



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 06:46 am BST

PDB ID : 8P9Y
EMDB ID : EMD-17578
Title : SARS-CoV-2 S protein S:D614G mutant in 3-down with binding site of an entry inhibitor
Authors : Adhav, A.; Forcada-Nadal, A.; Marco-Marin, C.; Lopez-Redondo, M.L.; Llacer, J.L.
Deposited on : 2023-06-06
Resolution : 4.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

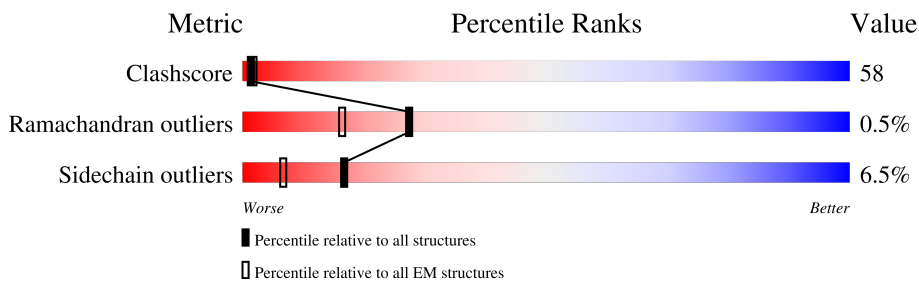
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	1270	 9% 42% 39% 15%
1	B	1270	 41% 40% 15%
1	C	1270	 5% 41% 38% 5% 15%
2	D	2	 100%
2	E	2	 50% 50%
2	F	2	 50% 50%
2	G	2	 100%
2	H	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	J	2	 50% 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%

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
2	NAG	F	1	X	-	-	-
2	NAG	H	1	X	-	-	-
2	NAG	I	1	X	-	-	-
2	NAG	L	1	X	-	-	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 25937 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 protein S1,Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1080	8425	5378	1403	1606	38	0	0
1	B	1081	8426	5379	1403	1606	38	0	0
1	C	1076	8374	5346	1395	1595	38	0	0

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P0DTC2
A	-4	VAL	-	expression tag	UNP P0DTC2
A	-3	SER	-	expression tag	UNP P0DTC2
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	ILE	-	expression tag	UNP P0DTC2
A	0	VAL	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	TYR	-	expression tag	UNP P0DTC2
A	3	VAL	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	ALA	-	expression tag	UNP P0DTC2
A	7	ALA	-	expression tag	UNP P0DTC2
A	8	ALA	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	HIS	-	expression tag	UNP P0DTC2
A	11	SER	-	expression tag	UNP P0DTC2
A	12	ALA	-	expression tag	UNP P0DTC2
A	13	PHE	-	expression tag	UNP P0DTC2
A	14	ALA	-	expression tag	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	685	ALA	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	VAL	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	SER	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	TYR	-	expression tag	UNP P0DTC2
A	1222	ILE	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLU	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	ARG	-	expression tag	UNP P0DTC2
A	1228	ASP	-	expression tag	UNP P0DTC2
A	1229	GLY	-	expression tag	UNP P0DTC2
A	1230	GLN	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	TYR	-	expression tag	UNP P0DTC2
A	1233	VAL	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	LYS	-	expression tag	UNP P0DTC2
A	1236	ASP	-	expression tag	UNP P0DTC2
A	1237	GLY	-	expression tag	UNP P0DTC2
A	1238	GLU	-	expression tag	UNP P0DTC2
A	1239	TRP	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	PHE	-	expression tag	UNP P0DTC2
A	1242	LEU	-	expression tag	UNP P0DTC2
A	1243	SER	-	expression tag	UNP P0DTC2
A	1244	THR	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	LEU	-	expression tag	UNP P0DTC2
A	1247	SER	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	GLN	-	expression tag	UNP P0DTC2
A	1260	LYS	-	expression tag	UNP P0DTC2
A	1261	LEU	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2
A	1263	SER	-	expression tag	UNP P0DTC2
A	1264	GLU	-	expression tag	UNP P0DTC2
A	1265	GLU	-	expression tag	UNP P0DTC2
A	1266	ASP	-	expression tag	UNP P0DTC2
A	1267	LEU	-	expression tag	UNP P0DTC2
B	-5	MET	-	initiating methionine	UNP P0DTC2
B	-4	VAL	-	expression tag	UNP P0DTC2
B	-3	SER	-	expression tag	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	ILE	-	expression tag	UNP P0DTC2
B	0	VAL	-	expression tag	UNP P0DTC2
B	1	LEU	-	expression tag	UNP P0DTC2
B	2	TYR	-	expression tag	UNP P0DTC2
B	3	VAL	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	ALA	-	expression tag	UNP P0DTC2
B	7	ALA	-	expression tag	UNP P0DTC2
B	8	ALA	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	HIS	-	expression tag	UNP P0DTC2
B	11	SER	-	expression tag	UNP P0DTC2
B	12	ALA	-	expression tag	UNP P0DTC2
B	13	PHE	-	expression tag	UNP P0DTC2
B	14	ALA	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	VAL	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	ARG	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	TYR	-	expression tag	UNP P0DTC2
B	1222	ILE	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLU	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	PRO	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	ASP	-	expression tag	UNP P0DTC2
B	1229	GLY	-	expression tag	UNP P0DTC2
B	1230	GLN	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	TYR	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	LYS	-	expression tag	UNP P0DTC2
B	1236	ASP	-	expression tag	UNP P0DTC2
B	1237	GLY	-	expression tag	UNP P0DTC2
B	1238	GLU	-	expression tag	UNP P0DTC2
B	1239	TRP	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	PHE	-	expression tag	UNP P0DTC2
B	1242	LEU	-	expression tag	UNP P0DTC2
B	1243	SER	-	expression tag	UNP P0DTC2
B	1244	THR	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	LEU	-	expression tag	UNP P0DTC2
B	1247	SER	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	GLN	-	expression tag	UNP P0DTC2
B	1260	LYS	-	expression tag	UNP P0DTC2
B	1261	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1262	ILE	-	expression tag	UNP P0DTC2
B	1263	SER	-	expression tag	UNP P0DTC2
B	1264	GLU	-	expression tag	UNP P0DTC2
B	1265	GLU	-	expression tag	UNP P0DTC2
B	1266	ASP	-	expression tag	UNP P0DTC2
B	1267	LEU	-	expression tag	UNP P0DTC2
C	-5	MET	-	initiating methionine	UNP P0DTC2
C	-4	VAL	-	expression tag	UNP P0DTC2
C	-3	SER	-	expression tag	UNP P0DTC2
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	ILE	-	expression tag	UNP P0DTC2
C	0	VAL	-	expression tag	UNP P0DTC2
C	1	LEU	-	expression tag	UNP P0DTC2
C	2	TYR	-	expression tag	UNP P0DTC2
C	3	VAL	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	ALA	-	expression tag	UNP P0DTC2
C	7	ALA	-	expression tag	UNP P0DTC2
C	8	ALA	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	HIS	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	ALA	-	expression tag	UNP P0DTC2
C	13	PHE	-	expression tag	UNP P0DTC2
C	14	ALA	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	VAL	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	ARG	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	SER	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	TYR	-	expression tag	UNP P0DTC2
C	1222	ILE	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLU	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	PRO	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	ASP	-	expression tag	UNP P0DTC2
C	1229	GLY	-	expression tag	UNP P0DTC2
C	1230	GLN	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	TYR	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	LYS	-	expression tag	UNP P0DTC2
C	1236	ASP	-	expression tag	UNP P0DTC2
C	1237	GLY	-	expression tag	UNP P0DTC2
C	1238	GLU	-	expression tag	UNP P0DTC2
C	1239	TRP	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	PHE	-	expression tag	UNP P0DTC2
C	1242	LEU	-	expression tag	UNP P0DTC2
C	1243	SER	-	expression tag	UNP P0DTC2
C	1244	THR	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	LEU	-	expression tag	UNP P0DTC2
C	1247	SER	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	GLN	-	expression tag	UNP P0DTC2
C	1260	LYS	-	expression tag	UNP P0DTC2
C	1261	LEU	-	expression tag	UNP P0DTC2
C	1262	ILE	-	expression tag	UNP P0DTC2
C	1263	SER	-	expression tag	UNP P0DTC2
C	1264	GLU	-	expression tag	UNP P0DTC2
C	1265	GLU	-	expression tag	UNP P0DTC2
C	1266	ASP	-	expression tag	UNP P0DTC2
C	1267	LEU	-	expression tag	UNP P0DTC2

- 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
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0
2	J	2	28	16	2	10	0	0
2	K	2	28	16	2	10	0	0
2	L	2	28	16	2	10	0	0
2	M	2	28	16	2	10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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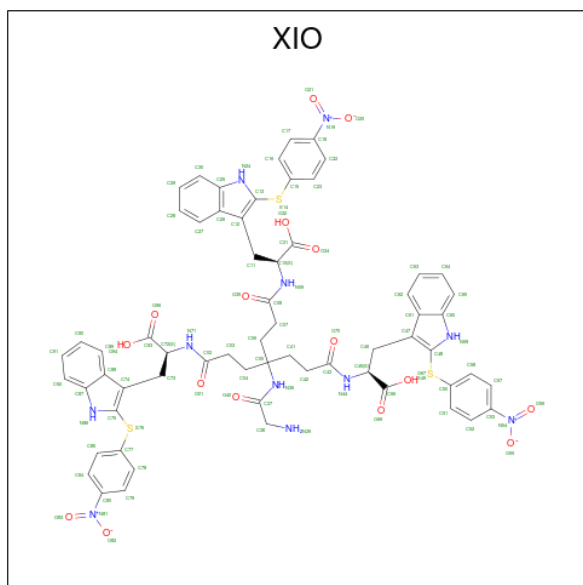
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
4	A	2	Total 2	Na 2	0
4	C	1	Total 1	Na 1	0

- Molecule 5 is [(2 {S})-2-[[4-(2-azanylethanoylamino)-7-[[[(2 {S})-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]-1-oxidanylidene-1-sodiooxy-propan-2-yl]amino]-4-[3-[[[(2 {S})-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]-1-oxidanylidene-1-sodiooxy-propan-2-yl]amino]-3-oxidanylidene-propyl]-7-oxidanylidene-heptanoyl]amino]-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]propanoyl]oxysodium (three-letter code: XIO) (formula: C₆₃H₅₉N₁₁O₁₆S₃) (labeled as "Ligand of Interest" by depositor).

