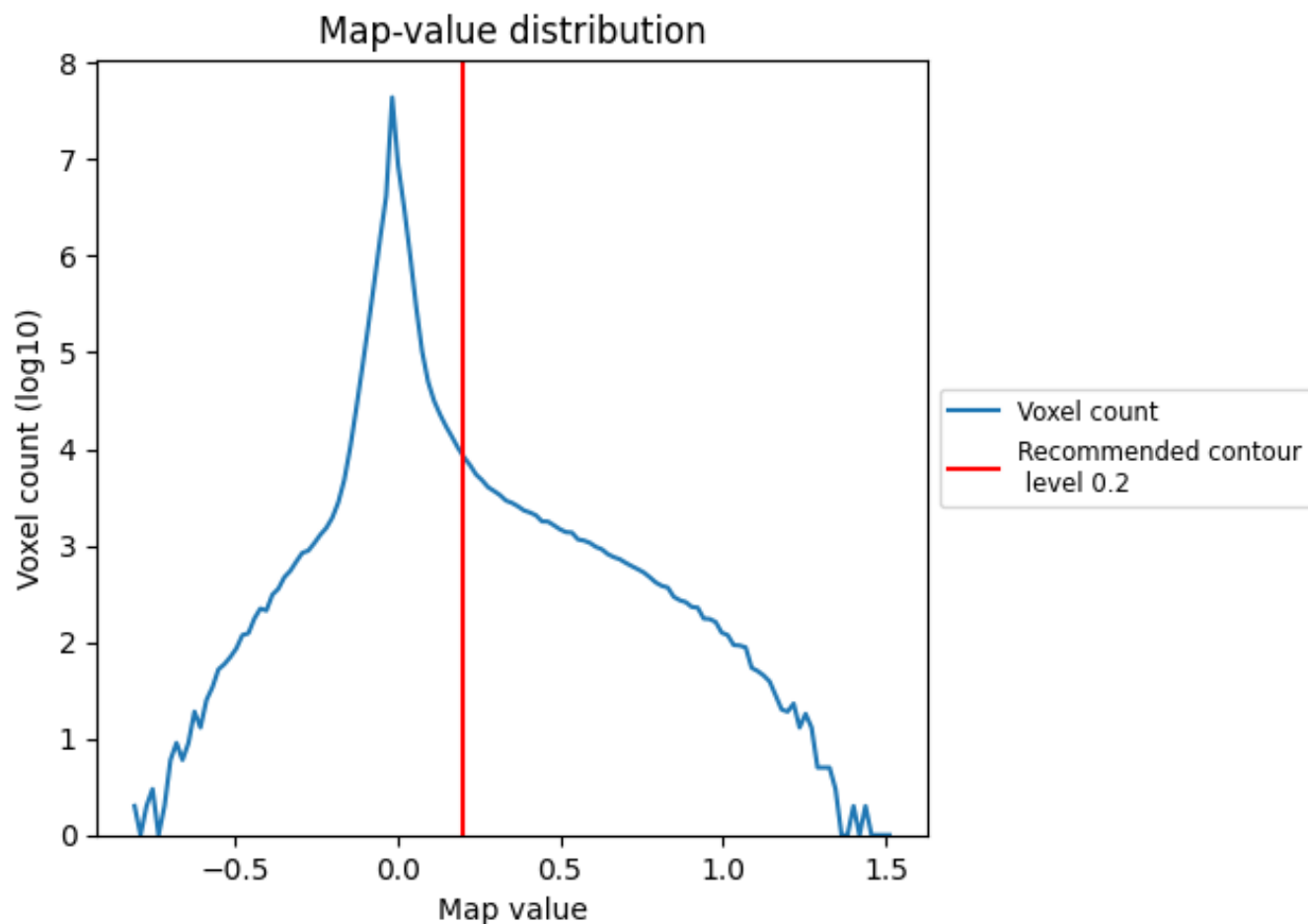


Z

7 Map analysis [i](#)

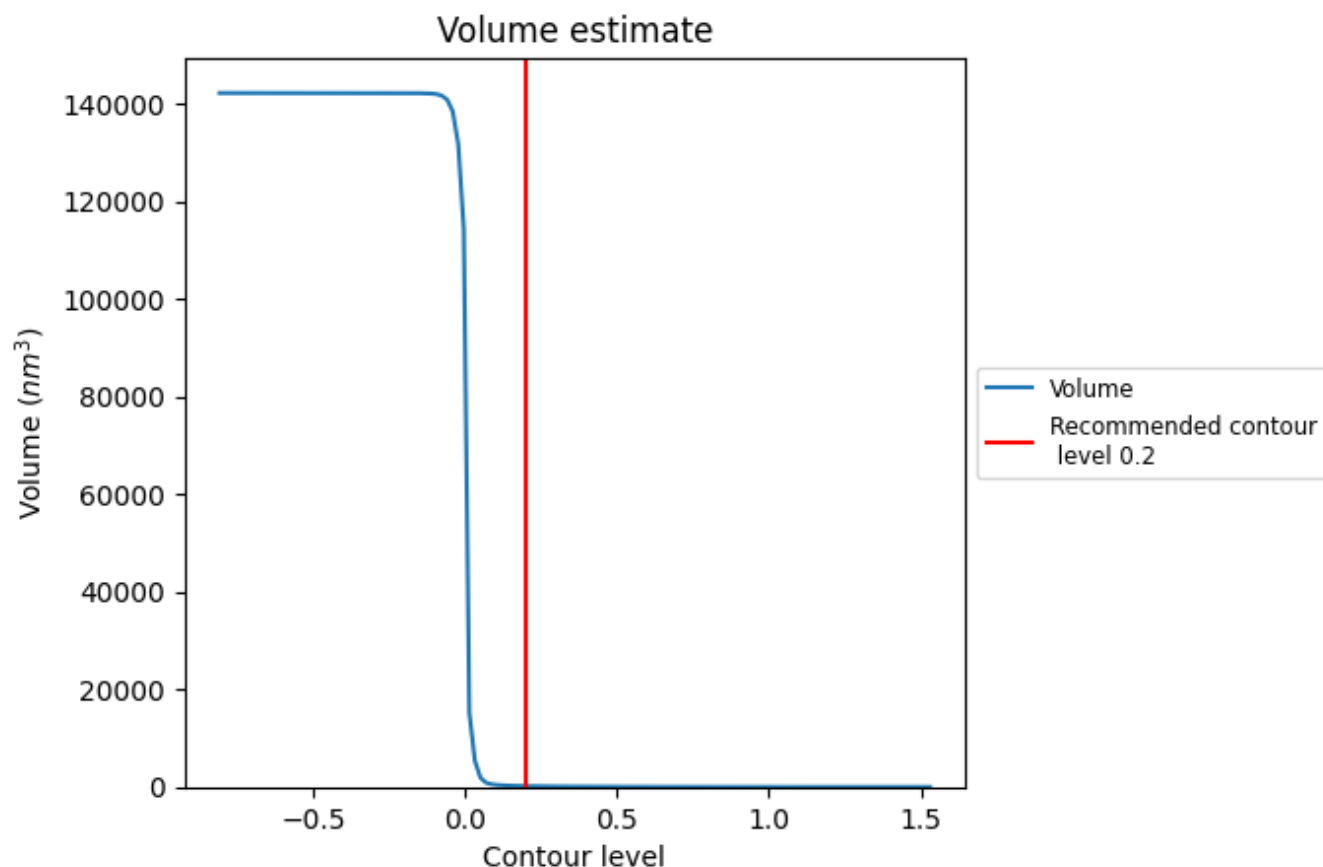
This section contains the results of statistical analysis of the map.

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.

