



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:07 AM UTC

PDB ID : 7QDG / pdb_00007qdg
EMDB ID : EMD-13916
Title : SARS-CoV-2 S protein S:A222V + 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.; Gougéard, 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 : 3.40 Å(reported)
Based on initial model : 7BNN

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)

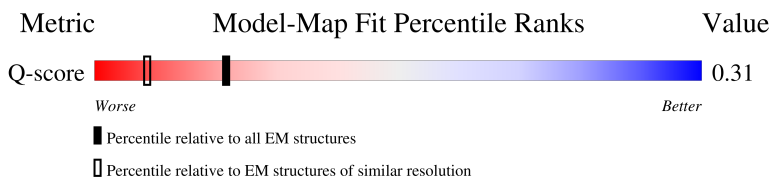
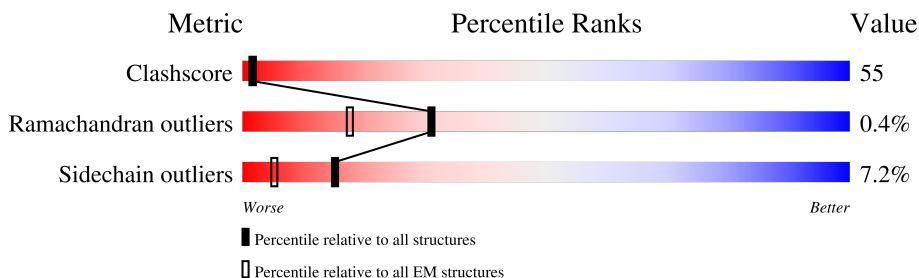
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1250	
1	B	1250	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	C	1250	
2	E	2	
2	G	2	
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
3	Q	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25570 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
			8356	5334	1392	1592	38		
1	B	1049	Total	C	N	O	S	0	0
			8191	5230	1365	1560	36		
1	C	1074	Total	C	N	O	S	0	0
			8365	5342	1393	1592	38		

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	VAL	ALA	conflict	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1259	GLN	-	expression tag	UNP P10104
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	222	VAL	ALA	conflict	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	222	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
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		
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	G	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	I	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 an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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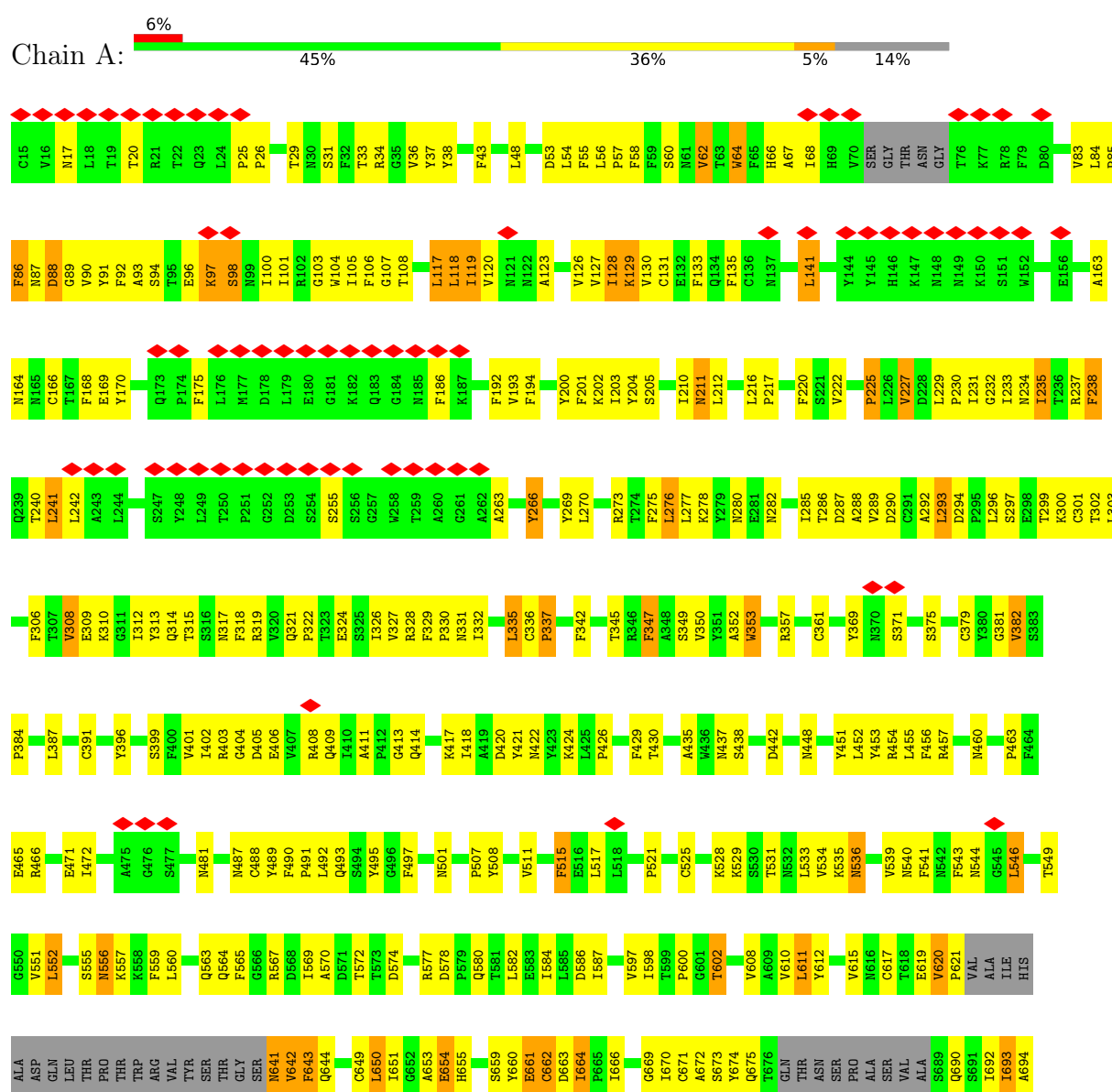
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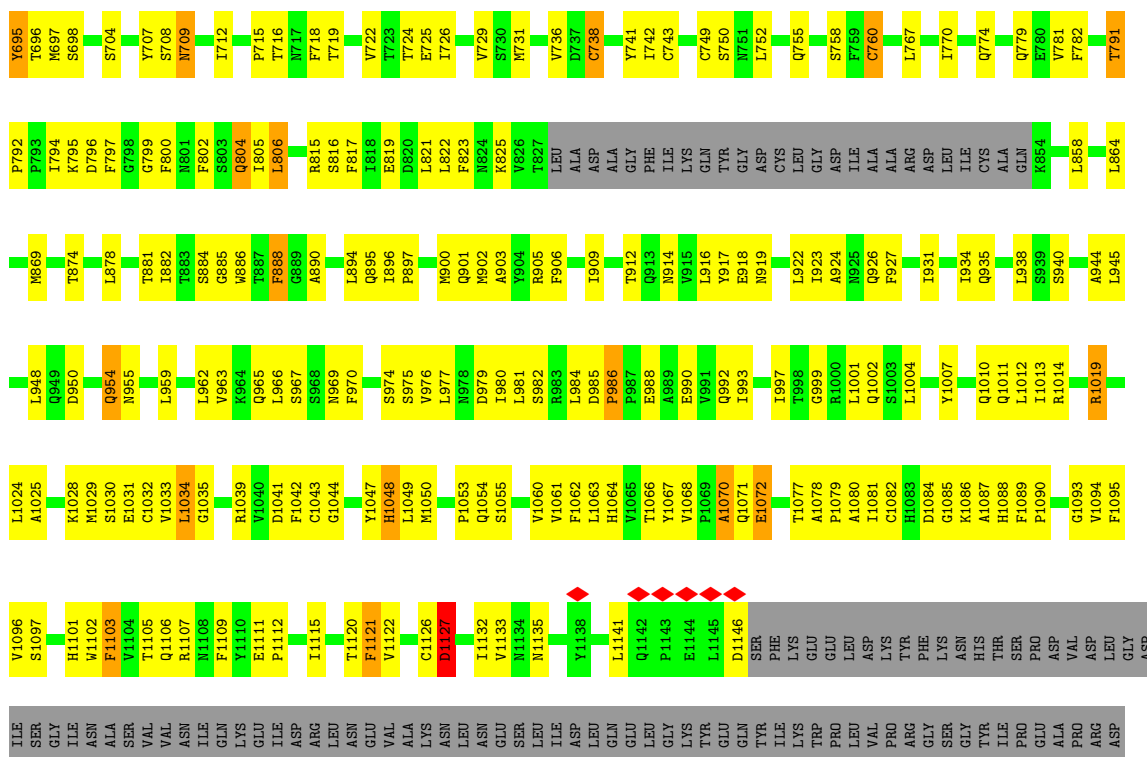
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C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

3 Residue-property plots

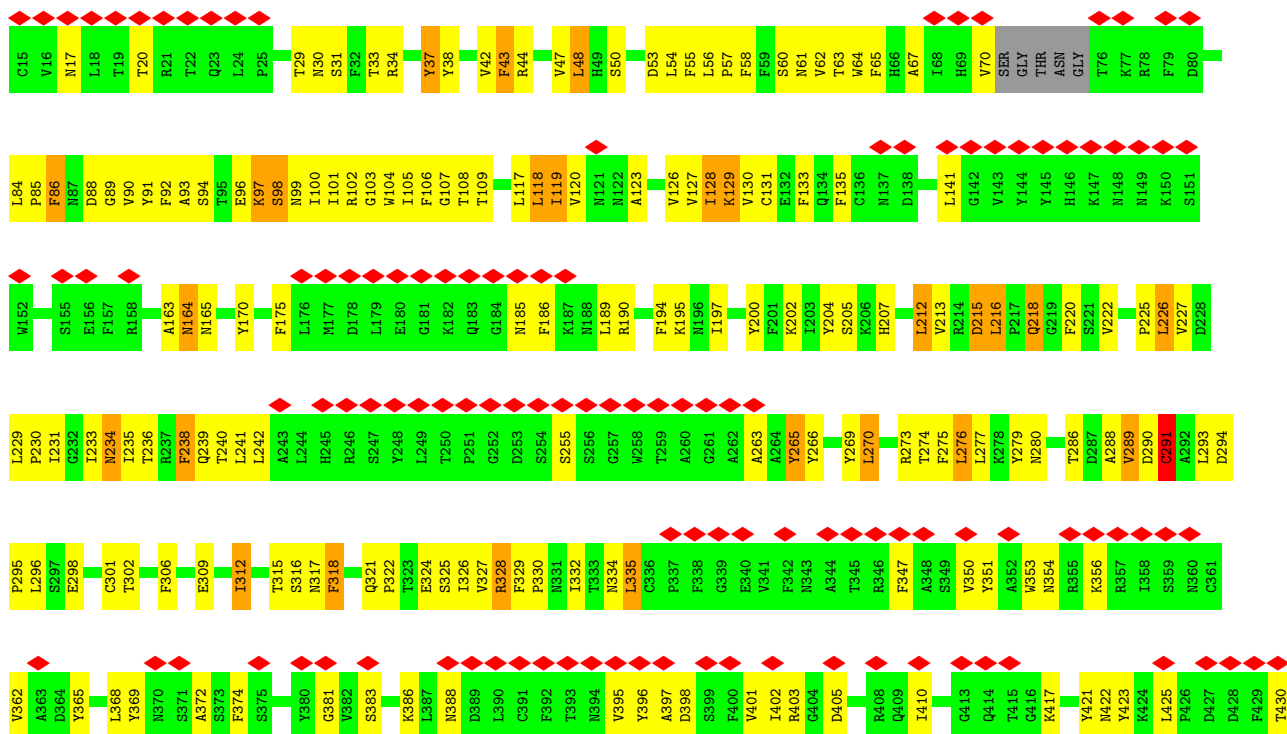
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

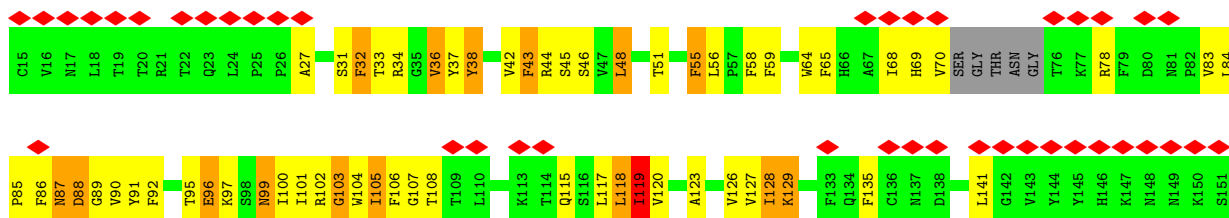
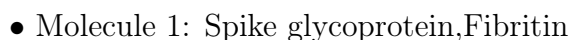
• Molecule 1: Spike glycoprotein,Fibritin





