wwPDB EM Validation Summary Report (i)

Mar 9, 2026 – 05:07 PM UTC

PDB ID	:	8P9Y / pdb_00008p9y
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 (i) symbol.

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

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

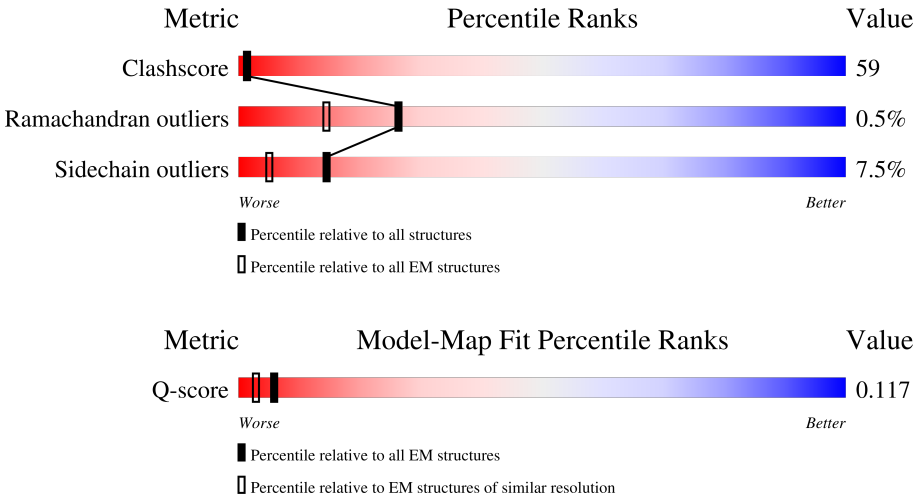
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	1270	9% 42% 38% 5% 15%
1	B	1270	41% 39% 5% 15%
1	C	1270	5% 40% 38% 6% 15%
2	D	2	100%

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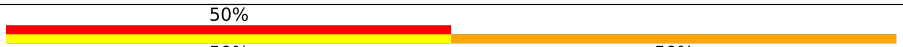
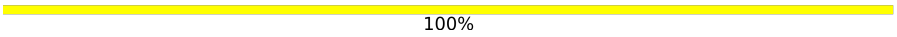
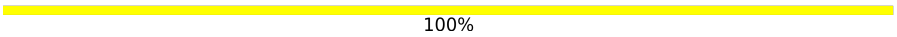
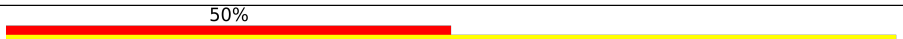
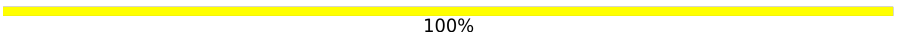
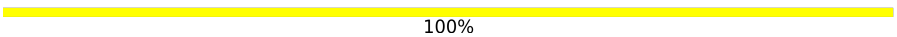
Mol	Chain	Length	Quality of chain
2	E	2	
2	F	2	
2	G	2	
2	H	2	
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	

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
1	A	1080	Total	C	N	O	S	0	0
			8425	5378	1403	1606	38		
1	B	1081	Total	C	N	O	S	0	0
			8426	5379	1403	1606	38		
1	C	1076	Total	C	N	O	S	0	0
			8374	5346	1395	1595	38		

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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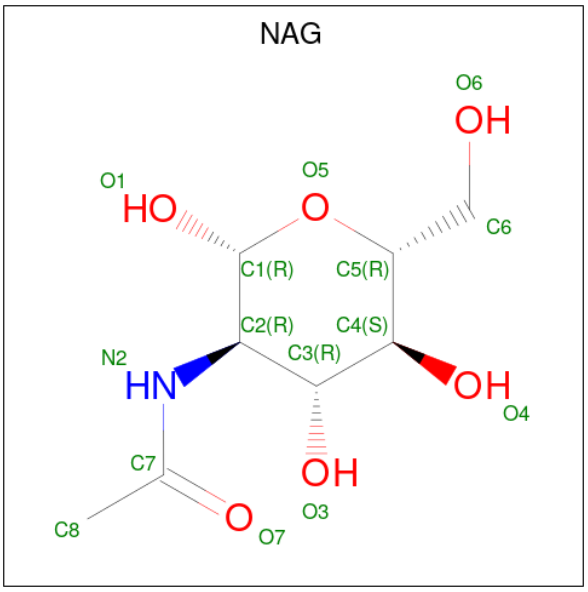
Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	PRO	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	ASP	-	expression tag	UNP P0DTC2
C	1229	GLY	-	expression tag	UNP P0DTC2
C	1230	GLN	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	TYR	-	expression 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	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	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

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



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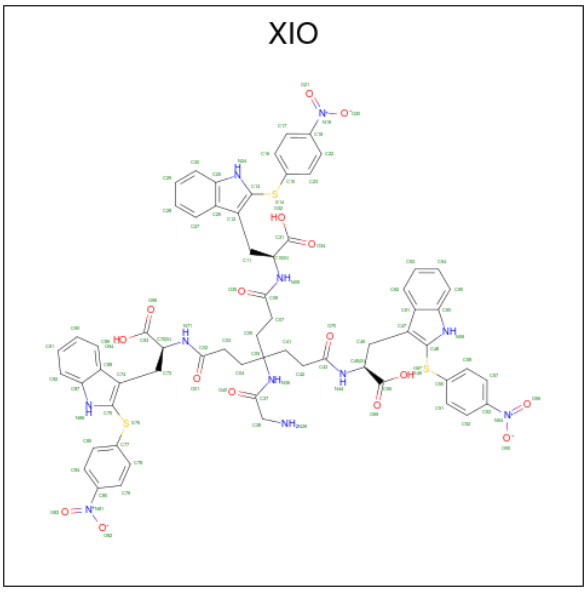
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C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

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

Mol	Chain	Residues	Atoms		AltConf
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 (CCD ID: XIO) (formula: $C_{63}H_{59}N_{11}O_{16}S_3$) (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