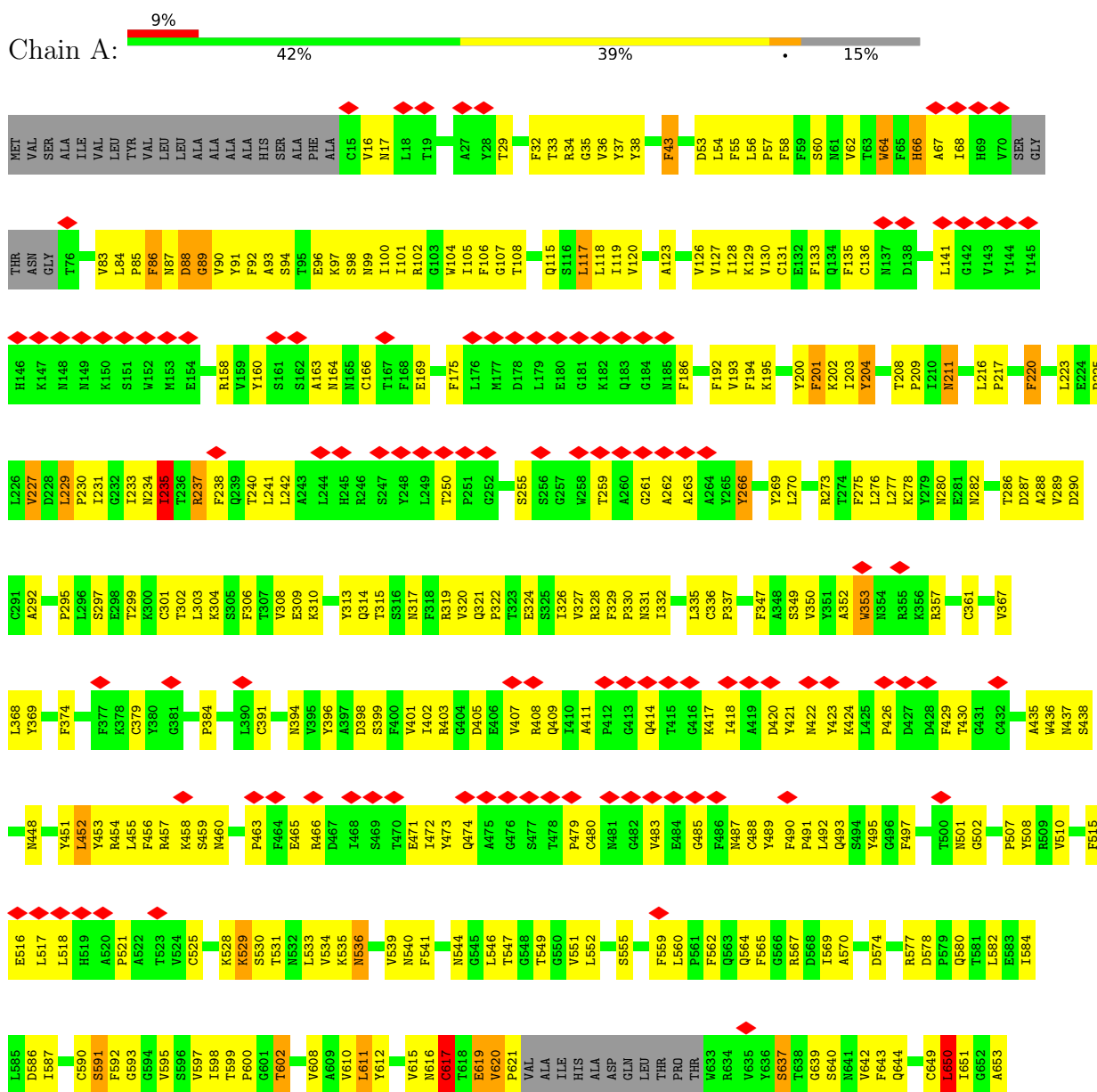


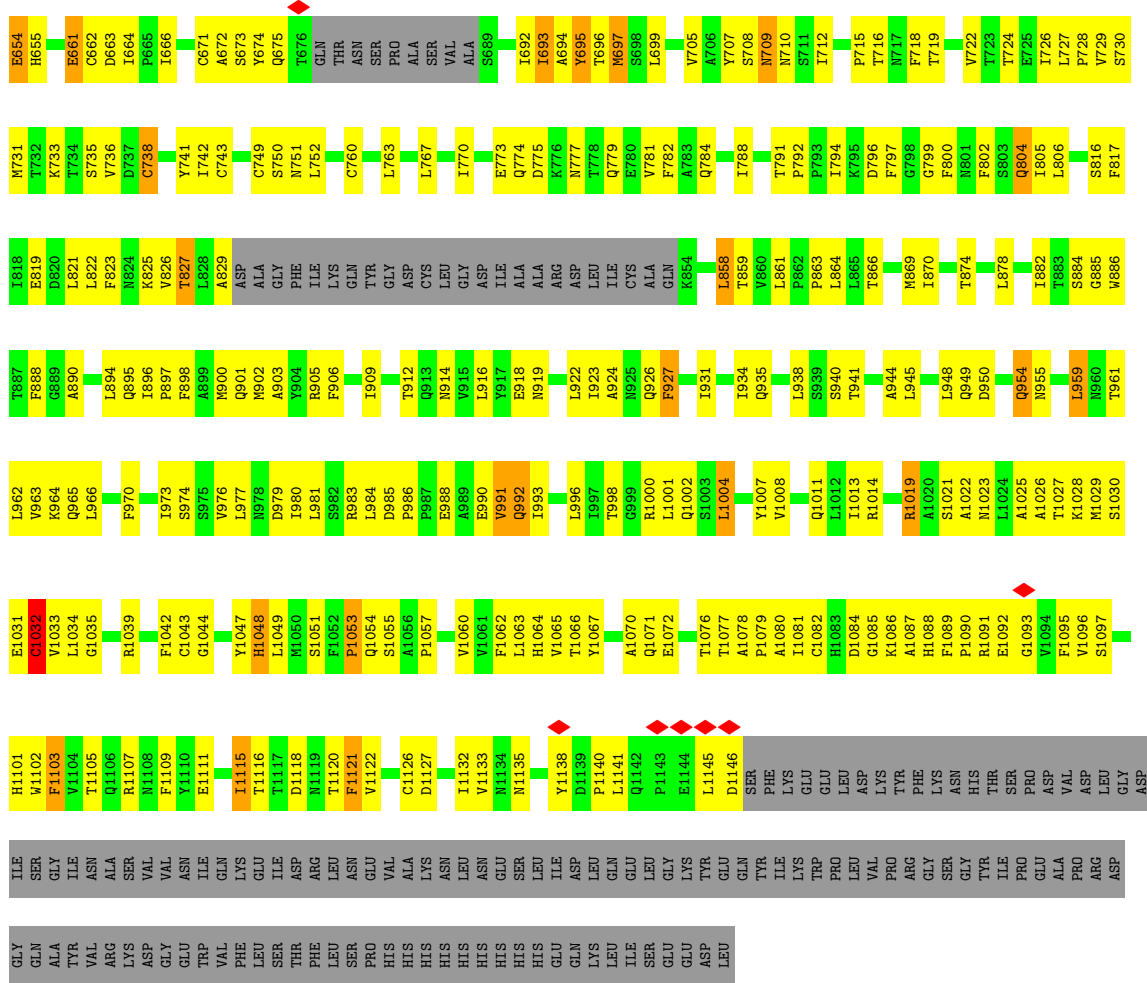
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		S
5	C	1	93	63	11	16	3	0

3 Residue-property plots

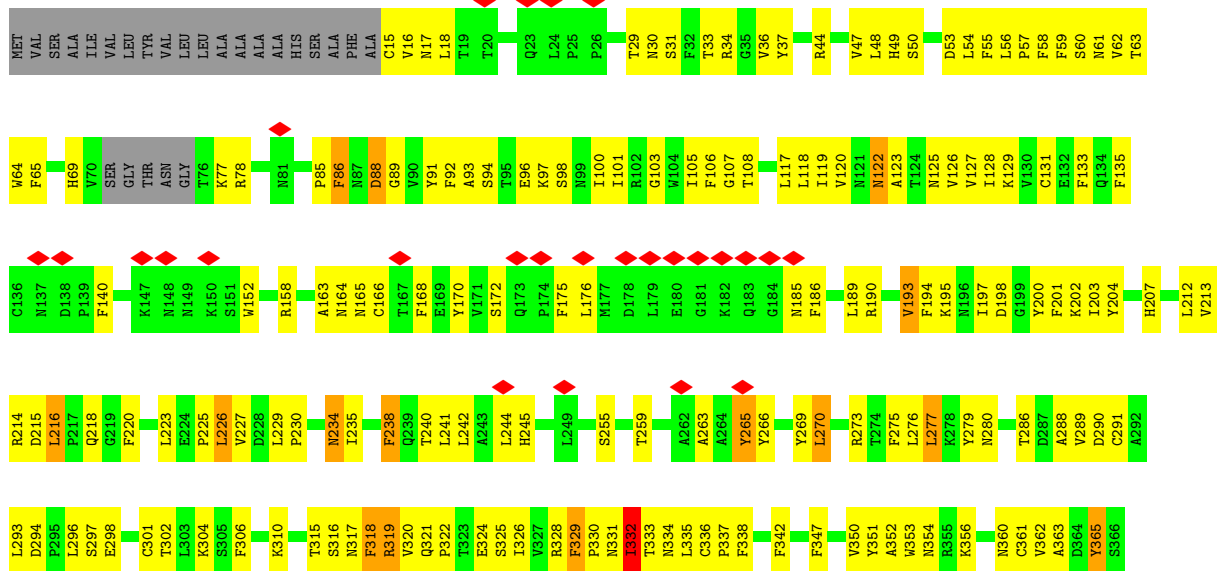
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

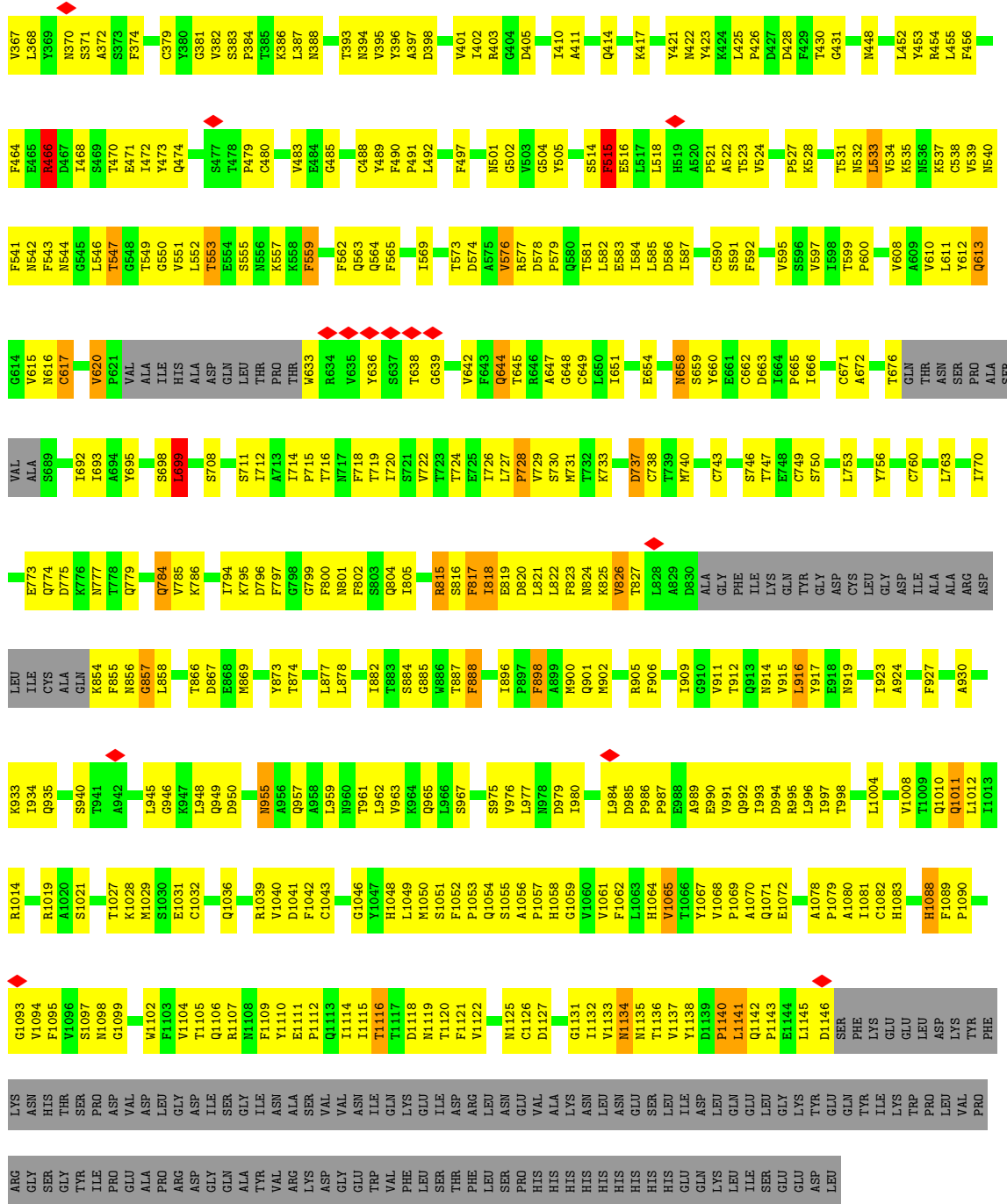
• Molecule 1: Spike protein S1,Spike glycoprotein



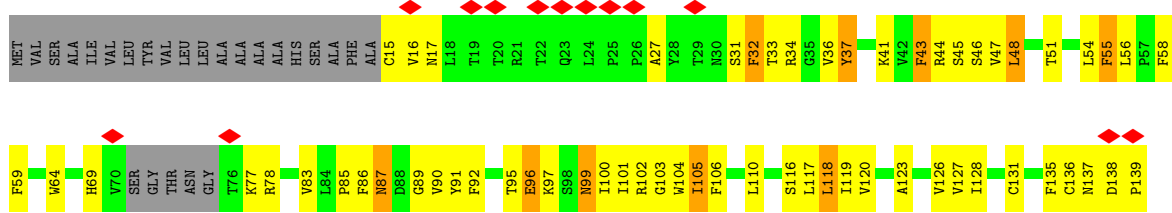


• Molecule 1: Spike protein S1, Spike glycoprotein






• Molecule 1: Spike protein S1,Spike glycoprotein



VAL	G1124	M1050	S975	M886	P809	S730	H655	L587	G502	F429	N560	D290	P225	F140
ALA	M125	P1053	V976	A890	S810	M731	N658	L588	V503	T930	C361	C291	L226	L141
ASN	C1126	Q1054	L977	P812	K811	T732	S659	P589	G601	T936	V362	A292	V227	Y145
ASN	I1132	G1059	I980	S813	K733	T734	S658	C590	Q506	C432	D364	D294	L229	H146
ASP	M1135	V1060	S982	P817	S735	T736	E661	S591	P507	V433	D365	P295	P230	K147
ASP	T1137	F1062	R983	L818	F892	W736	C662	F892	Y508	I434	S366	L296	I231	K150
ASP	V1138	F1063	L984	L821	G594	D737	P665	G594	R509	A435	V367	G232	G233	S151
ASP	D1139	N900	L822	L822	V595	I742	I666	S596	V511	N448	N370	C301	N234	W152
ASP	P1140	Q901	L825	V599	V512	C743	G667	S597	V513	Y449	L303	T302	I235	F157
ASN	Q1142	M902	K825	T599	L514	E748	C671	L598	S514	M450	F374	R237	T236	R158
ASN	P1143	R905	V826	T599	F515	C749	A672	P600	F515	Y451	F306	R237	F238	F157
ASP	L1144	T912	T627	C749	E516	C749	S673	S605	E516	L452	T307	T307	Q239	R158
ASP	D1146	Y915	Y674	L753	L517	L753	Y674	N606	L517	K378	V308	T240	T240	M164
SER	SER	L916	A629	L756	L518	L756	Q675	Q607	L518	C379	E309	R454	L241	M165
PHE	PHE	L917	D830	G757	H519	G757	T676	Q608	H519	L455	Y380	K310	L242	C166
LYS	LYS	Y917	ALA	G757	A520	G757	GLN	Q607	A520	F456	G881	G811	A243	T167
GLU	GLU	K921	GLY	S758	A521	S758	THR	A609	A521	K457	I312	I312	L244	F168
ILE	ILE	L922	PHE	F759	P521	F759	ASN	A609	P521	K458	Q134	Q134	R246	F175
ILE	ILE	L923	LYS	C760	L611	C760	SER	V610	L611	K458	T315	T315	R246	L176
TRP	TRP	I923	GLN	T761	V612	T761	PRO	V612	V612	S459	N316	N316	Y248	M177
PRO	PRO	A930	LYS	G762	V615	G762	ALA	V615	G525	L461	L387	L387	Y248	M177
LEU	LEU	Q1005	TVR	L763	N616	L763	VAL	N616	G525	K462	N317	N317	Y248	M177
VAL	VAL	T1006	GLY	M764	N617	M764	ALA	N617	P527	P463	F818	F818	L249	M177
ARG	ARG	Y1007	ASP	R765	C617	R765	ALA	C617	P527	F464	D889	D889	L249	M177
LYS	LYS	V1008	CYS	L766	K528	L766	VAL	K528	K529	E465	C391	C391	T250	L179
ASN	ASN	K1086	LEU	A766	E619	A766	VAL	E619	S530	R466	F392	F392	P251	E180
HIS	HIS	A1087	GLY	T768	V620	T768	ALA	V620	T531	D467	T393	T393	G252	G181
SER	SER	F1088	ASP	G768	P621	G768	ASP	P621	N532	L468	N394	N394	D253	K182
THR	THR	P1089	ASP	D775	ALA	D775	ASP	ALA	N533	S469	Y396	Y396	S254	Q183
SER	SER	P1090	ILE	K776	ALA	K776	GLN	GLN	V534	S469	R328	R328	S255	G184
PRO	PRO	R1013	ALA	F781	ILE	F781	THR	THR	V539	T470	D398	D398	T259	M185
ASP	ASP	R1014	ALA	F782	ILE	F782	THR	THR	N540	I472	F329	F329	T259	M185
VAL	VAL	A1015	ARG	F782	THR	F782	THR	THR	N541	I473	S399	S399	T259	F186
ASP	ASP	A1016	ASP	F782	THR	F782	THR	THR	F543	Q474	F400	F400	T259	F186
LEU	LEU	F1095	LEU	F782	THR	F782	THR	THR	G545	G475	M334	M334	T259	F186
GLY	GLY	Y1096	ILE	F782	THR	F782	THR	THR	L546	S477	L335	L335	T259	F186
ASP	ASP	S1097	ILE	F782	THR	F782	THR	THR	G550	C480	C336	C336	T259	F186
ILE	ILE	N1098	ASP	F782	THR	F782	THR	THR	V551	C480	D405	D405	T259	F186
GLY	GLY	A1022	ASP	F782	THR	F782	THR	THR	L546	S477	E406	E406	T259	F186
ILE	ILE	A1022	ASP	F782	THR	F782	THR	THR	G550	C480	Q409	Q409	T259	F186
GLY	GLY	H1101	ASP	F782	THR	F782	THR	THR	V551	C480	I410	I410	T259	F186
GLY	GLY	F1102	ASP	F782	THR	F782	THR	THR	L552	G482	A411	A411	T259	F186
ASN	ASN	F1103	ASP	F782	THR	F782	THR	THR	L552	G482	A411	A411	T259	F186
ALA	ALA	Q1106	ASP	F782	THR	F782	THR	THR	S655	V483	T345	T345	T259	F186
SER	SER	M1029	ASP	F782	THR	F782	THR	THR	V576	F486	R346	R346	T270	Y200
VAL	VAL	S1030	ASP	F782	THR	F782	THR	THR	D578	N487	G414	G414	L270	F201
VAL	VAL	E1031	ASP	F782	THR	F782	THR	THR	P643	C488	Q414	Q414	L270	K202
GLY	GLY	F1109	ASP	F782	THR	F782	THR	THR	Q644	Y489	Q414	Q414	L270	Y204
ASN	ASN	Y1110	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	I203
ILE	ILE	E1111	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	I203
VAL	VAL	L1114	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
LYS	LYS	I1115	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
LEU	LEU	T1116	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
THR	THR	N969	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
THR	THR	F970	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
PHE	PHE	G571	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
LEU	LEU	Y1047	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
LEU	LEU	F1122	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
SER	SER	N1048	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
ASN	ASN	L1048	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
PRO	PRO	L1049	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
PRO	PRO	S1123	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204
PRO	PRO	S974	ASP	F782	THR	F782	THR	THR	V641	N487	T345	T345	L270	Y204

