wwPDB EM Validation Summary Report

Aug 6, 2022 – 09:13 am BST

PDB ID	:	7QDH
EMDB ID	:	EMD-13919
Title	:	SARS-CoV-2 S protein S:D614G mutant 1-up
Authors	:	Ginex, T.; Marco-Marin, C.; Wieczor, M.; Mata, C.P.; Krieger, J.; Lopez-Redondo, M.L.; Frances-Gomez, C.; Ruiz-Rodriguez, P.; Melero, R.; Sanchez-Sorzano, C.O.; Martinez, M.; Gougeard, N.; Forcada-Nadal, A.; Zamora-Caballero, S.; Gozalbo-Rovira, R.; Sanz-Frasquet, C.; Bravo, J.; Rubio, V.; Marina, A.; Geller, R.; Comas, I.; Gil, C.; Coscolla, M.; Orozco, M.; LLacer, J.L.; Carazo, J.M.
Deposited on	:	2021-11-27
Resolution	:	4.20 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

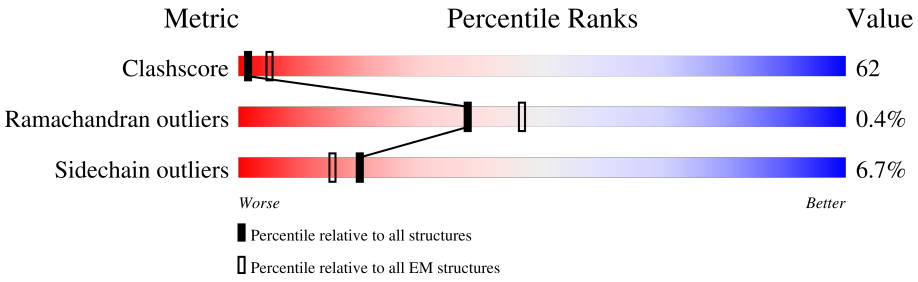
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1250	16% 42% 40% · 14%
1	B	1250	16% 42% 40% · 14%
1	C	1250	18% 40% 42% 5% 14%
2	E	2	50% 50%
2	G	2	50% 100%
2	I	2	100% 100%
2	J	2	100%
2	K	2	50% 50%

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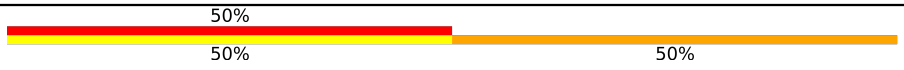
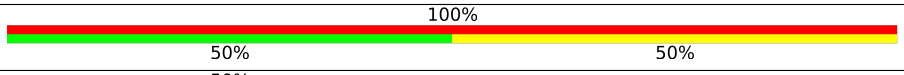
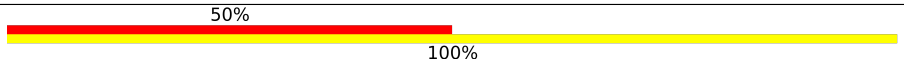
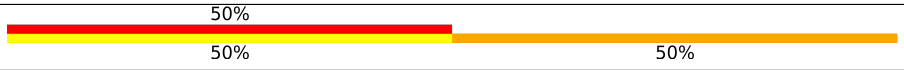
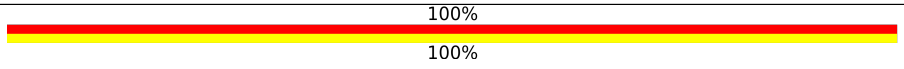
Mol	Chain	Length	Quality of chain
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1070	Total	C	N	O	S	0	0
			8354	5332	1392	1592	38		
1	B	1073	Total	C	N	O	S	0	0
			8369	5342	1393	1596	38		
1	C	1076	Total	C	N	O	S	0	0
			8373	5346	1395	1594	38		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	conflict	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1214	LEU	-	linker	UNP P0DTC2
A	1215	VAL	-	linker	UNP P0DTC2
A	1216	PRO	-	linker	UNP P0DTC2
A	1217	ARG	-	linker	UNP P0DTC2
A	1218	GLY	-	linker	UNP P0DTC2
A	1219	SER	-	linker	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	GLU	-	expression tag	UNP P10104
A	1259	GLN	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1260	LYS	-	expression tag	UNP P10104
A	1261	LEU	-	expression tag	UNP P10104
A	1262	ILE	-	expression tag	UNP P10104
A	1263	SER	-	expression tag	UNP P10104
A	1264	GLU	-	expression tag	UNP P10104
A	1265	GLU	-	expression tag	UNP P10104
A	1266	ASP	-	expression tag	UNP P10104
A	1267	LEU	-	expression tag	UNP P10104
B	614	GLY	ASP	conflict	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1214	LEU	-	linker	UNP P0DTC2
B	1215	VAL	-	linker	UNP P0DTC2
B	1216	PRO	-	linker	UNP P0DTC2
B	1217	ARG	-	linker	UNP P0DTC2
B	1218	GLY	-	linker	UNP P0DTC2
B	1219	SER	-	linker	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	GLU	-	expression tag	UNP P10104
B	1259	GLN	-	expression tag	UNP P10104
B	1260	LYS	-	expression tag	UNP P10104
B	1261	LEU	-	expression tag	UNP P10104
B	1262	ILE	-	expression tag	UNP P10104
B	1263	SER	-	expression tag	UNP P10104
B	1264	GLU	-	expression tag	UNP P10104
B	1265	GLU	-	expression tag	UNP P10104
B	1266	ASP	-	expression tag	UNP P10104
B	1267	LEU	-	expression tag	UNP P10104
C	614	GLY	ASP	conflict	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1214	LEU	-	linker	UNP P0DTC2
C	1215	VAL	-	linker	UNP P0DTC2
C	1216	PRO	-	linker	UNP P0DTC2
C	1217	ARG	-	linker	UNP P0DTC2
C	1218	GLY	-	linker	UNP P0DTC2
C	1219	SER	-	linker	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P10104
C	1250	HIS	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104
C	1253	HIS	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	GLU	-	expression tag	UNP P10104
C	1259	GLN	-	expression tag	UNP P10104
C	1260	LYS	-	expression tag	UNP P10104
C	1261	LEU	-	expression tag	UNP P10104
C	1262	ILE	-	expression tag	UNP P10104
C	1263	SER	-	expression tag	UNP P10104
C	1264	GLU	-	expression tag	UNP P10104
C	1265	GLU	-	expression tag	UNP P10104
C	1266	ASP	-	expression tag	UNP P10104
C	1267	LEU	-	expression tag	UNP P10104

- Molecule 2 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
2	E	2	Total	C	N	O	0	0
			28	16	2	10		

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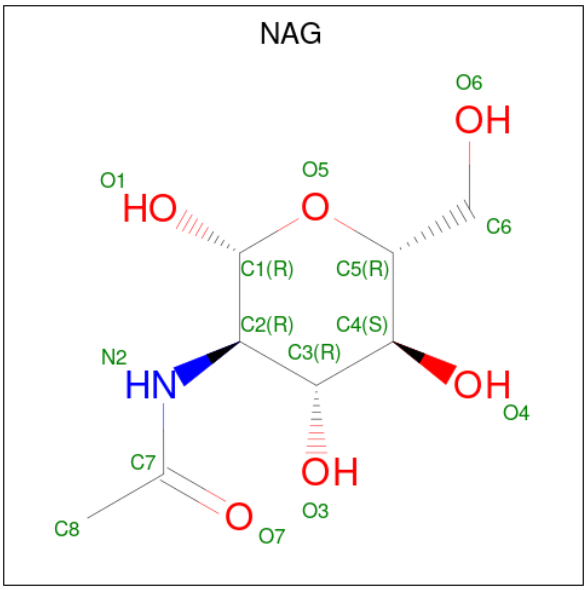
Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			126	72	9	45	
3	A	1	Total	C	N	O	0
			126	72	9	45	

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Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 126 72 9 45	0
3	A	1	Total C N O 126 72 9 45	0
3	A	1	Total C N O 126 72 9 45	0
3	A	1	Total C N O 126 72 9 45	0
3	A	1	Total C N O 126 72 9 45	0
3	A	1	Total C N O 126 72 9 45	0
3	A	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	B	1	Total C N O 126 72 9 45	0
3	C	1	Total C N O 84 48 6 30	0
3	C	1	Total C N O 84 48 6 30	0
3	C	1	Total C N O 84 48 6 30	0
3	C	1	Total C N O 84 48 6 30	0
3	C	1	Total C N O 84 48 6 30	0

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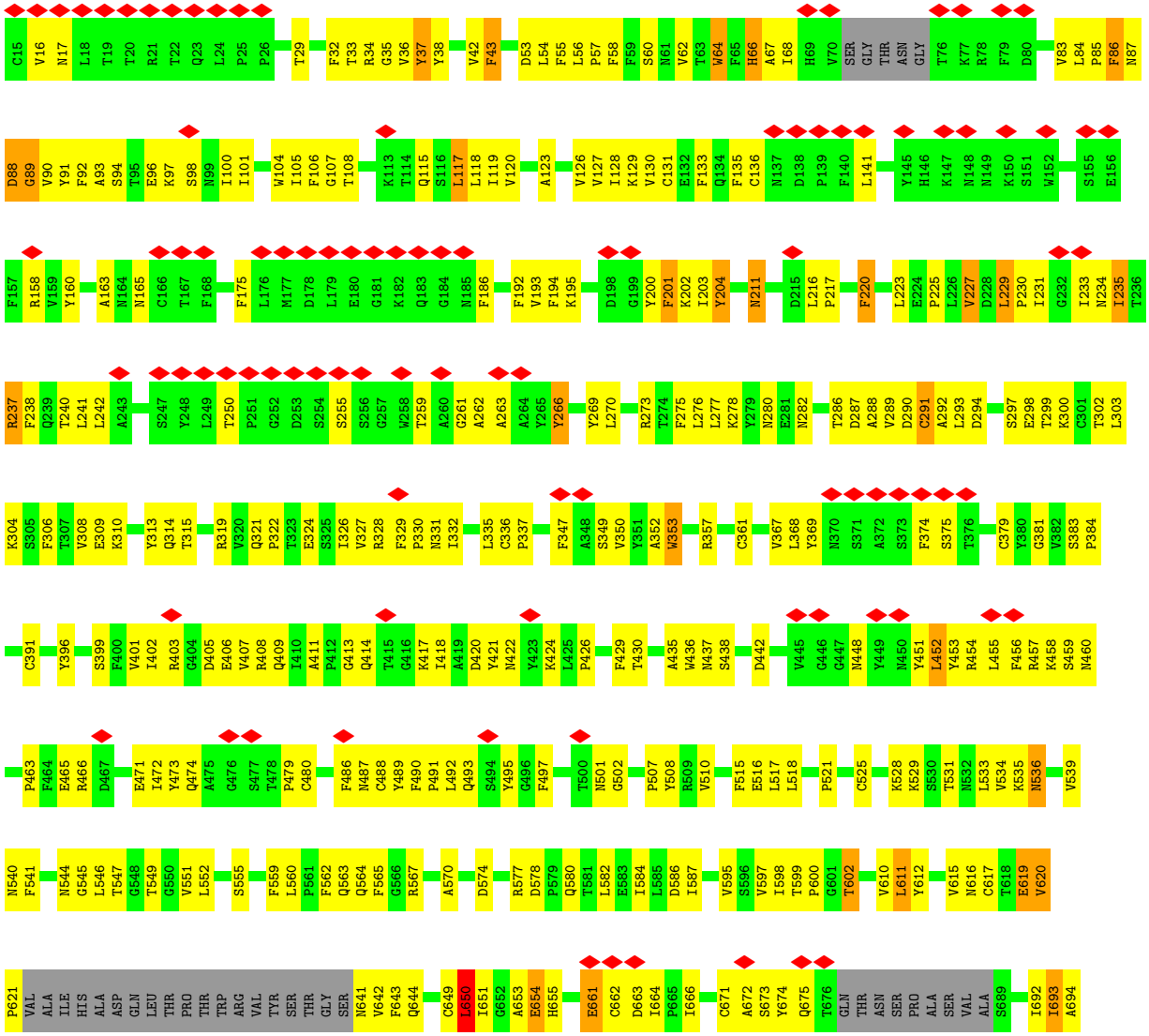
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			84	48	6	30	