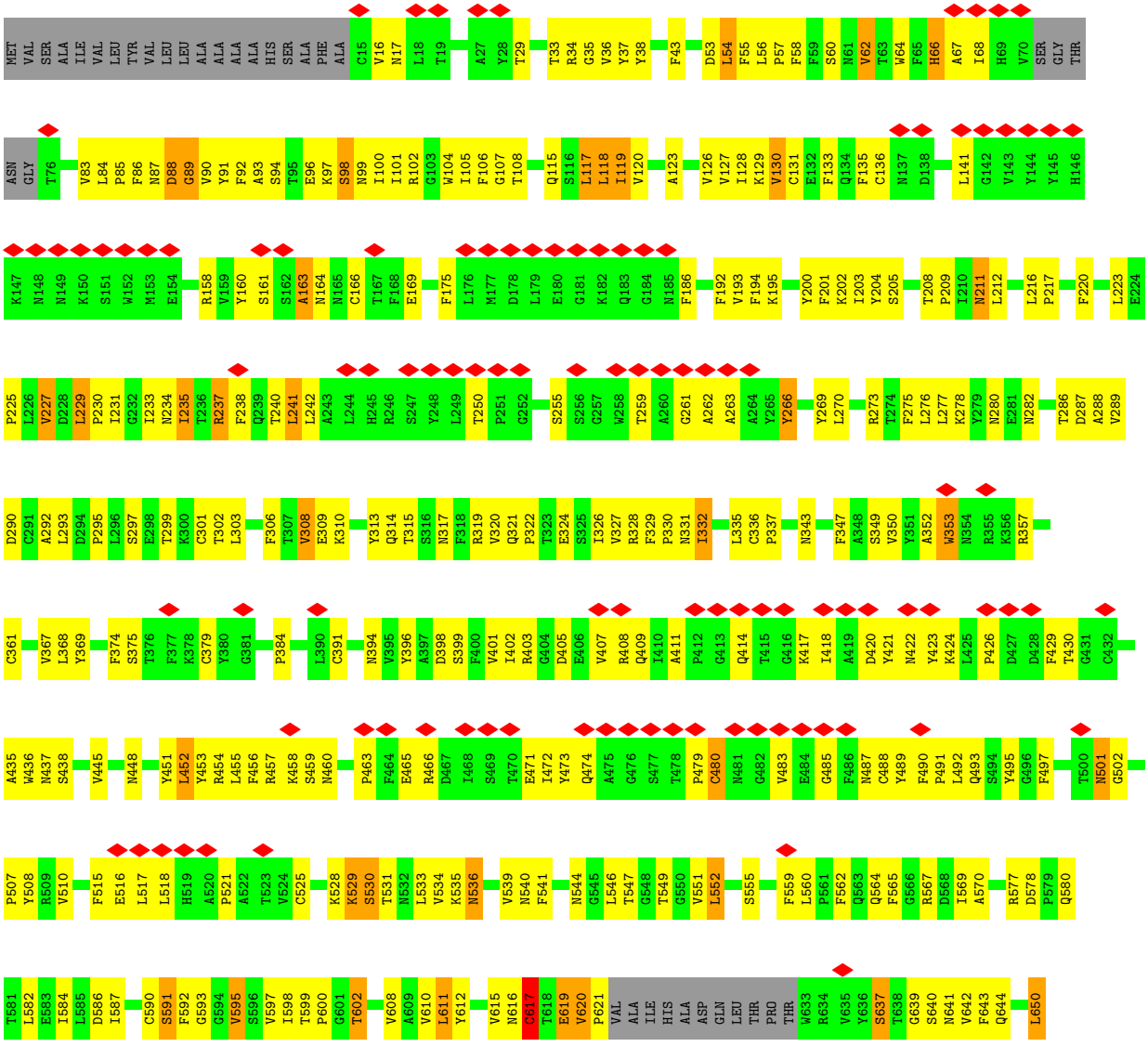
3 Residue-property plots (i)

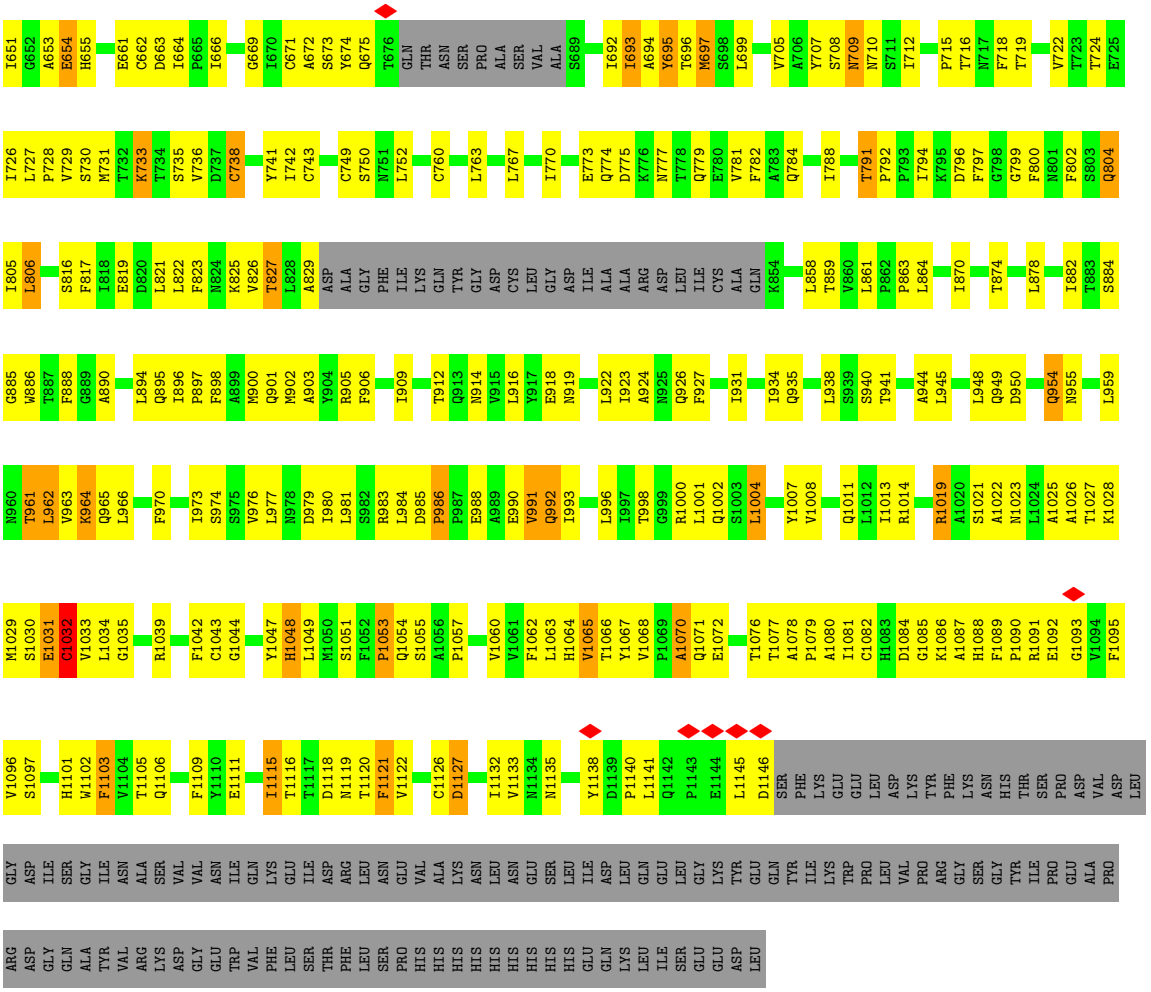
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Spike protein S1,Spike glycoprotein

Chain A:



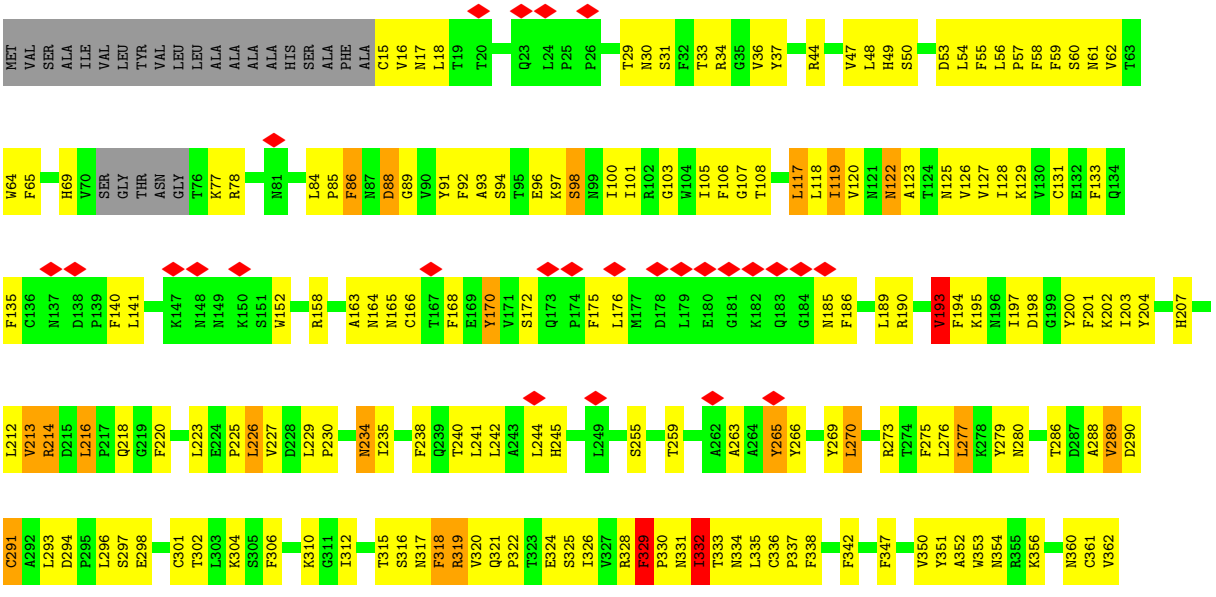


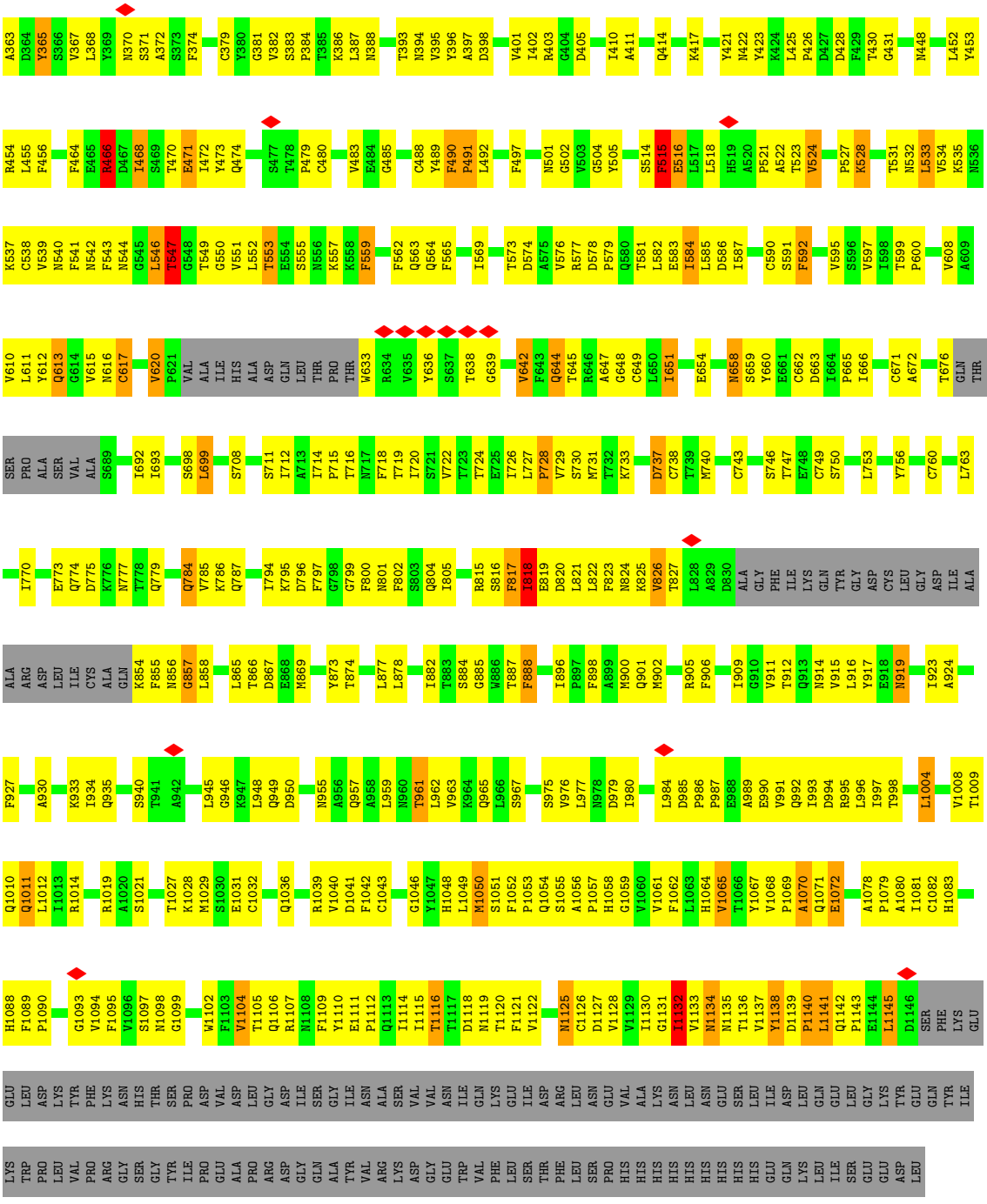


• Molecule 1: Spike protein S1,Spike glycoprotein

Chain B:



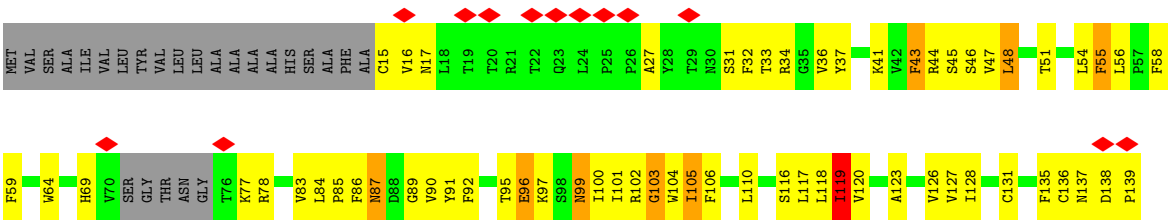


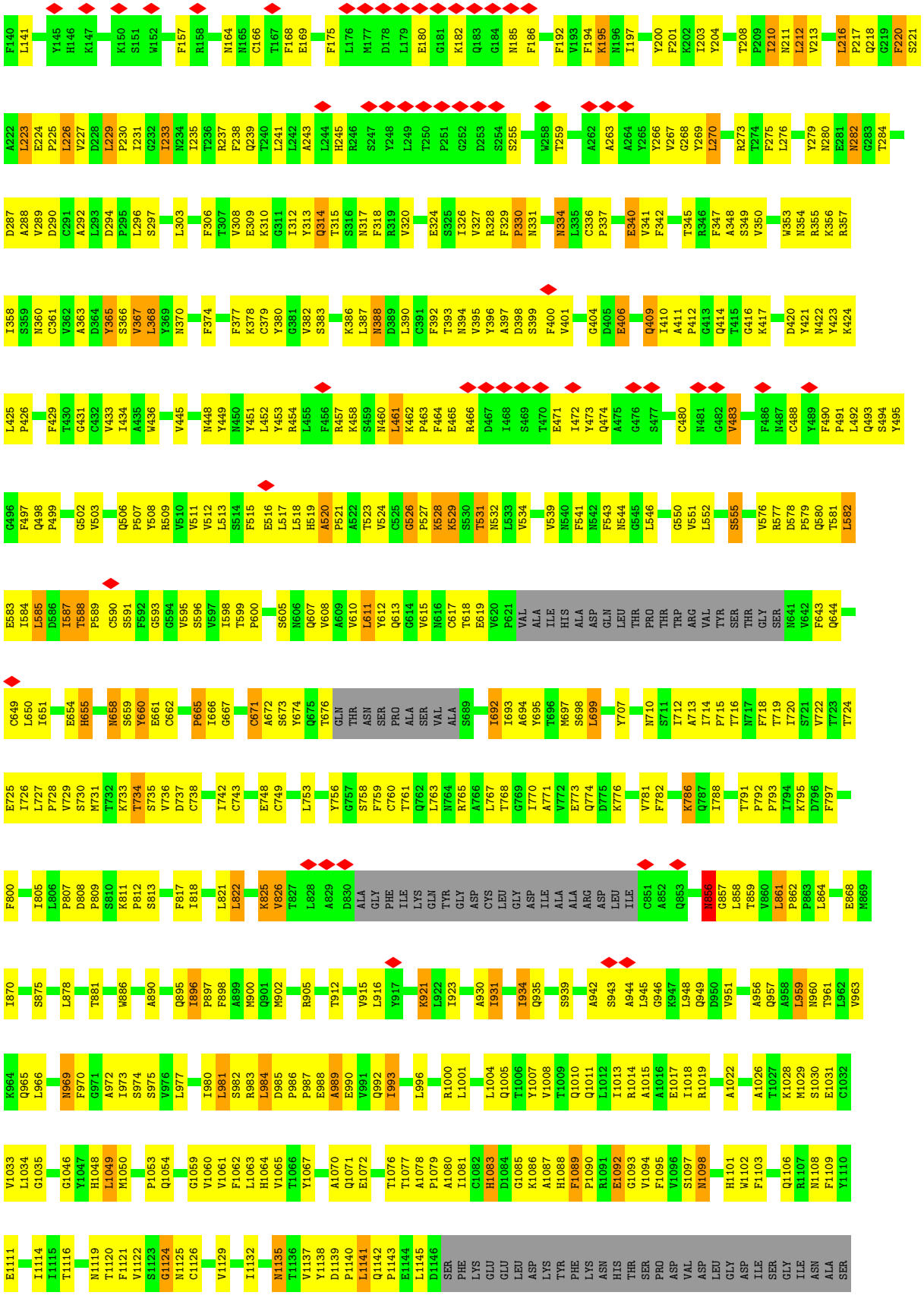


• Molecule 1: Spike protein S1,Spike glycoprotein

Chain C:





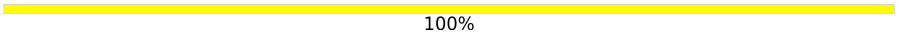

F140 L141 Y145 H146 K147 K150 S151 W152 F157 R158 N164 N165 C166 T167 F168 E169 F175 L176 M177 D178 L179 E180 G181 K182 Q183 G184 N185 F186 F192 V193 F194 K195 N196 I197 Y200 F201 K202 I203 Y204 T208 P209 I210 N211 L212 V213 L216 P217 Q218 G219 F220 S221
A222 L223 E224 P225 L226 V227 D228 L229 P230 I231 G232 T233 N234 I235 T236 R237 F238 Q239 T240 L241 L242 A243 L244 H245 R246 S247 Y248 L249 T250 P251 G252 D253 S254 S255 W258 T259 A262 A263 A264 Y265 Y266 V267 G268 Y269 L270 R273 T274 F275 L276 Y279 N280 E281 N282 G283 T284
D287 A288 V289 D290 C291 A292 L293 D294 P295 L296 S297 L303 F306 T307 V308 E309 K310 G311 I312 Y313 Q314 T315 S316 N317 F318 R319 V320 E324 S325 T326 V327 R328 F329 P330 N331 N334 L335 C336 P337 E340 V341 F342 T345 R346 F347 A348 S349 V350 W353 N354 R355 K356 R357
I358 S359 N360 C361 V362 A363 D364 Y365 S366 V367 L368 Y369 N370 F374 F377 K378 C379 Y380 G381 V382 S383 K386 L387 N388 D389 L390 G391 F392 T393 N394 V395 Y396 A397 D398 S399 F400 V401 G404 D405 E406 Q409 I410 A411 P412 G413 Q414 T415 G416 K417 D420 Y421 N422 Y423 K424
L425 P426 F429 T430 G431 C432 V433 I434 A435 W436 V445 N448 Y449 N450 Y451 L452 Y453 R454 L455 F456 R457 K458 S459 N460 L461 K462 P463 F464 E465 R466 D467 I468 S469 T470 E471 I472 Y473 Q474 A475 G476 S477 C480 N481 G482 V483 F486 N487 C488 Y489 F490 P491 L492 Q493 S494 Y495
G496 F497 Q498 P499 G502 V503 Q506 P507 Y508 R509 V510 V511 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 T523 V524 C525 G526 P527 K528 K529 S530 T531 N532 L533 V534 V539 N540 F541 N542 F543 N544 G545 L546 G550 V551 L552 S555 V576 R577 D578 P579 Q580 T581 L582
E583 I584 L585 D586 I587 T588 P589 C590 S591 F592 G593 G594 V595 S596 V597 I598 T599 P600 S605 N606 Q607 V608 A609 V610 L611 Y612 Q613 G614 V615 N616 C617 T618 E619 V620 P621 VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER N641 V642 F643 Q644
C649 L650 I651 E654 H655 N658 S659 Y660 E661 C662 P665 I666 G667 G671 A672 S673 Y674 D675 T676 GLN THR ASN SER PRO ALA VAL ALA S689 I692 I693 A694 Y695 I696 M697 S698 L699 Y707 N710 S711 I712 A713 I714 P715 T716 N717 F718 T719 I720 S721 V722 T723 T724
E725 I726 L727 P728 V729 S730 M731 T732 K733 T734 S735 V736 D737 C738 I742 C743 E748 C749 L753 Y756 G757 S758 F759 C760 T761 Q762 L763 N764 R765 A766 L767 T768 G769 I770 A771 V772 E773 Q774 D775 K776 V781 F782 K786 Q787 I788 T791 P792 P793 I794 K795 D796 F797
F800 I805 L806 P807 D808 P809 S810 K811 P812 S813 F817 I818 L821 L822 K825 V826 T827 L828 A829 D830 ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE C851 A852 Q853 N856 G857 L858 T859 V860 L861 P862 P863 L864 E868 M869
I870 S875 L878 T881 W886 A890 Q895 I896 P897 F898 A899 M900 Q901 M902 R905 T912 V915 L916 Y917 K921 L922 I923 A930 I931 I934 Q935 S939 A942 S943 A944 L945 G946 K947 L948 Q949 D950 V951 A956 Q957 A958 L959 N960 T961 L962 V963
K964 Q965 L966 N969 F970 G971 A972 I973 S974 S975 V976 L977 I980 L981 S982 R983 L984 D985 P986 P987 E988 A989 E990 V991 Q992 I993 L996 R1000 L1001 L1004 Q1005 T1006 Y1007 V1008 T1009 Q1010 Q1011 L1012 I1013 R1014 A1015 A1016 E1017 I1018 R1019 A1022 A1026 T1027 K1028 M1029 S1030 E1031 C1032
V1033 L1034 G1035 G1046 Y1047 H1048 L1049 M1050 P1053 Q1054 G1059 V1060 V1061 F1062 L1063 H1064 V1065 T1066 Y1067 A1070 Q1071 E1072 T1076 T1077 A1078 P1079 A1080 I1081 C1082 H1083 D1084 G1085 K1086 A1087 H1088 F1089 P1090 R1091 E1092 G1093 V1094 F1095 V1096 S1097 N1098 H1101 W1102 F1103 Q1106 R1107 N1108 F1109 Y1110
E1111 I1114 I1115 T1116 N1119 T1120 F1121 V1122 S1123 G1124 N1125 C1126 V1129 I1132 N1135 T1136 V1137 Y1138 D1139 P1140 L1141 Q1142 P1143 E1144 L1145 D1146 SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER

VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO LEU VAL PRO ARG GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS

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





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

Chain E:





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

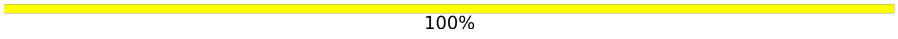
Chain F:





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

Chain G:





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

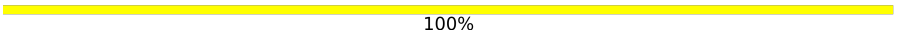
Chain H:





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

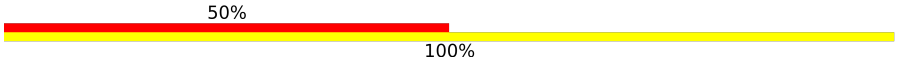
Chain I:





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

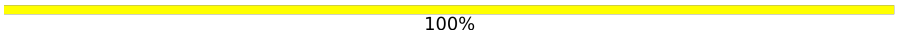
Chain J:





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

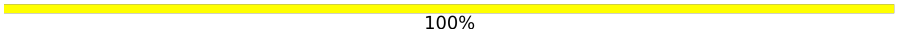
Chain K:





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

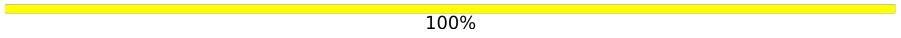
Chain L:





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

Chain M:





4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

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

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	0.72	9/8624 (0.1%)	0.97	30/11744 (0.3%)
1	B	0.78	10/8625 (0.1%)	1.00	33/11746 (0.3%)
1	C	0.70	6/8570 (0.1%)	1.01	28/11670 (0.2%)
All	All	0.73	25/25819 (0.1%)	0.99	91/35160 (0.3%)

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 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	940	SER	C-O	-29.95	0.88	1.24
1	A	940	SER	C-O	-22.37	0.94	1.24
1	B	617	CYS	C-O	-11.75	1.09	1.24
1	A	617	CYS	C-O	11.20	1.38	1.24
1	C	676	THR	C-O	-11.18	1.01	1.23

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	526	GLY	CA-C-N	20.38	140.35	119.56
1	C	526	GLY	C-N-CA	20.38	140.35	119.56
1	B	515	PHE	O-C-N	-13.35	104.84	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1146	ASP	CA-C-O	-11.43	101.37	120.80
1	B	617	CYS	CA-C-O	-10.98	107.69	120.10

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	955	0
1	B	8426	0	8179	1096	0
1	C	8374	0	8124	1042	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	3010	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 59.

The worst 5 of 3010 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%)	18	55
1	B	1071/1270 (84%)	1025 (96%)	38 (4%)	8 (1%)	18	55
1	C	1066/1270 (84%)	1020 (96%)	44 (4%)	2 (0%)	43	77
All	All	3207/3810 (84%)	3062 (96%)	128 (4%)	17 (0%)	26	62

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%)	16	38
1	B	937/1102 (85%)	866 (92%)	71 (8%)	12	33
1	C	929/1102 (84%)	849 (91%)	80 (9%)	10	30
All	All	2804/3306 (85%)	2593 (92%)	211 (8%)	14	33

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	950	ASP
1	C	212	LEU
1	C	981	LEU
1	B	1050	MET
1	B	1145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1011	GLN
1	C	394	ASN
1	B	1058	HIS
1	C	164	ASN
1	C	493	GLN

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	0.80	0	17,19,21	3.07	7 (41%)
2	NAG	D	2	2	14,14,15	0.66	0	17,19,21	1.12	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.79	0	17,19,21	2.96	6 (35%)
2	NAG	E	2	2	14,14,15	0.66	0	17,19,21	1.12	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.81	0	17,19,21	2.98	7 (41%)
2	NAG	F	2	2	14,14,15	0.65	0	17,19,21	1.13	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.76	0	17,19,21	3.02	6 (35%)
2	NAG	G	2	2	14,14,15	0.65	0	17,19,21	1.14	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.86	1 (7%)	17,19,21	3.02	7 (41%)
2	NAG	H	2	2	14,14,15	0.63	0	17,19,21	1.13	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.82	0	17,19,21	2.97	7 (41%)
2	NAG	I	2	2	14,14,15	0.63	0	17,19,21	1.12	2 (11%)
2	NAG	J	1	1,2	14,14,15	0.79	0	17,19,21	3.04	7 (41%)
2	NAG	J	2	2	14,14,15	0.66	0	17,19,21	1.10	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.78	0	17,19,21	3.11	7 (41%)
2	NAG	K	2	2	14,14,15	0.67	0	17,19,21	1.11	2 (11%)
2	NAG	L	1	1,2	14,14,15	0.80	0	17,19,21	2.99	7 (41%)
2	NAG	L	2	2	14,14,15	0.66	0	17,19,21	1.14	2 (11%)
2	NAG	M	1	1,2	14,14,15	0.81	0	17,19,21	3.18	6 (35%)
2	NAG	M	2	2	14,14,15	0.69	0	17,19,21	1.15	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O7-C7	-2.02	1.18	1.23

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C8-C7-N2	7.72	128.91	116.12
2	K	1	NAG	C8-C7-N2	7.63	128.78	116.12
2	H	1	NAG	C8-C7-N2	7.58	128.69	116.12
2	J	1	NAG	C8-C7-N2	7.56	128.66	116.12
2	D	1	NAG	C8-C7-N2	7.49	128.54	116.12

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

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Mol	Chain	Res	Type	Atom
2	L	1	NAG	C1

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7

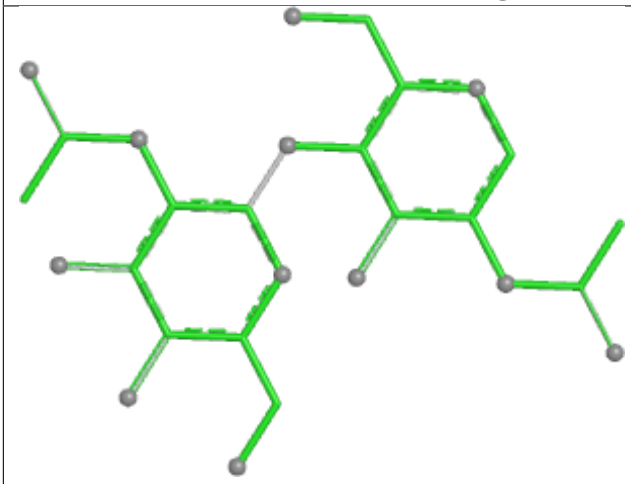
There are no ring outliers.