HIS
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LYS
LEU
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

Chain D:  100%

MAG1
MAG2

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

Chain E:  50%


MAG1
MAG2

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

Chain F:  50%

MAG1
MAG2

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

Chain G:  100%


MAG1
MAG2

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

Chain H:  50%

MAG1
MAG2

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

Chain I:  100%

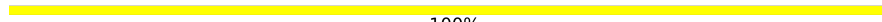
MAG1
MAG2

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

Chain J:  50%
100%

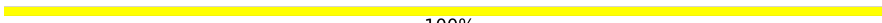


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

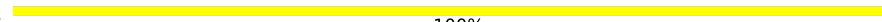


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%



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

Chain M:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97094	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.867	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	420.66, 420.66, 420.66	wwPDB
Map dimensions	492, 492, 492	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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, XIO, NA

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	0.55	7/8624 (0.1%)	0.72	9/11744 (0.1%)
1	B	0.57	4/8625 (0.0%)	0.72	13/11746 (0.1%)
1	C	0.58	11/8570 (0.1%)	0.72	14/11670 (0.1%)
All	All	0.57	22/25819 (0.1%)	0.72	36/35160 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	940	SER	C-O	-18.36	0.88	1.23
1	A	940	SER	C-O	-15.06	0.94	1.23
1	C	676	THR	C-O	-11.67	1.01	1.23
1	A	1146	ASP	C-O	8.43	1.39	1.23
1	A	617	CYS	C-O	7.76	1.38	1.23

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	515	PHE	O-C-N	-11.16	104.84	122.70
1	A	1146	ASP	CA-C-O	-8.92	101.37	120.10
1	A	1032	CYS	CA-CB-SG	8.58	129.45	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	590	CYS	CA-CB-SG	-7.69	100.15	114.00
1	A	650	LEU	CA-CB-CG	6.91	131.20	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	617	CYS	Mainchain
1	B	515	PHE	Mainchain

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	8425	0	8181	937	0
1	B	8426	0	8179	1080	0
1	C	8374	0	8124	1031	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
3	A	126	0	117	2	0
3	B	126	0	117	2	0
3	C	84	0	78	1	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	C	93	0	0	0	0
All	All	25937	0	25046	2968	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 58.

The worst 5 of 2968 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	1.28	1.65
1:C:541:PHE:CZ	1:C:587:ILE:HD13	1.31	1.61
1:B:543:PHE:CB	1:B:576:VAL:HG21	1.17	1.60
1:A:317:ASN:HB3	1:A:592:PHE:CZ	1.36	1.56
1:B:543:PHE:HB3	1:B:576:VAL:CG2	1.31	1.55

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	1070/1270 (84%)	1017 (95%)	46 (4%)	7 (1%)	19	56
1	B	1071/1270 (84%)	1025 (96%)	38 (4%)	8 (1%)	19	56
1	C	1066/1270 (84%)	1020 (96%)	44 (4%)	2 (0%)	44	78
All	All	3207/3810 (84%)	3062 (96%)	128 (4%)	17 (0%)	27	63

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	SER
1	A	620	VAL
1	B	332	ILE
1	B	371	SER
1	B	857	GLY

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	938/1102 (85%)	878 (94%)	60 (6%)	14	36
1	B	937/1102 (85%)	884 (94%)	53 (6%)	17	40
1	C	929/1102 (84%)	859 (92%)	70 (8%)	11	31
All	All	2804/3306 (85%)	2621 (94%)	183 (6%)	17	36

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	LEU
1	C	365	TYR
1	C	87	ASN
1	C	226	LEU
1	C	517	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	394	ASN
1	C	992	GLN
1	C	414	GLN
1	C	644	GLN
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	D	1	1,2	14,14,15	0.79	0	17,19,21	2.97	7 (41%)
2	NAG	D	2	2	14,14,15	0.64	0	17,19,21	1.09	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.79	0	17,19,21	2.86	6 (35%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.10	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.81	0	17,19,21	2.88	7 (41%)
2	NAG	F	2	2	14,14,15	0.63	0	17,19,21	1.11	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.75	0	17,19,21	2.92	6 (35%)
2	NAG	G	2	2	14,14,15	0.63	0	17,19,21	1.12	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.86	0	17,19,21	2.92	7 (41%)
2	NAG	H	2	2	14,14,15	0.62	0	17,19,21	1.10	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.81	0	17,19,21	2.88	6 (35%)
2	NAG	I	2	2	14,14,15	0.62	0	17,19,21	1.09	2 (11%)
2	NAG	J	1	1,2	14,14,15	0.80	0	17,19,21	2.95	6 (35%)
2	NAG	J	2	2	14,14,15	0.65	0	17,19,21	1.07	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.77	0	17,19,21	3.00	7 (41%)
2	NAG	K	2	2	14,14,15	0.65	0	17,19,21	1.08	2 (11%)
2	NAG	L	1	1,2	14,14,15	0.80	0	17,19,21	2.89	7 (41%)
2	NAG	L	2	2	14,14,15	0.64	0	17,19,21	1.12	2 (11%)
2	NAG	M	1	1,2	14,14,15	0.80	0	17,19,21	3.07	6 (35%)
2	NAG	M	2	2	14,14,15	0.68	0	17,19,21	1.13	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	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	1/1/5/7	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	1,2	-	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	1,2	-	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	1/1/5/7	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	1,2	-	3/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C8-C7-N2	7.57	128.91	116.10
2	K	1	NAG	C8-C7-N2	7.49	128.78	116.10
2	H	1	NAG	C8-C7-N2	7.44	128.69	116.10
2	J	1	NAG	C8-C7-N2	7.42	128.66	116.10
2	D	1	NAG	C8-C7-N2	7.35	128.54	116.10

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1
2	H	1	NAG	C1
2	I	1	NAG	C1
2	L	1	NAG	C1

5 of 50 torsion outliers are listed below:

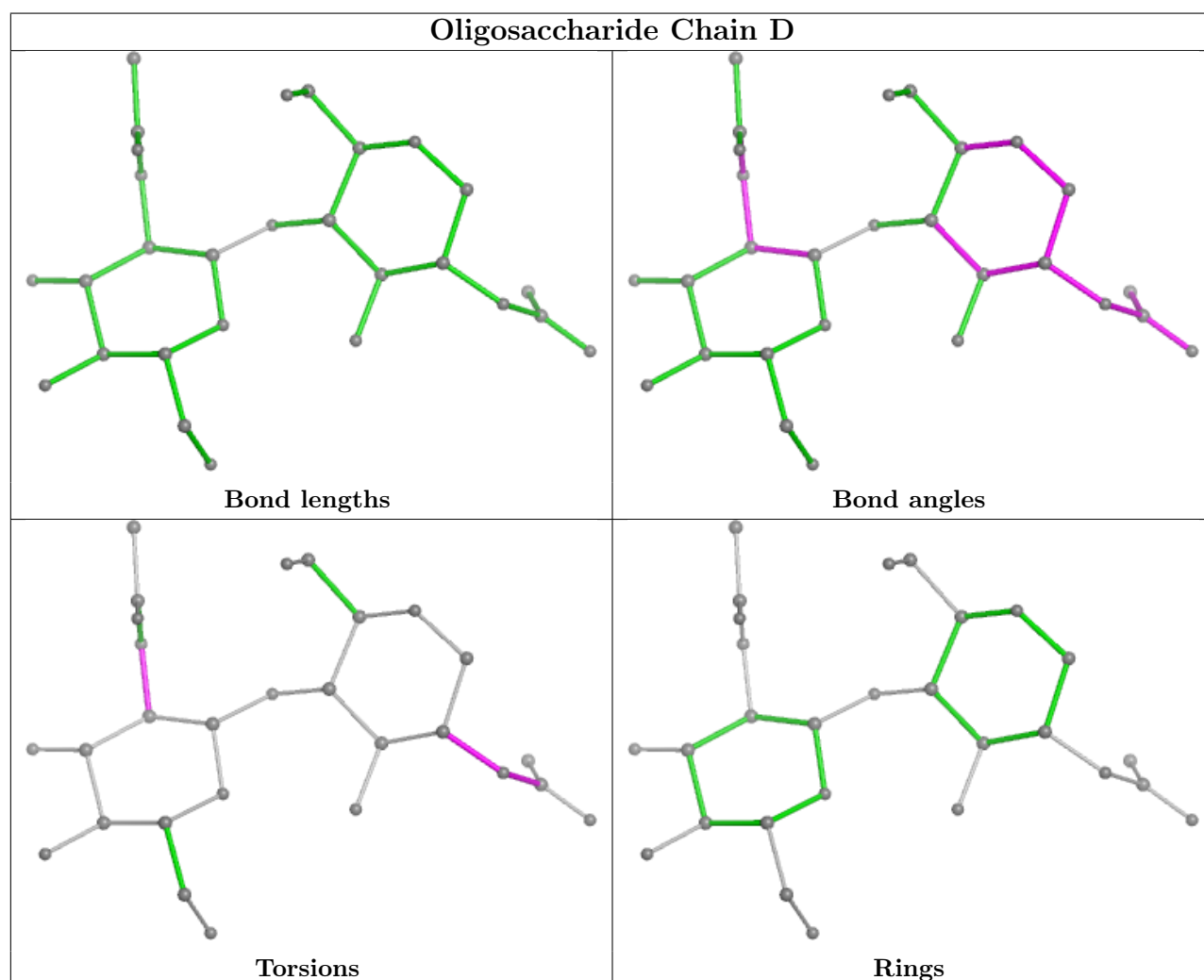
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2

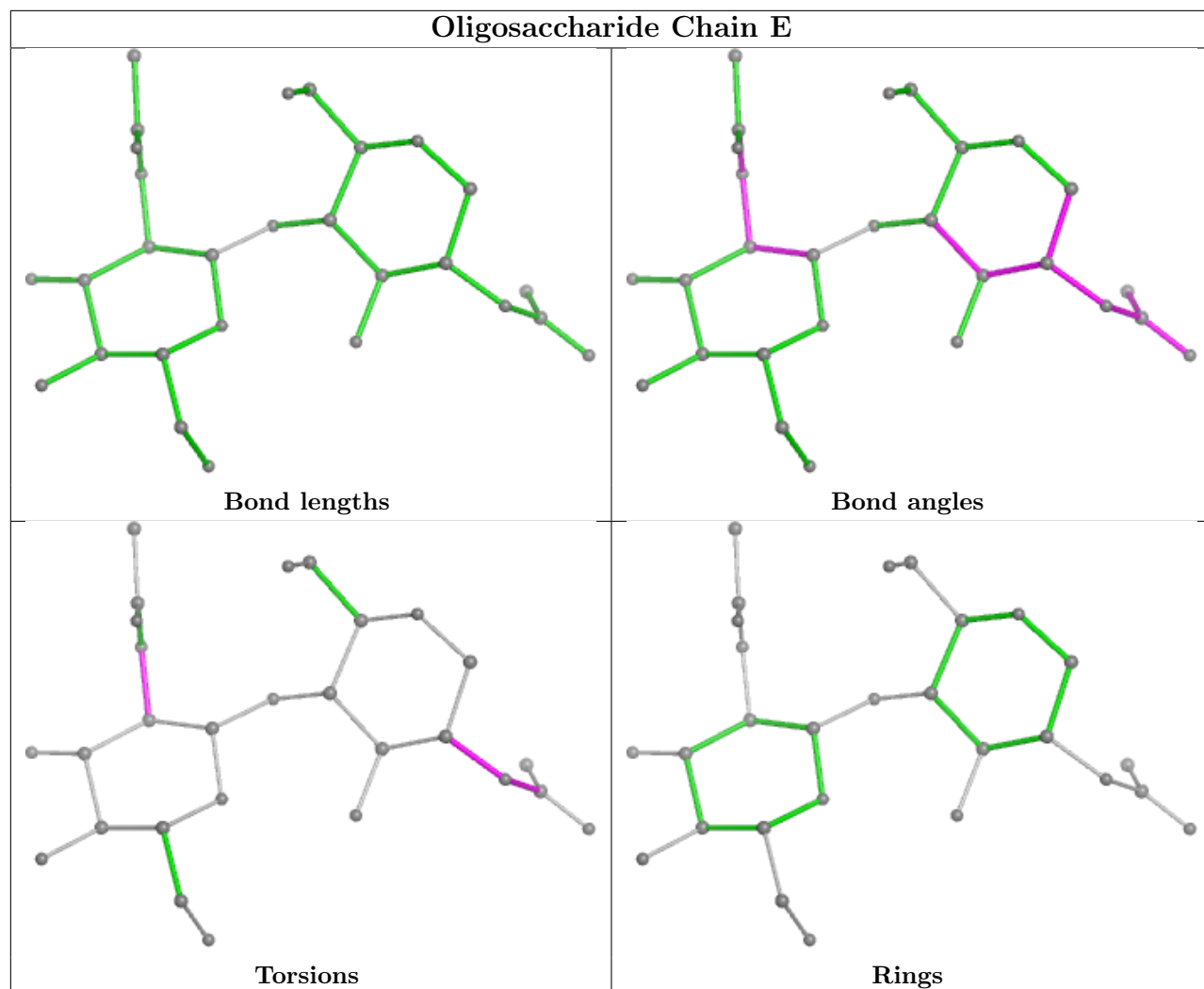
There are no ring outliers.