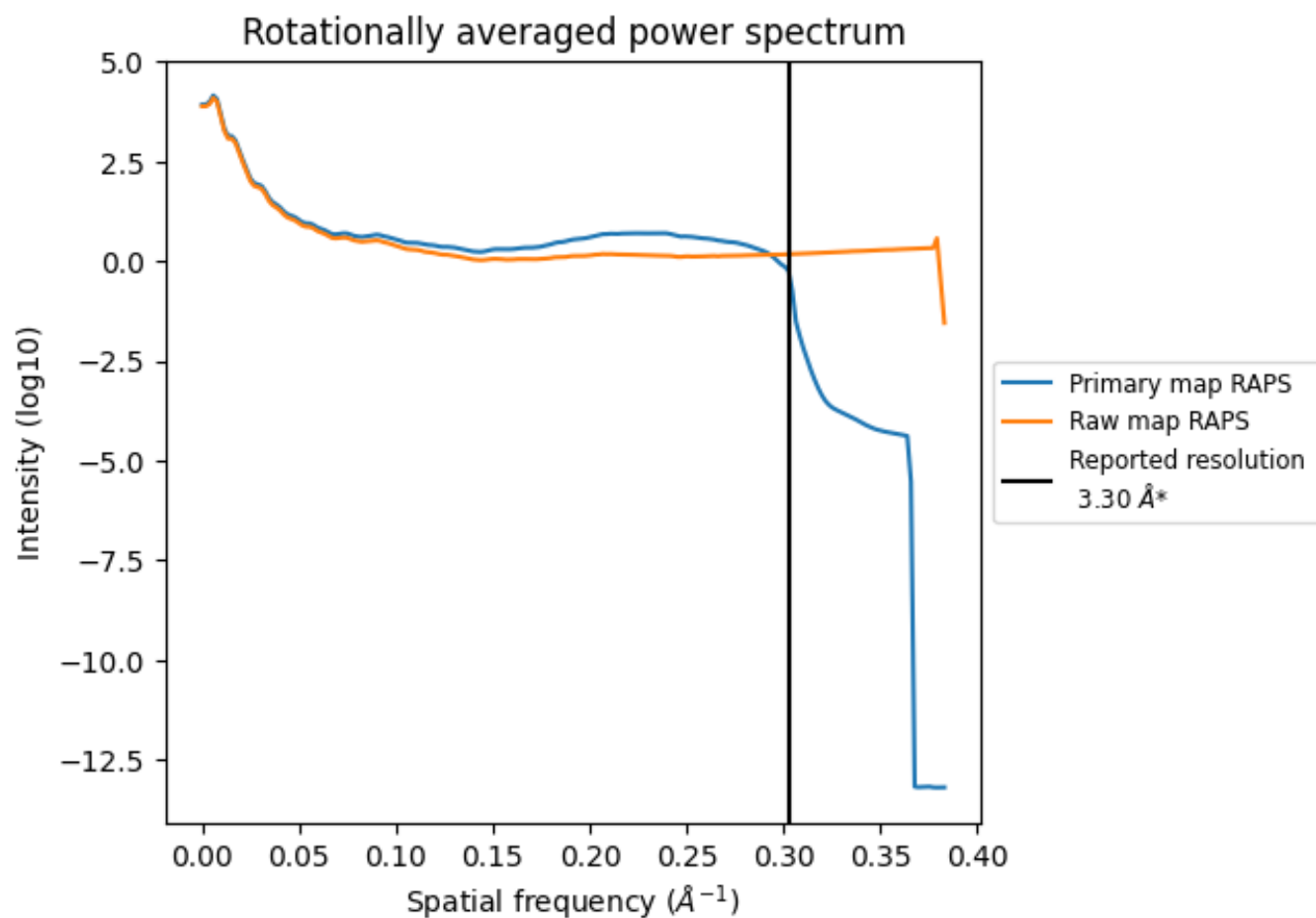
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 171 nm^3 ; this corresponds to an approximate mass of 155 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 ⓘ