3 monomers are involved in 3 short contacts:

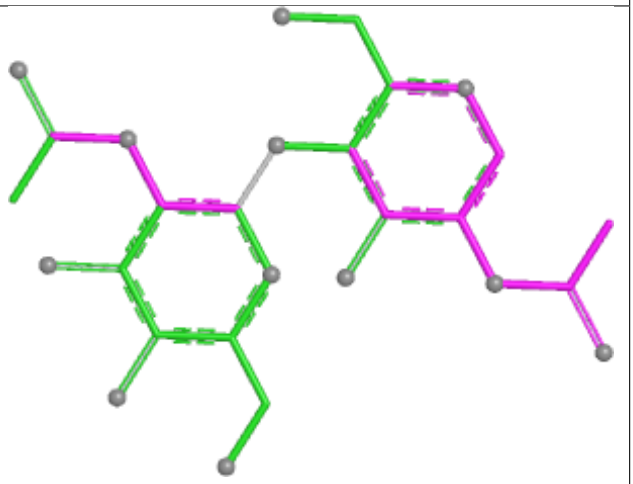
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	E	1	NAG	1	0
2	F	1	NAG	1	0

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

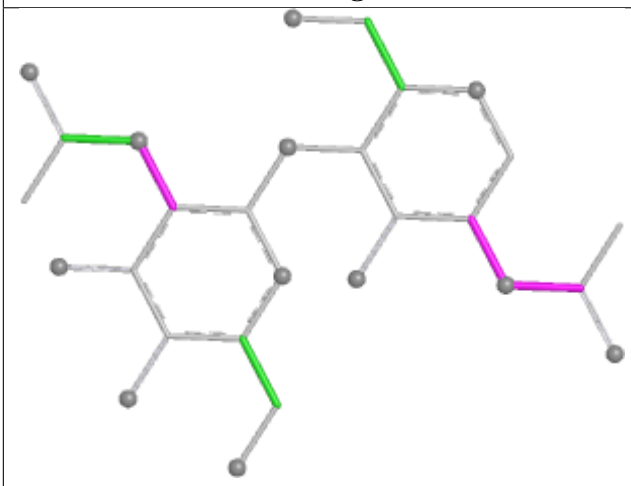
Oligosaccharide Chain D



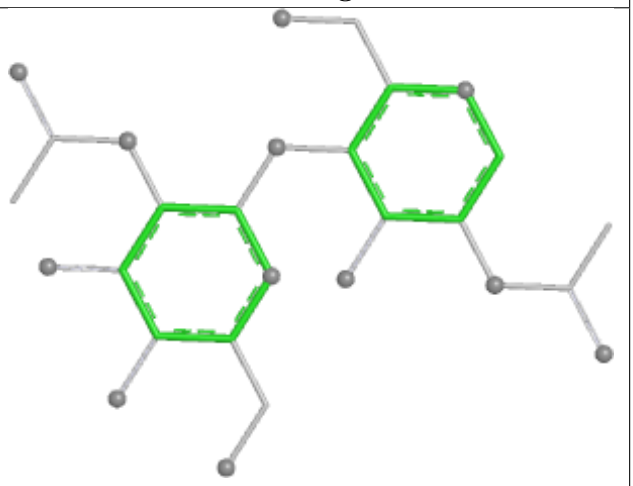
Bond lengths



Bond angles

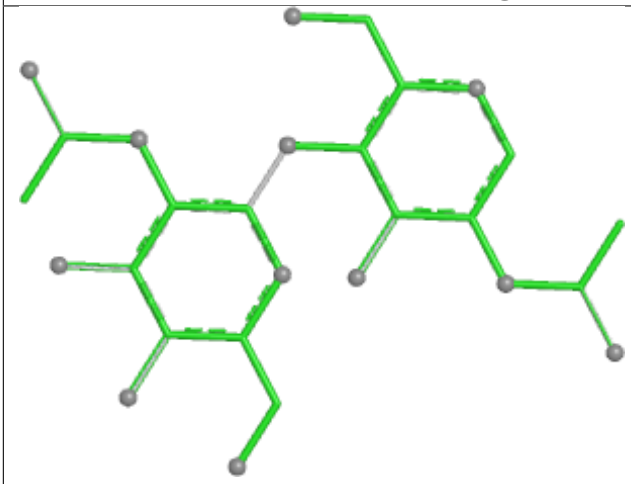


Torsions

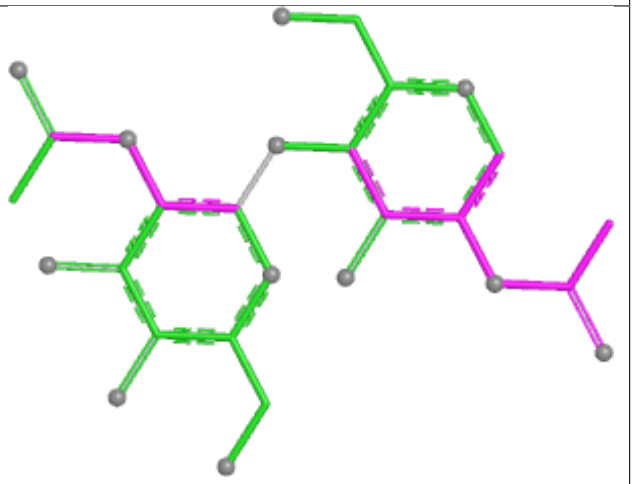


Rings

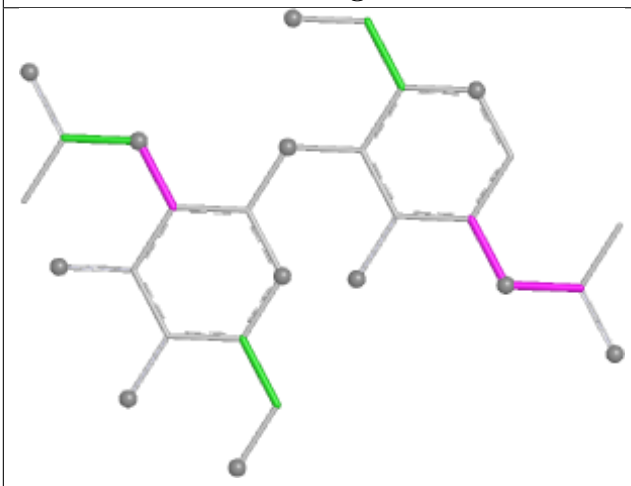
Oligosaccharide Chain E



Bond lengths



Bond angles



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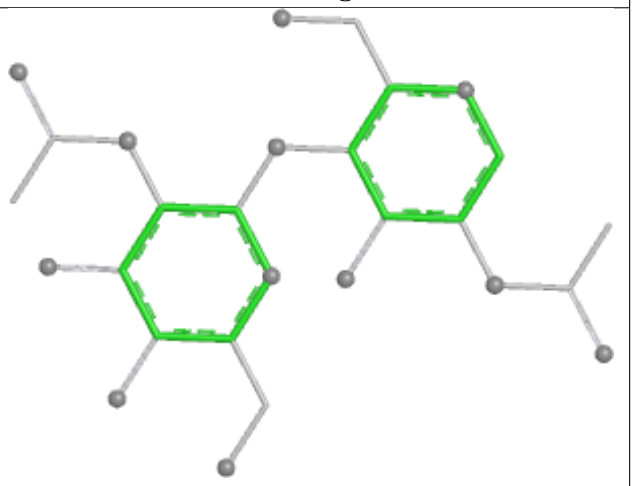
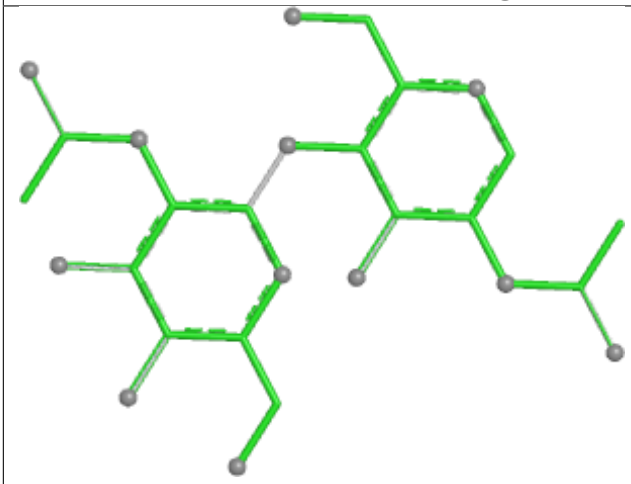
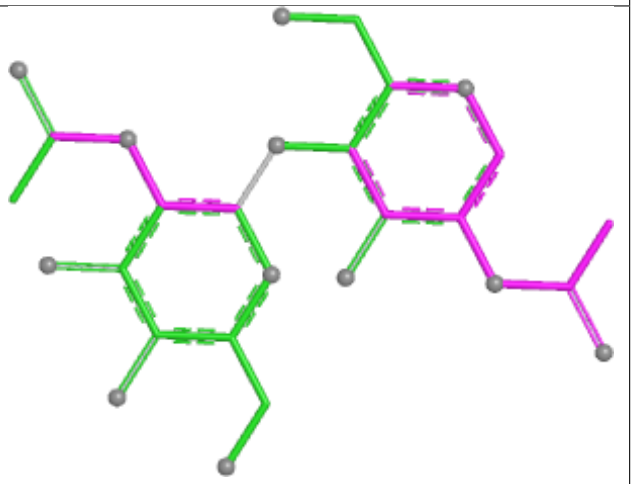