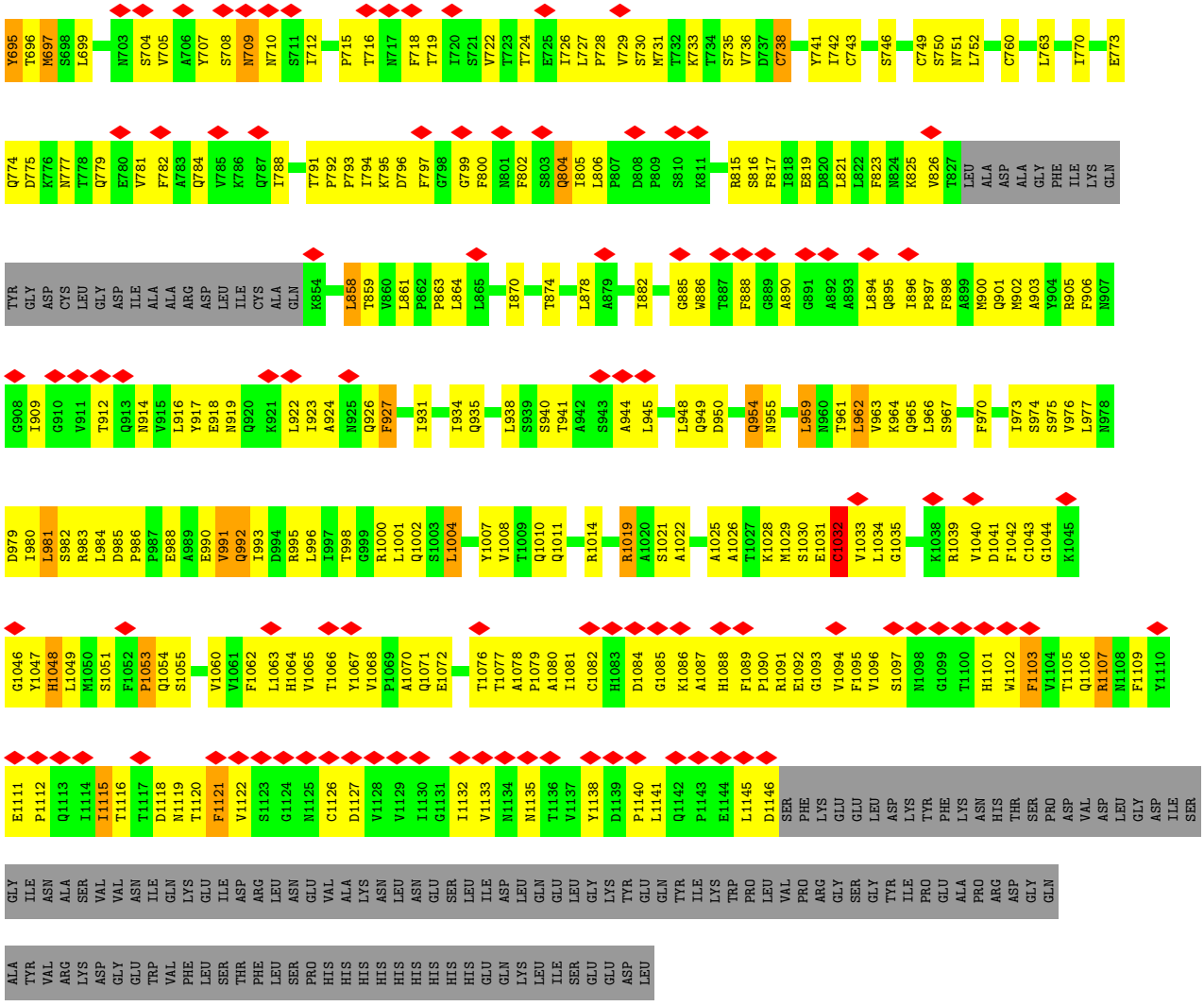
3 Residue-property plots (i)

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: Spike glycoprotein,Fibritin

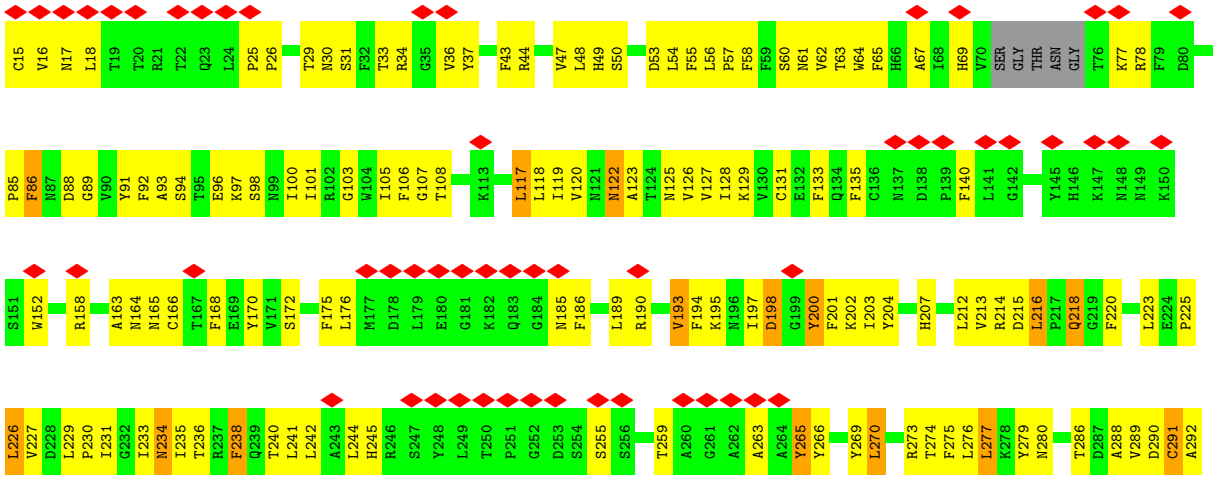
Chain A:

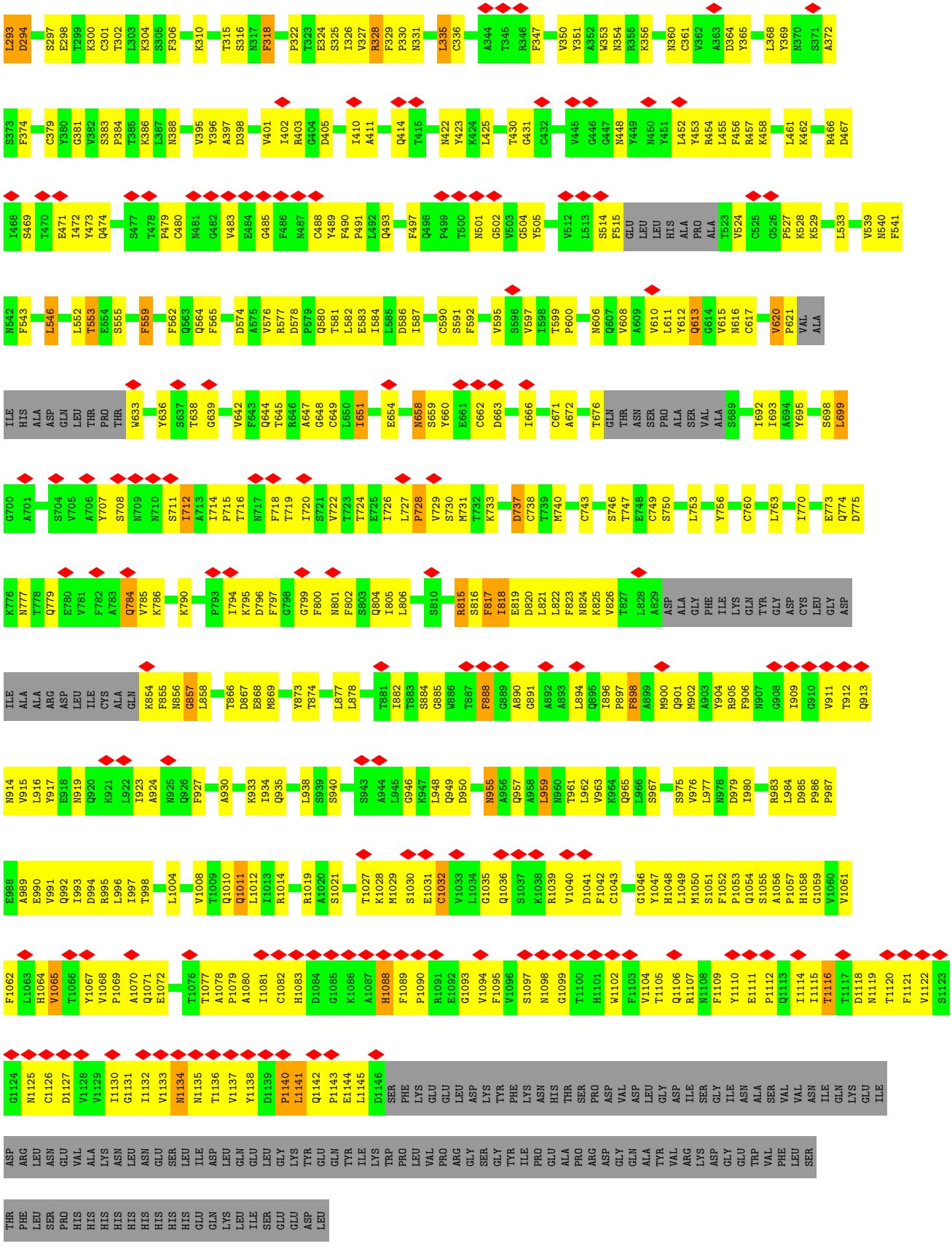




• Molecule 1: Spike glycoprotein,Fibritin

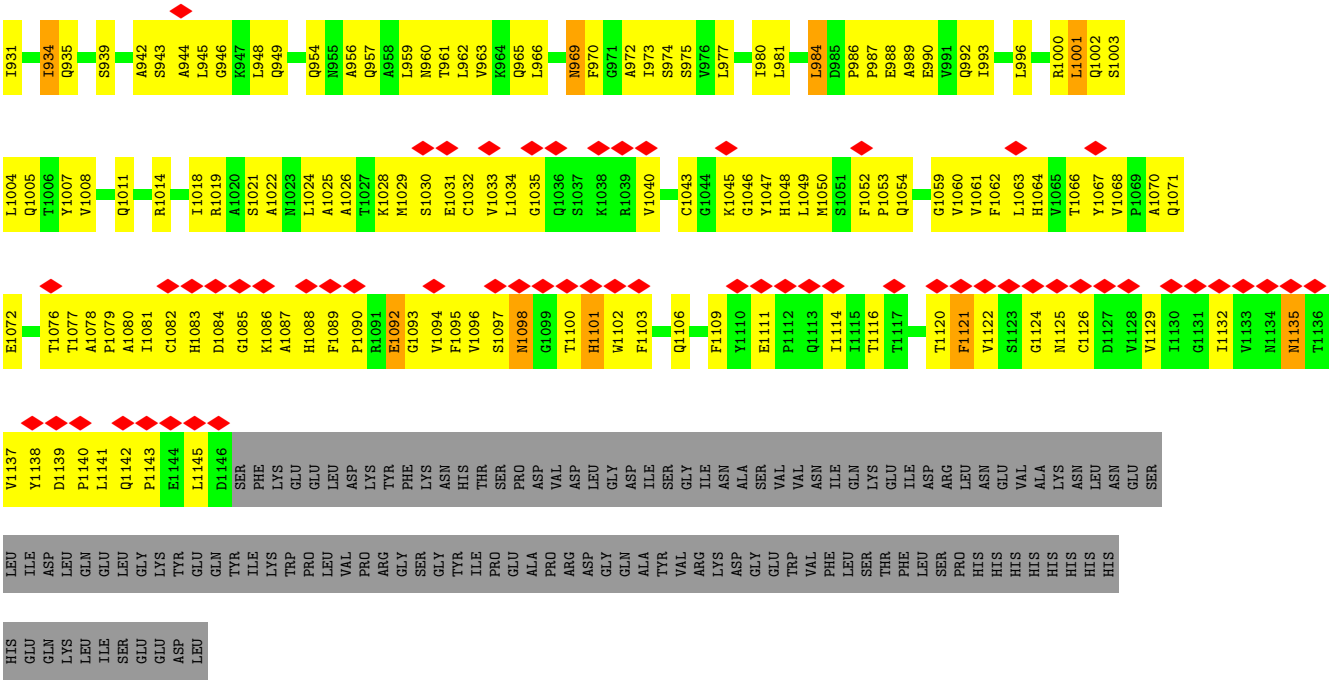
Chain B:





- Molecule 1: Spike glycoprotein,Fibritin

Chain C:

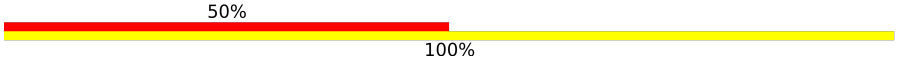


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

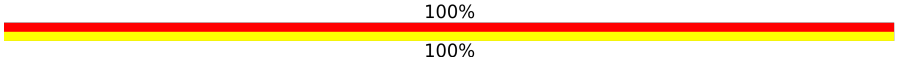
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



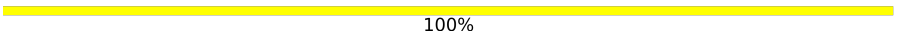
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain J:



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

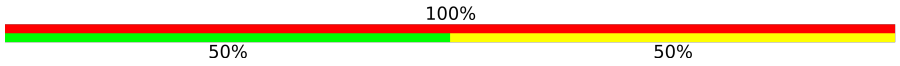
Chain K:

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

Chain L:

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

Chain M:



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

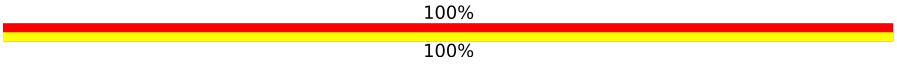
Chain N:

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

Chain O:

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

Chain P:




NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82102	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	32.4	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.513	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.057	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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	0.53	7/8550 (0.1%)	0.71	4/11641 (0.0%)
1	B	0.56	4/8565 (0.0%)	0.68	2/11661 (0.0%)
1	C	0.54	5/8569 (0.1%)	0.69	3/11669 (0.0%)
All	All	0.54	16/25684 (0.1%)	0.69	9/34971 (0.0%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	676	THR	C-O	-17.56	0.90	1.23
1	B	940	SER	C-O	-17.20	0.90	1.23
1	A	940	SER	C-O	-10.93	1.02	1.23
1	C	432	CYS	CB-SG	8.21	1.96	1.82
1	C	423	TYR	CE1-CZ	-7.37	1.28	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1032	CYS	CA-CB-SG	8.54	129.38	114.00
1	A	650	LEU	CA-CB-CG	7.41	132.35	115.30
1	C	526	GLY	C-N-CD	-6.64	105.98	120.60
1	C	1032	CYS	CA-CB-SG	-6.39	102.50	114.00
1	B	1032	CYS	CA-CB-SG	6.04	124.87	114.00

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	8354	0	8126	1043	0
1	B	8369	0	8130	1018	0
1	C	8373	0	8126	1174	0
2	E	28	0	25	1	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	2	0
2	L	28	0	25	2	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	1	0
2	P	28	0	25	0	0
3	A	126	0	117	2	0
3	B	126	0	117	6	0
3	C	84	0	78	1	0
All	All	25712	0	24944	3122	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 62.