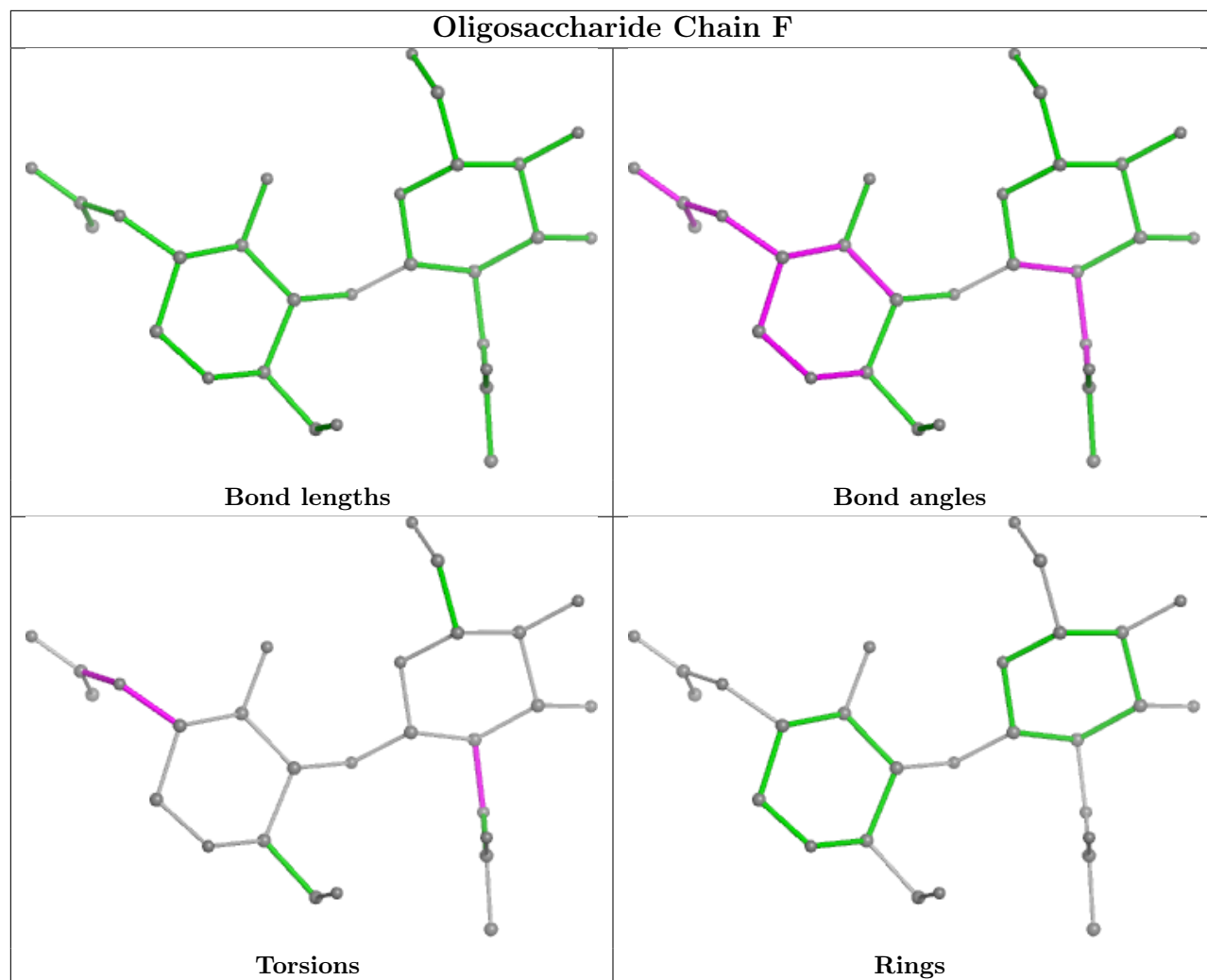
3 monomers are involved in 3 short contacts:

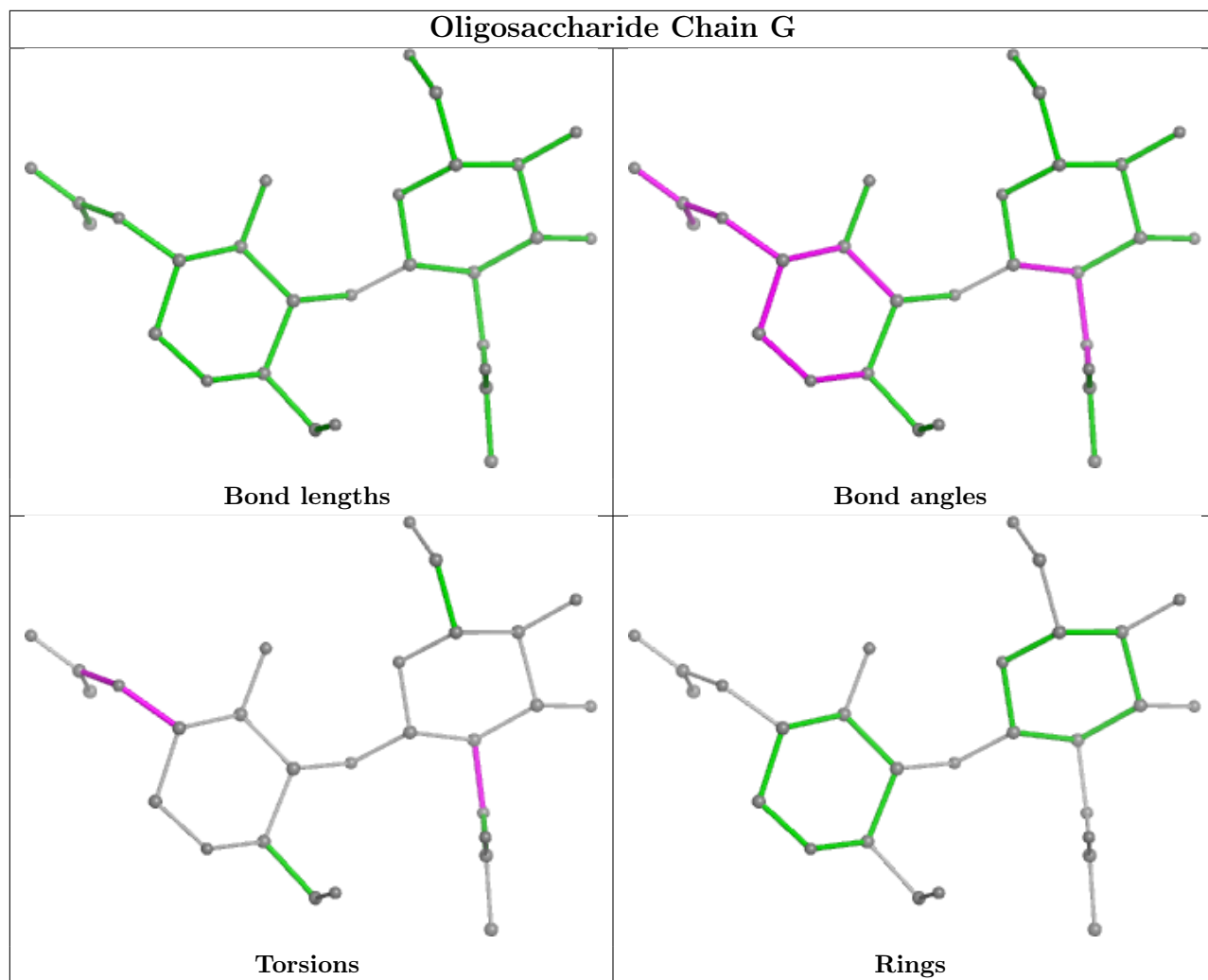
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	E	1	NAG	1	0
2	F	1	NAG	1	0

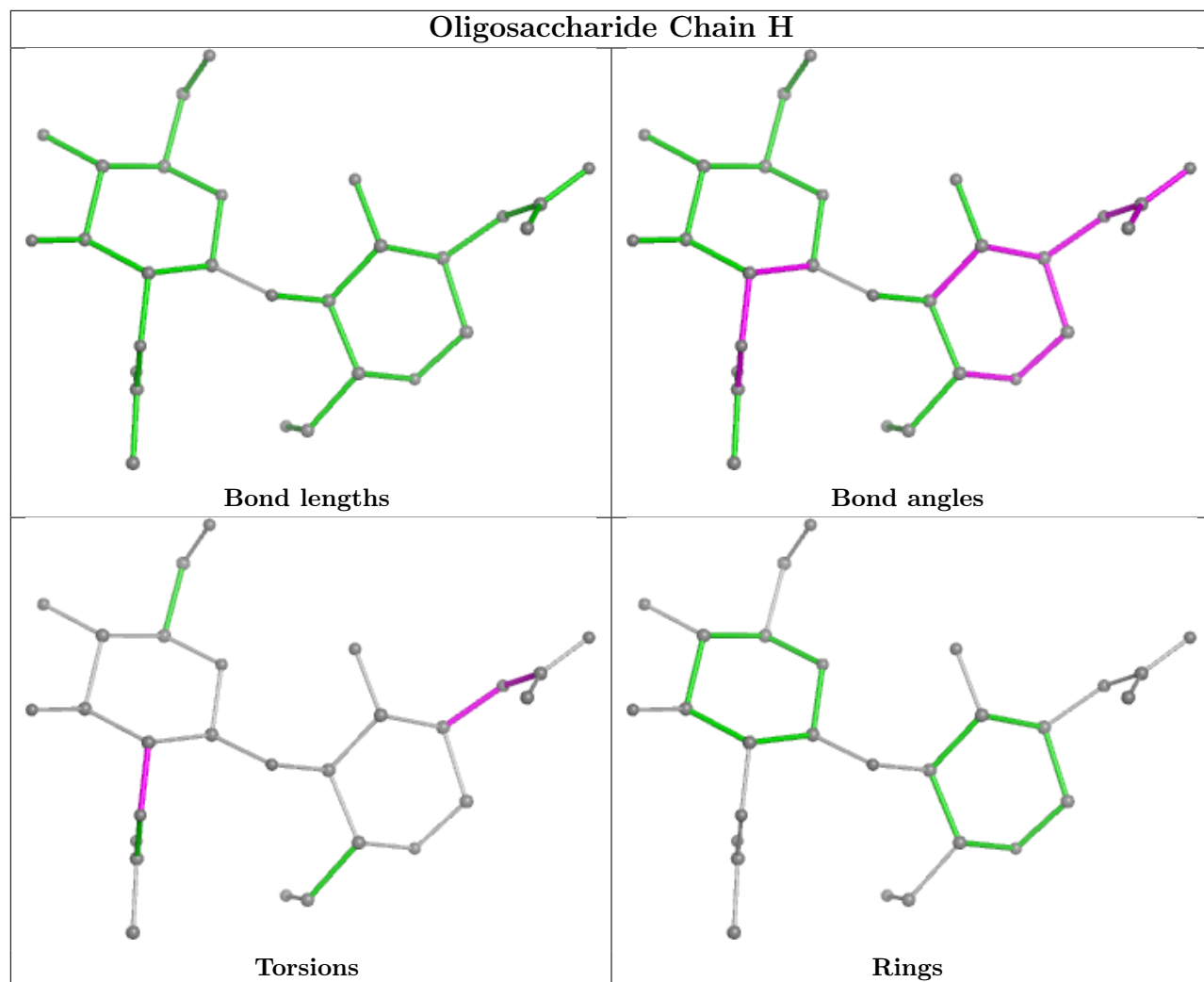
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