Rings

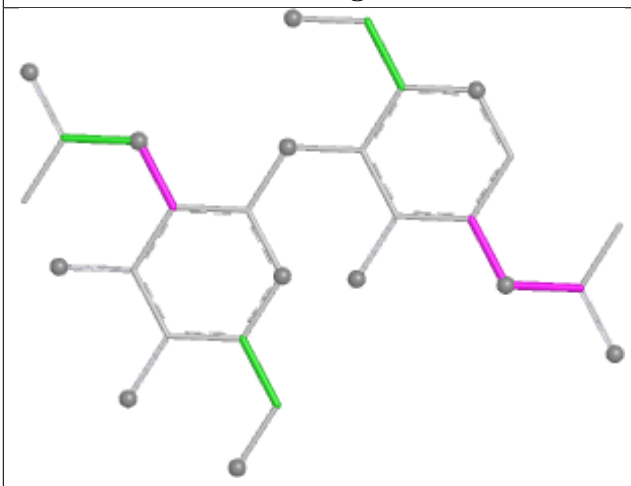
Oligosaccharide Chain F



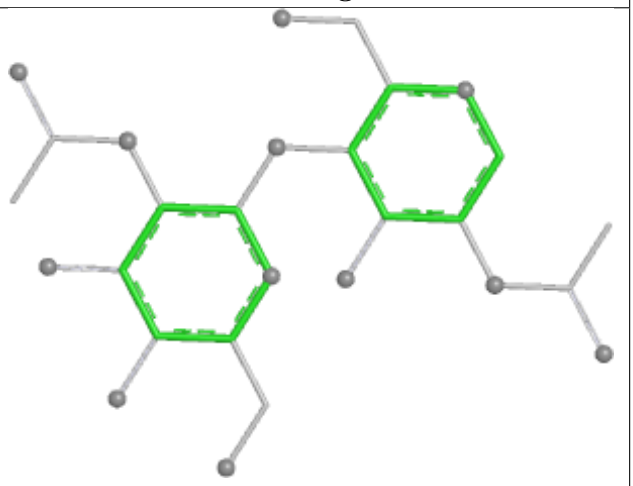
Bond lengths



Bond angles

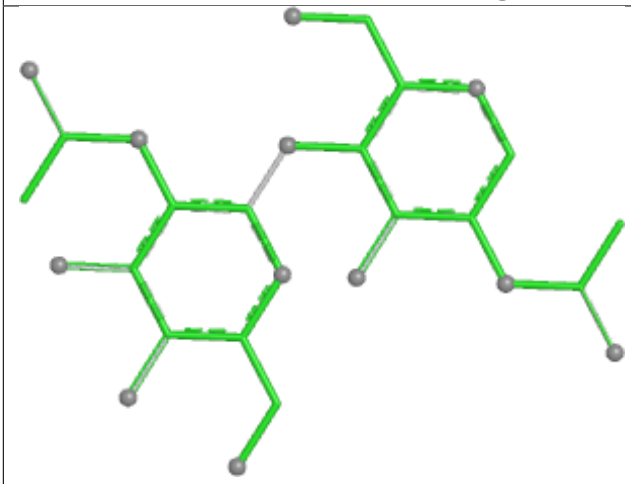


Torsions

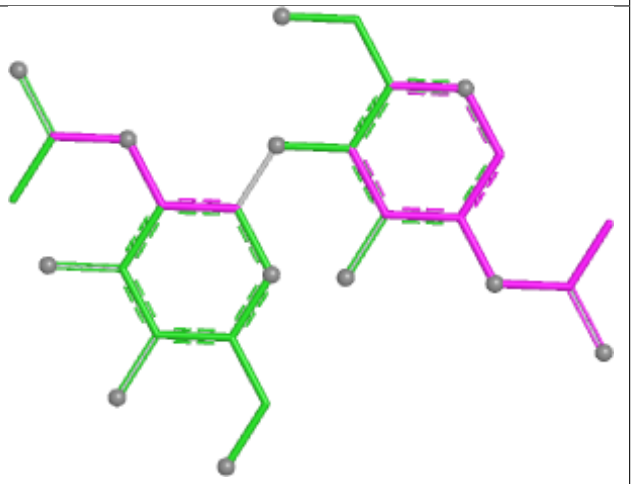


Rings

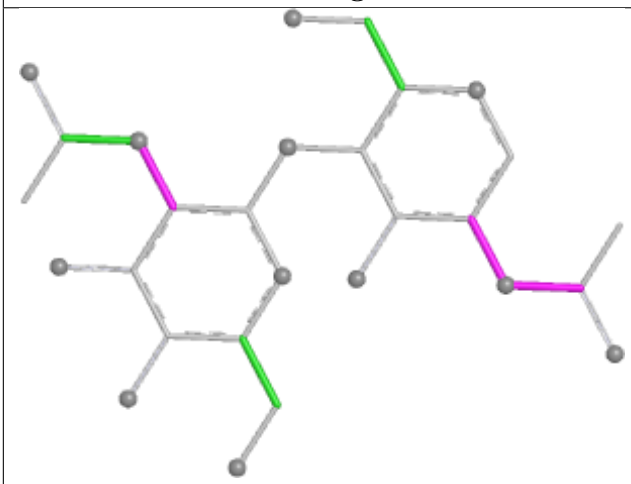
Oligosaccharide Chain G



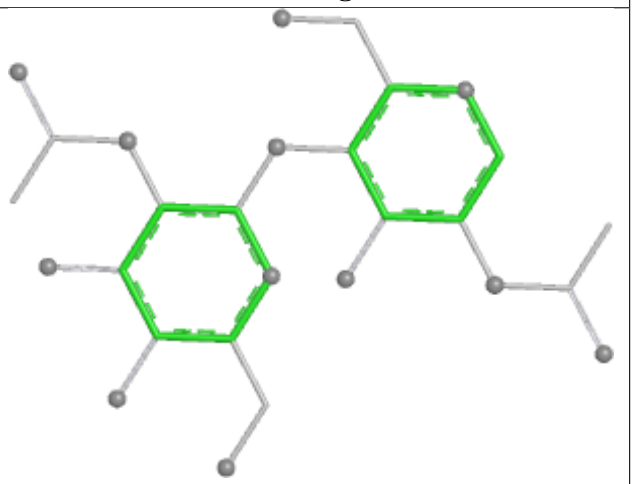