• Molecule 1: Spike glycoprotein,Fibrin







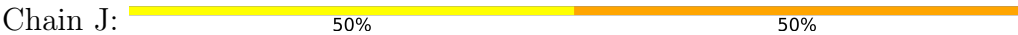
ASP GLY GLU TRP VAL PHE LEU SER THR PHE LEU SER PRO HIS HIS HIS HIS HIS HIS HIS GLN LYS LEU ILE SER SER GLU GLU ASP LEU

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



NAG1
NAG2

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



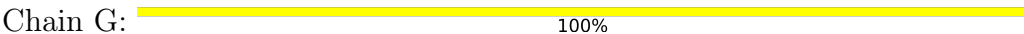
NAG1
NAG2

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



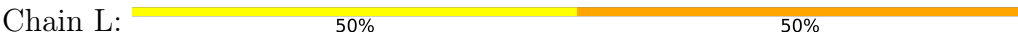
NAG1
NAG2

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



NAG1
NAG2

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



NAG1
NAG2

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



NAG1
NAG2

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



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



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



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



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145681	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 ($e^-/\text{\AA}^2$)	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	1.176	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.048	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.70	6/8552 (0.1%)	0.97	25/11644 (0.2%)
1	B	0.70	9/8379 (0.1%)	0.95	33/11404 (0.3%)
1	C	0.77	10/8561 (0.1%)	0.99	36/11658 (0.3%)
All	All	0.72	25/25492 (0.1%)	0.97	94/34706 (0.3%)

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1146	ASP	C-O	-20.25	0.83	1.23
1	B	1146	ASP	C-O	-13.24	0.97	1.23
1	C	165	ASN	CA-C	9.98	1.63	1.53
1	A	940	SER	C-O	-9.83	1.12	1.24
1	C	129	LYS	N-CA	-8.18	1.35	1.46

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	526	GLY	CA-C-N	9.76	130.02	119.87
1	C	526	GLY	C-N-CA	9.76	130.02	119.87
1	A	791	THR	CA-C-N	8.93	126.18	119.66
1	A	791	THR	C-N-CA	8.93	126.18	119.66
1	C	208	THR	CA-C-N	8.61	128.60	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8356	0	8129	945	0
1	B	8191	0	7974	752	0
1	C	8365	0	8121	1123	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	4	0
2	K	28	0	25	4	0
2	L	28	0	25	1	0
2	M	28	0	25	1	0
2	N	28	0	25	0	0
2	O	28	0	25	3	0
2	P	28	0	25	2	0
3	Q	28	0	24	2	0
4	A	140	0	129	6	0
4	B	112	0	103	1	0
4	C	98	0	91	2	0
All	All	25570	0	24821	2751	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 55.

The worst 5 of 2751 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:118:LEU:HD22	1:C:135:PHE:CZ	1.27	1.67
1:A:87:ASN:ND2	1:A:269:TYR:CD2	1.69	1.55
1:A:33:THR:HG22	1:A:58:PHE:CD2	1.47	1.49
1:B:718:PHE:HB2	1:B:1067:TYR:CE1	1.46	1.49
1:B:1104:VAL:CG1	1:B:1119:ASN:HD21	1.27	1.48

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	1060/1250 (85%)	1001 (94%)	52 (5%)	7 (1%)	18	47
1	B	1035/1250 (83%)	986 (95%)	45 (4%)	4 (0%)	30	59
1	C	1064/1250 (85%)	1015 (95%)	48 (4%)	1 (0%)	48	78
All	All	3159/3750 (84%)	3002 (95%)	145 (5%)	12 (0%)	31	59

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	620	VAL
1	B	946	GLY
1	A	347	PHE
1	A	501	ASN
1	A	643	PHE

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	933/1090 (86%)	878 (94%)	55 (6%)	18	44
1	B	915/1090 (84%)	859 (94%)	56 (6%)	17	43
1	C	929/1090 (85%)	841 (90%)	88 (10%)	8	29
All	All	2777/3270 (85%)	2578 (93%)	199 (7%)	15	39

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	51	THR
1	C	365	TYR
1	C	96	GLU
1	C	223	LEU
1	C	445	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	207	HIS
1	C	690	GLN
1	C	343	ASN
1	C	493	GLN
1	C	824	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](#)

22 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	1,2	14,14,15	0.96	1 (7%)	17,19,21	2.37	4 (23%)
2	NAG	E	2	2	14,14,15	0.78	0	17,19,21	1.13	2 (11%)
2	NAG	G	1	1,2	14,14,15	1.06	2 (14%)	17,19,21	1.94	5 (29%)
2	NAG	G	2	2	14,14,15	0.73	1 (7%)	17,19,21	1.09	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	1	1,2	14,14,15	1.14	2 (14%)	17,19,21	2.28	5 (29%)
2	NAG	I	2	2	14,14,15	0.90	1 (7%)	17,19,21	1.72	3 (17%)
2	NAG	J	1	1,2	14,14,15	0.74	0	17,19,21	1.10	2 (11%)
2	NAG	J	2	2	14,14,15	0.77	1 (7%)	17,19,21	1.73	4 (23%)
2	NAG	K	1	1,2	14,14,15	0.66	0	17,19,21	1.34	2 (11%)
2	NAG	K	2	2	14,14,15	0.91	0	17,19,21	1.83	4 (23%)
2	NAG	L	1	1,2	14,14,15	0.69	0	17,19,21	1.27	1 (5%)
2	NAG	L	2	2	14,14,15	0.72	1 (7%)	17,19,21	1.58	3 (17%)
2	NAG	M	1	1,2	14,14,15	0.61	0	17,19,21	1.27	2 (11%)
2	NAG	M	2	2	14,14,15	0.29	0	17,19,21	0.60	0
2	NAG	N	1	1,2	14,14,15	1.26	2 (14%)	17,19,21	2.19	6 (35%)
2	NAG	N	2	2	14,14,15	0.24	0	17,19,21	0.79	0
2	NAG	O	1	1,2	14,14,15	2.13	4 (28%)	17,19,21	3.94	8 (47%)
2	NAG	O	2	2	14,14,15	0.86	1 (7%)	17,19,21	1.71	4 (23%)
2	NAG	P	1	1,2	14,14,15	1.12	1 (7%)	17,19,21	2.30	6 (35%)
2	NAG	P	2	2	14,14,15	0.95	0	17,19,21	1.70	2 (11%)
3	NDG	Q	1	3	14,14,15	1.19	2 (14%)	17,19,21	2.18	6 (35%)
3	NAG	Q	2	3	14,14,15	0.91	2 (14%)	17,19,21	1.88	4 (23%)

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

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

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1	NAG	C2-N2	-5.96	1.36	1.46
2	N	1	NAG	C2-N2	-3.35	1.40	1.46
2	N	1	NAG	C8-C7	-2.87	1.44	1.50
2	I	2	NAG	C8-C7	-2.86	1.44	1.50
3	Q	1	NDG	C2-N2	-2.61	1.41	1.46

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	NAG	O7-C7-N2	10.01	139.67	121.98
2	E	1	NAG	C1-O5-C5	-7.94	101.54	112.19
2	O	1	NAG	C8-C7-N2	-7.01	104.50	116.12
2	O	1	NAG	C1-O5-C5	6.37	120.72	112.19
2	N	1	NAG	C8-C7-N2	-6.21	105.83	116.12

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

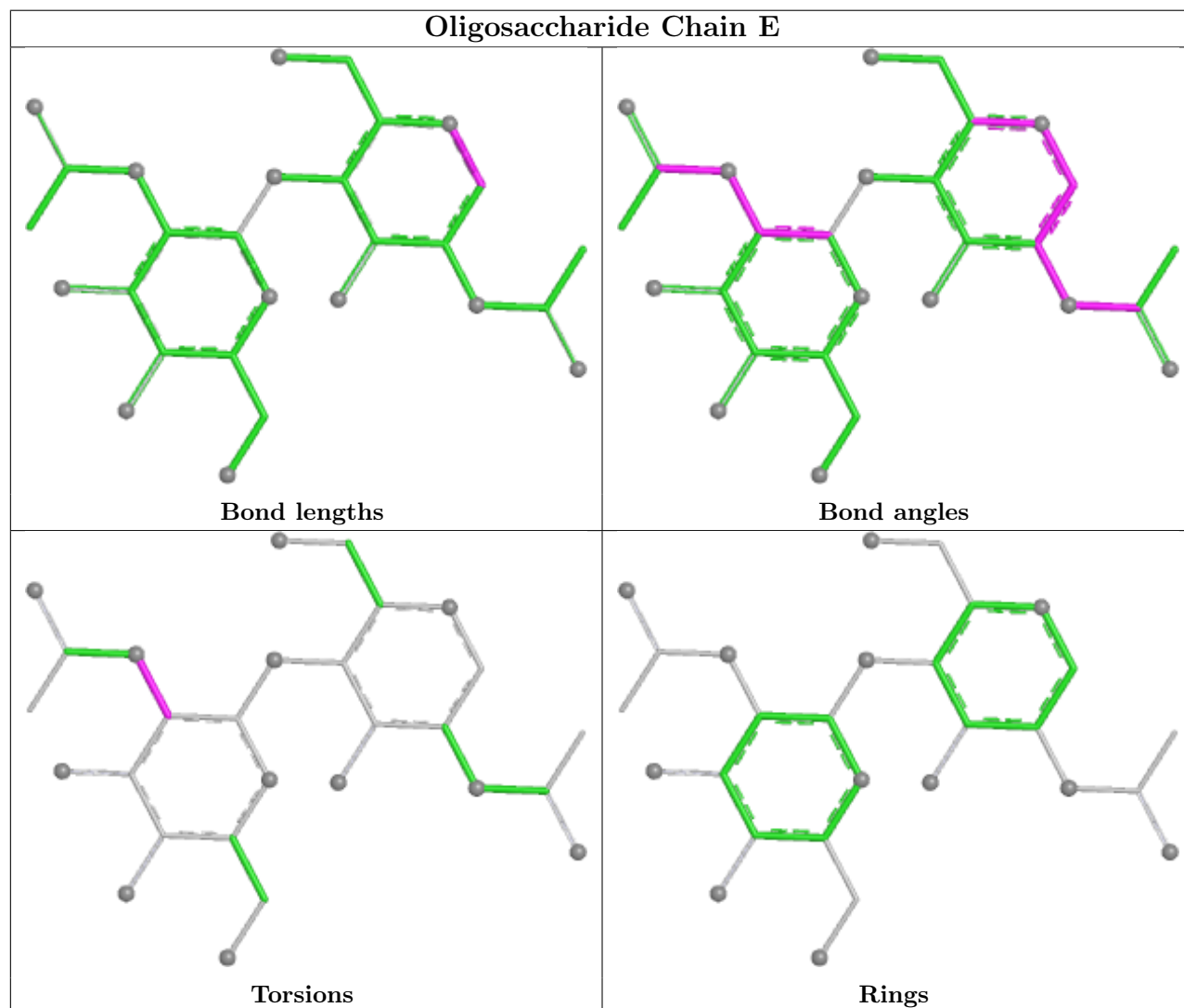
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C1-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C1-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7

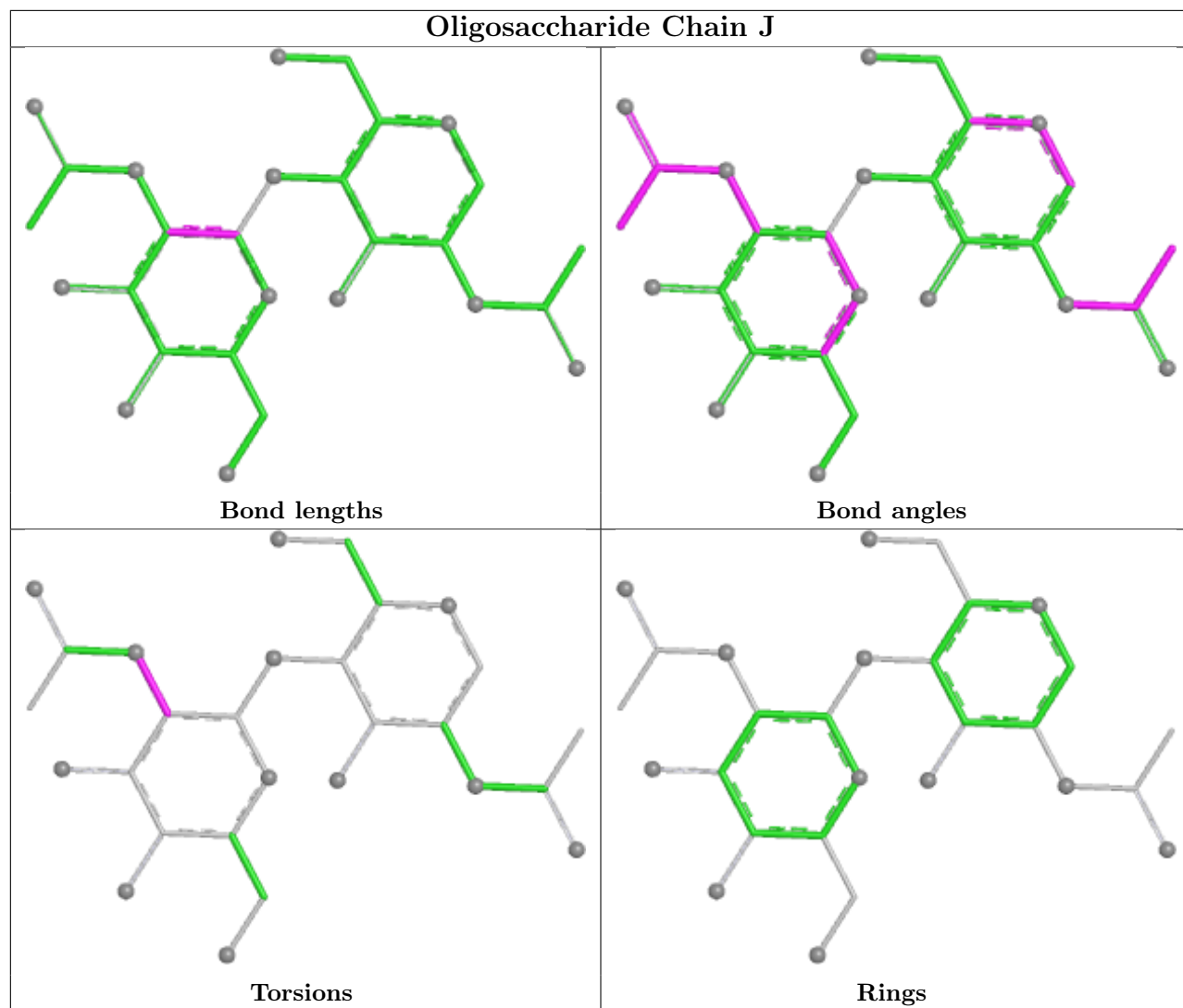
There are no ring outliers.