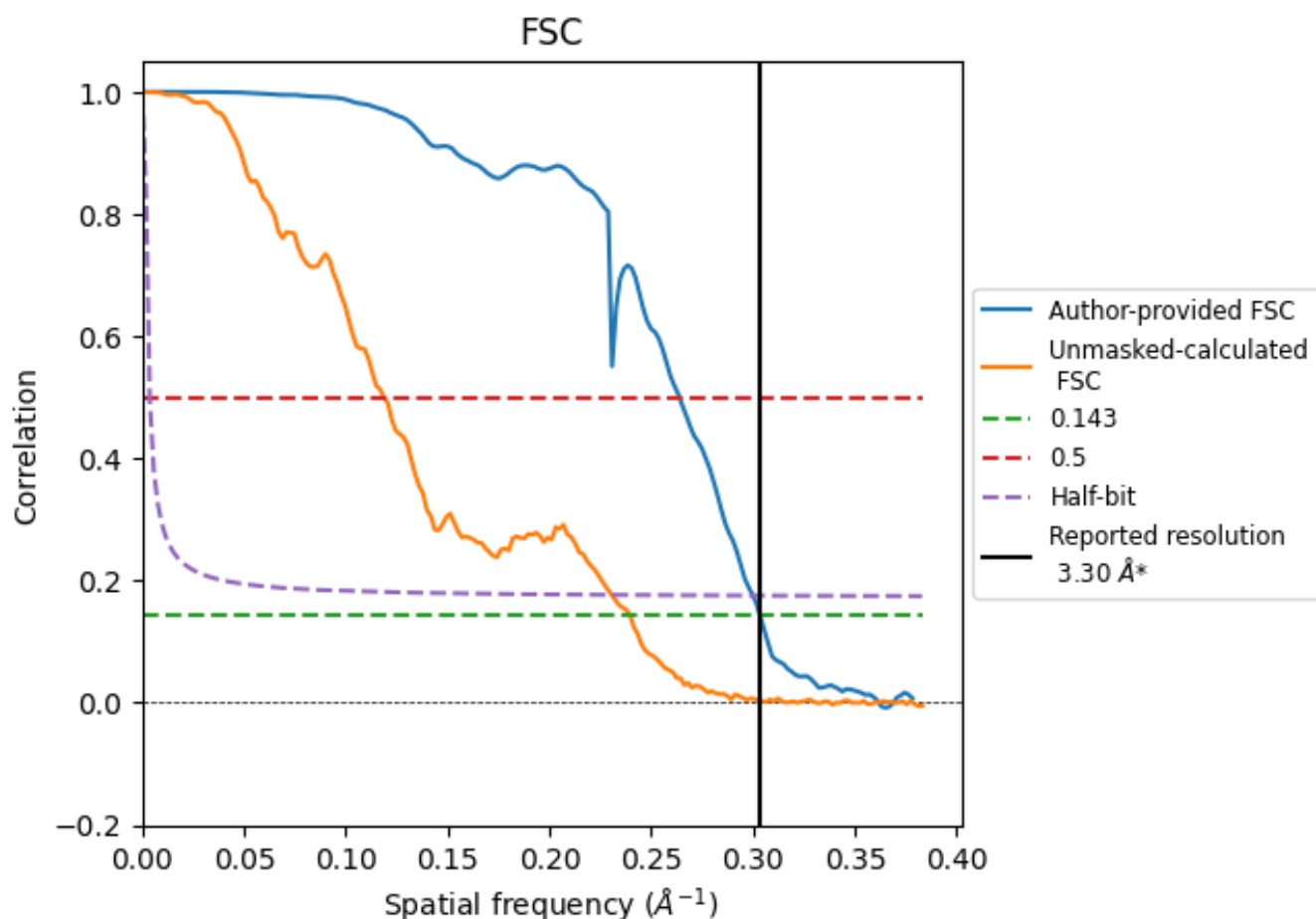


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

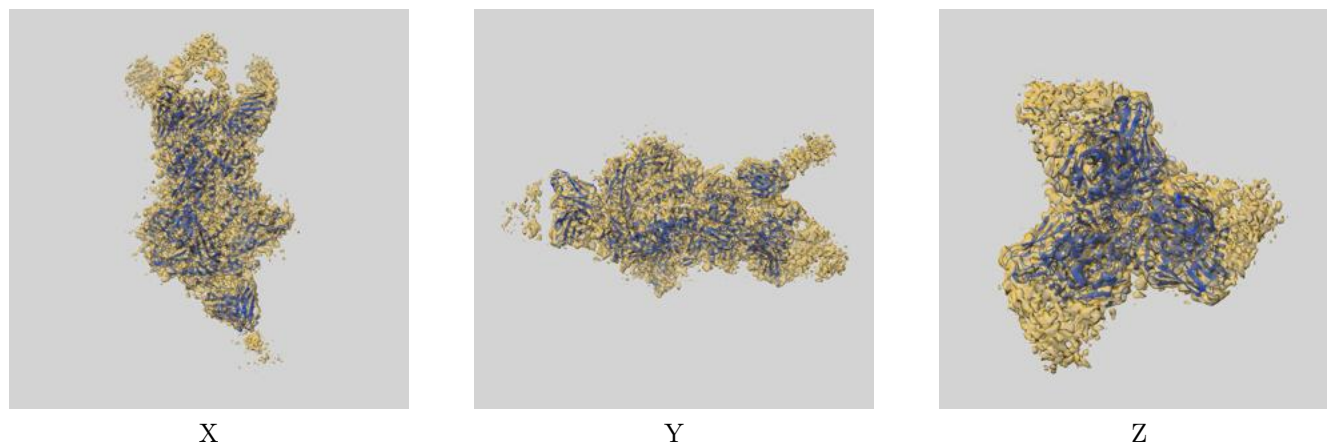
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.79	3.33
Unmasked-calculated*	4.17	8.43	4.34