The worst 5 of 3122 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:C:33:THR:HA	1:C:58:PHE:CE1	1.21	1.70
1:C:320:VAL:CG2	1:C:591:SER:HB2	1.28	1.58
1:B:1141:LEU:CD2	1:B:1145:LEU:HD21	1.37	1.54
1:B:195:LYS:HG3	1:B:197:ILE:CD1	1.34	1.52
1:C:118:LEU:HD22	1:C:135:PHE:CZ	1.46	1.50

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1060/1250 (85%)	1010 (95%)	44 (4%)	6 (1%)	25	64
1	B	1061/1250 (85%)	1015 (96%)	41 (4%)	5 (0%)	29	68
1	C	1066/1250 (85%)	1022 (96%)	43 (4%)	1 (0%)	51	85
All	All	3187/3750 (85%)	3047 (96%)	128 (4%)	12 (0%)	38	72

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	620	VAL
1	B	857	GLY
1	B	946	GLY
1	A	502	GLY
1	A	619	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	932/1089 (86%)	871 (94%)	61 (6%)	17	44
1	B	932/1089 (86%)	877 (94%)	55 (6%)	19	47
1	C	928/1089 (85%)	858 (92%)	70 (8%)	13	40
All	All	2792/3267 (86%)	2606 (93%)	186 (7%)	20	43

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1141	LEU
1	C	318	PHE
1	C	51	THR
1	C	213	VAL
1	C	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	493	GLN
1	C	544	ASN
1	C	824	ASN
1	B	207	HIS
1	B	165	ASN

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)

20 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	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.96	0	17,19,21	3.24	7 (41%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.12	2 (11%)
2	NAG	G	1	2,1	14,14,15	0.91	0	17,19,21	3.19	6 (35%)
2	NAG	G	2	2	14,14,15	0.66	0	17,19,21	1.14	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	I	1	2,1	14,14,15	0.91	0	17,19,21	3.23	6 (35%)
2	NAG	I	2	2	14,14,15	0.65	0	17,19,21	1.13	2 (11%)
2	NAG	J	1	2,1	14,14,15	1.01	1 (7%)	17,19,21	3.19	6 (35%)
2	NAG	J	2	2	14,14,15	0.66	0	17,19,21	1.14	2 (11%)
2	NAG	K	1	2	14,14,15	0.43	0	17,19,21	0.84	1 (5%)
2	NAG	K	2	2	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	L	1	2	14,14,15	0.93	1 (7%)	17,19,21	3.10	7 (41%)
2	NAG	L	2	2	14,14,15	0.68	0	17,19,21	1.14	2 (11%)
2	NAG	M	1	2,1	14,14,15	0.42	0	17,19,21	1.20	2 (11%)
2	NAG	M	2	2	14,14,15	0.27	0	17,19,21	0.56	0
2	NAG	N	1	2,1	14,14,15	1.00	1 (7%)	17,19,21	3.24	7 (41%)
2	NAG	N	2	2	14,14,15	0.67	0	17,19,21	1.10	2 (11%)
2	NAG	O	1	2,1	14,14,15	0.76	0	17,19,21	2.02	2 (11%)
2	NAG	O	2	2	14,14,15	0.55	0	17,19,21	2.22	5 (29%)
2	NAG	P	1	2,1	14,14,15	1.04	1 (7%)	17,19,21	3.46	7 (41%)
2	NAG	P	2	2	14,14,15	0.69	0	17,19,21	1.11	2 (11%)

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
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2	-	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	N	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	NAG	O7-C7	-2.56	1.17	1.23
2	P	1	NAG	O7-C7	-2.14	1.18	1.23
2	N	1	NAG	O7-C7	-2.06	1.18	1.23
2	L	1	NAG	O7-C7	-2.05	1.18	1.23

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	1	NAG	C2-N2-C7	8.02	134.32	122.90
2	J	1	NAG	C8-C7-N2	7.89	129.46	116.10
2	I	1	NAG	C8-C7-N2	7.63	129.01	116.10
2	E	1	NAG	C8-C7-N2	7.50	128.79	116.10
2	G	1	NAG	C8-C7-N2	7.45	128.71	116.10

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	2	0

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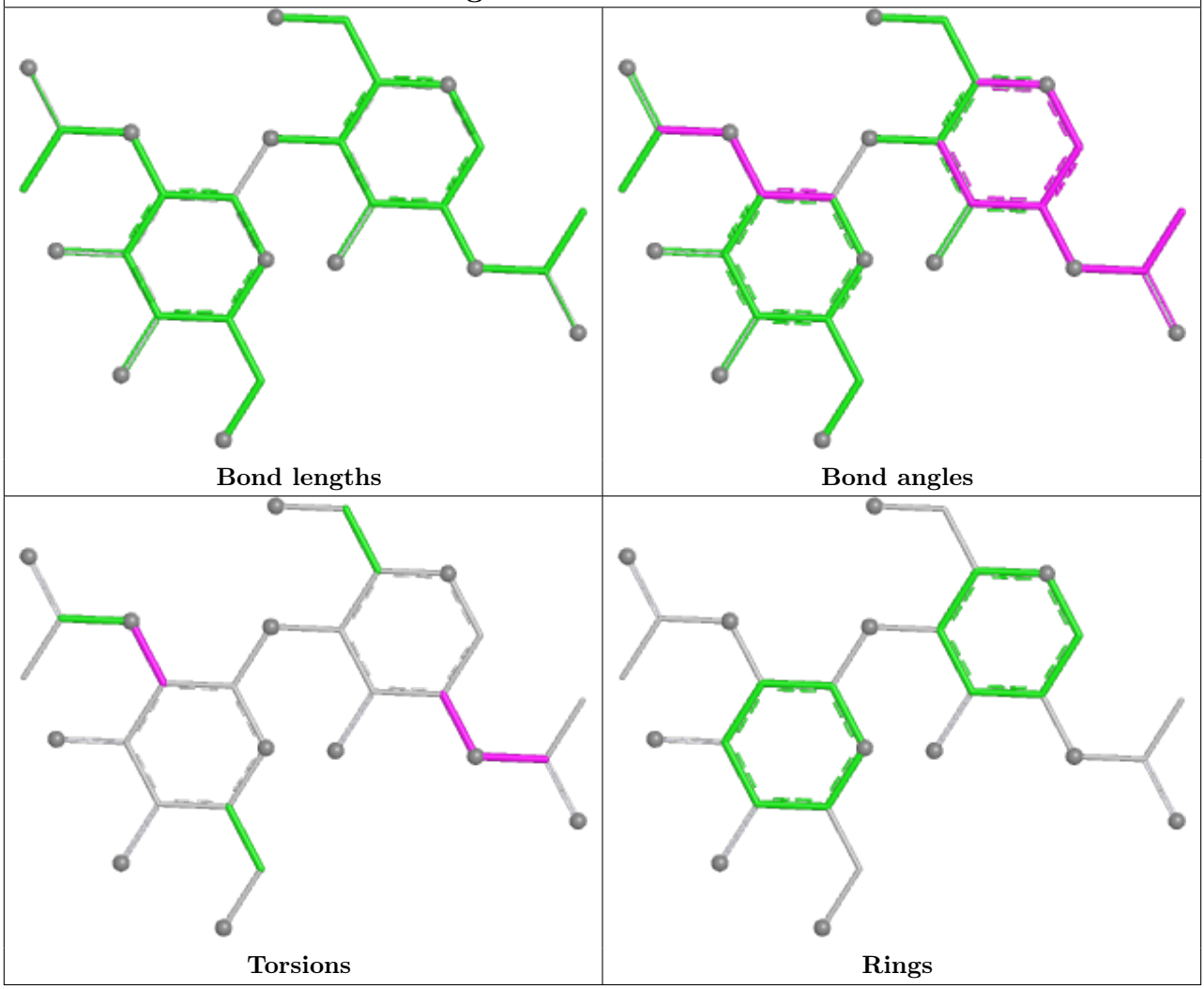
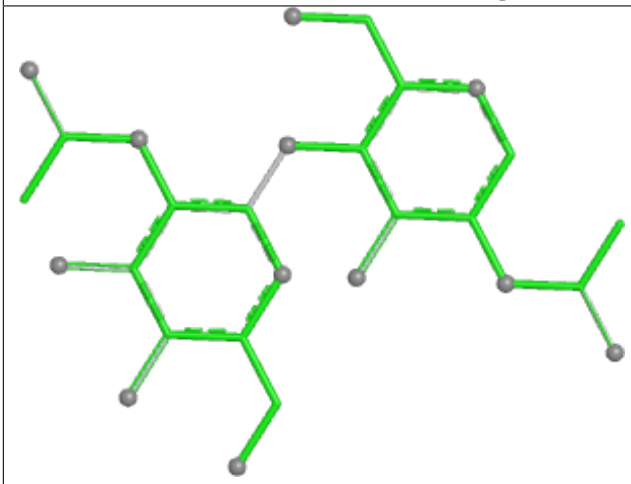
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	NAG	1	0
2	E	1	NAG	1	0
2	O	2	NAG	1	0
2	L	1	NAG	2	0