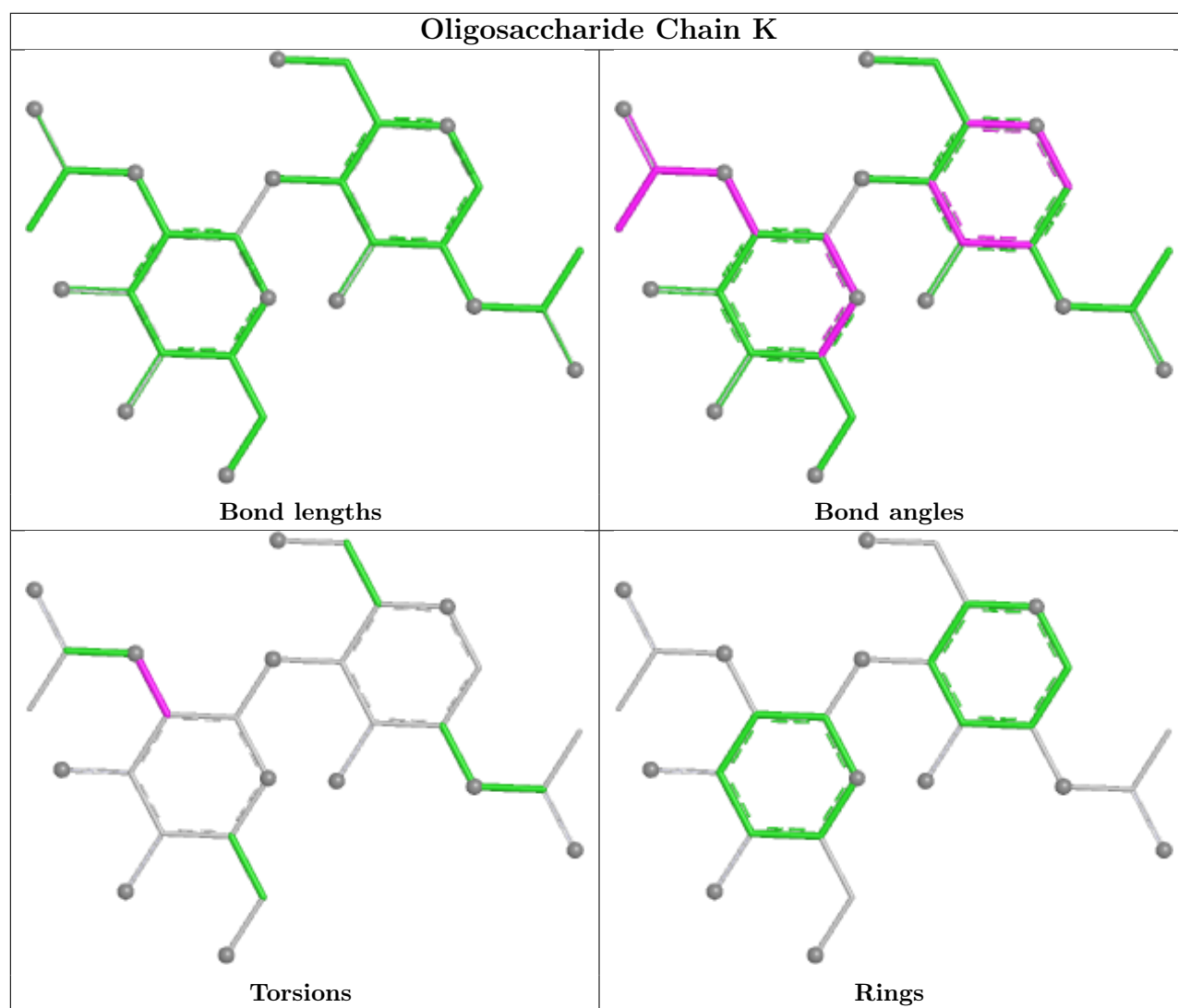
10 monomers are involved in 18 short contacts:

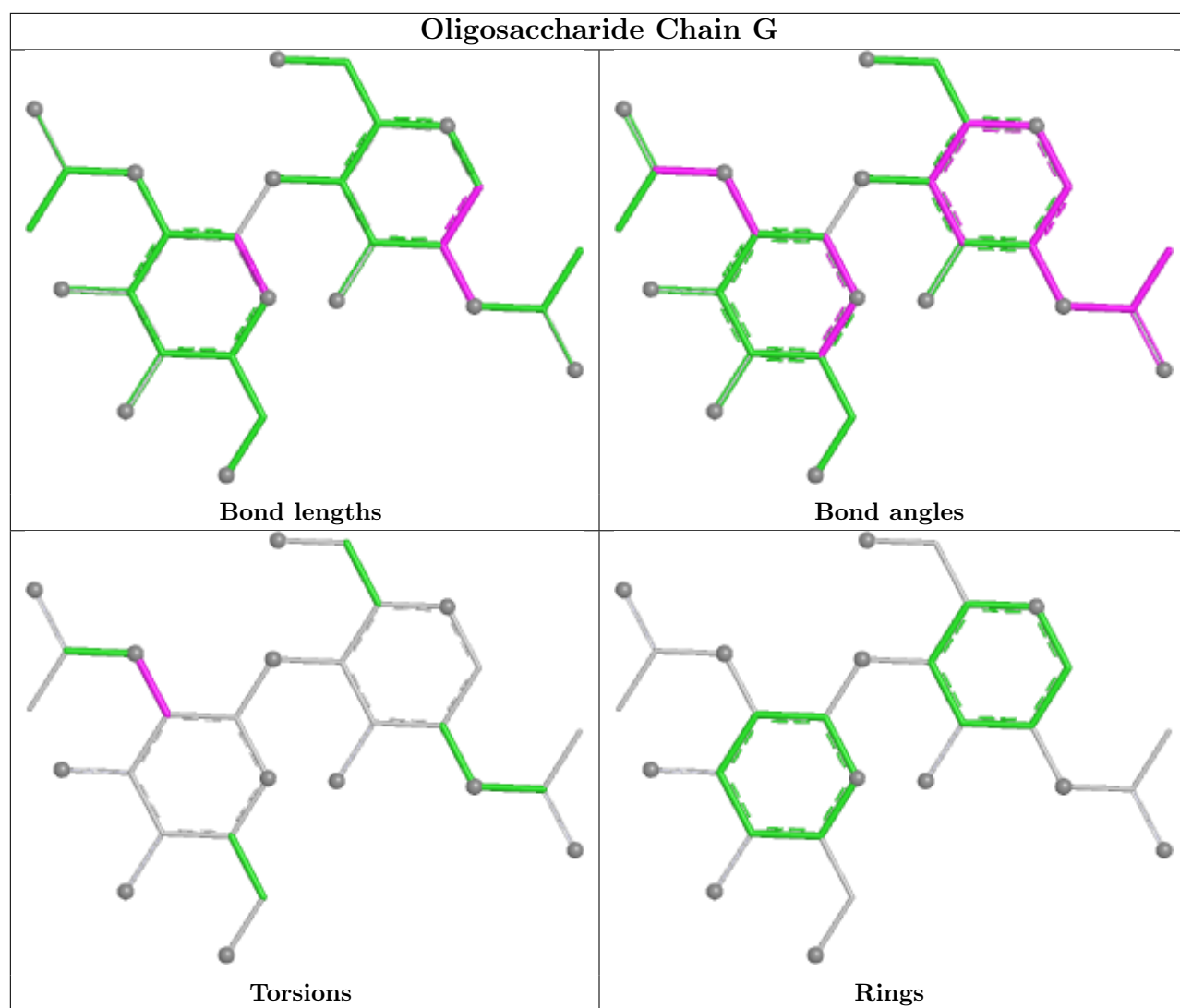
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	2	NAG	2	0
2	K	1	NAG	3	0
2	P	1	NAG	2	0
2	J	2	NAG	4	0
2	K	2	NAG	1	0
3	Q	1	NDG	2	0
2	L	2	NAG	1	0
2	M	1	NAG	1	0
2	O	1	NAG	1	0
2	I	2	NAG	1	0

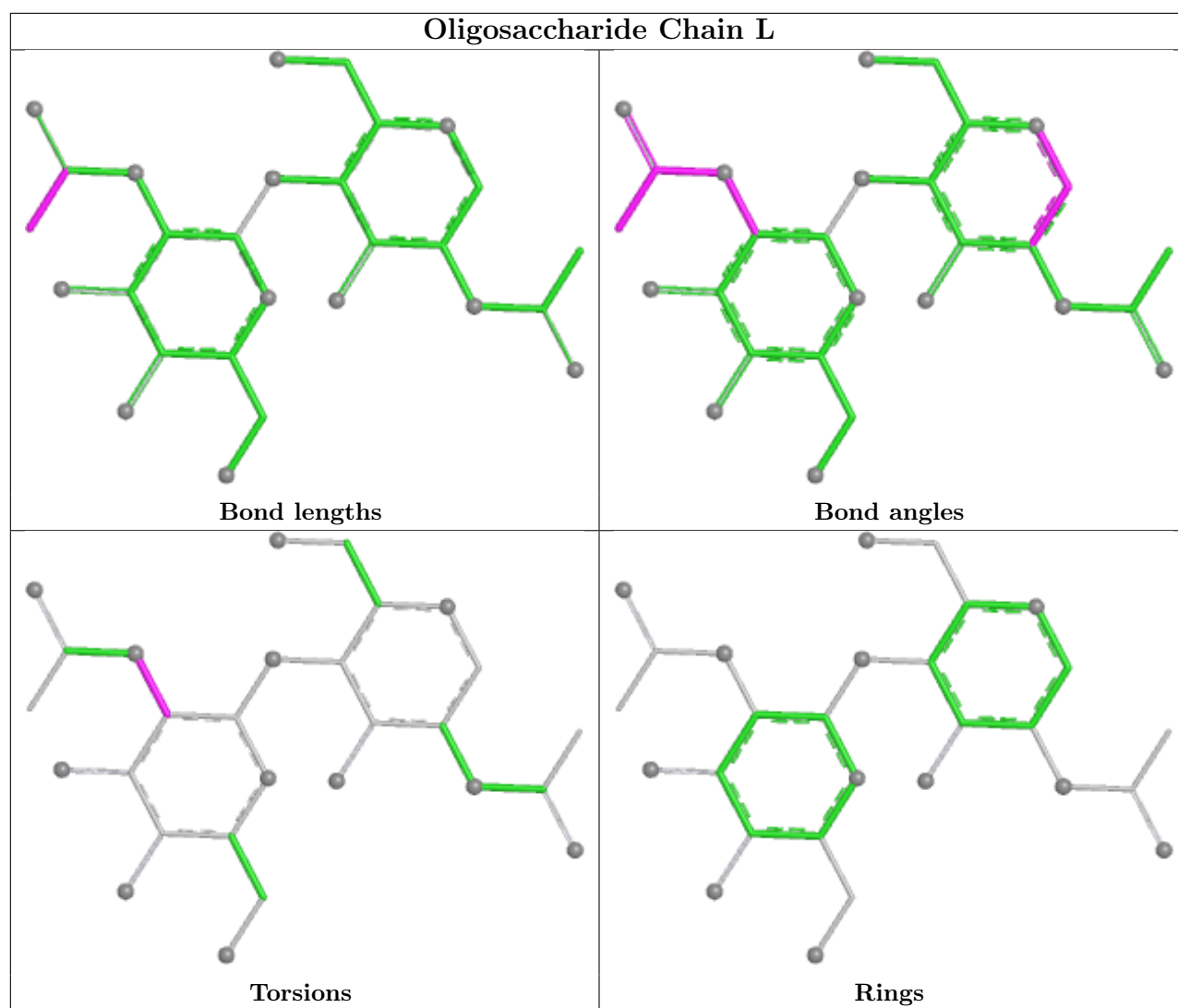
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