*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 4.17 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

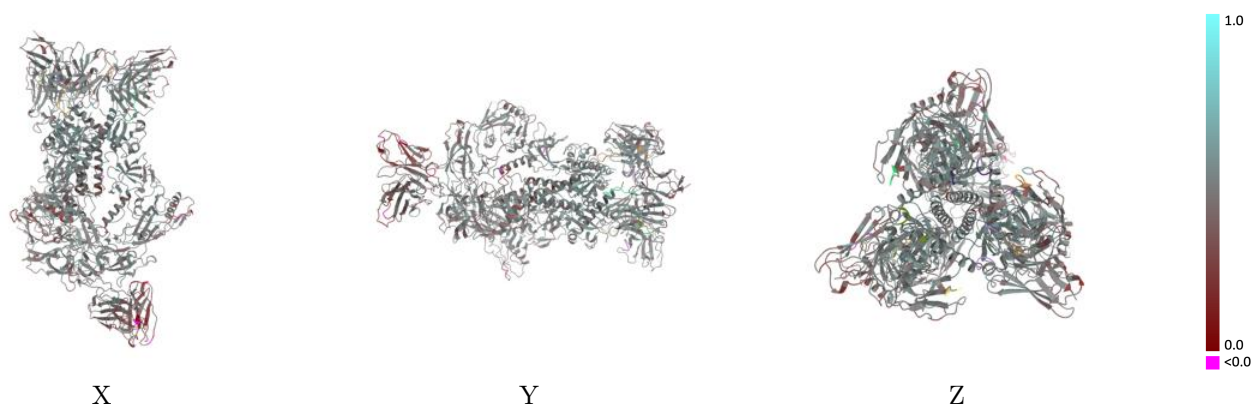
This section contains information regarding the fit between EMDB map EMD-44342 and PDB model 9B8C. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



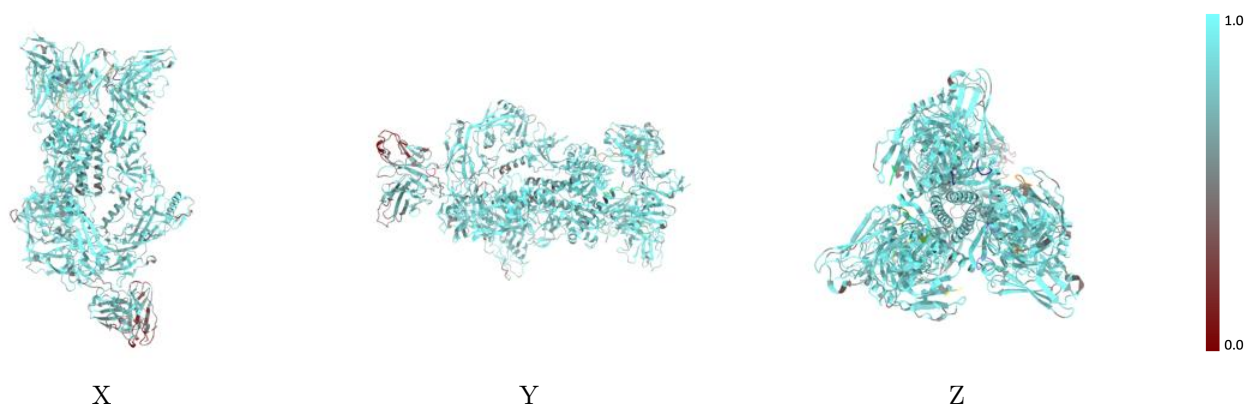
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