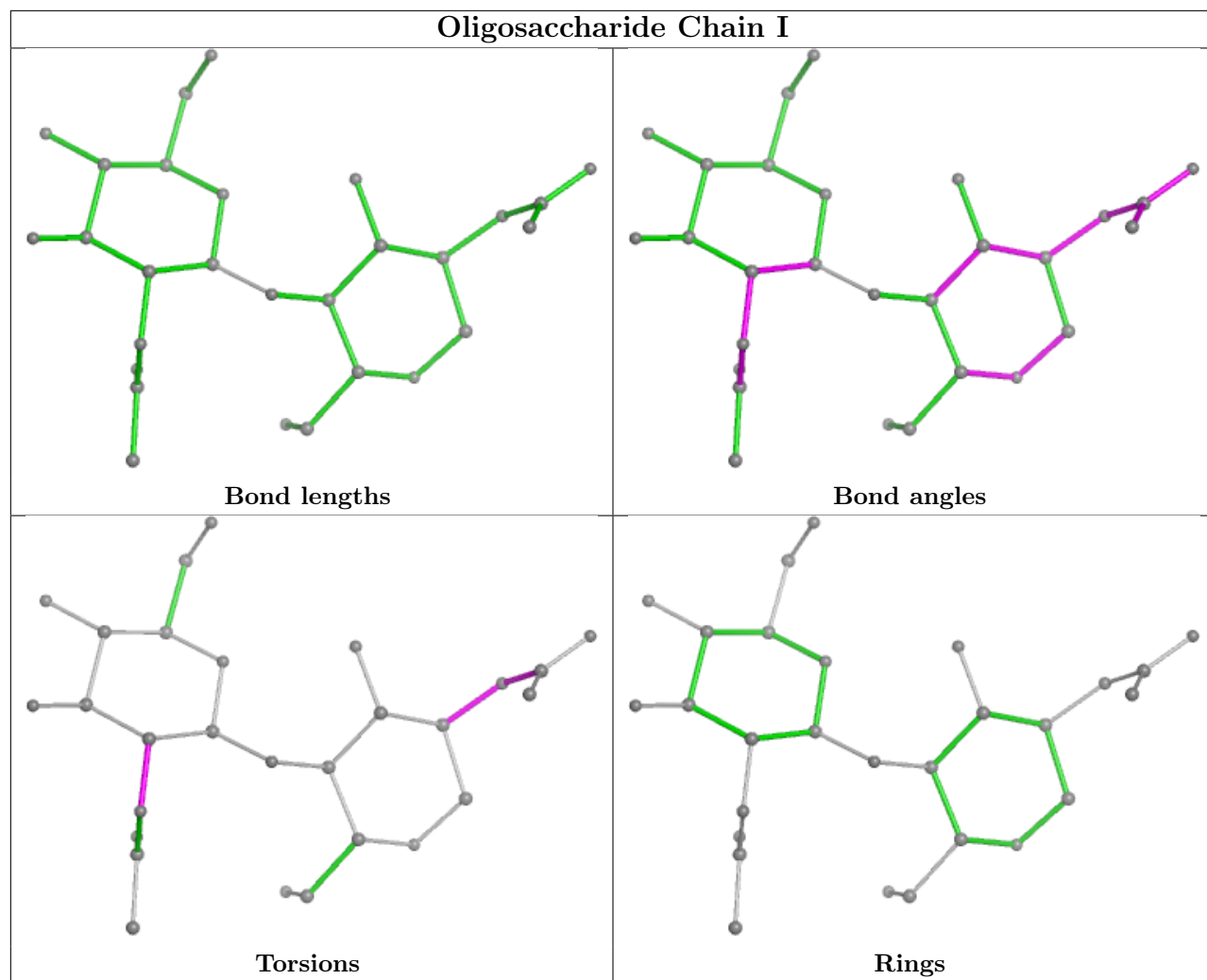


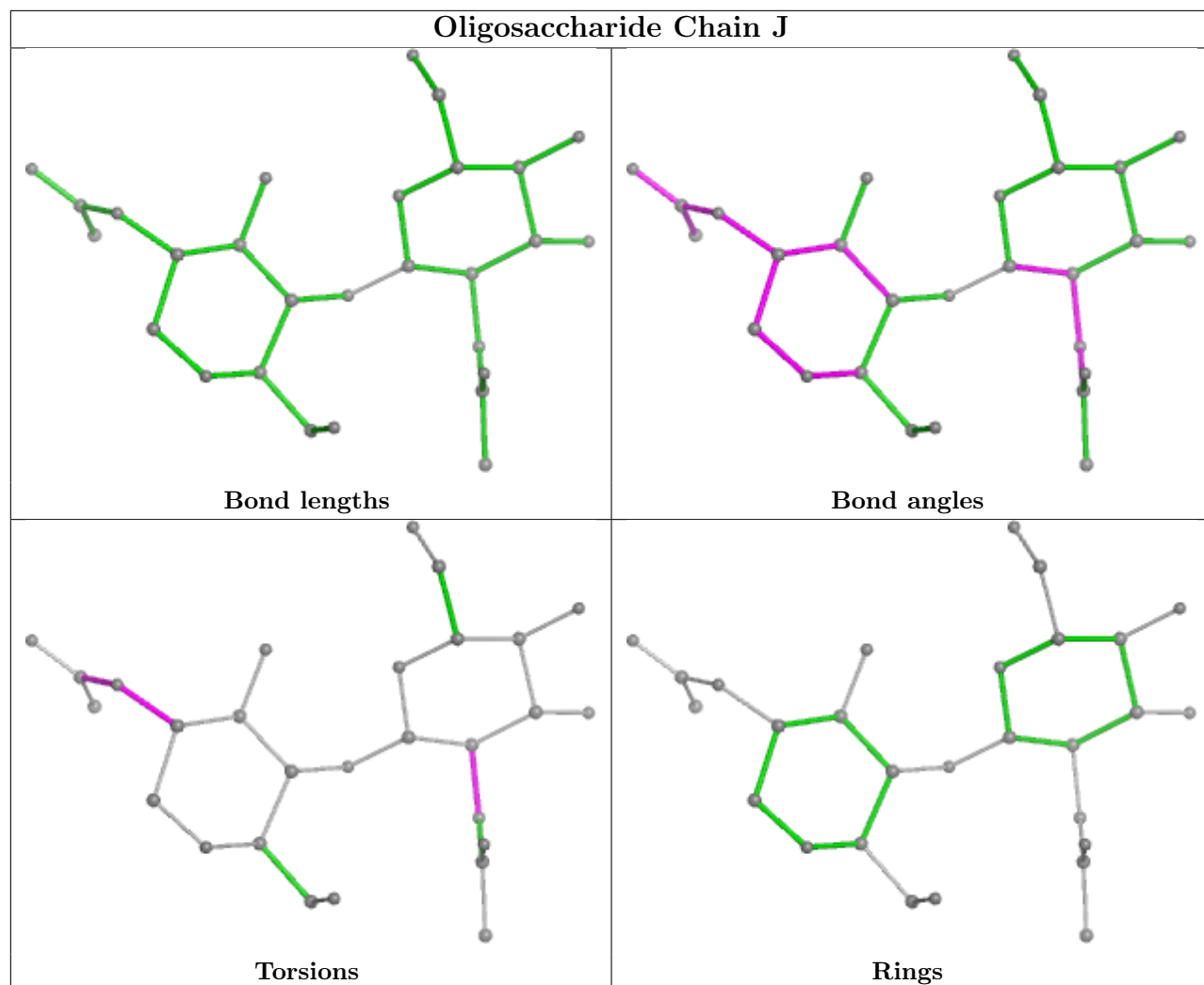


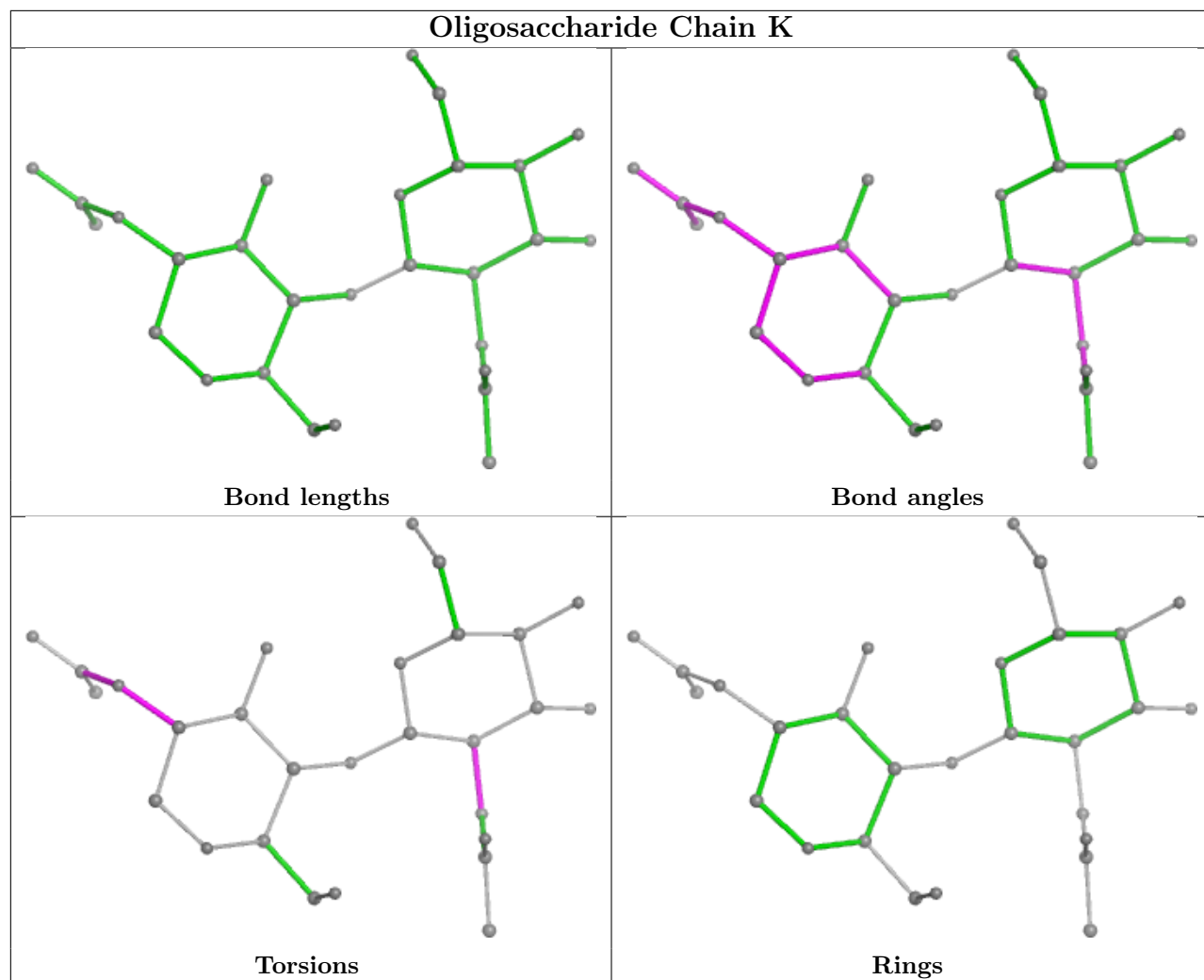


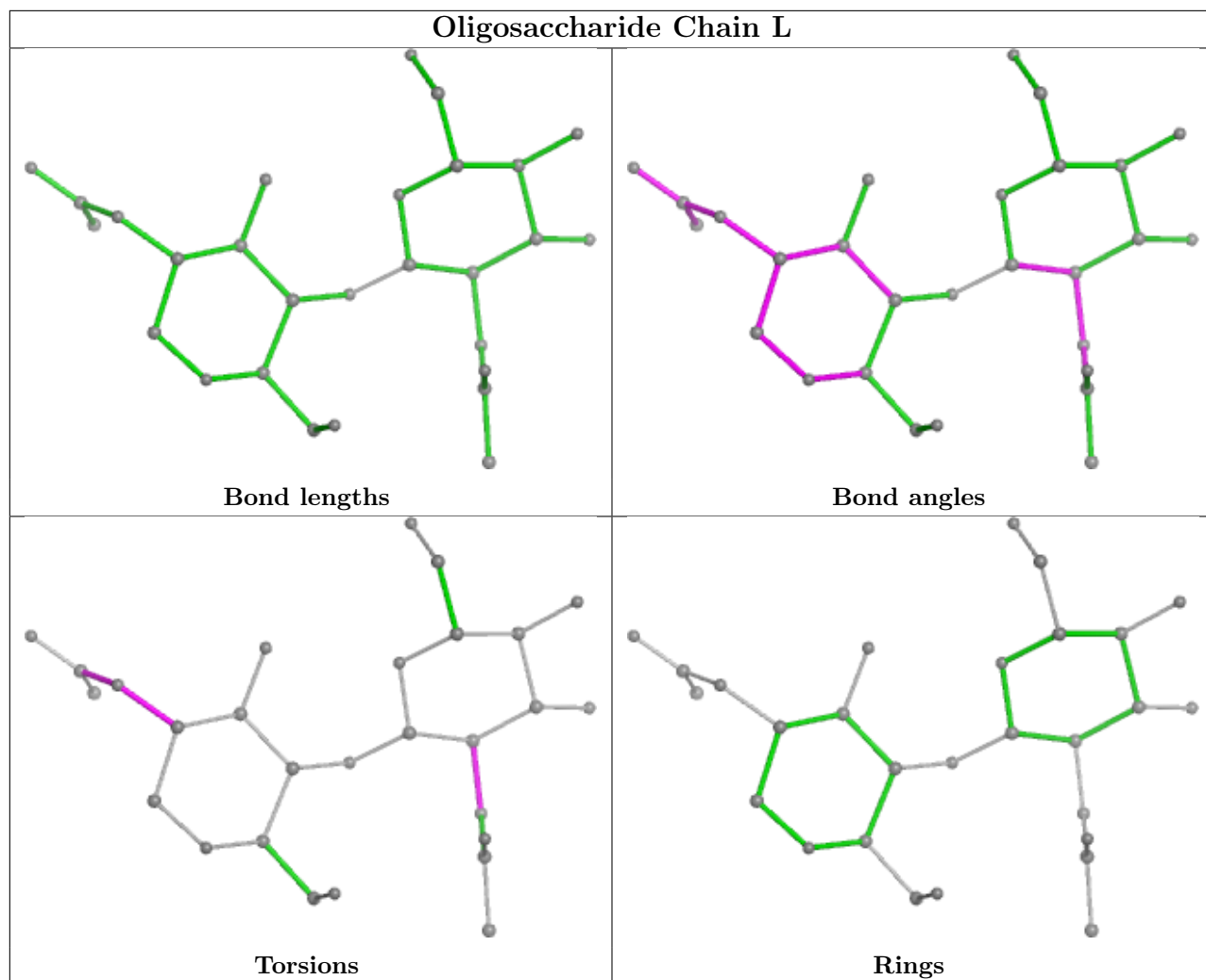


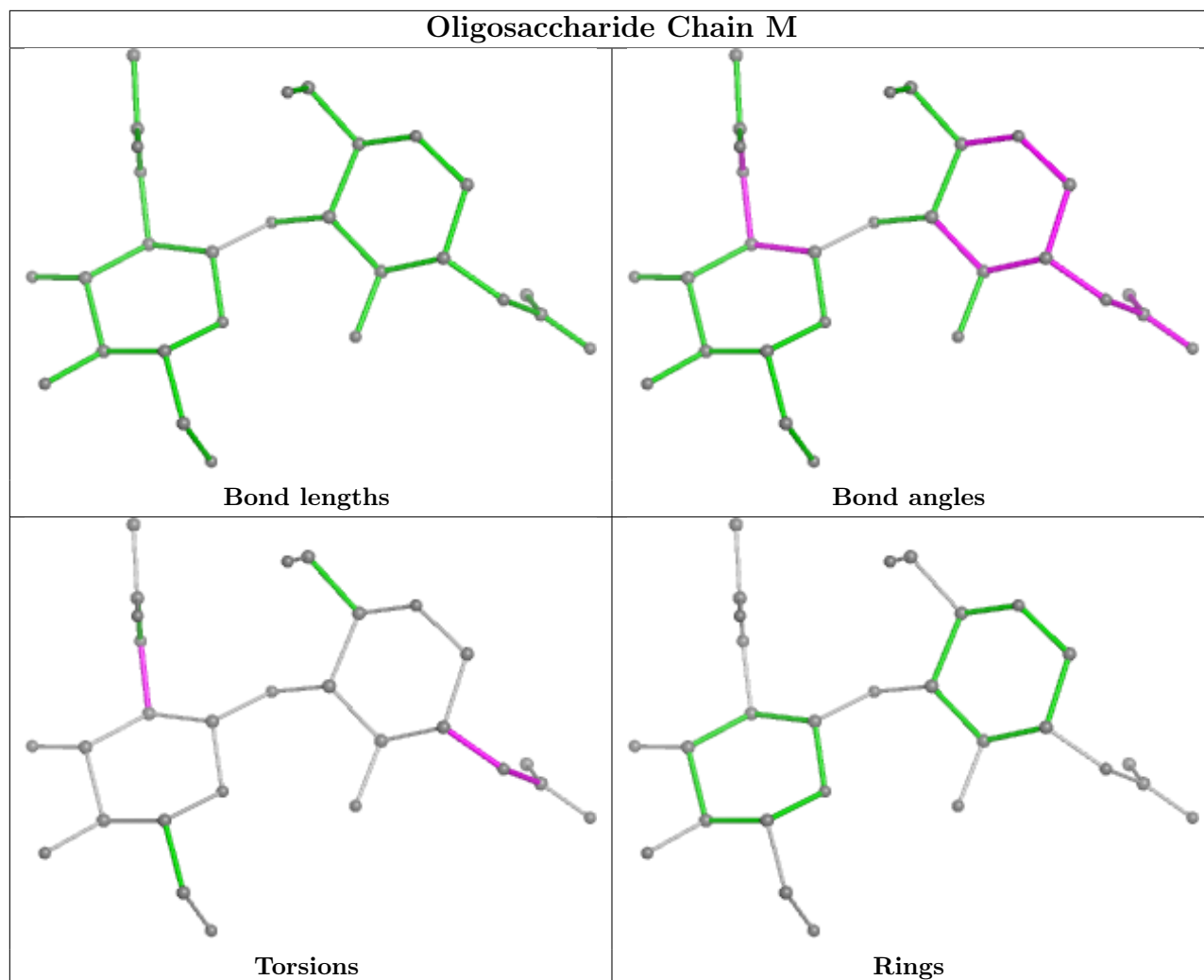












5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 for Mogul analysis.