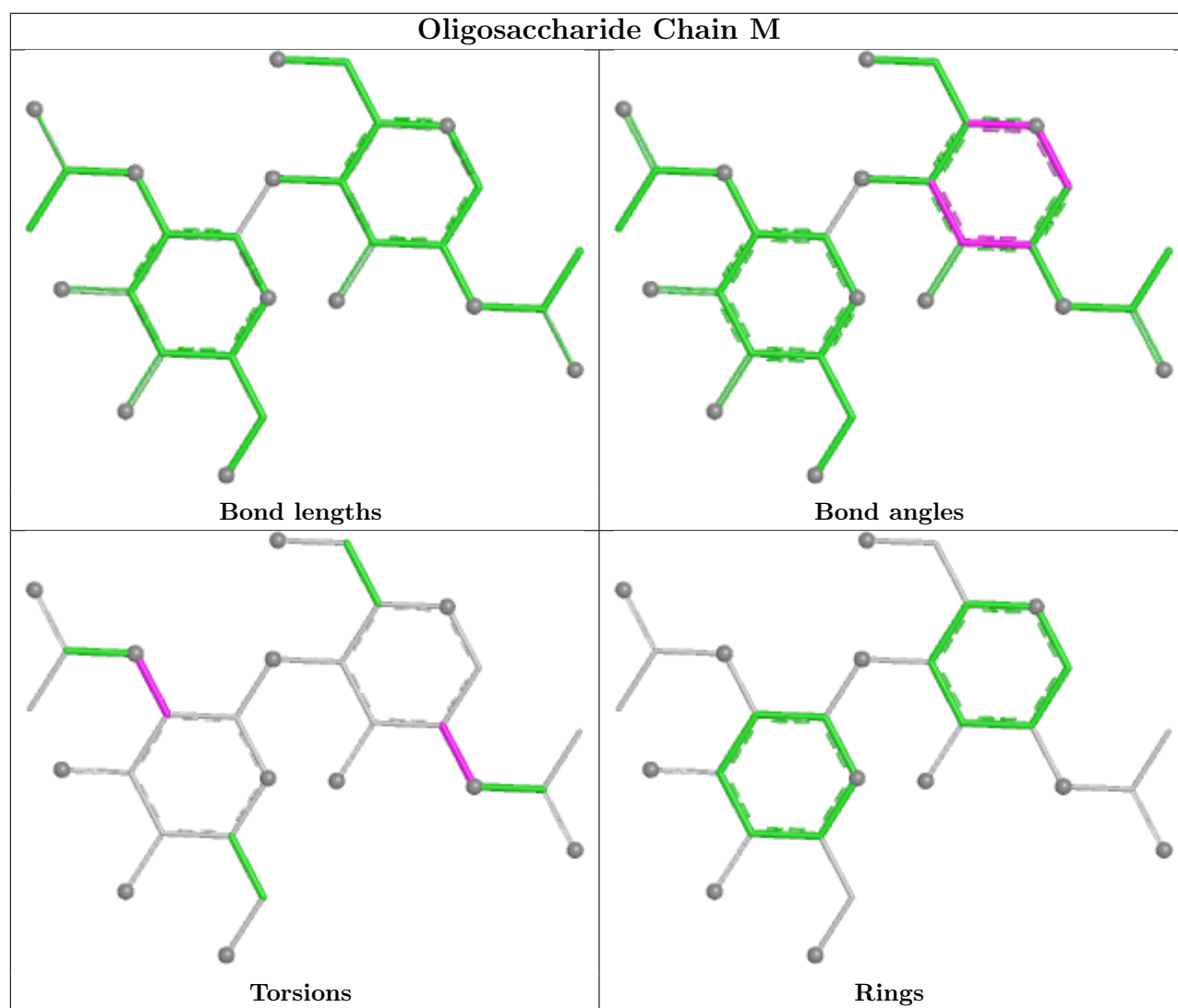


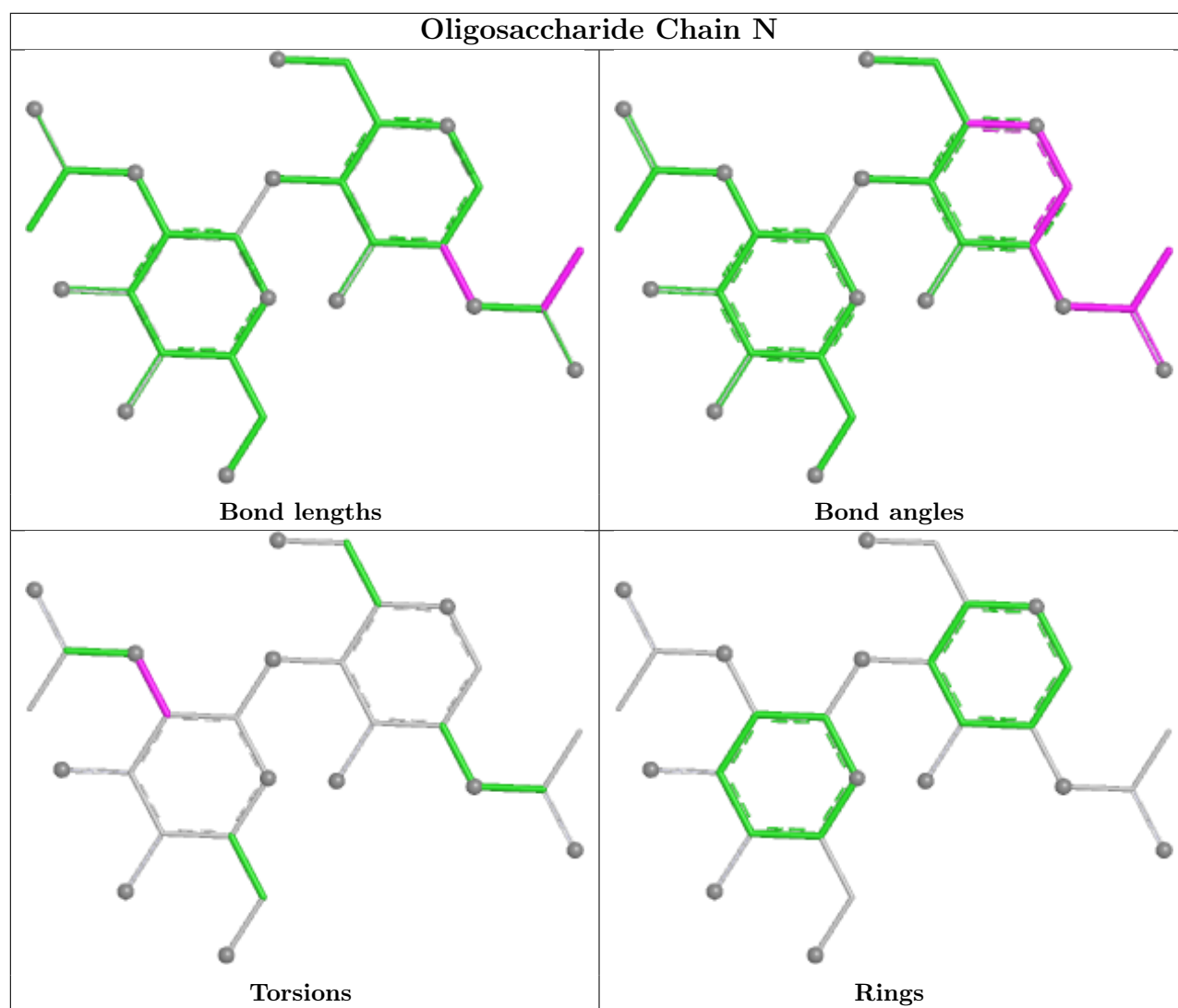


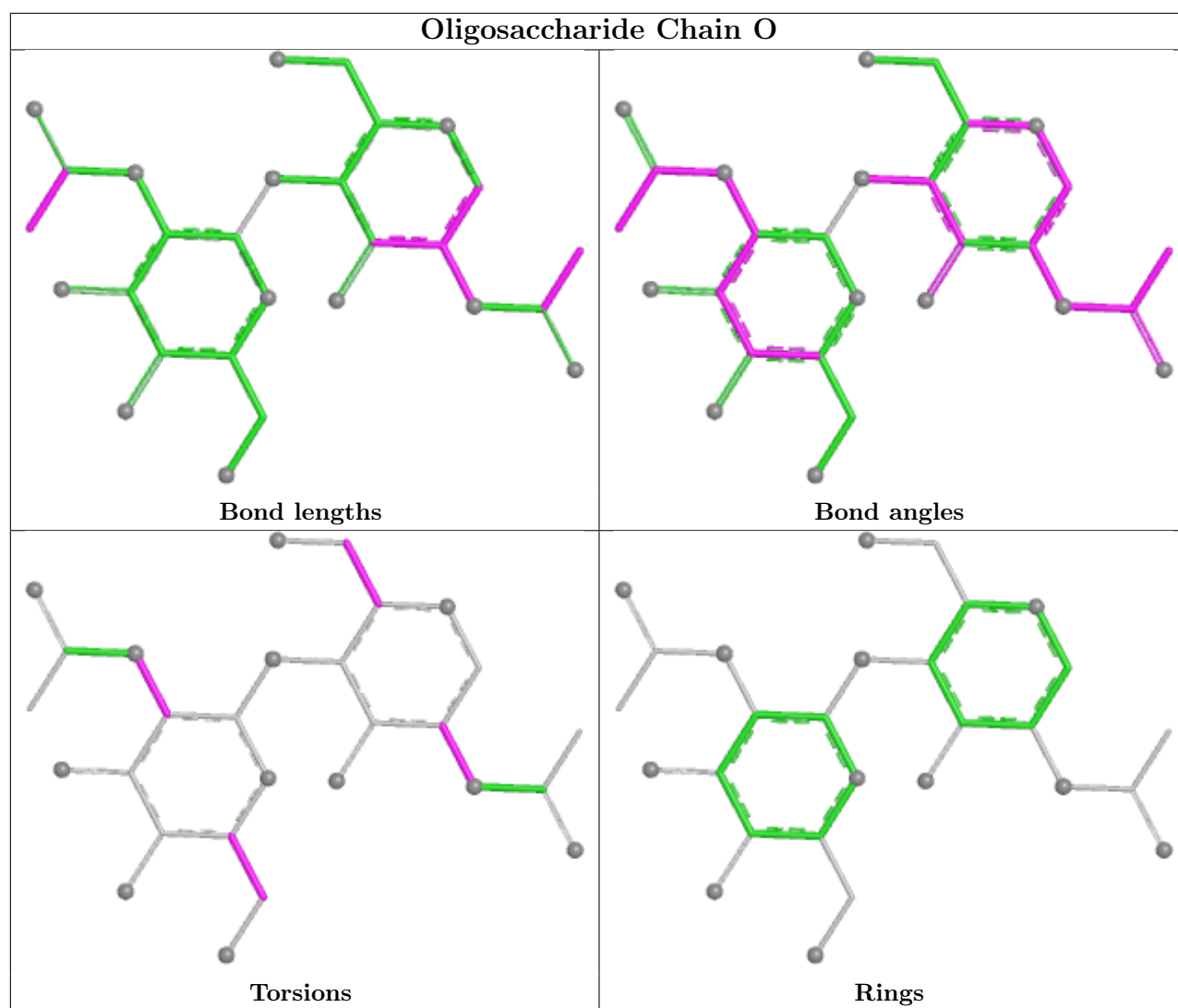


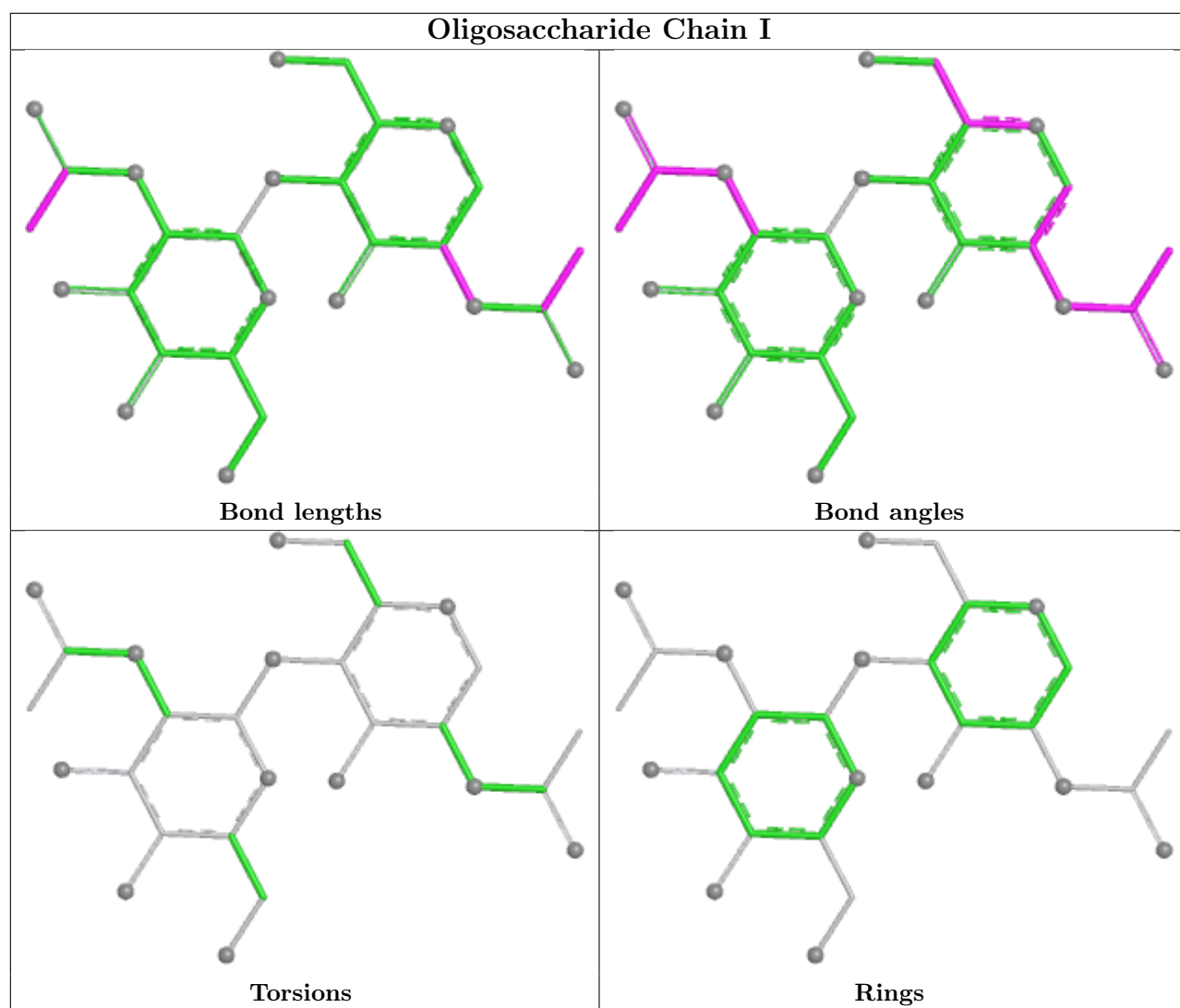


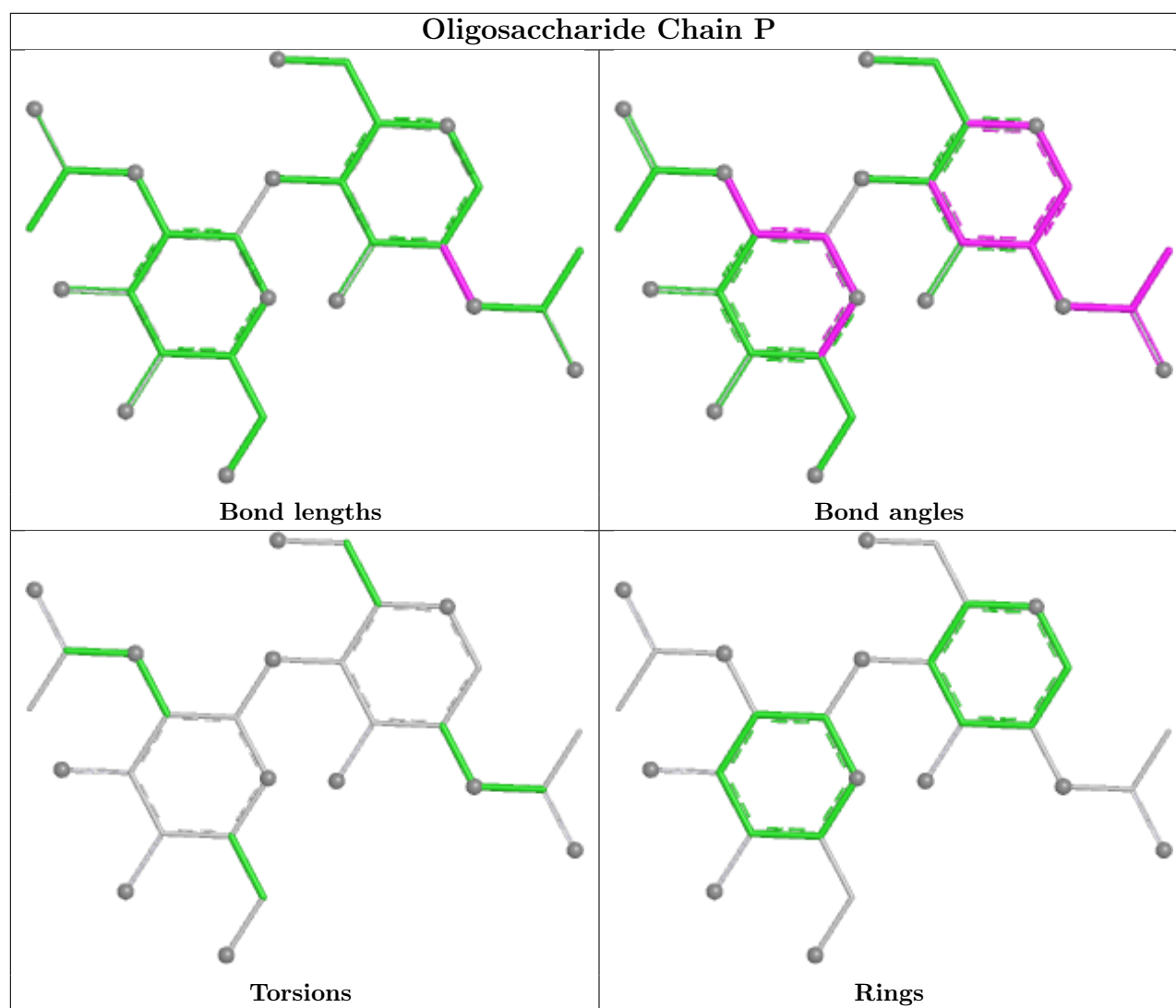


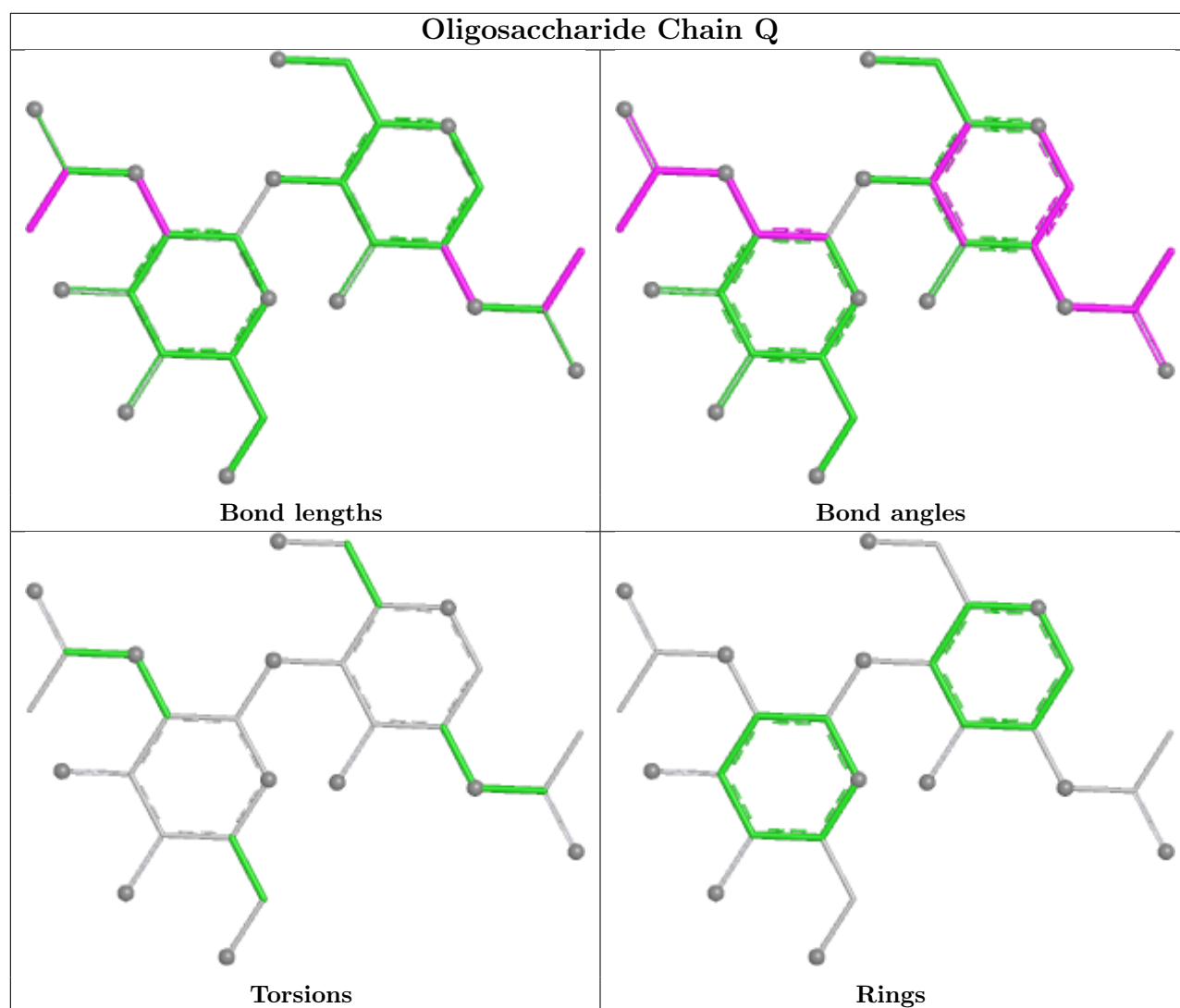












5.6 Ligand geometry [i](#)

25 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	$\# Z > 2$
4	NAG	B	1307	1	14,14,15	1.00	0	17,19,21	4.55	5 (29%)
4	NAG	B	1308	1	14,14,15	1.33	3 (21%)	17,19,21	3.52	5 (29%)
4	NAG	B	1305	1	14,14,15	0.85	0	17,19,21	3.96	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1304	1	14,14,15	0.66	0	17,19,21	1.97	3 (17%)
4	NAG	B	1306	1	14,14,15	0.81	0	17,19,21	1.83	2 (11%)
4	NAG	A	1303	1	14,14,15	0.49	0	17,19,21	0.62	0
4	NAG	A	1306	1	14,14,15	1.09	1 (7%)	17,19,21	1.57	3 (17%)
4	NAG	A	1301	1	14,14,15	1.15	0	17,19,21	4.36	9 (52%)
4	NAG	C	1303	1	14,14,15	0.85	1 (7%)	17,19,21	1.57	2 (11%)
4	NAG	A	1308	1	14,14,15	0.69	1 (7%)	17,19,21	1.25	3 (17%)
4	NAG	C	1302	1	14,14,15	0.80	0	17,19,21	3.77	8 (47%)
4	NAG	C	1305	1	14,14,15	0.61	0	17,19,21	0.88	1 (5%)
4	NAG	B	1304	1	14,14,15	0.83	0	17,19,21	3.61	7 (41%)
4	NAG	B	1303	1	14,14,15	0.44	0	17,19,21	0.88	1 (5%)
4	NAG	A	1310	1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
4	NAG	B	1301	1	14,14,15	0.53	0	17,19,21	1.02	0
4	NAG	B	1302	1	14,14,15	0.33	0	17,19,21	1.28	1 (5%)
4	NAG	C	1307	1	14,14,15	0.53	0	17,19,21	2.49	7 (41%)