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

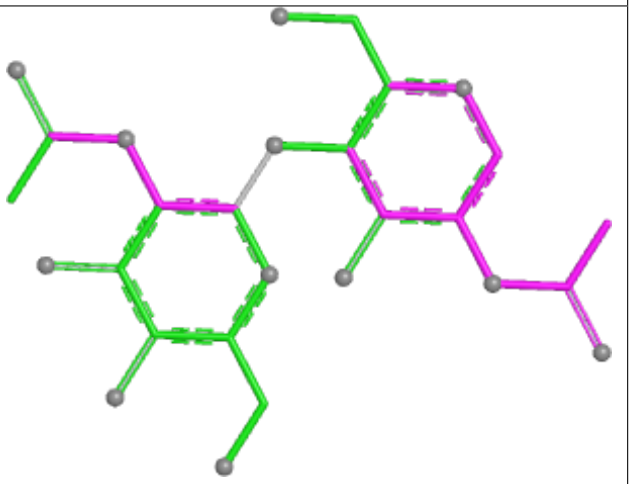
Oligosaccharide Chain E



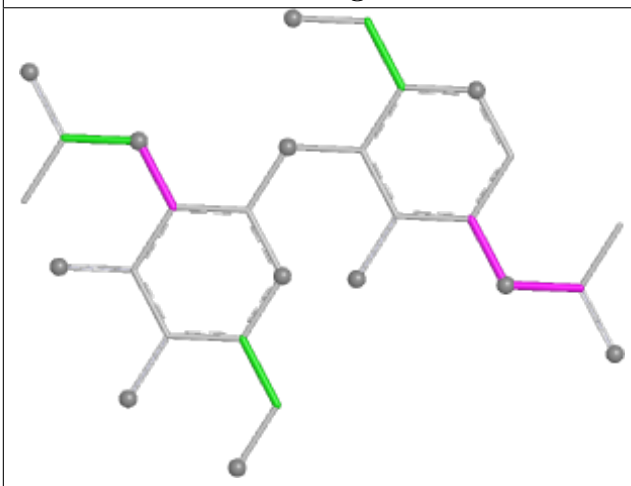
Oligosaccharide Chain G



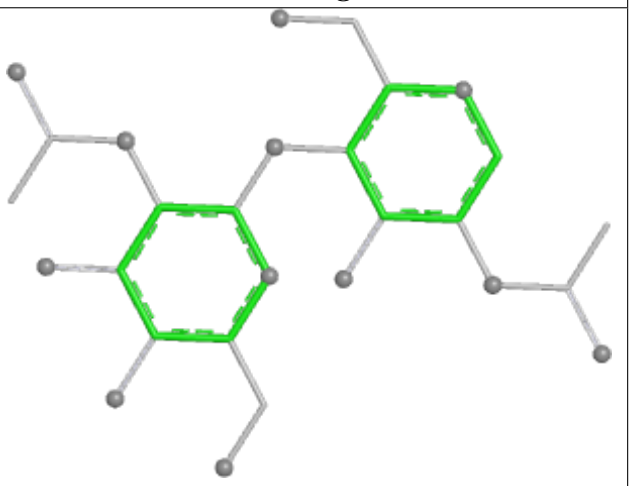
Bond lengths



Bond angles

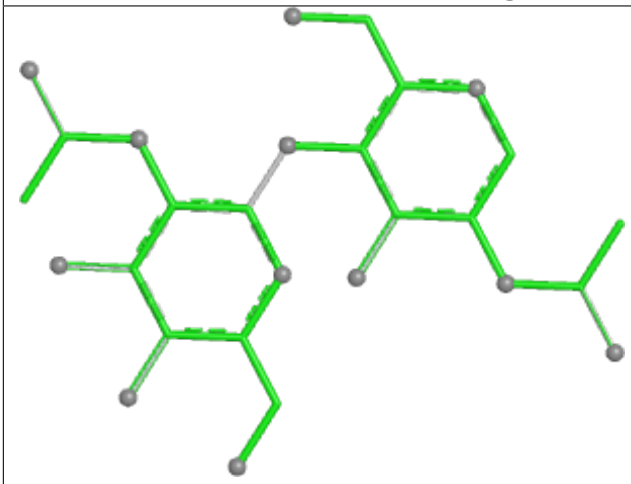


Torsions

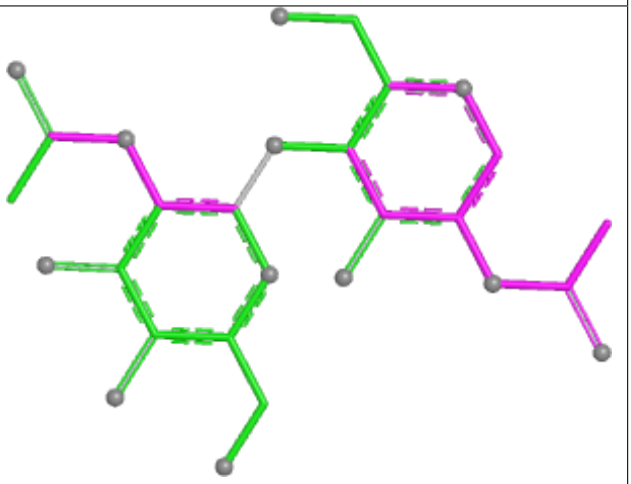


Rings

Oligosaccharide Chain I



Bond lengths



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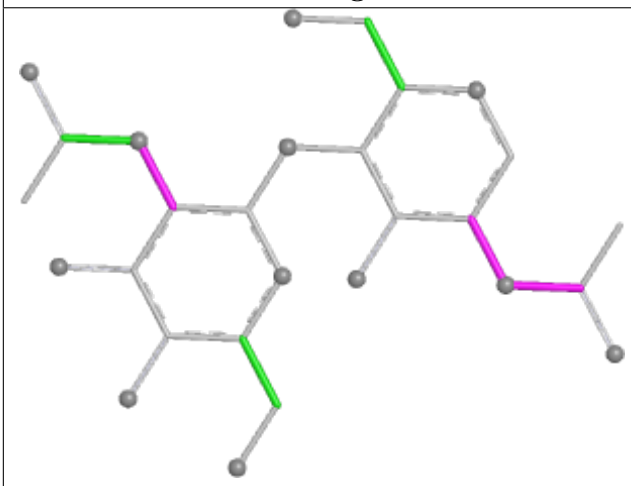

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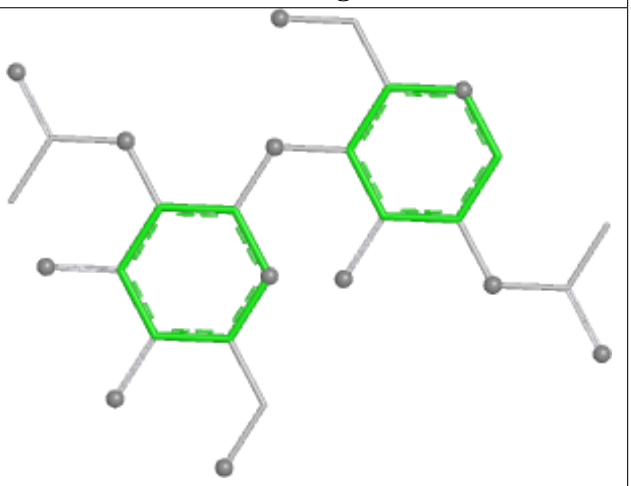
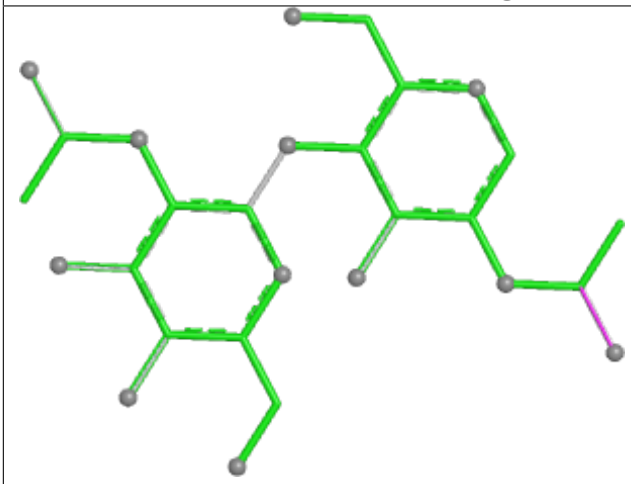
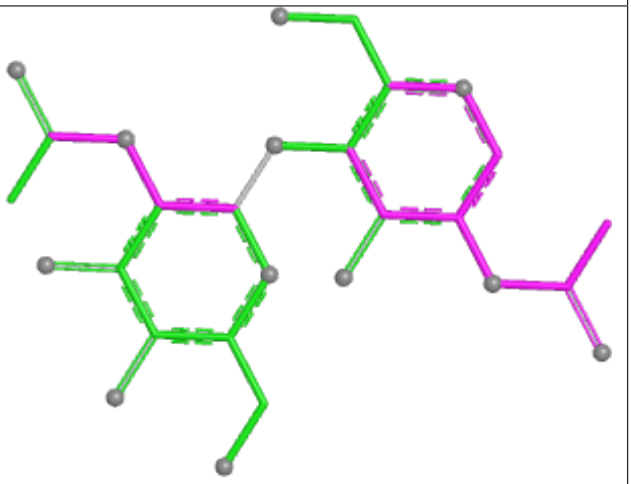