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	1308	1	14,14,15	0.46	0	17,19,21	1.96	5 (29%)
3	NAG	A	1305	1	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
3	NAG	C	1304	1	14,14,15	0.46	0	17,19,21	1.58	3 (17%)
3	NAG	B	1305	1	14,14,15	0.54	0	17,19,21	1.45	3 (17%)

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	0.47	0	17,19,21	1.00	0
3	NAG	B	1309	1	14,14,15	0.90	1 (7%)	17,19,21	1.72	4 (23%)
3	NAG	C	1301	1	14,14,15	0.47	0	17,19,21	1.42	3 (17%)
3	NAG	A	1302	1	14,14,15	0.34	0	17,19,21	0.70	0
3	NAG	B	1307	1	14,14,15	0.56	0	17,19,21	1.26	2 (11%)
3	NAG	B	1302	1	14,14,15	0.89	0	17,19,21	1.23	1 (5%)
3	NAG	A	1309	1	14,14,15	0.47	0	17,19,21	1.13	1 (5%)
3	NAG	A	1306	1	14,14,15	0.42	0	17,19,21	2.45	6 (35%)
3	NAG	C	1303	1	14,14,15	1.88	3 (21%)	17,19,21	3.23	4 (23%)
3	NAG	A	1301	1	14,14,15	0.33	0	17,19,21	0.75	1 (5%)
3	NAG	B	1301	1	14,14,15	0.59	0	17,19,21	1.51	2 (11%)
3	NAG	A	1308	1	14,14,15	0.35	0	17,19,21	0.68	0
3	NAG	A	1304	1	14,14,15	0.36	0	17,19,21	1.26	2 (11%)
3	NAG	C	1306	1	14,14,15	0.47	0	17,19,21	1.57	3 (17%)
3	NAG	A	1307	1	14,14,15	0.63	0	17,19,21	1.63	2 (11%)
3	NAG	C	1305	1	14,14,15	0.45	0	17,19,21	0.75	0
3	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	0.66	0
3	NAG	B	1303	1	14,14,15	0.59	0	17,19,21	0.93	1 (5%)
3	NAG	C	1302	1	14,14,15	0.46	0	17,19,21	1.48	3 (17%)
3	NAG	B	1306	1	14,14,15	0.57	0	17,19,21	1.13	3 (17%)
5	XIO	C	1307	4	88,101,101	2.10	24 (27%)	110,143,143	1.07	7 (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
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1304	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	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	XIO	C	1307	4	-	23/67/85/85	0/9/9/9

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1307	XIO	C08-N09	7.01	1.49	1.34
5	C	1307	XIO	C43-N44	6.82	1.48	1.34
5	C	1307	XIO	C02-N71	6.49	1.47	1.34
5	C	1307	XIO	C37-N36	6.45	1.45	1.34
3	C	1303	NAG	C1-C2	5.91	1.61	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1303	NAG	C1-O5-C5	11.52	127.80	112.19
3	A	1306	NAG	C2-N2-C7	6.02	131.47	122.90
3	A	1306	NAG	C8-C7-N2	5.76	125.85	116.10
3	B	1308	NAG	C8-C7-N2	5.14	124.81	116.10
3	A	1307	NAG	O5-C1-C2	-4.64	103.95	111.29

There are no chirality outliers.

5 of 67 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

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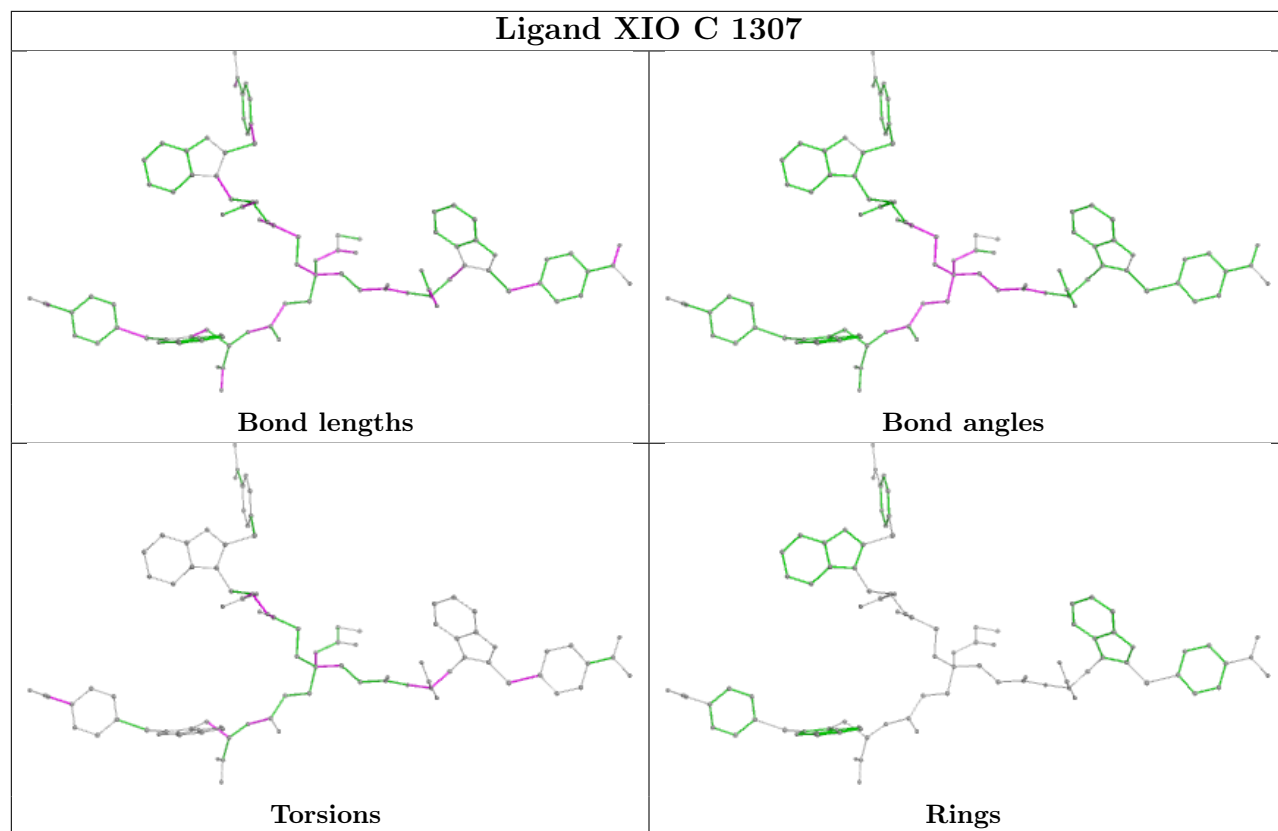
Mol	Chain	Res	Type	Atoms
5	C	1307	XIO	N09-C10-C11-C12
5	C	1307	XIO	C31-C10-N09-C08
5	C	1307	XIO	C06-C05-N36-C37

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1308	NAG	2	0
3	A	1306	NAG	1	0
3	A	1308	NAG	1	0
3	C	1305	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

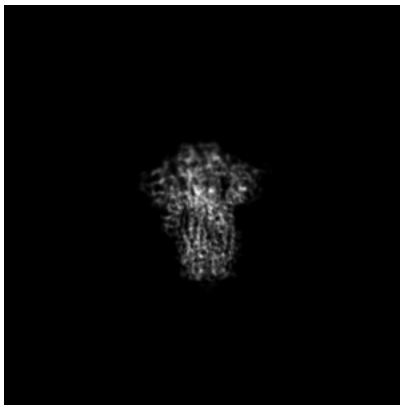
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17578. These allow visual inspection of the internal detail of the map and identification of artifacts.

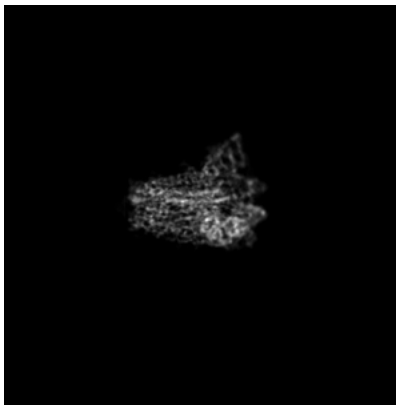
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

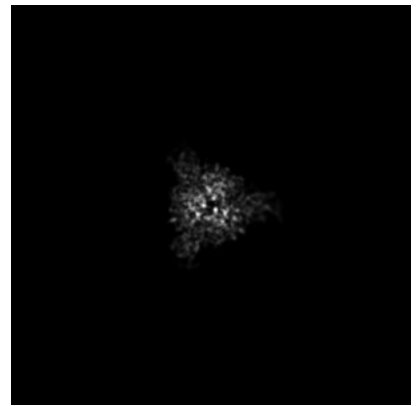
6.1.1 Primary map



X

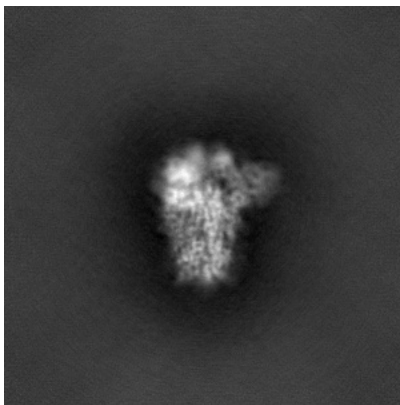


Y

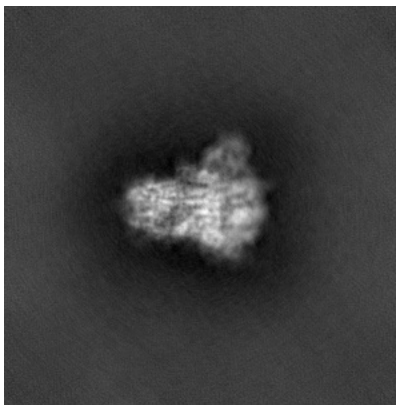


Z

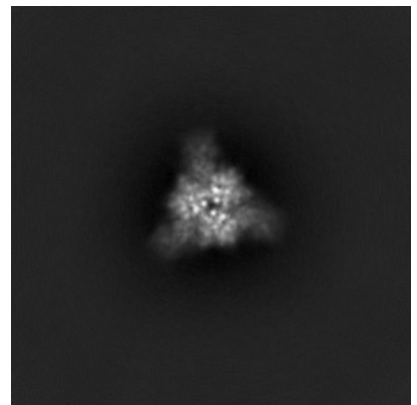
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