4	NAG	A	1307	1	14,14,15	1.18	1 (7%)	17,19,21	3.68	7 (41%)
4	NAG	A	1305	1	14,14,15	0.46	0	17,19,21	1.29	2 (11%)
4	NAG	C	1301	-	14,14,15	0.77	0	17,19,21	1.02	1 (5%)
4	NAG	C	1304	1	14,14,15	0.64	0	17,19,21	1.55	2 (11%)
4	NAG	A	1302	1	14,14,15	0.83	0	17,19,21	3.55	8 (47%)
4	NAG	C	1306	1	14,14,15	0.61	0	17,19,21	3.28	5 (29%)
4	NAG	A	1309	1	14,14,15	1.49	3 (21%)	17,19,21	5.39	7 (41%)

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	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1309	NAG	O5-C1	-3.63	1.37	1.43
4	B	1308	NAG	C2-N2	-3.57	1.40	1.46
4	A	1307	NAG	O7-C7	-3.35	1.15	1.23
4	A	1306	NAG	O5-C1	-3.18	1.38	1.43
4	C	1303	NAG	C1-C2	2.85	1.56	1.52

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1309	NAG	C2-N2-C7	15.02	143.03	122.90
4	A	1301	NAG	C8-C7-N2	-11.75	96.64	116.12
4	C	1306	NAG	C1-O5-C5	11.74	127.92	112.19
4	B	1307	NAG	C8-C7-N2	-11.70	96.71	116.12
4	B	1307	NAG	C2-N2-C7	10.68	137.22	122.90

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1304	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	A	1306	NAG	C1-C2-N2-C7
4	A	1307	NAG	C1-C2-N2-C7
4	A	1309	NAG	C1-C2-N2-C7
4	A	1307	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
4	B	1305	NAG	1	0
4	A	1306	NAG	1	0
4	A	1308	NAG	1	0
4	C	1305	NAG	1	0
4	A	1307	NAG	4	0
4	C	1304	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13916. These allow visual inspection of the internal detail of the map and identification of artifacts.