Rings

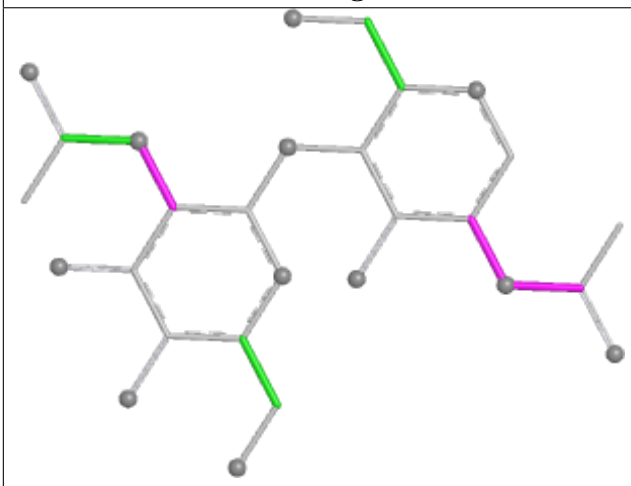
Oligosaccharide Chain J



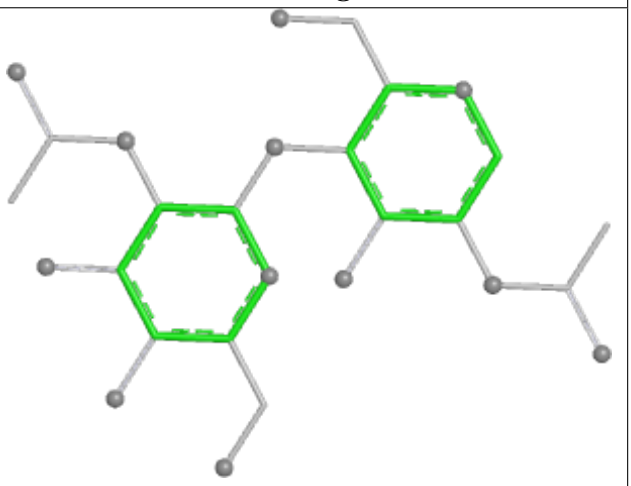
Bond lengths



Bond angles

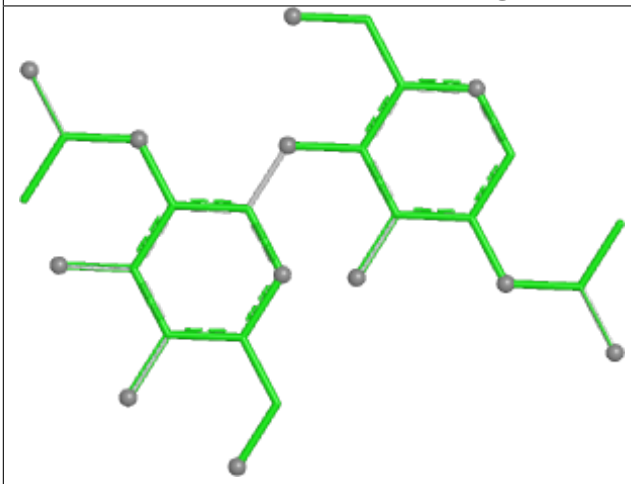


Torsions

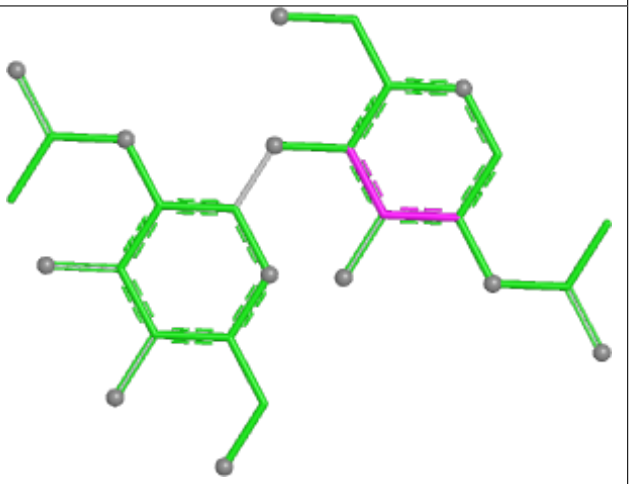


Rings

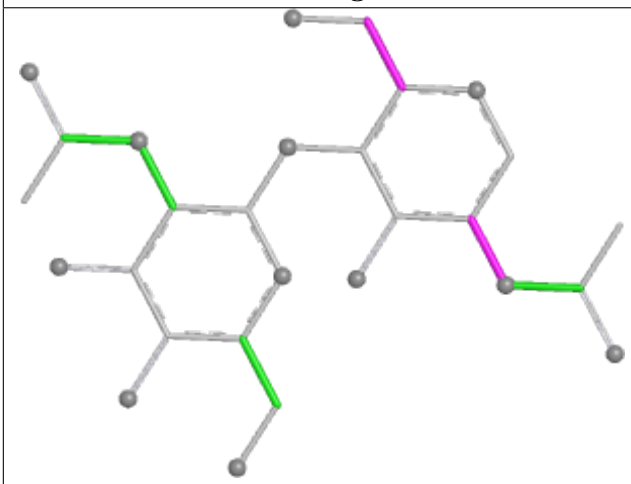
Oligosaccharide Chain K



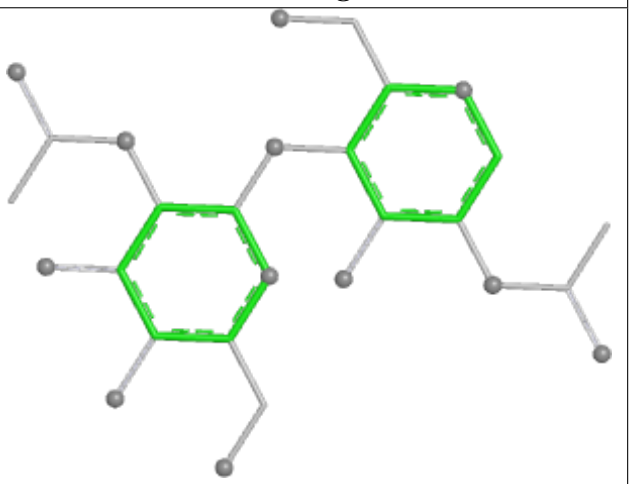
Bond lengths



Bond angles

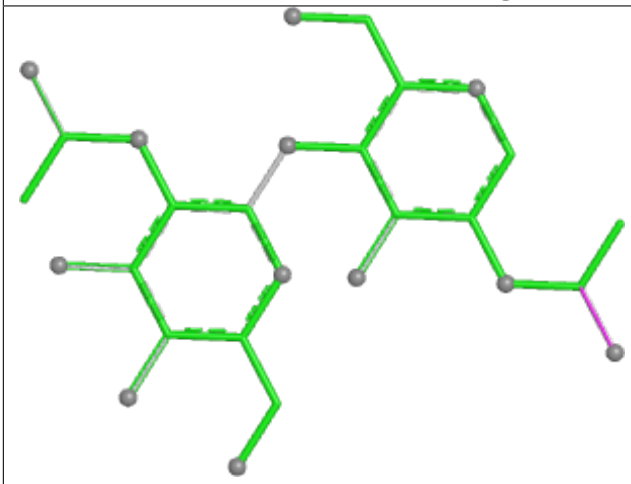


Torsions

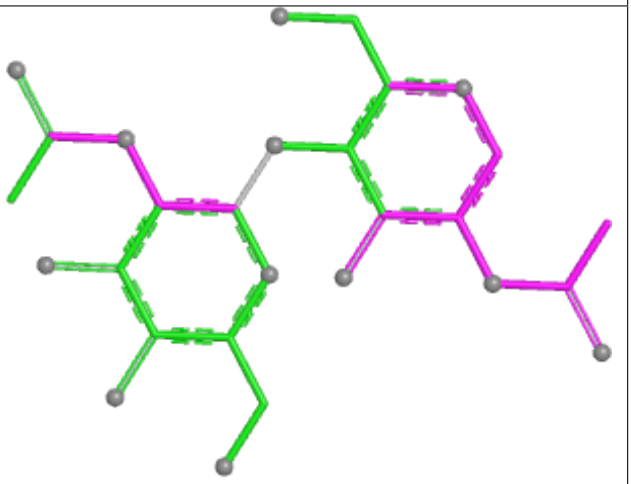


Rings

Oligosaccharide Chain L



Bond lengths



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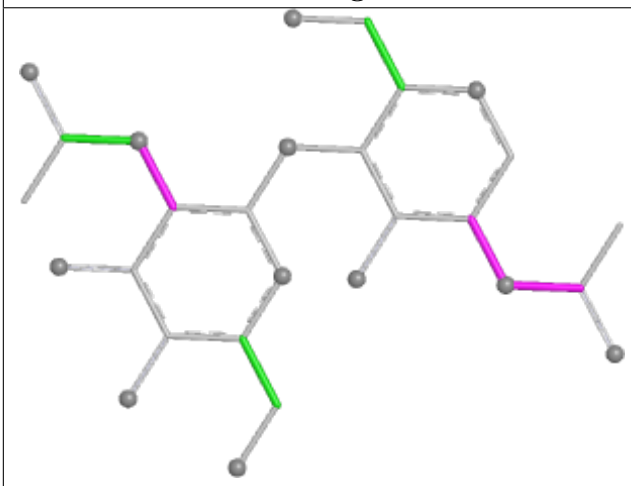
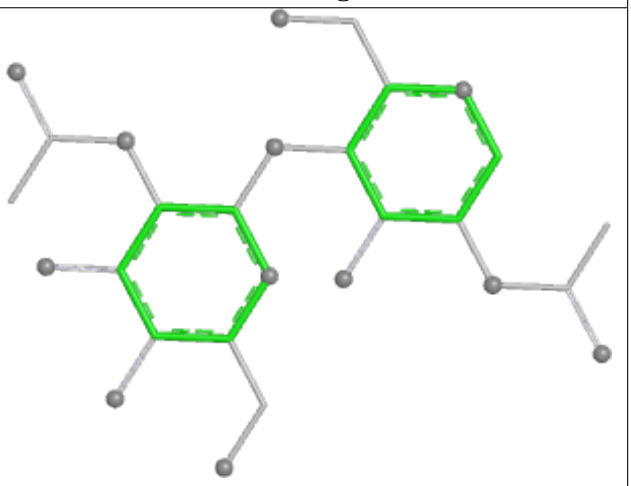
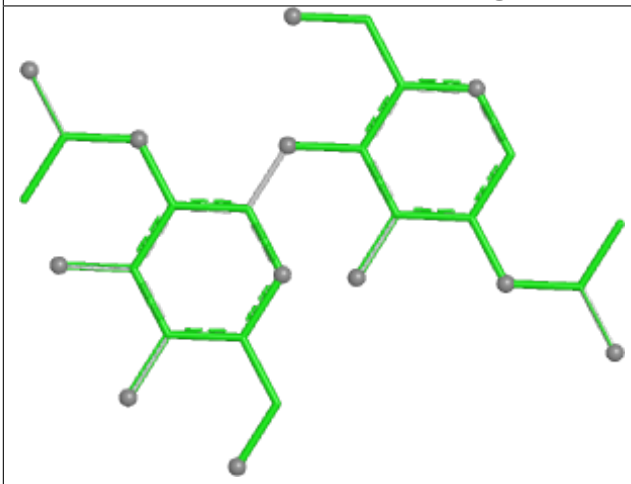
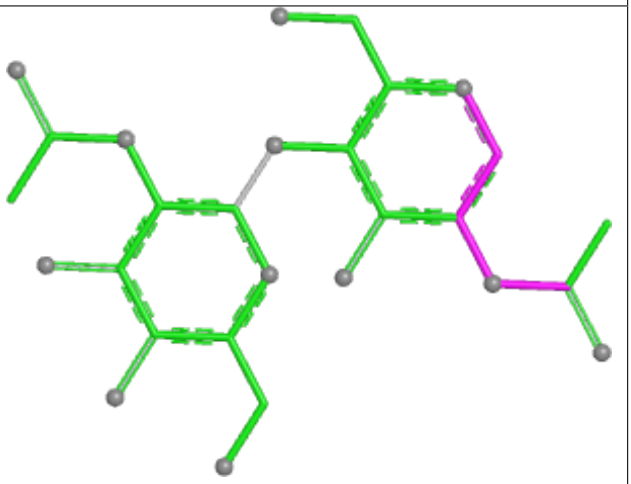
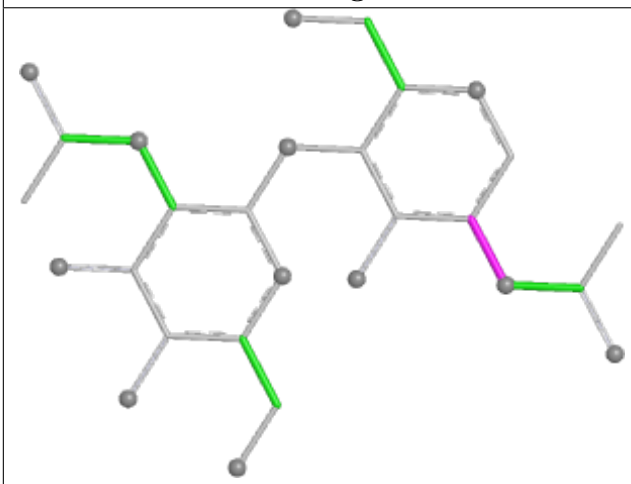
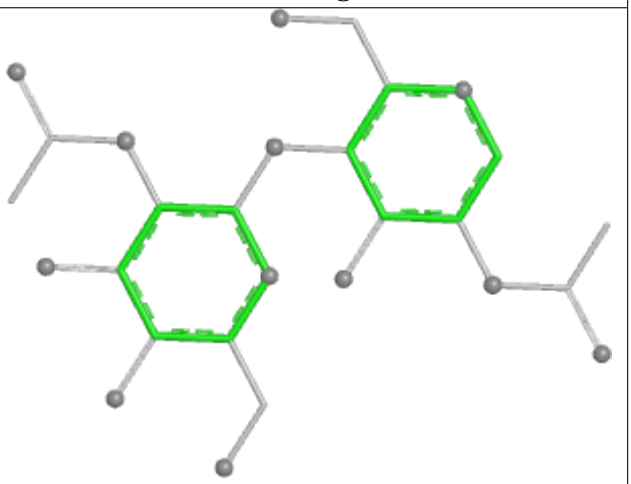