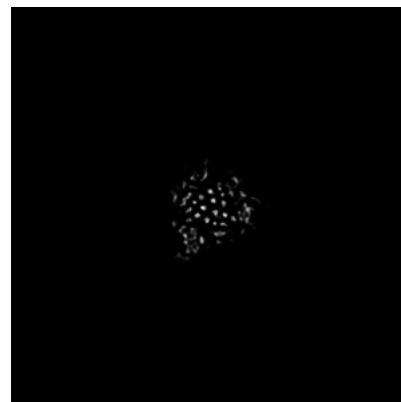
6.2.1 Primary map



X Index: 246

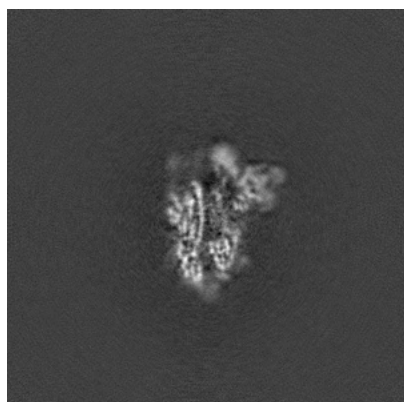


Y Index: 246

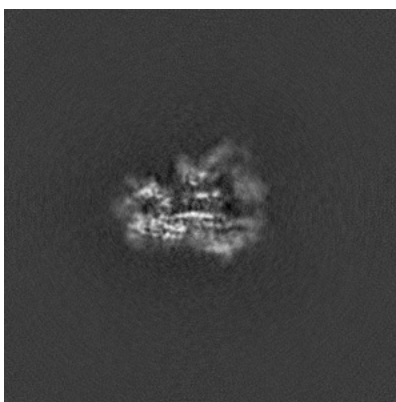


Z Index: 246

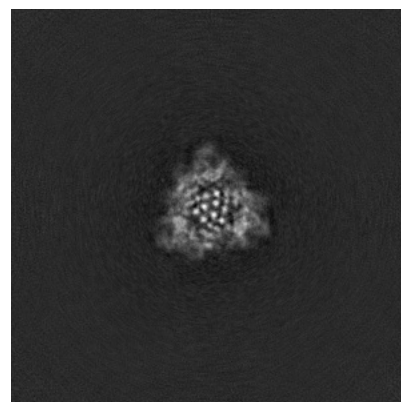
6.2.2 Raw map



X Index: 246



Y Index: 246



Z Index: 246

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: 251

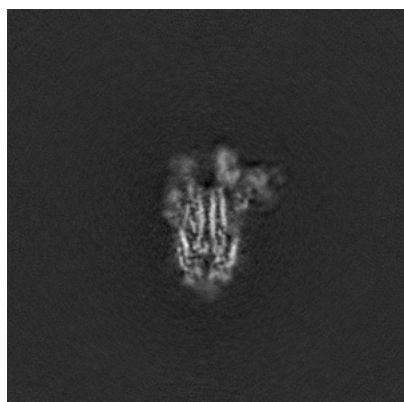


Y Index: 239

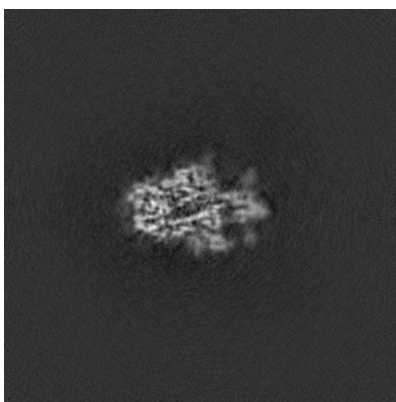


Z Index: 248

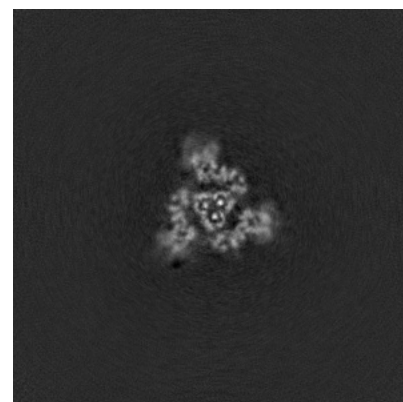
6.3.2 Raw map



X Index: 251



Y Index: 260

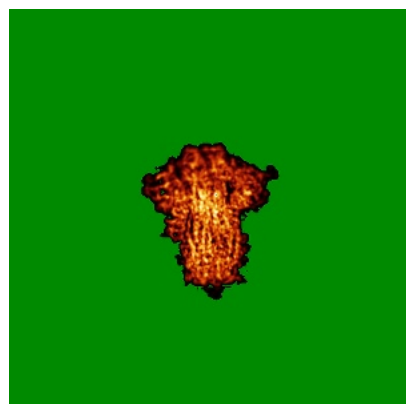


Z Index: 262

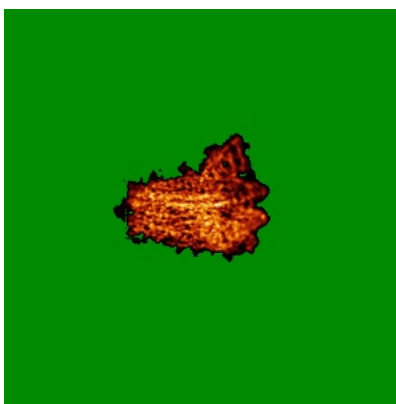
The images above show the largest variance slices of the map in three orthogonal directions.

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

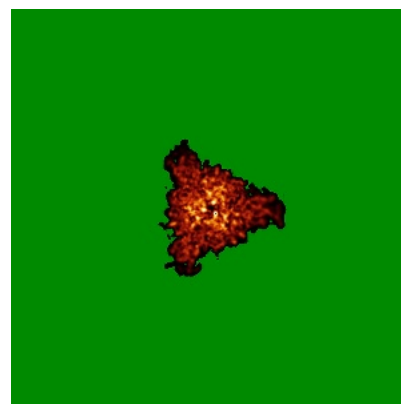
6.4.1 Primary map



X

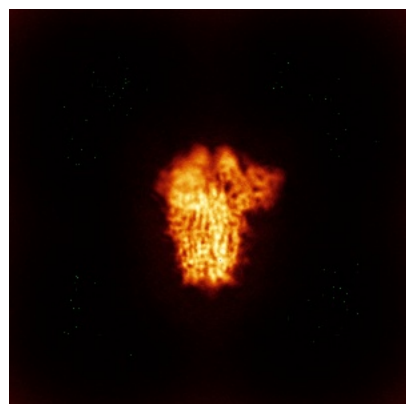


Y

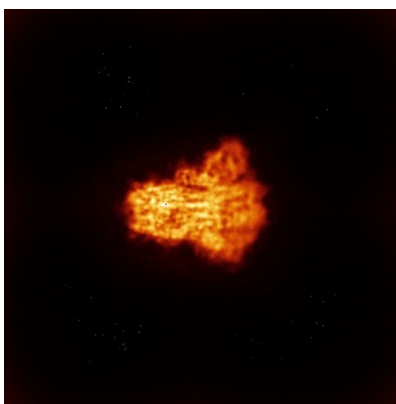


Z

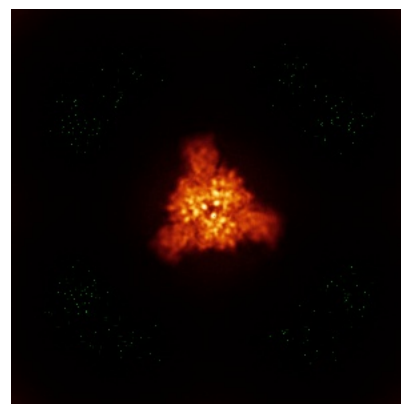
6.4.2 Raw map



X



Y



Z

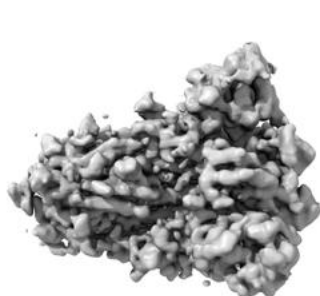
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

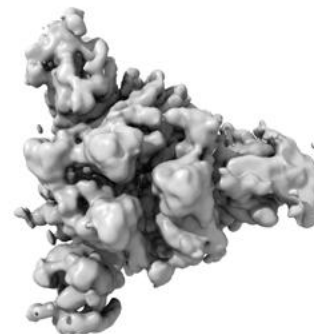
6.5.1 Primary map



X



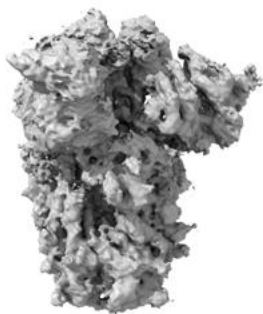
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

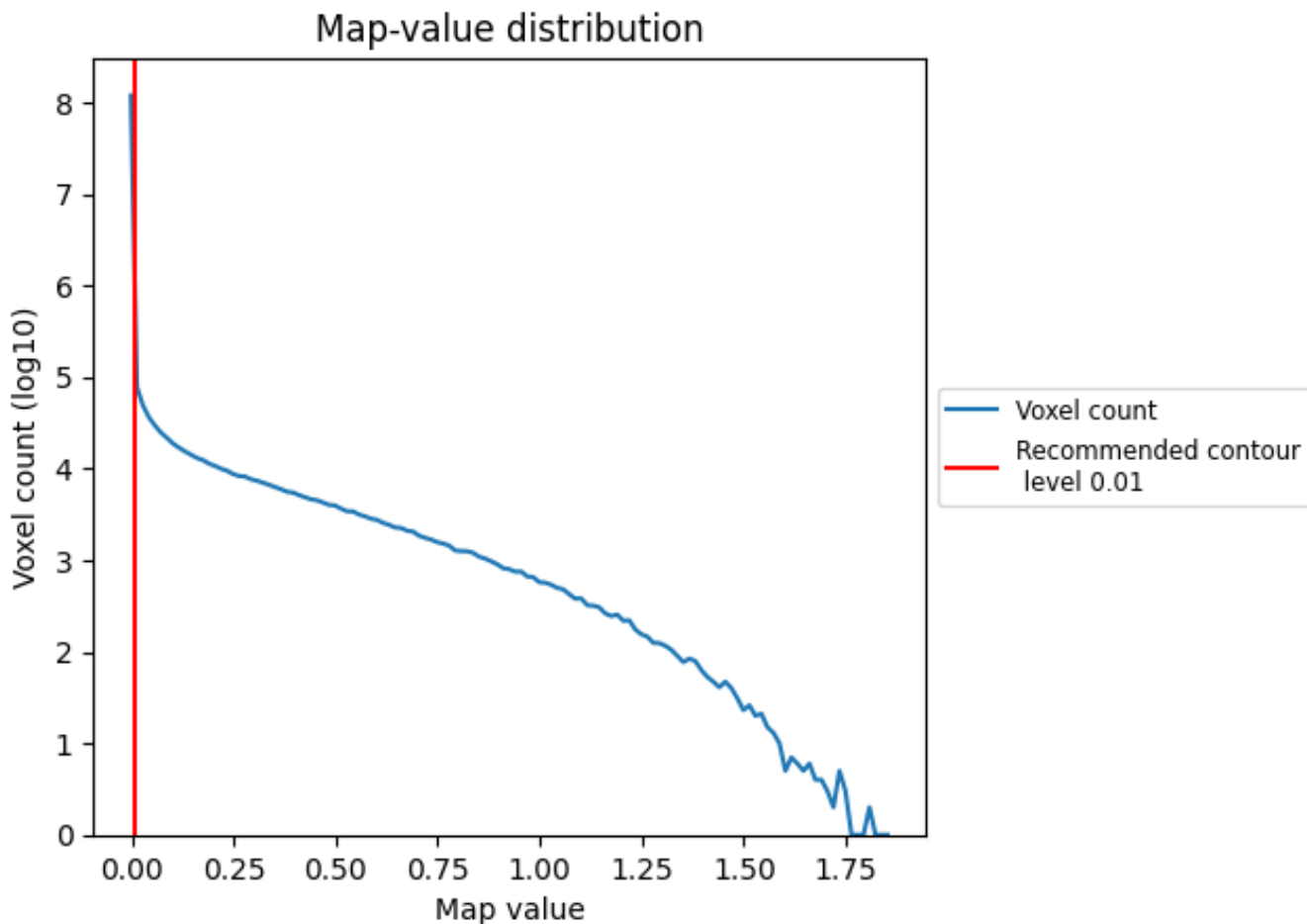
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

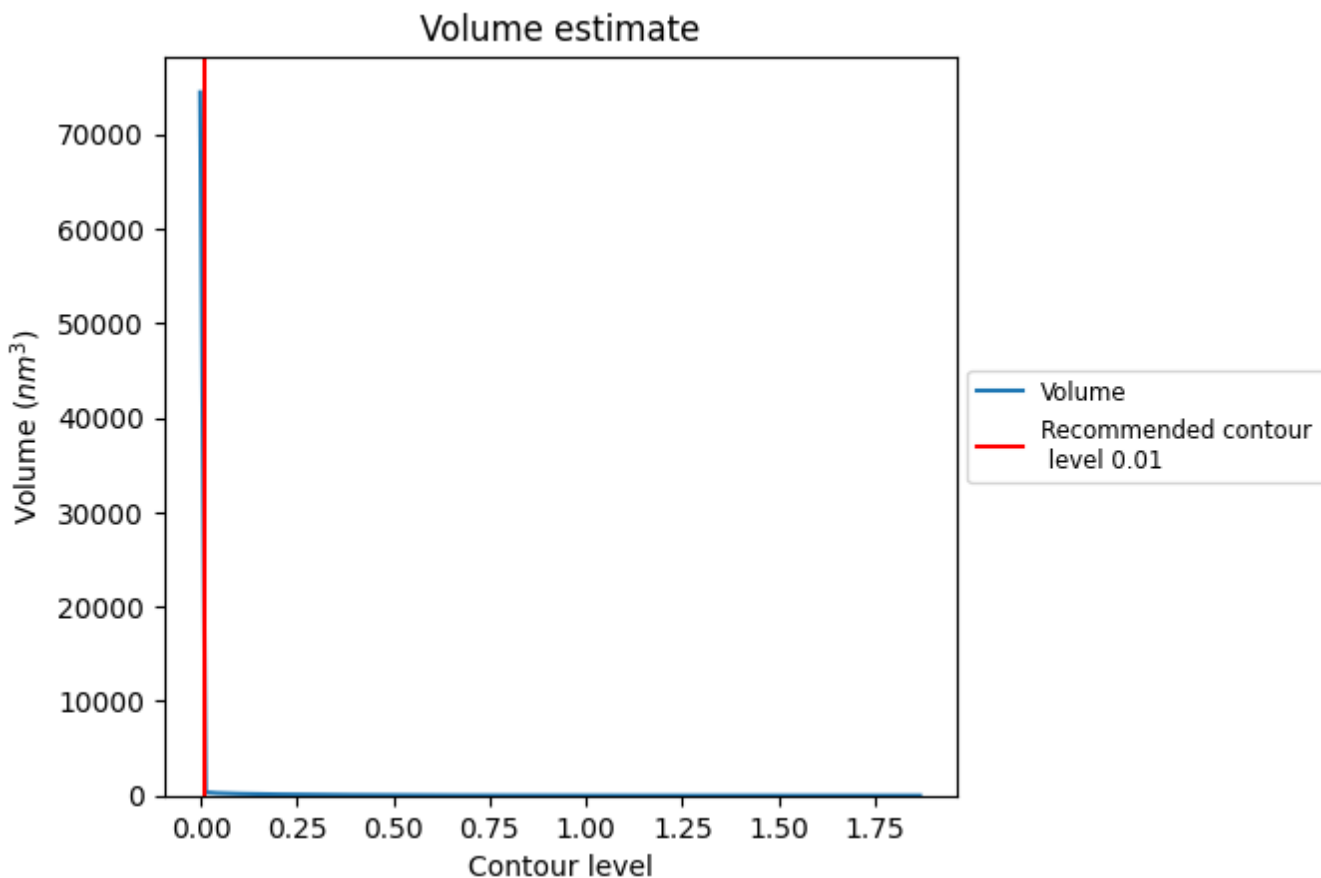
This section contains the results of statistical analysis of the map.

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.