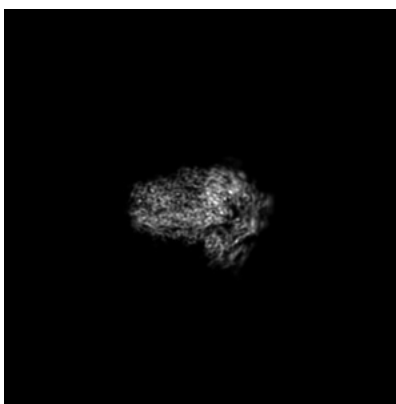
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

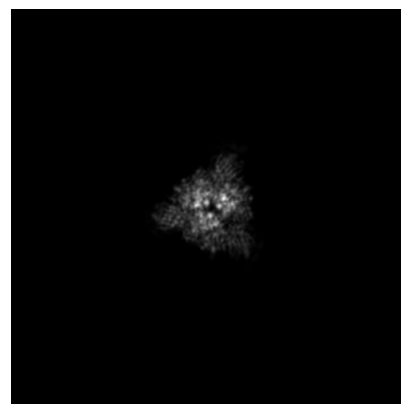
6.1.1 Primary map



X

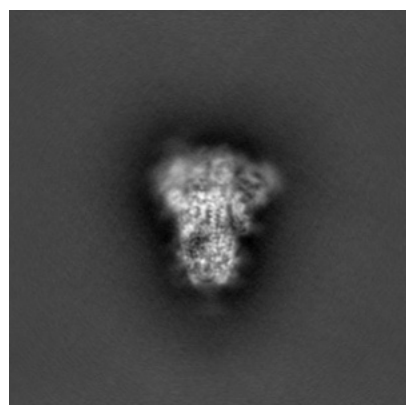


Y

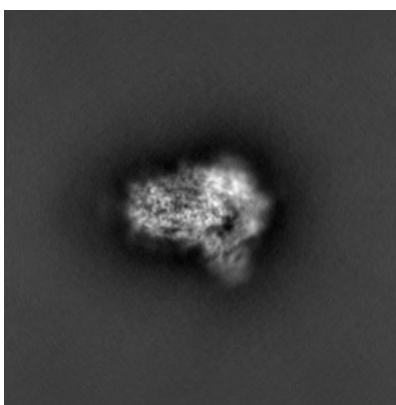


Z

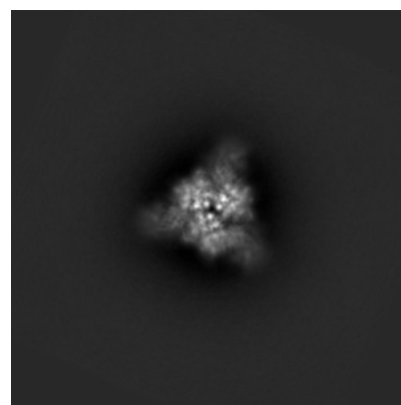
6.1.2 Raw map



X



Y

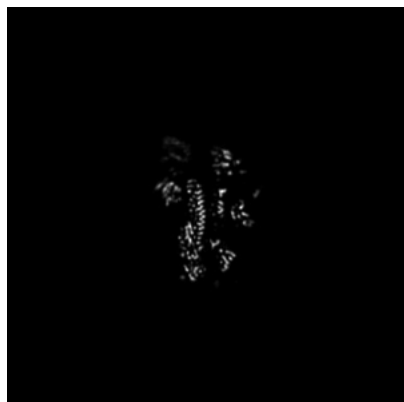


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150

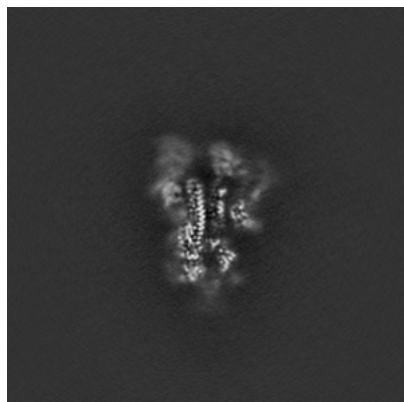


Y Index: 150

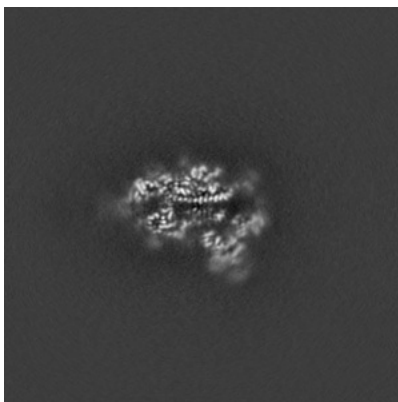


Z Index: 150

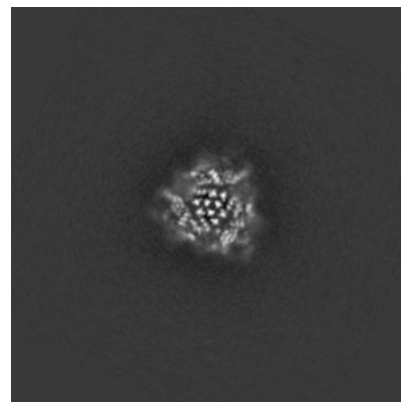
6.2.2 Raw map



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](#)

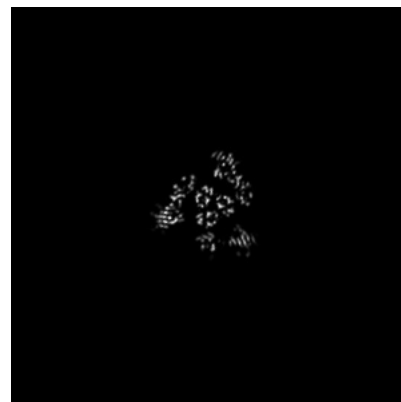
6.3.1 Primary map



X Index: 159

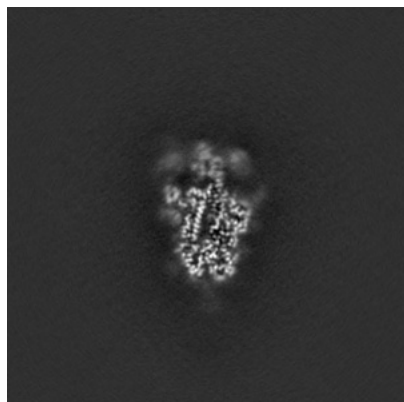


Y Index: 153

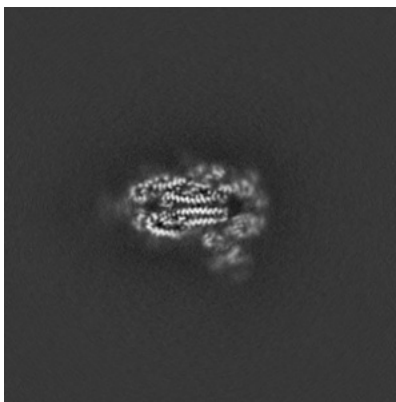


Z Index: 162

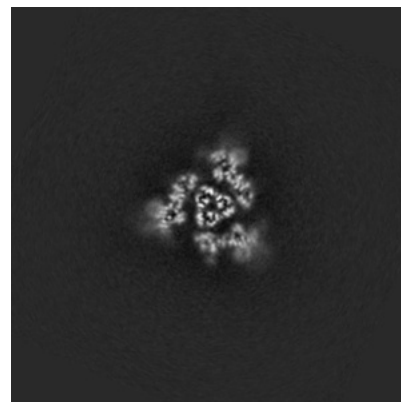
6.3.2 Raw map



X Index: 142



Y Index: 153

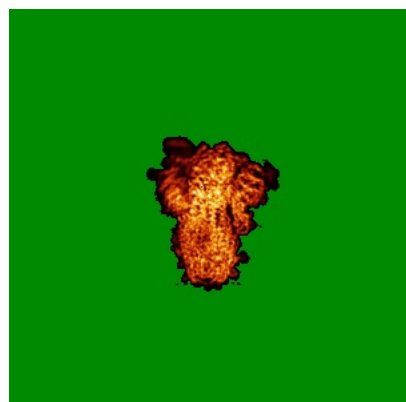


Z Index: 161

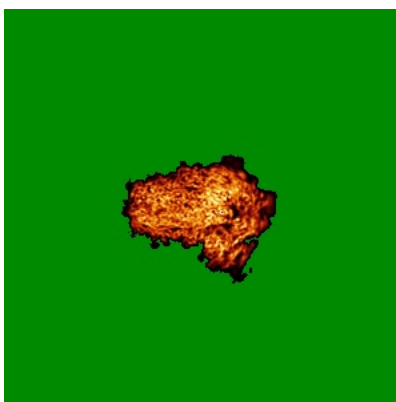
The images above show the largest variance slices of the map in three orthogonal directions.

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

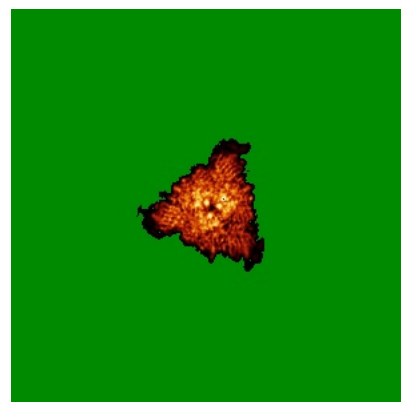
6.4.1 Primary map



X



Y

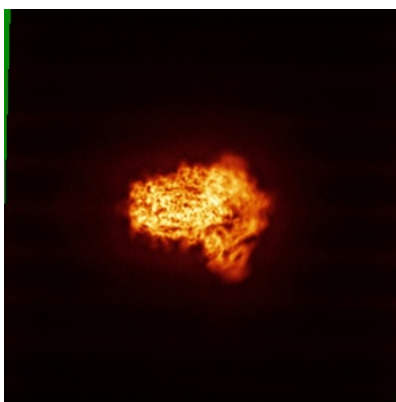


Z

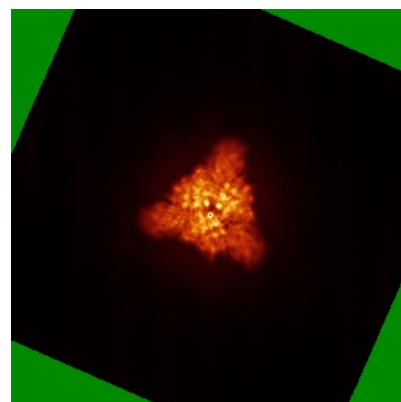
6.4.2 Raw map



X



Y

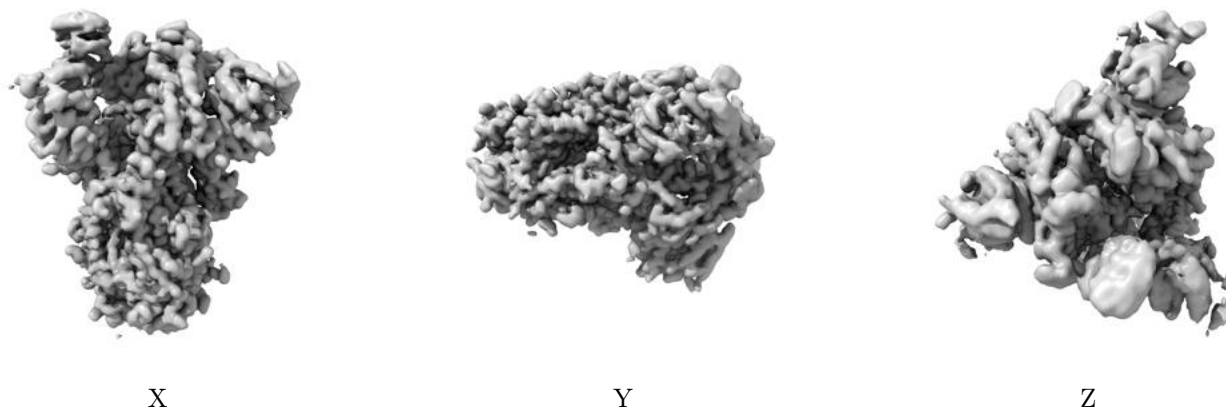


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.048. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