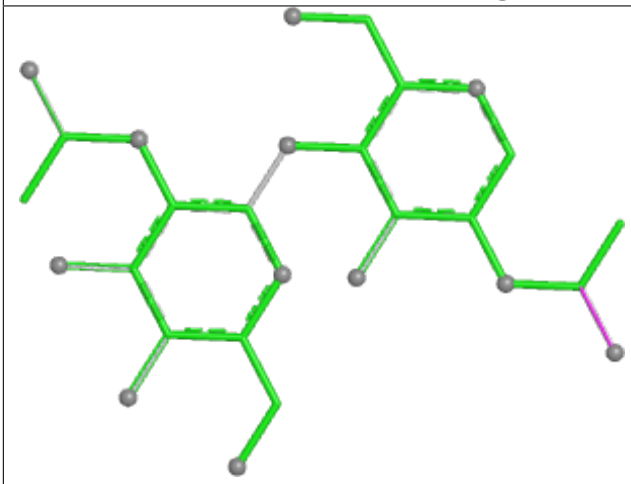
Torsions



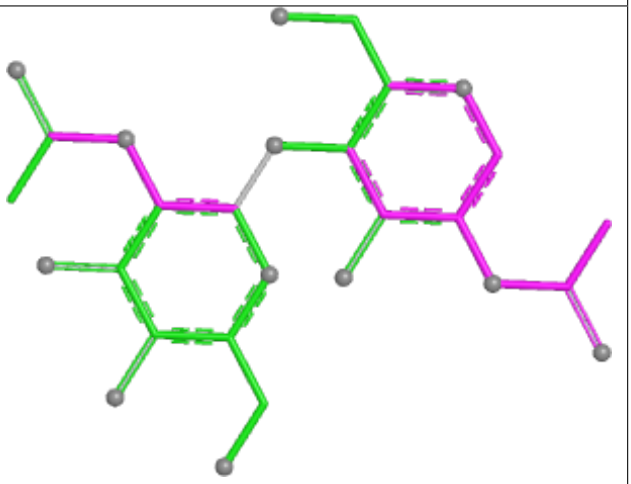
Rings

Oligosaccharide Chain M	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

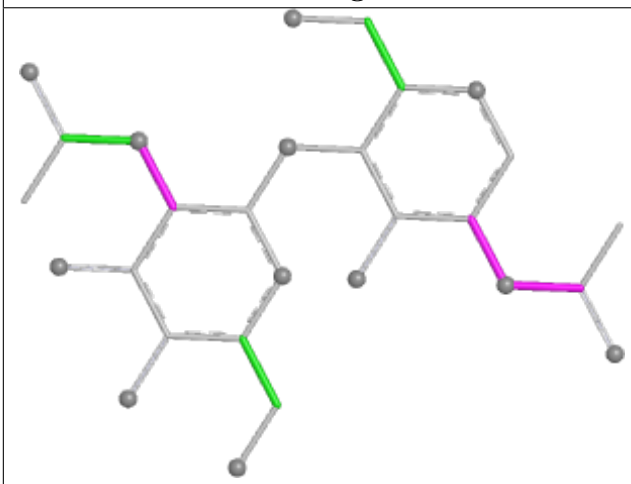
Oligosaccharide Chain N



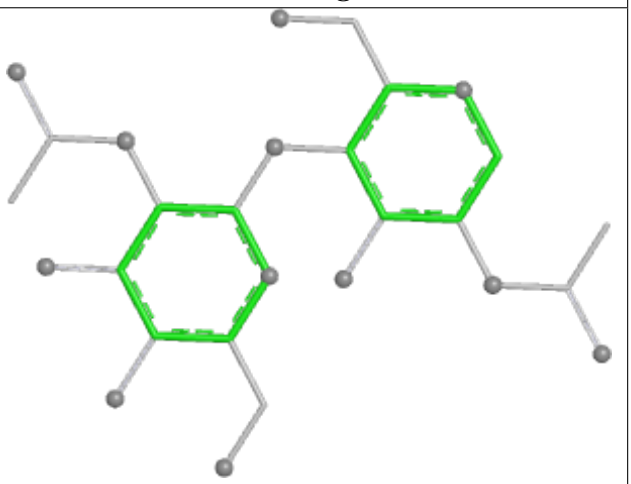
Bond lengths



Bond angles

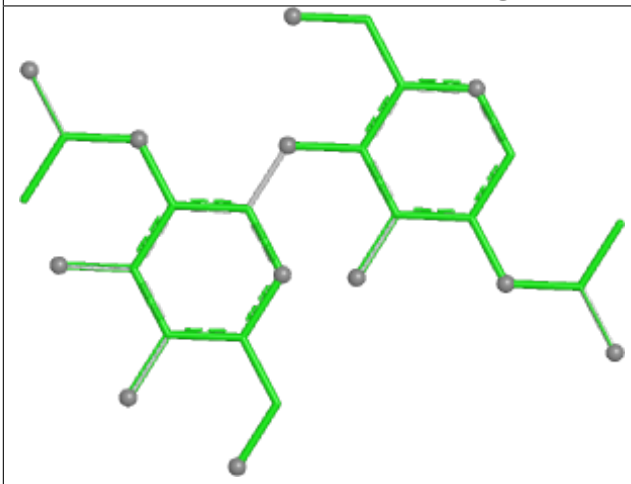


Torsions

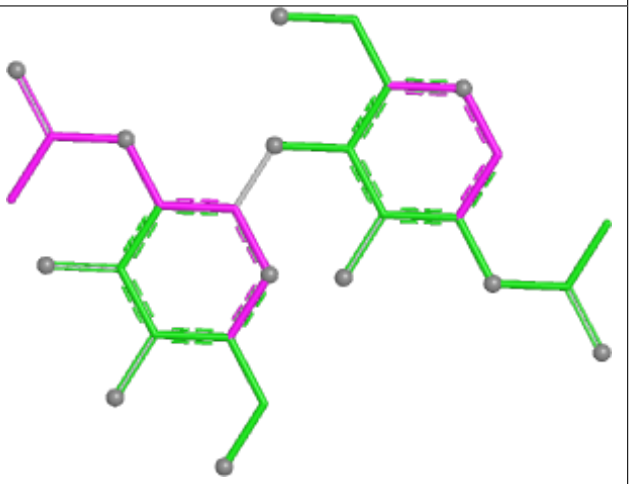


Rings

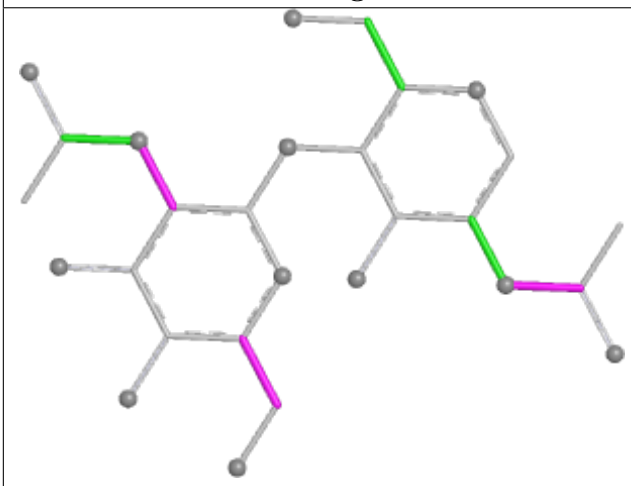
Oligosaccharide Chain O



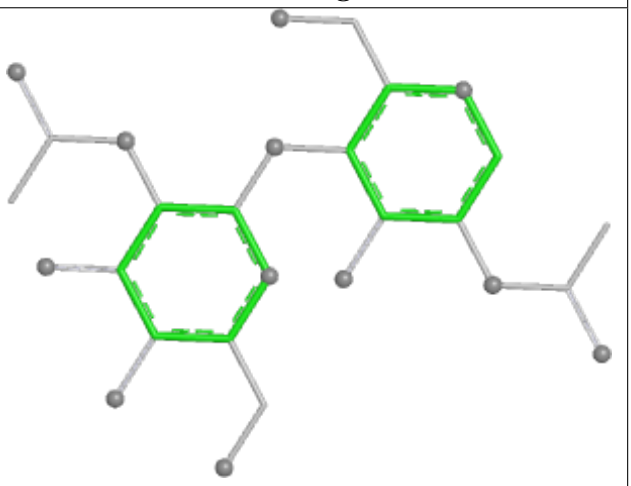
Bond lengths



Bond angles

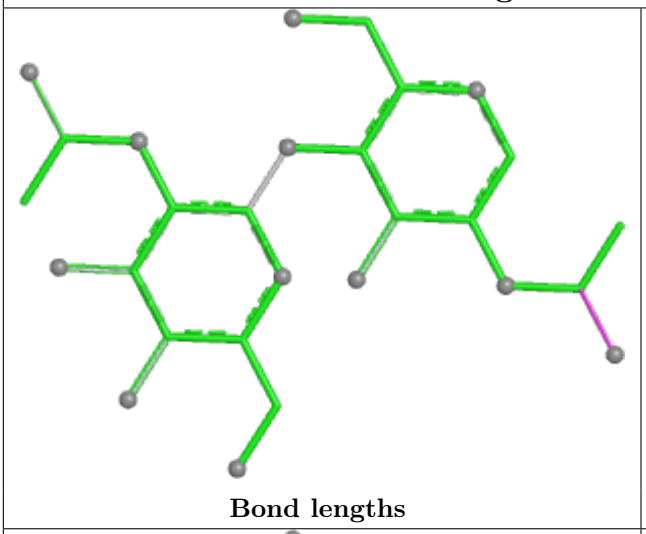


Torsions

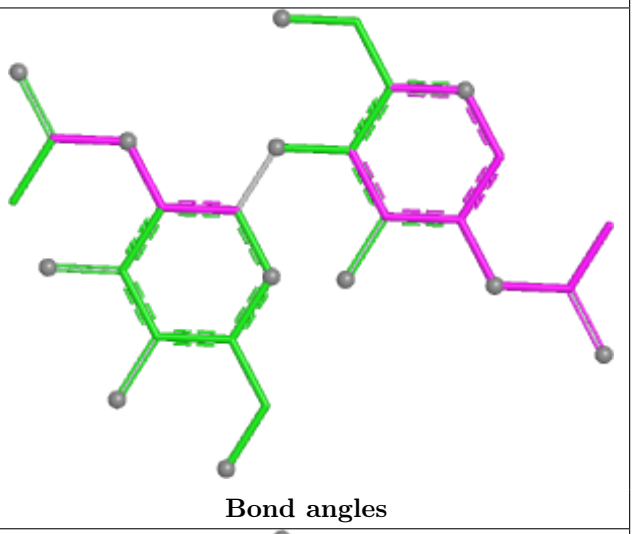


Rings

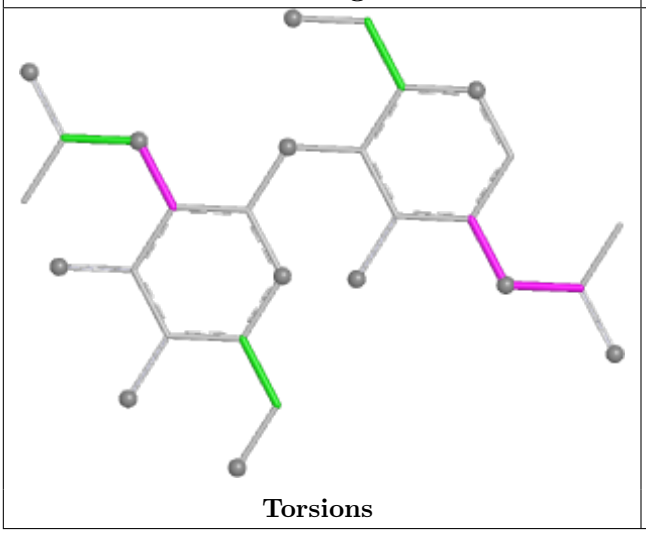
Oligosaccharide Chain P



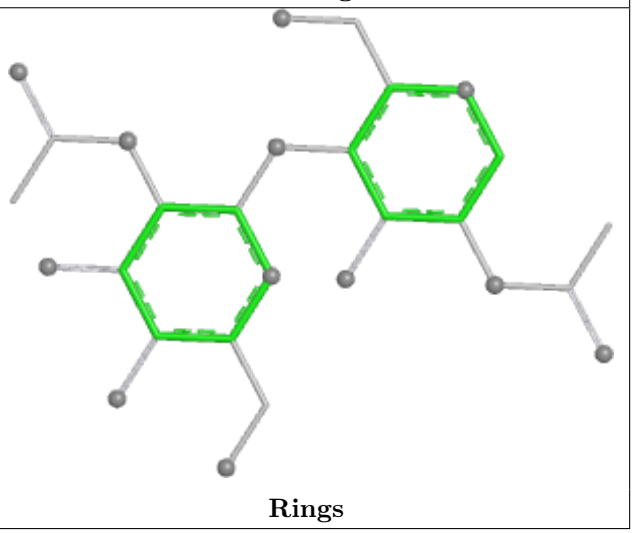
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
3	NAG	B	1304	1	14,14,15	0.57	0	17,19,21	1.34	2 (11%)
3	NAG	A	1306	1	14,14,15	0.43	0	17,19,21	2.53	6 (35%)
3	NAG	B	1305	1	14,14,15	0.56	0	17,19,21	1.49	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1301	1	14,14,15	0.50	0	17,19,21	1.58	3 (17%)
3	NAG	C	1302	1	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
3	NAG	C	1301	1	14,14,15	0.64	0	17,19,21	1.68	3 (17%)
3	NAG	B	1306	1	14,14,15	0.63	0	17,19,21	1.32	3 (17%)
3	NAG	C	1306	1	14,14,15	0.64	0	17,19,21	1.70	3 (17%)
3	NAG	A	1305	1	14,14,15	0.39	0	17,19,21	0.85	1 (5%)
3	NAG	B	1307	1	14,14,15	0.55	0	17,19,21	1.36	3 (17%)
3	NAG	A	1301	1	14,14,15	0.37	0	17,19,21	0.65	0
3	NAG	B	1308	1	14,14,15	0.49	0	17,19,21	2.14	4 (23%)
3	NAG	C	1304	1	14,14,15	0.61	0	17,19,21	1.68	3 (17%)
3	NAG	A	1302	1	14,14,15	0.38	0	17,19,21	0.69	0
3	NAG	A	1304	1	14,14,15	0.38	0	17,19,21	1.21	1 (5%)
3	NAG	A	1309	1	14,14,15	0.57	0	17,19,21	1.17	1 (5%)
3	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.71	0
3	NAG	B	1303	1	14,14,15	0.53	0	17,19,21	0.98	1 (5%)
3	NAG	A	1303	1	14,14,15	0.38	0	17,19,21	0.64	0
3	NAG	B	1309	1	14,14,15	0.37	0	17,19,21	1.76	4 (23%)
3	NAG	C	1303	1	14,14,15	0.78	0	17,19,21	2.99	7 (41%)
3	NAG	B	1302	1	14,14,15	0.75	0	17,19,21	1.22	4 (23%)
3	NAG	C	1305	1	14,14,15	0.53	0	17,19,21	0.87	0
3	NAG	A	1307	1	14,14,15	0.70	1 (7%)	17,19,21	1.74	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	5/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1307	NAG	C1-C2	2.20	1.55	1.52

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1303	NAG	C1-O5-C5	9.26	124.73	112.19
3	A	1306	NAG	C8-C7-N2	6.25	126.68	116.10
3	A	1306	NAG	C2-N2-C7	5.82	131.19	122.90
3	B	1308	NAG	C8-C7-N2	5.72	125.78	116.10
3	A	1307	NAG	O5-C1-C2	-5.02	103.36	111.29

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1304	NAG	C3-C2-N2-C7
3	A	1306	NAG	C1-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7
3	B	1308	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1306	NAG	1	0
3	B	1308	NAG	2	0
3	A	1308	NAG	1	0
3	B	1309	NAG	1	0
3	B	1302	NAG	3	0
3	C	1305	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

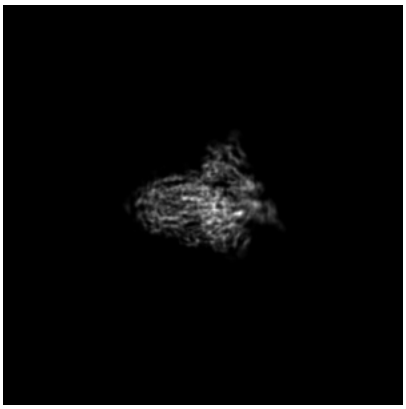
This section contains visualisations of the EMDB entry EMD-13919. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

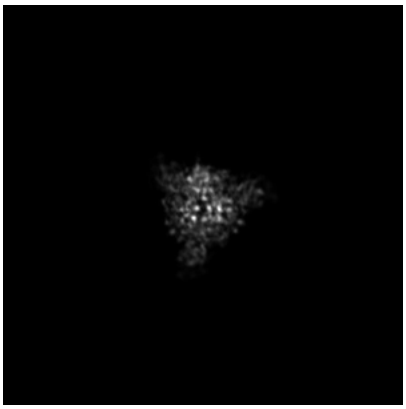
6.1 Orthogonal projections

6.1.1 Primary map

X

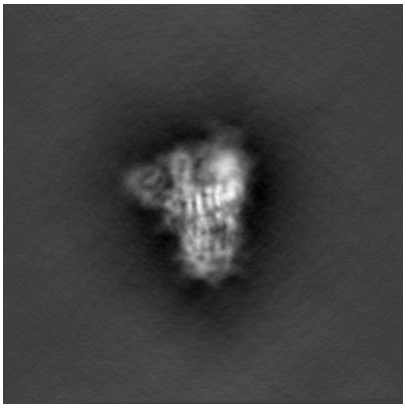


Y

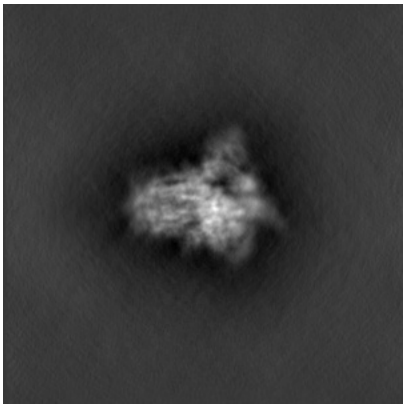


Z

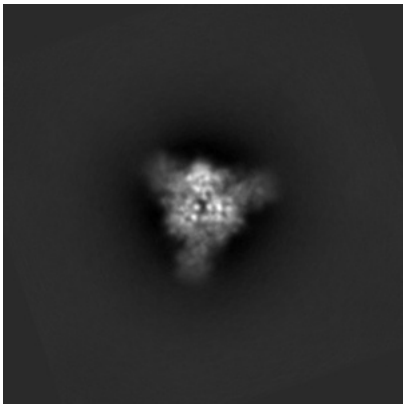
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