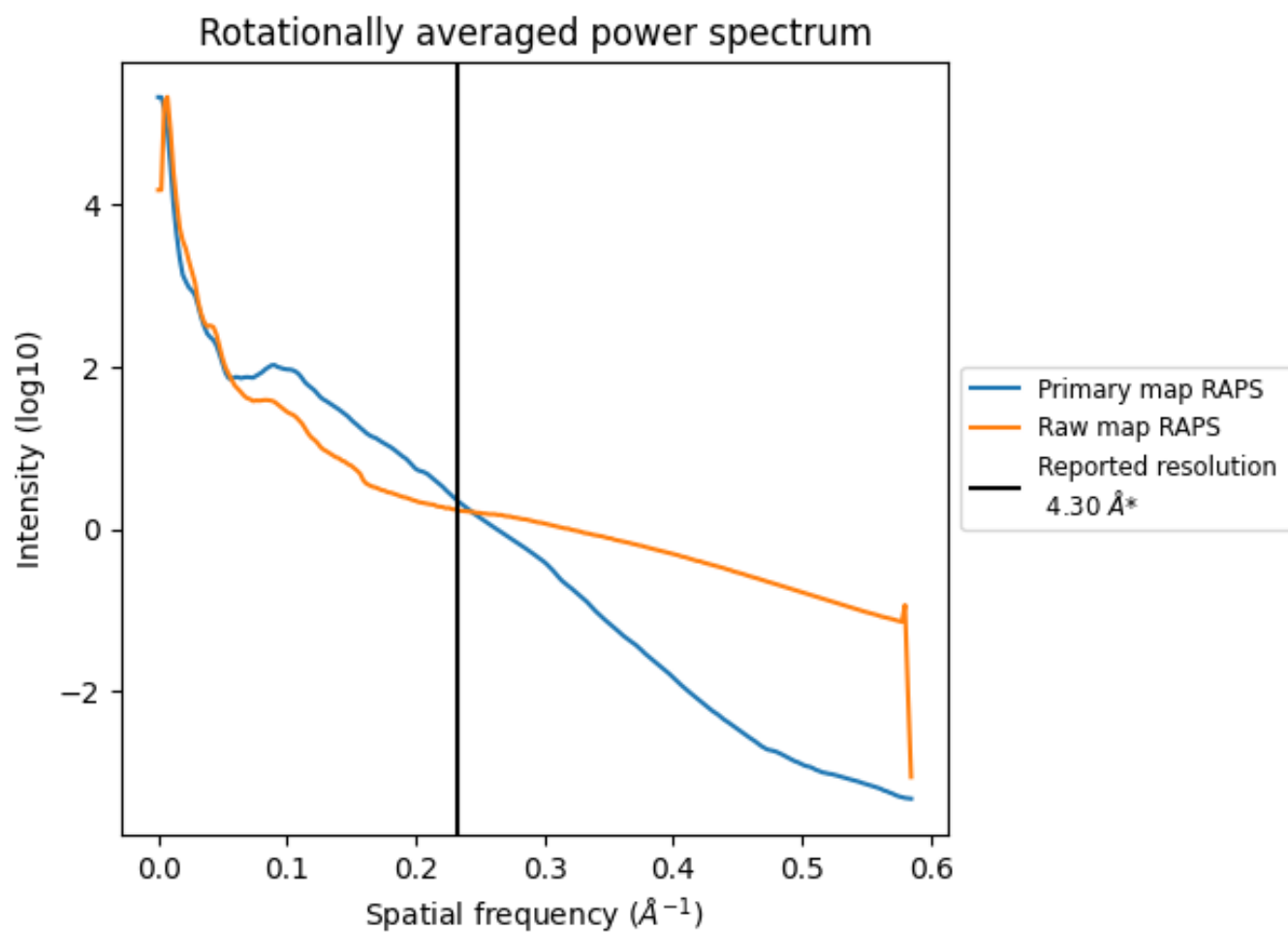
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 15139 nm³; this corresponds to an approximate mass of 13676 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](#)

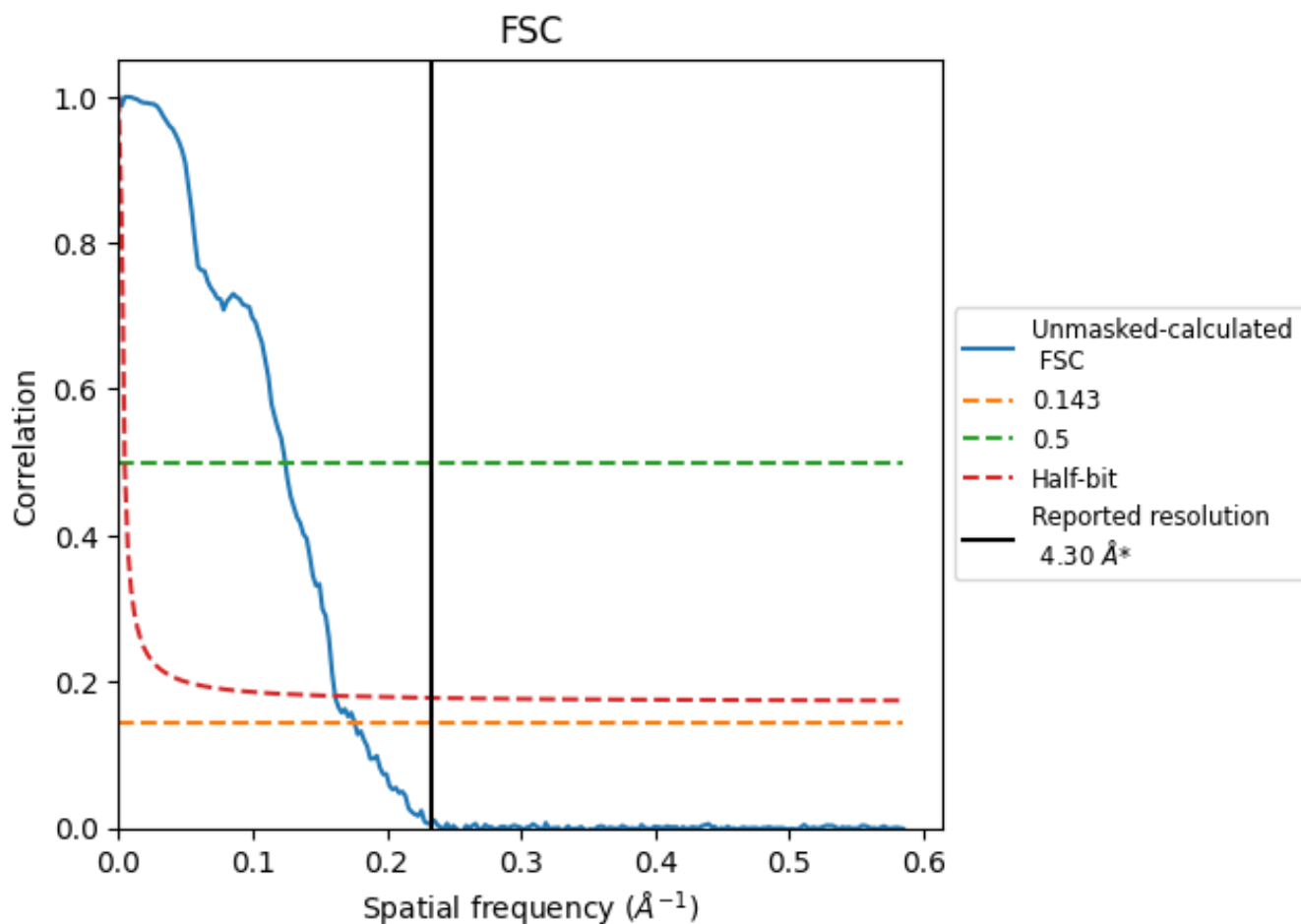


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

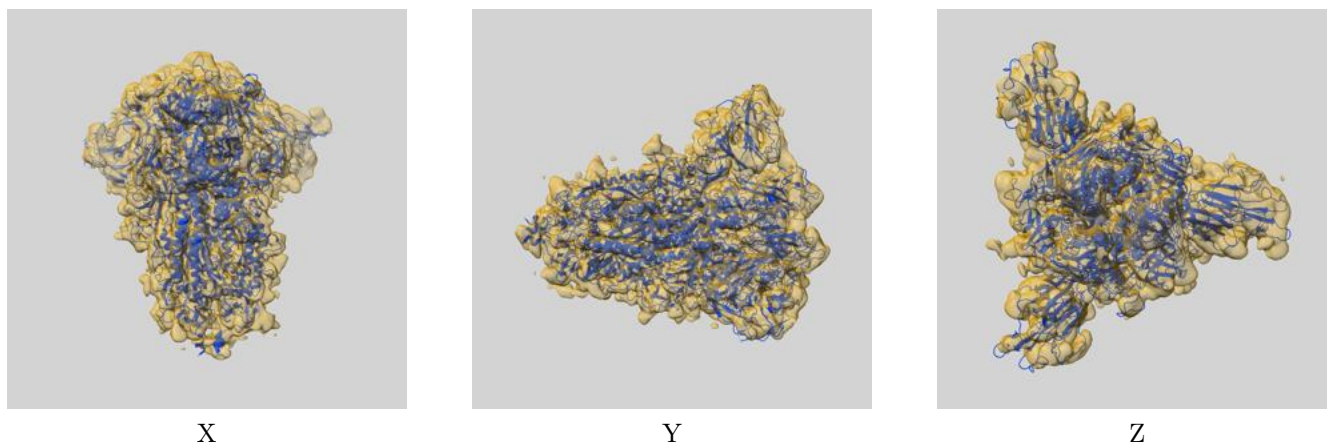
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.68	8.05	6.19

*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 5.68 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17578 and PDB model 8P9Y. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



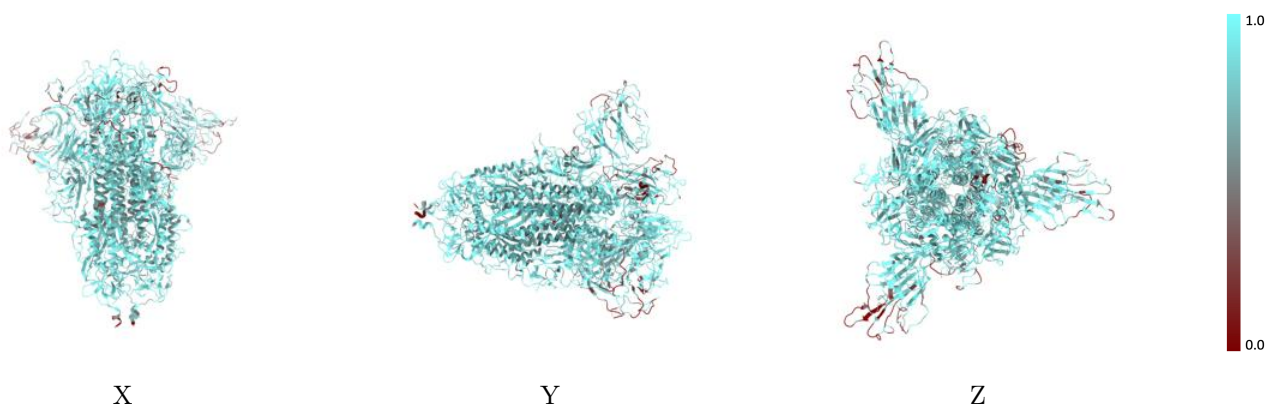
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



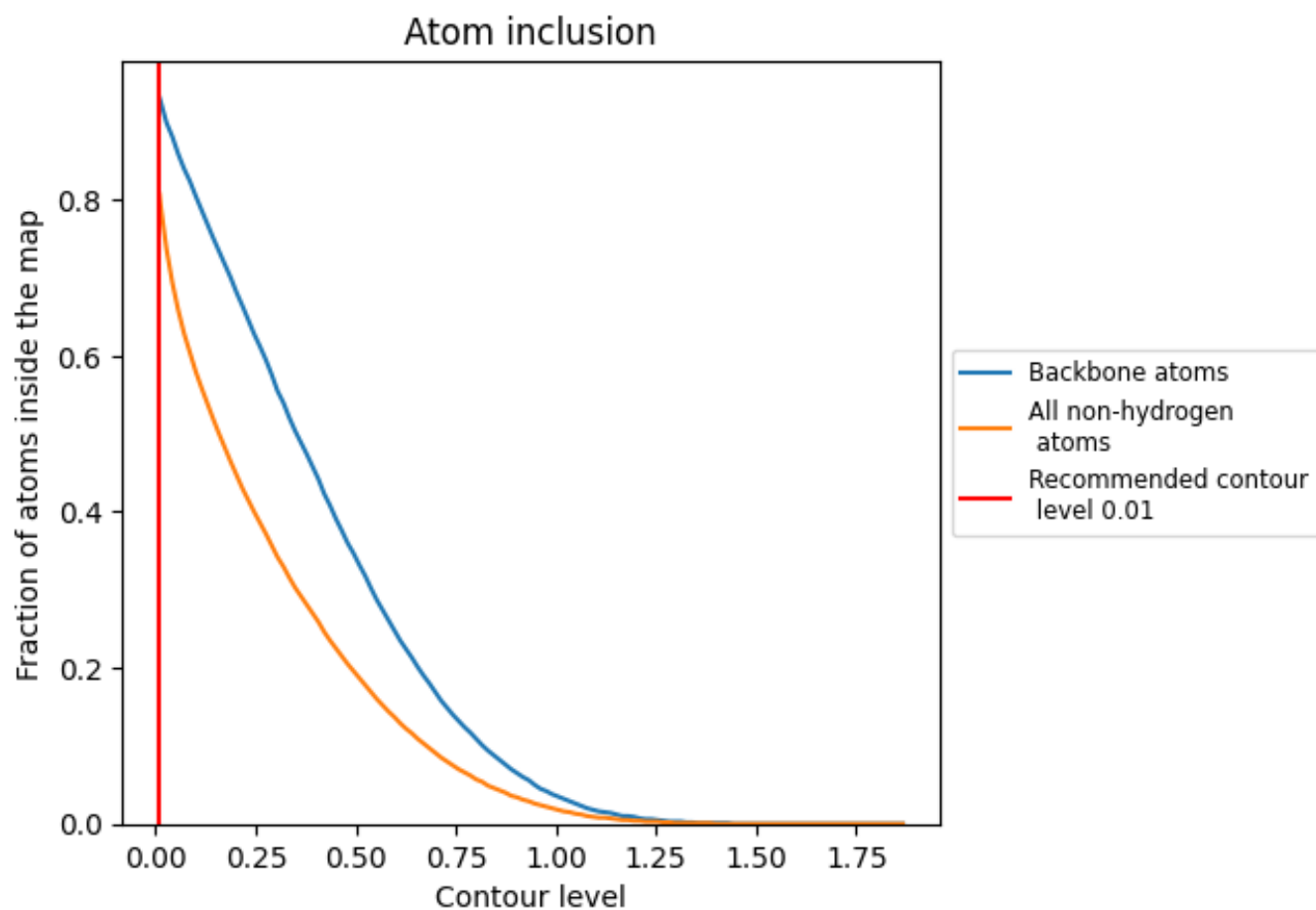
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 81% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.1170
A	 0.7830	 0.1110
B	 0.8340	 0.1200
C	 0.8070	 0.1170
D	 0.9640	 0.2830
E	 1.0000	 0.2490
F	 0.5710	 0.0870
G	 0.9290	 0.2820
H	 0.2860	 -0.0580
I	 1.0000	 0.2100
J	 0.4290	 0.0340
K	 0.8930	 0.2470
L	 0.6790	 0.1960
M	 1.0000	 0.2090