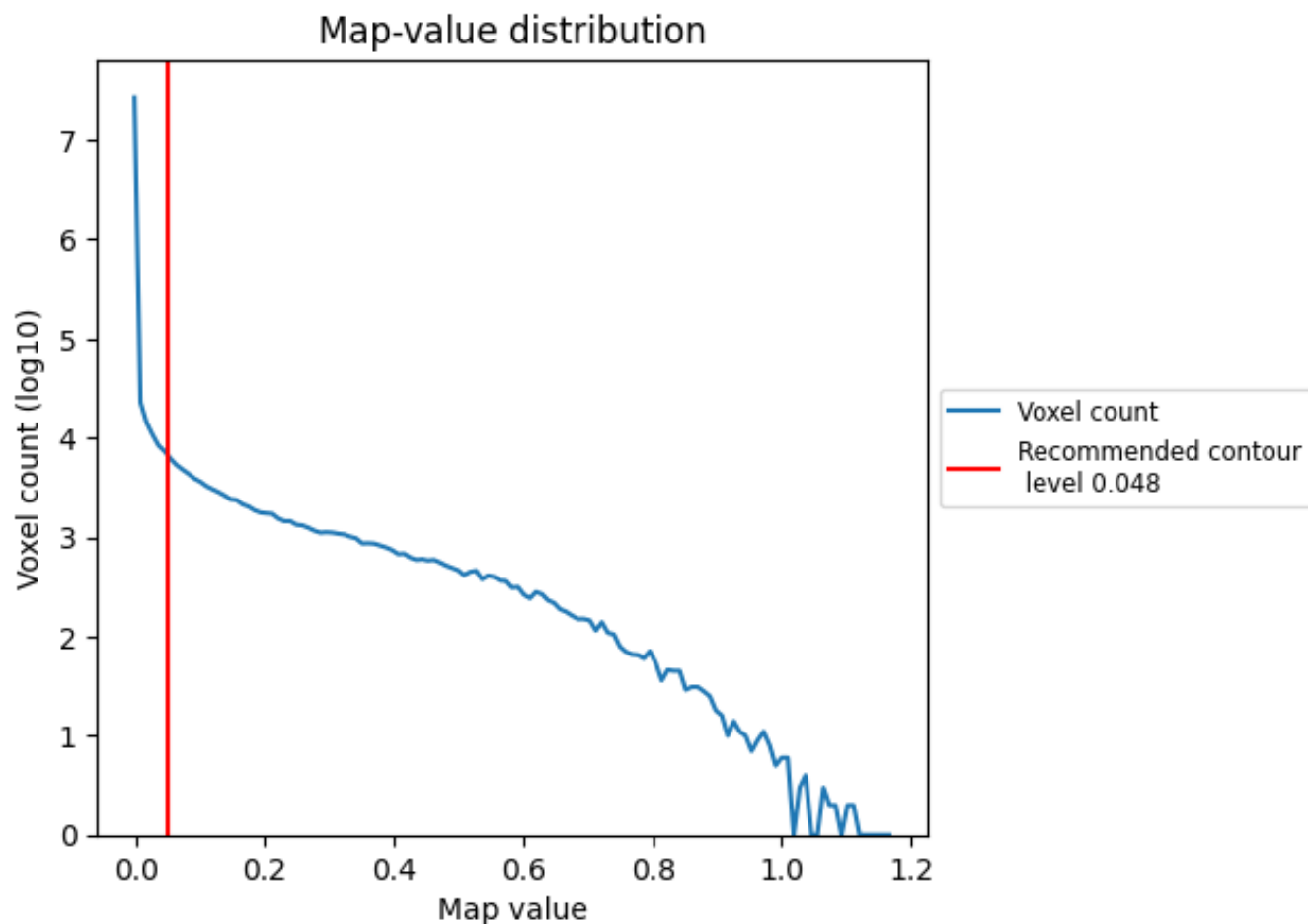
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

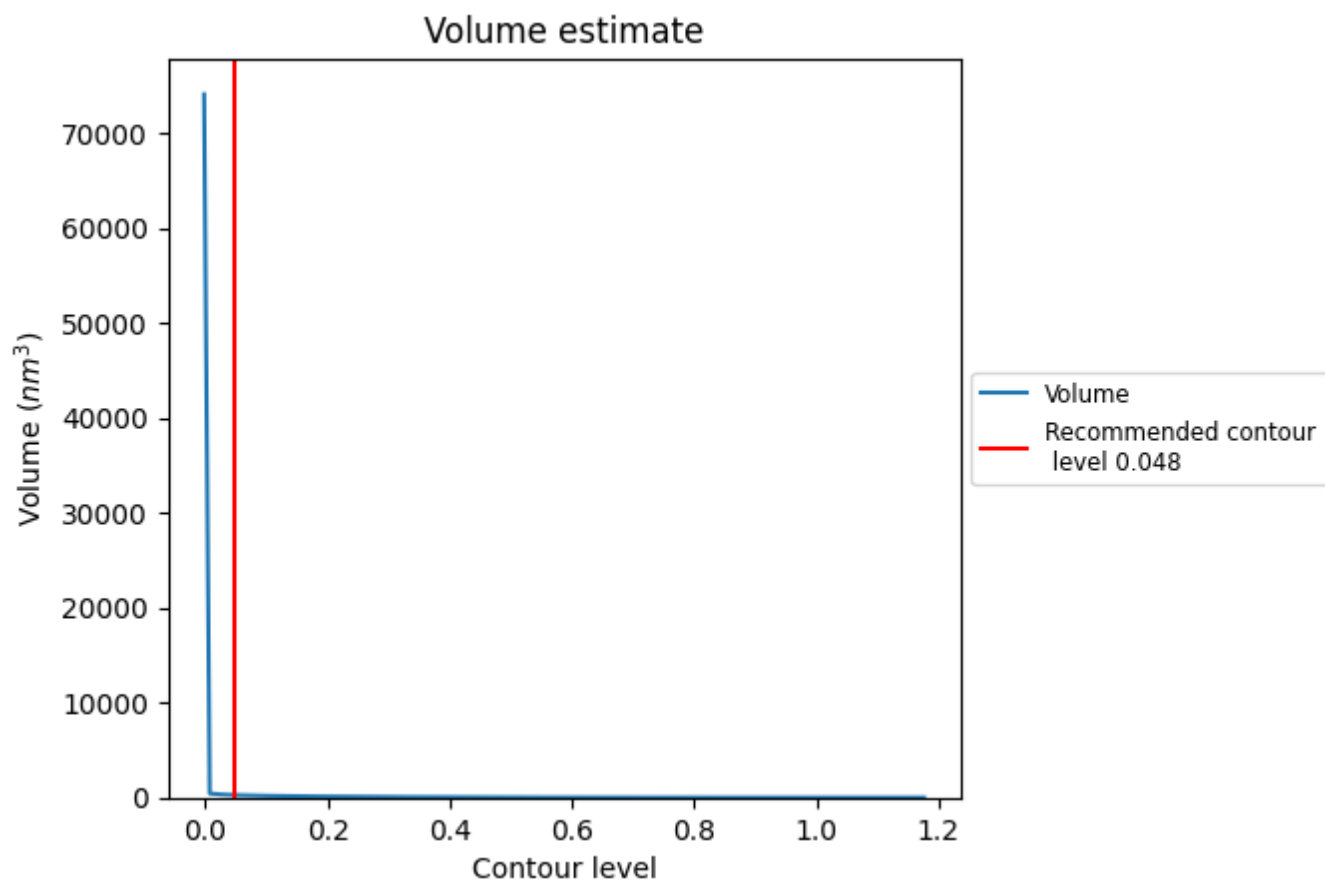
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

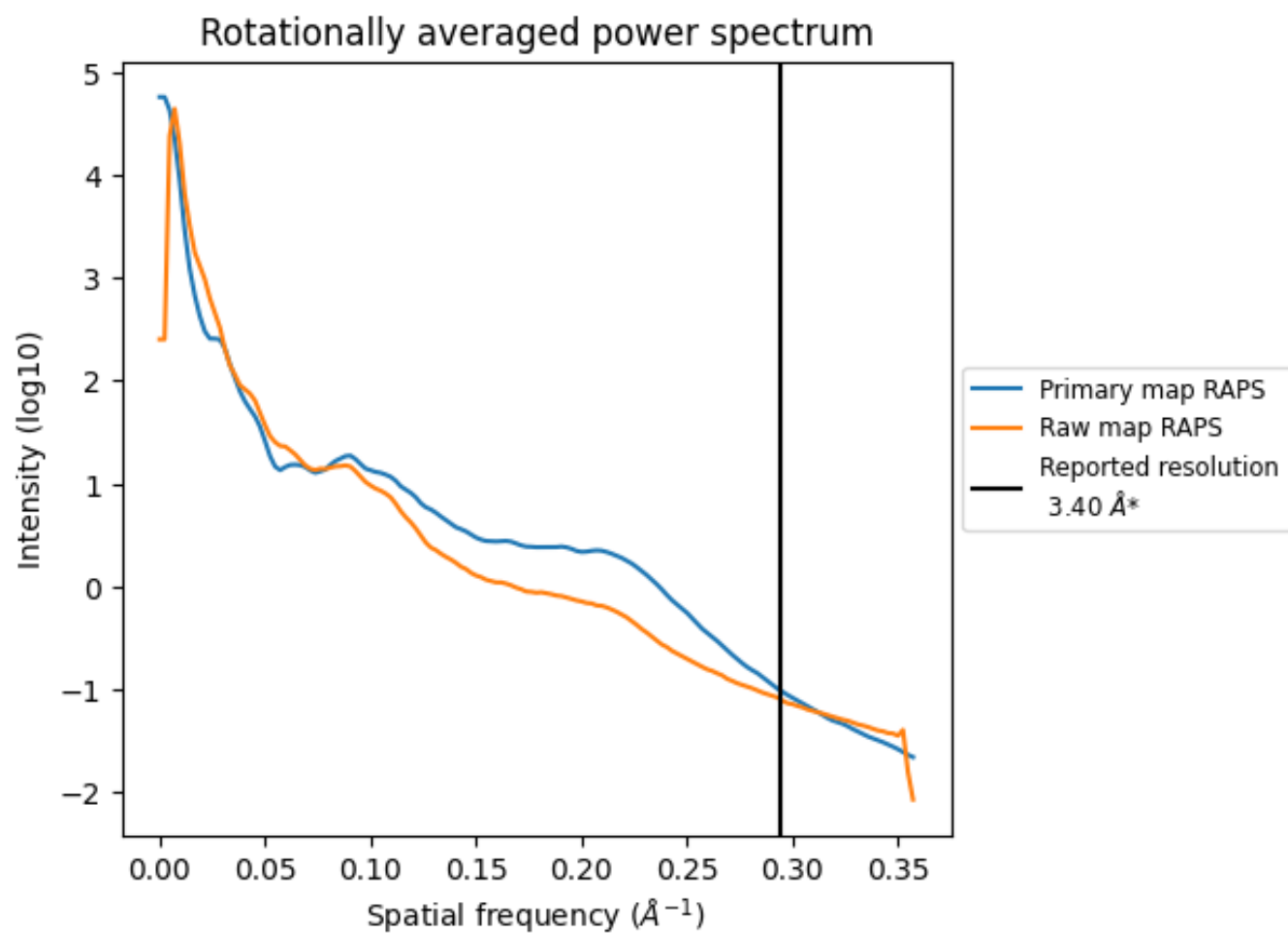
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm³; this corresponds to an approximate mass of 239 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 ⓘ