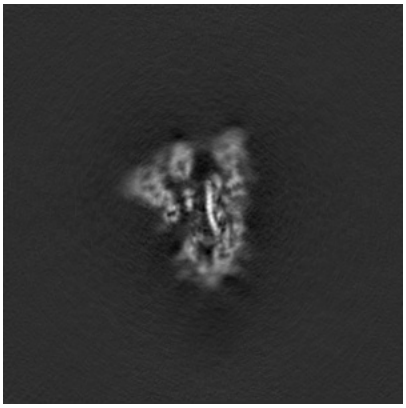
6.2.1 Primary map

X Index: 150

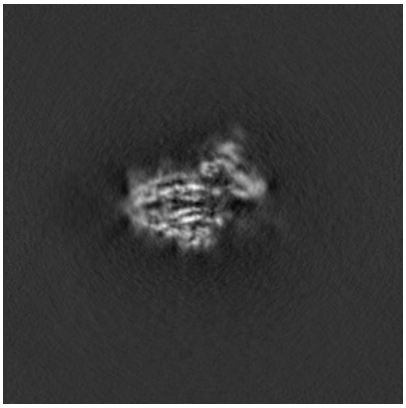
Y Index: 150

Z Index: 150

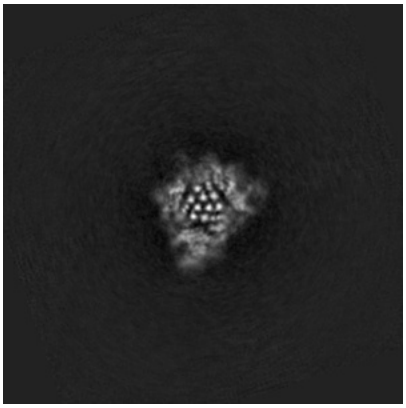
6.2.2 Raw map



X Index: 150



Y Index: 150



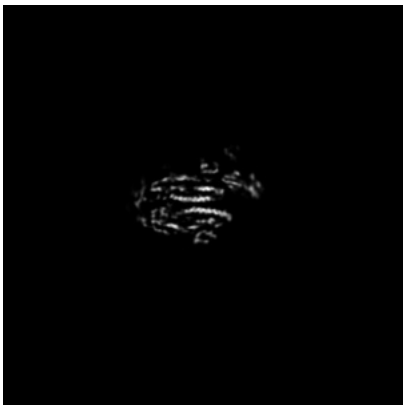
Z Index: 150

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

6.3 Largest variance slices (i)

6.3.1 Primary map

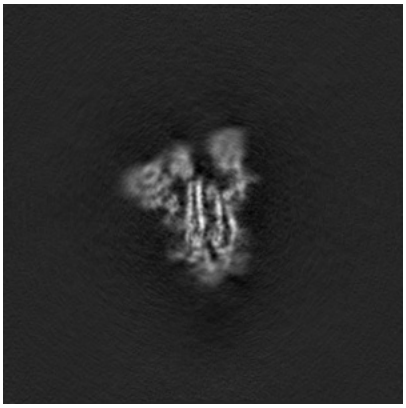
X Index: 151



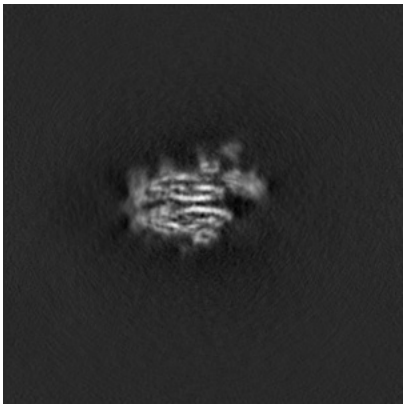
Y Index: 147

Z Index: 154

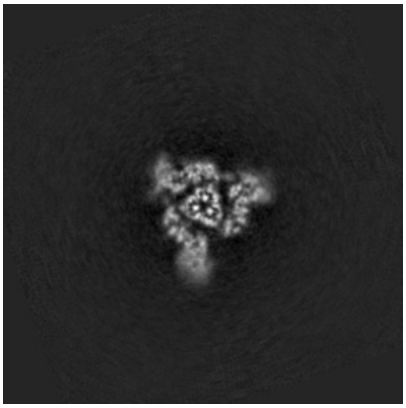
6.3.2 Raw map



X Index: 144



Y Index: 147

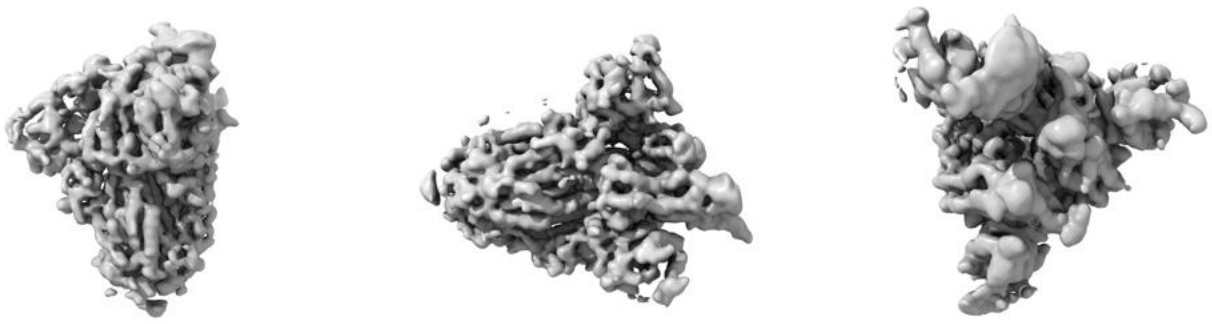


Z Index: 159

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

6.4 Orthogonal surface views (i)

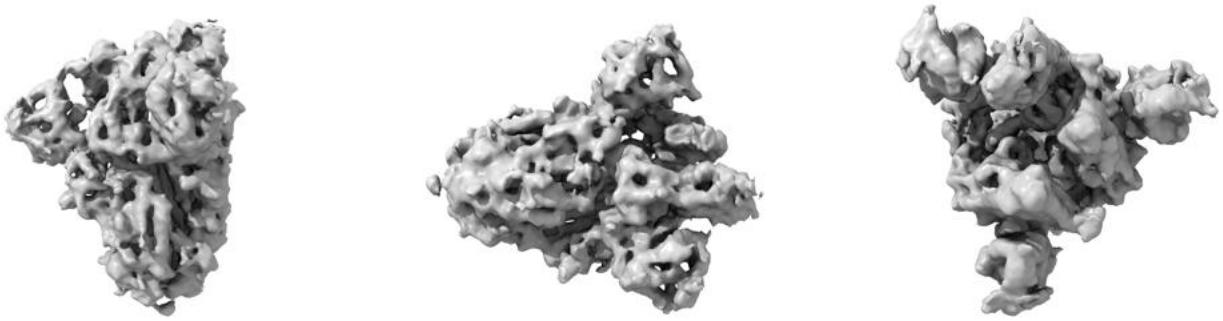
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.057. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

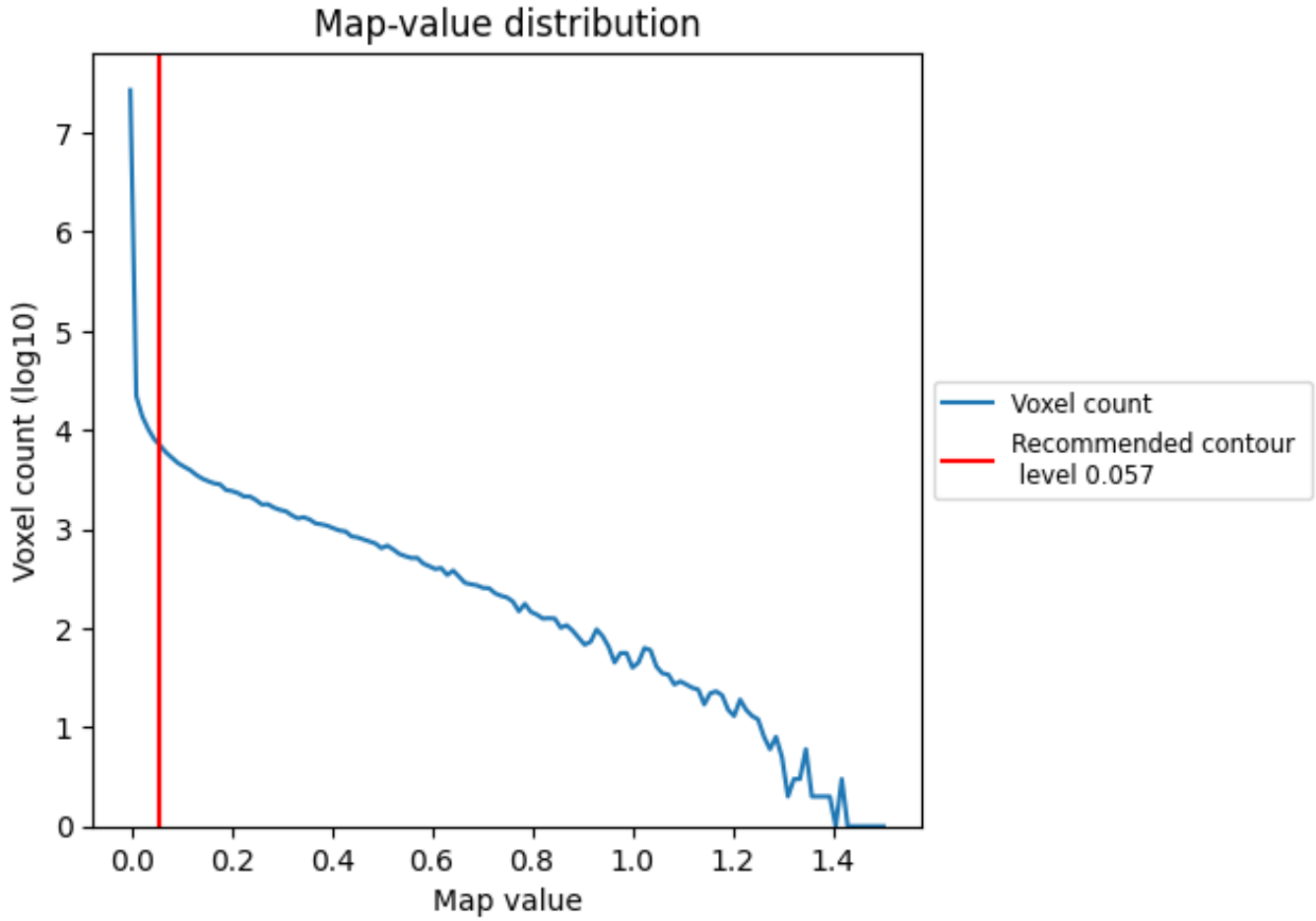
6.5 Mask visualisation (i)

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

7 Map analysis

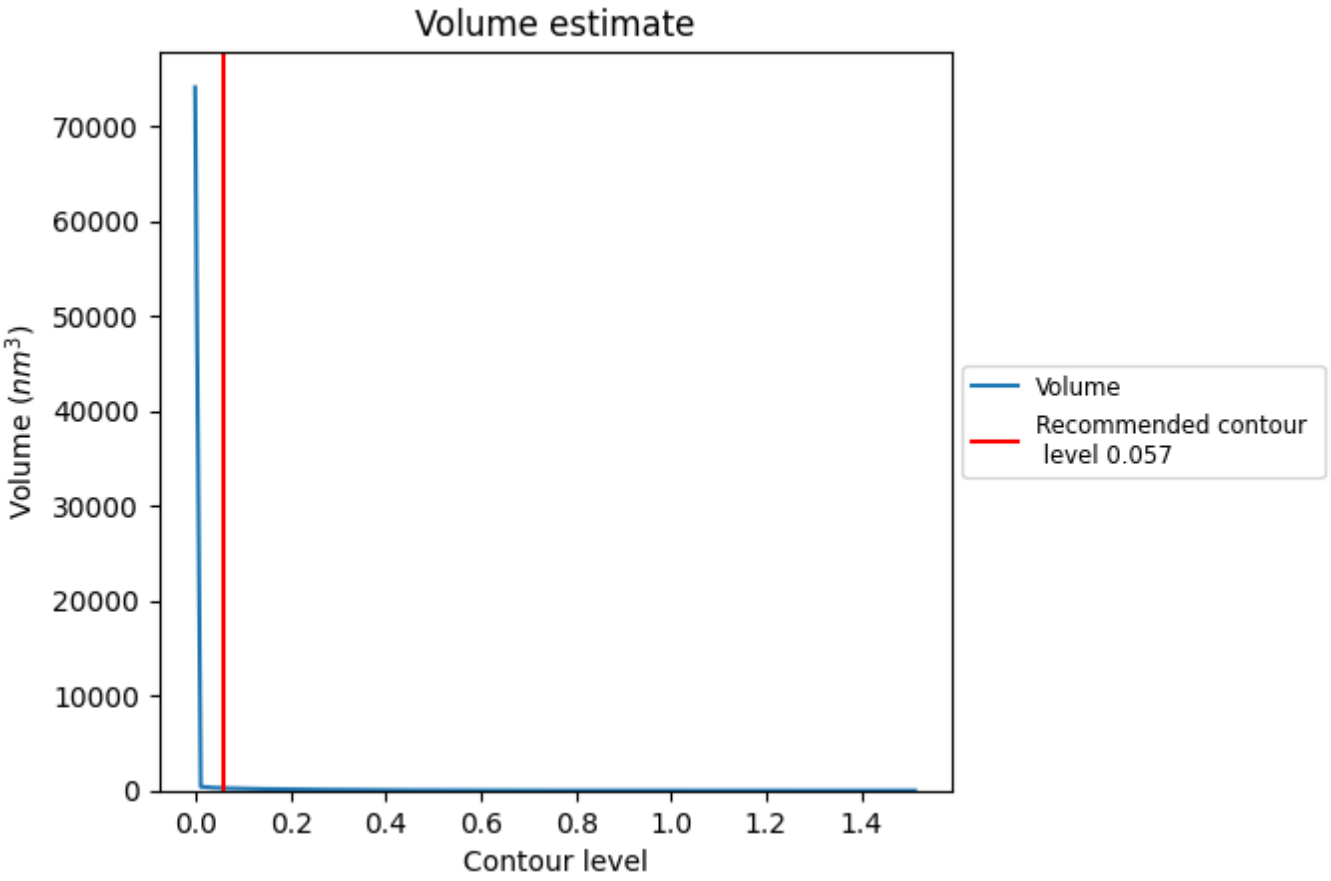
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