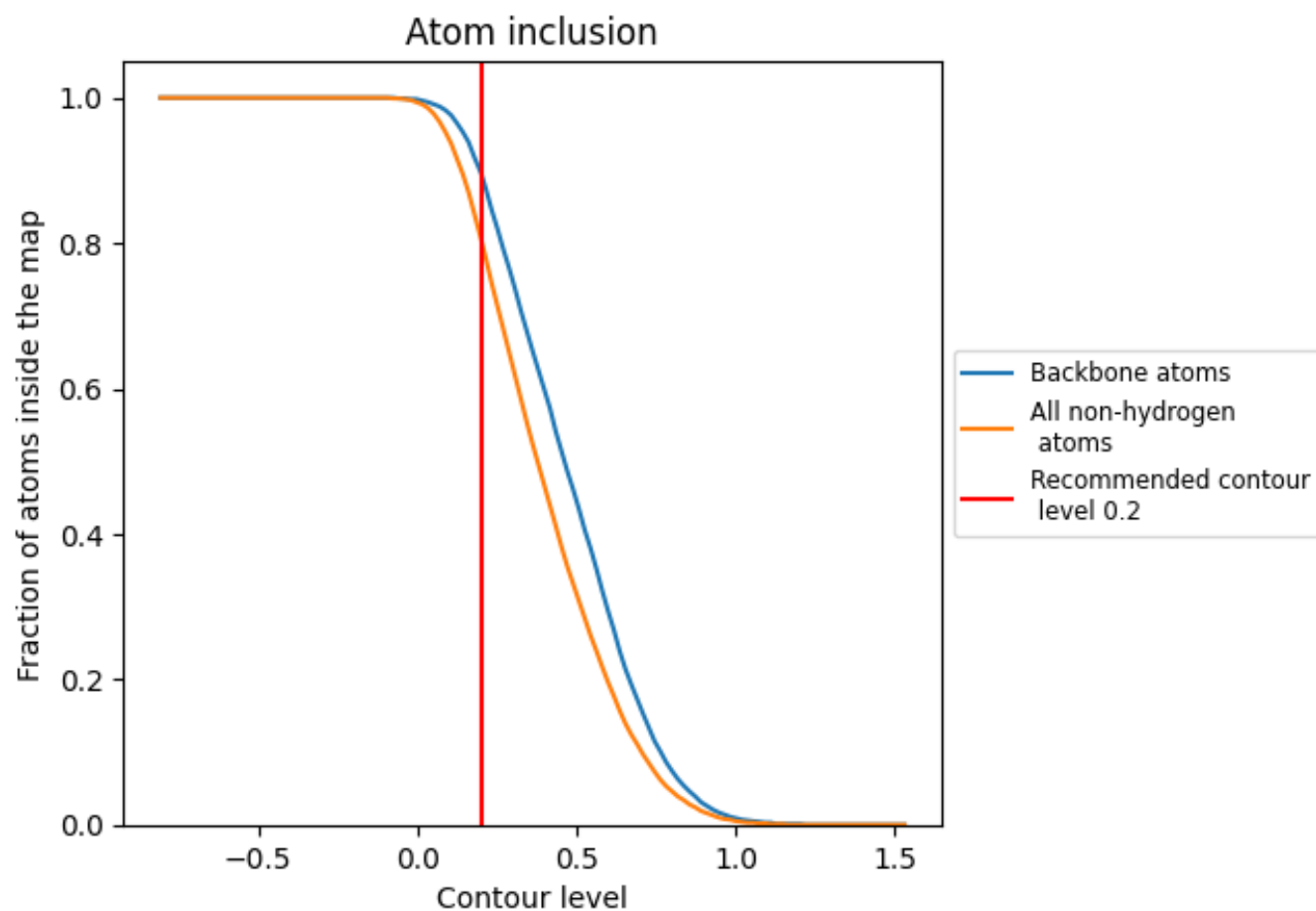
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.4640
A	 0.8190	 0.4780
B	 0.8590	 0.5060
C	 0.8100	 0.4610
D	 0.8050	 0.4600
E	 0.8560	 0.5070
F	 0.8410	 0.5000
G	 0.8170	 0.4570
H	 0.7180	 0.4100
I	 0.8490	 0.4870
J	 0.8250	 0.4630
K	 0.8490	 0.4860
L	 0.5100	 0.3150
M	 0.8310	 0.4810
N	 0.8220	 0.4630
O	 0.7980	 0.4410
P	 0.7500	 0.4830
Q	 0.5360	 0.3970
R	 0.7500	 0.4350
S	 0.7860	 0.4840
T	 0.8210	 0.4340
U	 0.6790	 0.4010
V	 0.3210	 0.2930
W	 0.6430	 0.3860
X	 0.8460	 0.4960