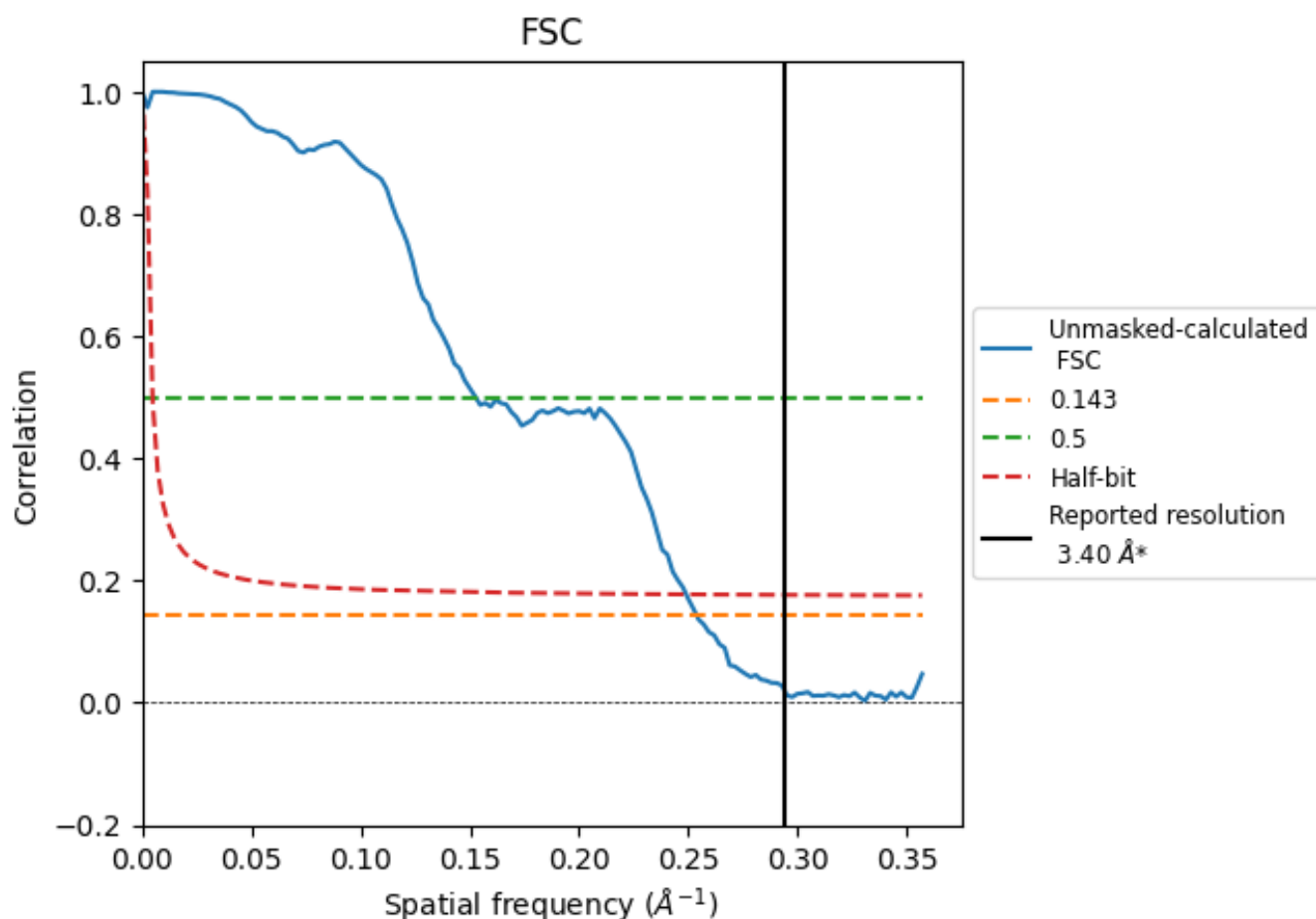


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

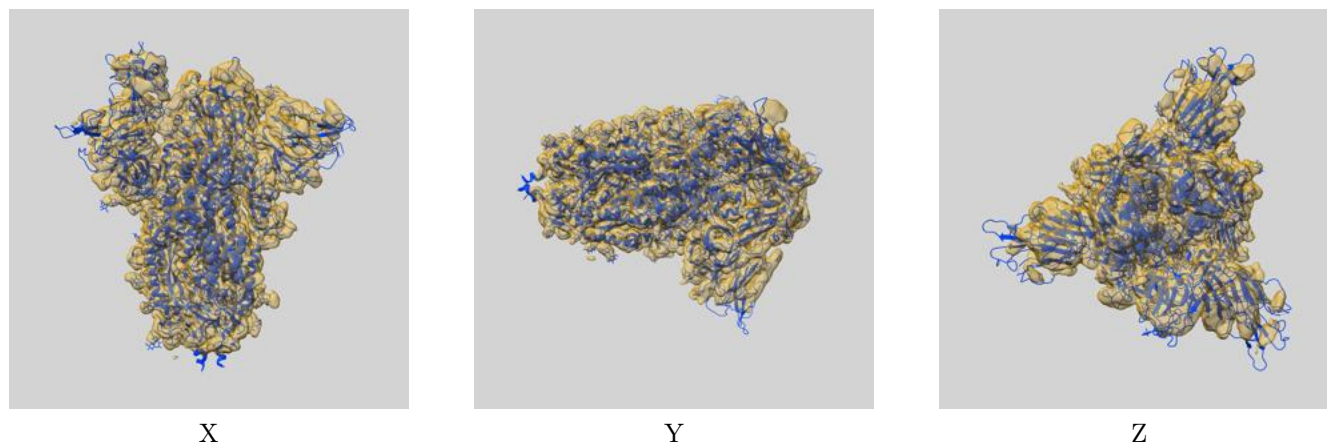
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	6.55	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

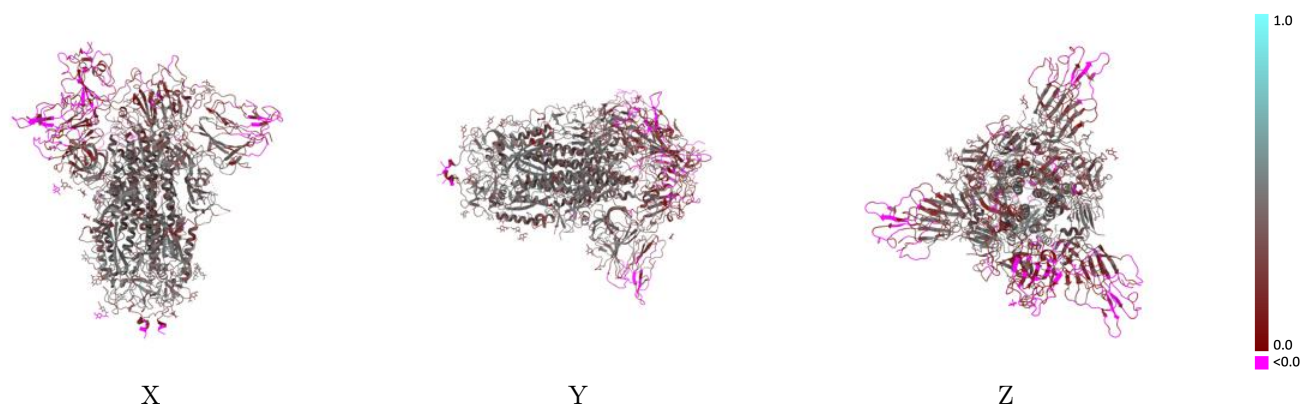
This section contains information regarding the fit between EMDB map EMD-13916 and PDB model 7QDG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



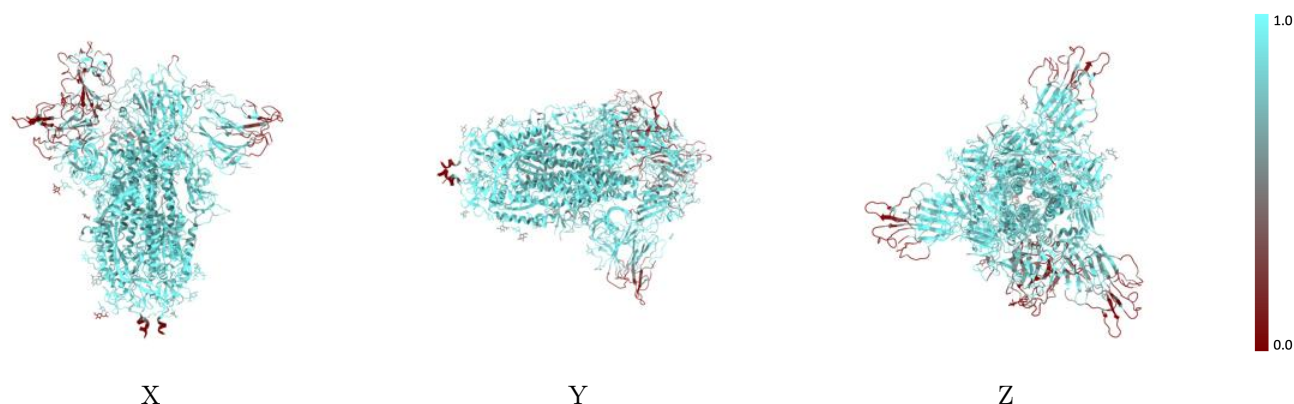
The images above show the 3D surface view of the map at the recommended contour level 0.048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



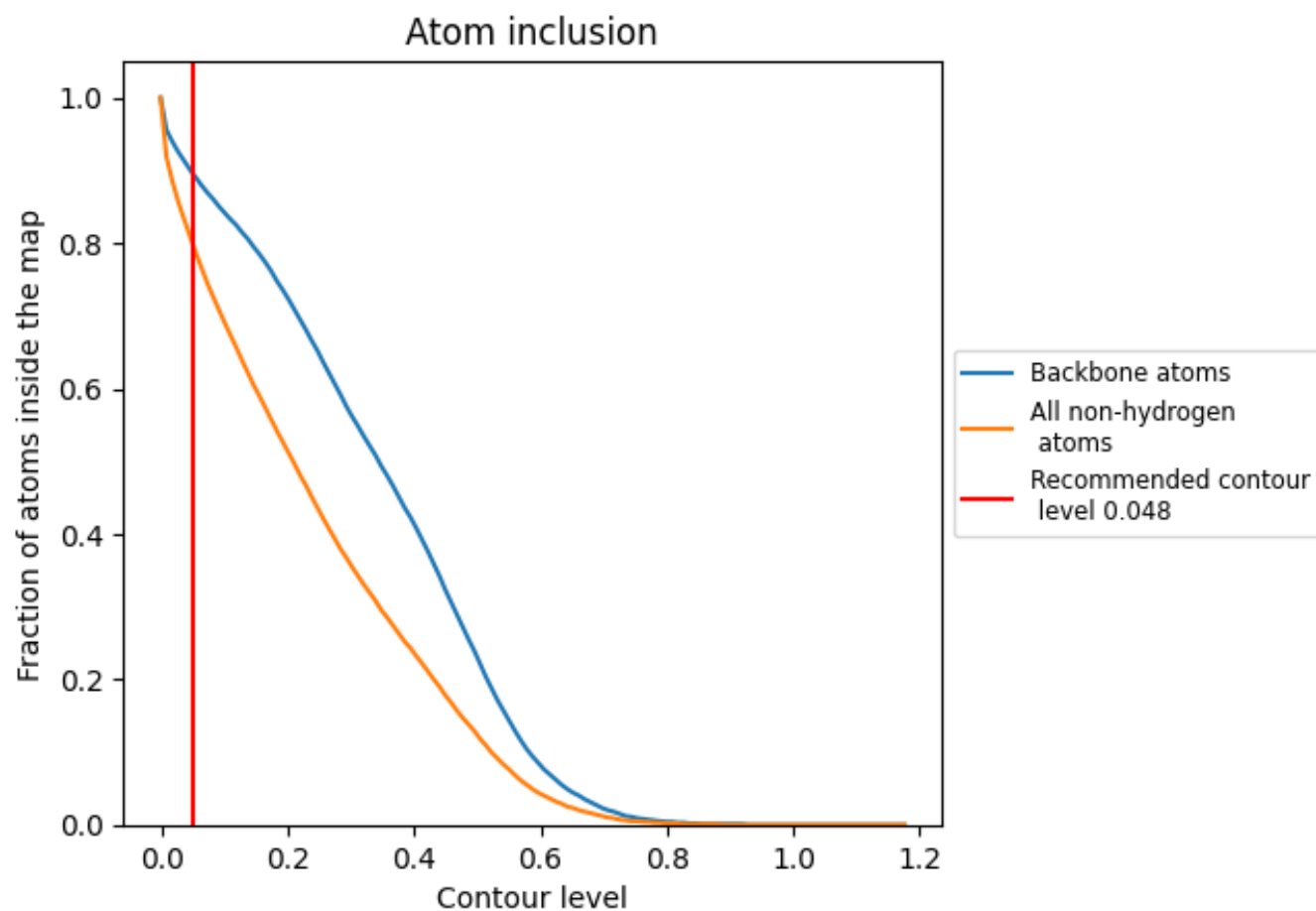
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.048).

9.4 Atom inclusion ⓘ



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 (0.048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.3100
A	 0.8380	 0.3210
B	 0.7640	 0.2940
C	 0.8110	 0.3170
E	 0.8930	 0.4040
G	 0.7140	 0.2580
I	 0.6790	 0.3310
J	 0.7140	 0.2020
K	 0.5710	 0.2560
L	 0.6430	 0.2520
M	 0.3930	 0.1580
N	 0.0000	 0.0930
O	 0.6430	 0.2920
P	 0.4290	 0.0380
Q	 0.6430	 0.2010