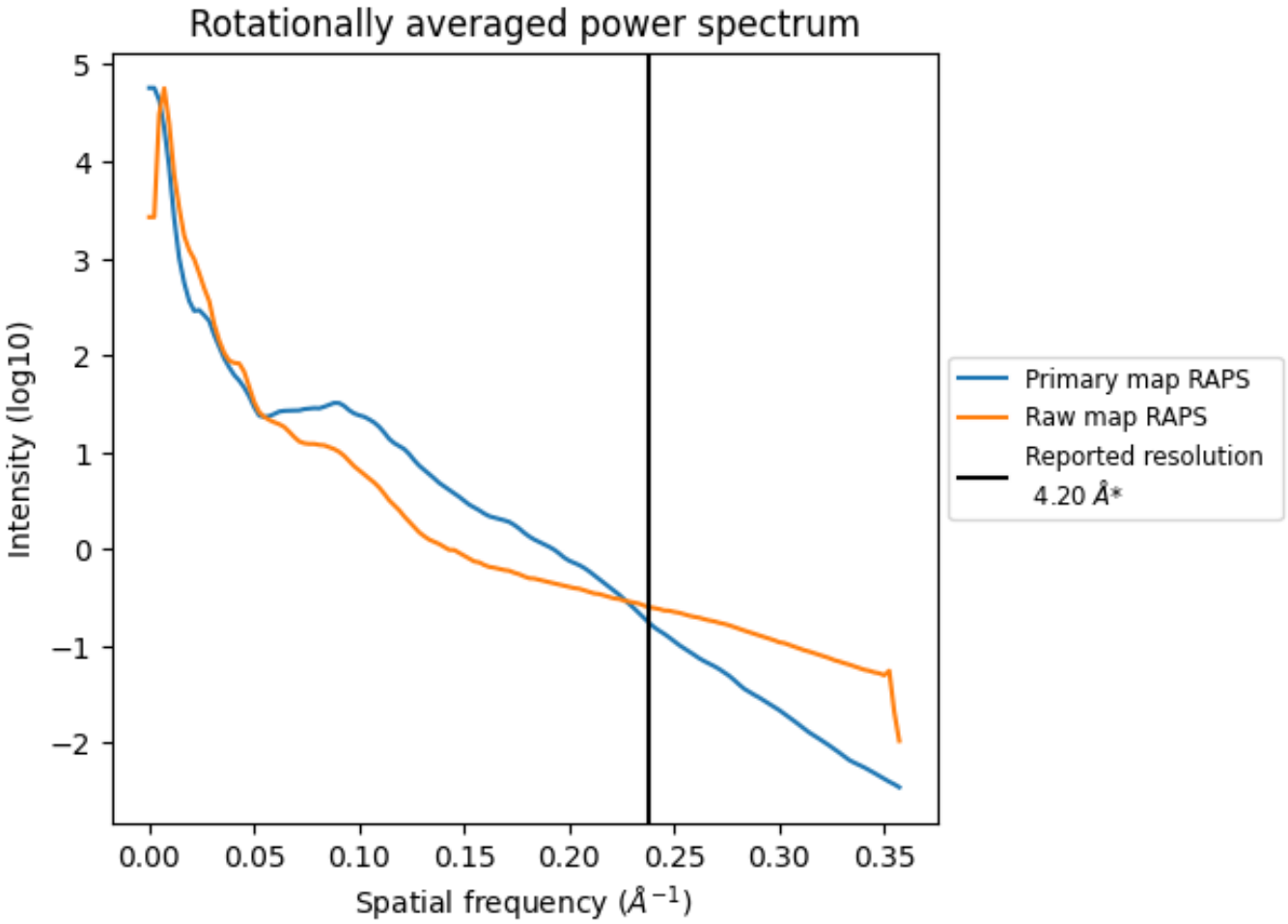
7.2 Volume estimate (i)



The volume at the recommended contour level is 263 nm^3; this corresponds to an approximate mass of 237 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

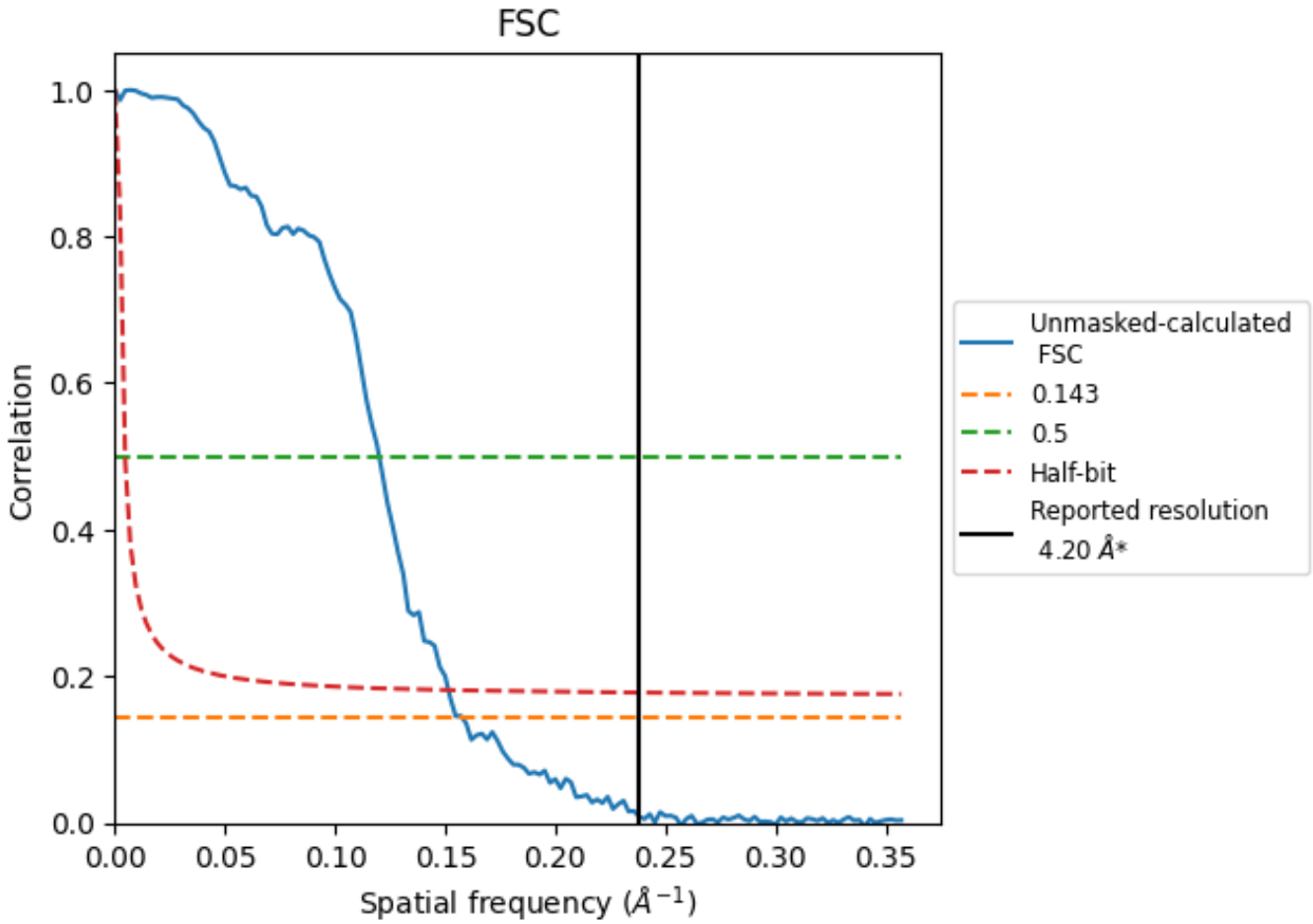


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

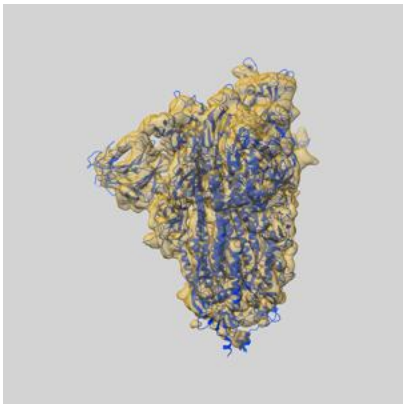
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.34	8.33	6.60

*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 6.34 differs from the reported value 4.2 by more than 10 %

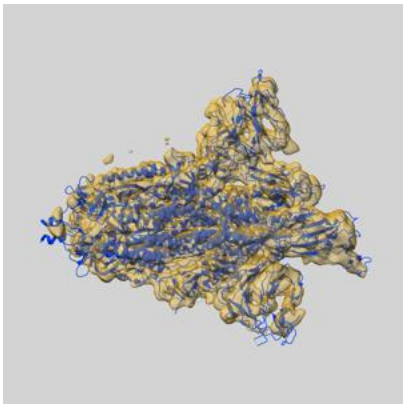
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13919 and PDB model 7QDH. Per-residue inclusion information can be found in section 3 on page 10.

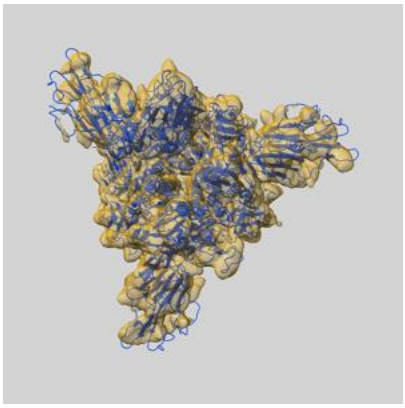
9.1 Map-model overlay



X



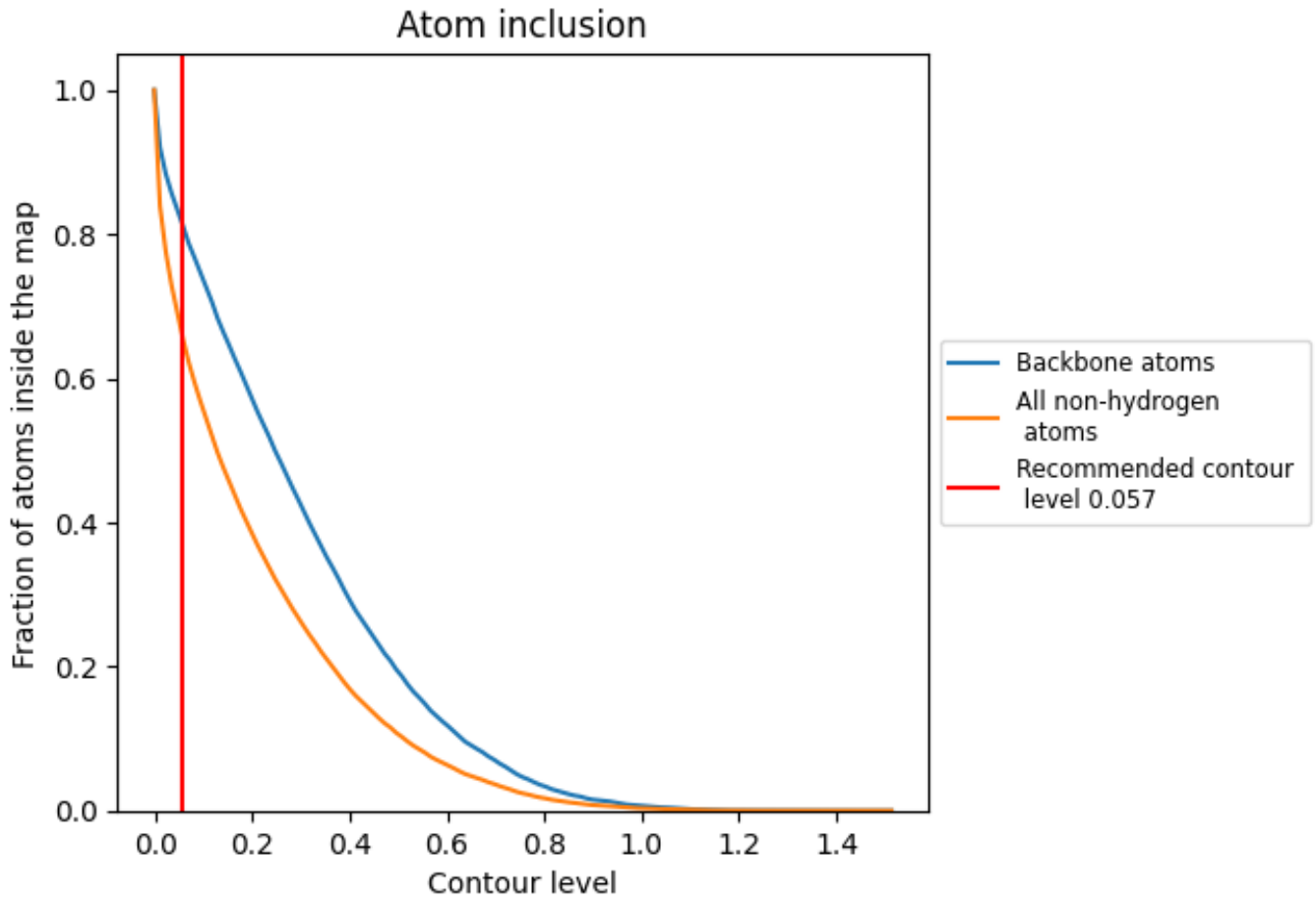
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.057 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 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.