Bond lengths



Bond angles

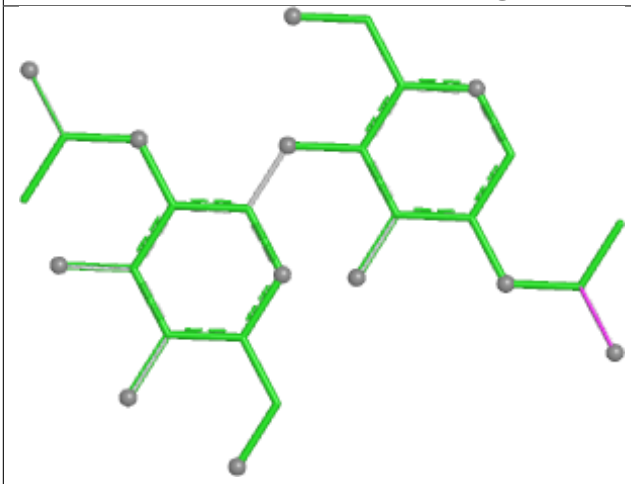


Torsions

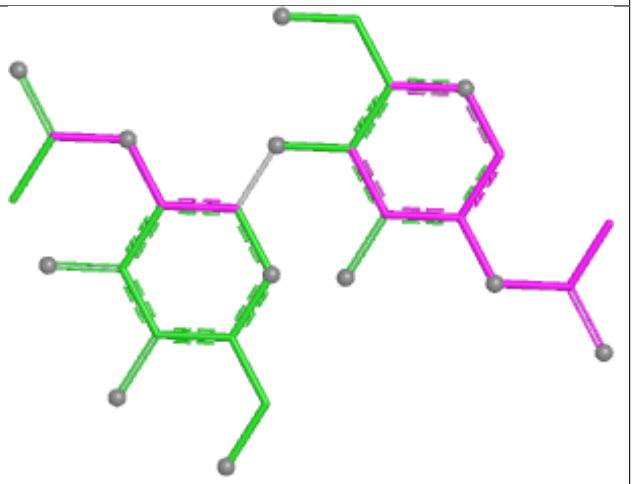


Rings

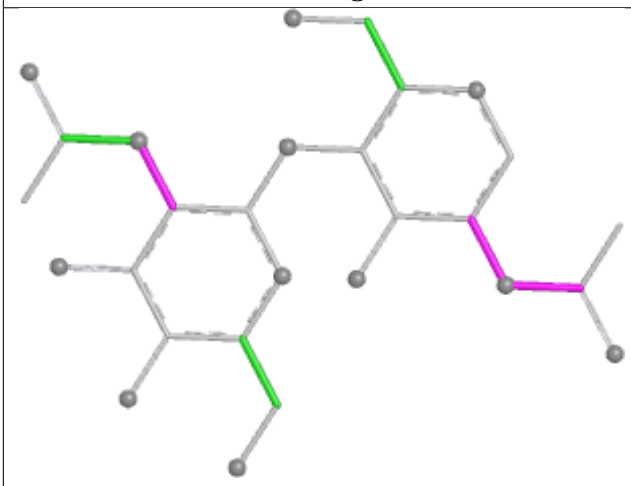
Oligosaccharide Chain H



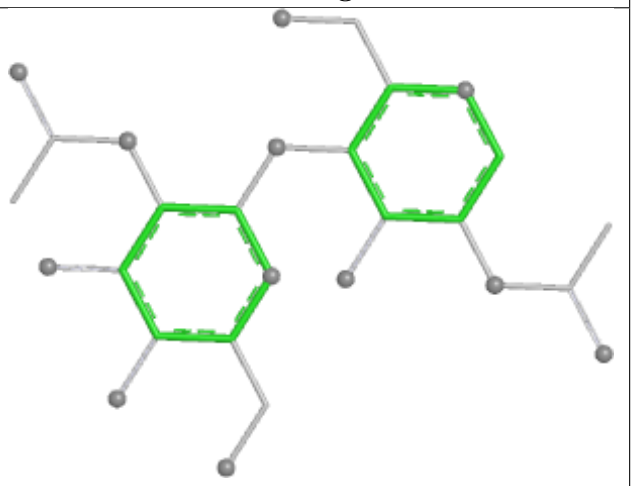
Bond lengths



Bond angles

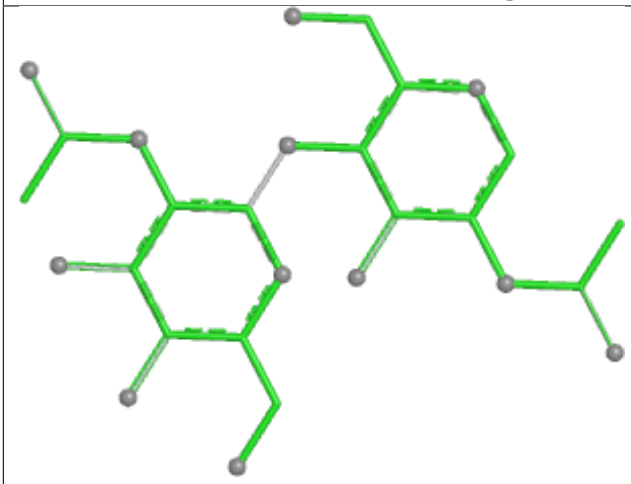


Torsions

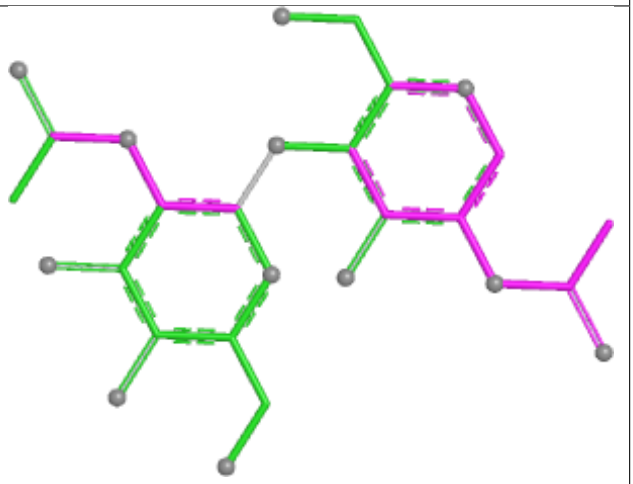


Rings

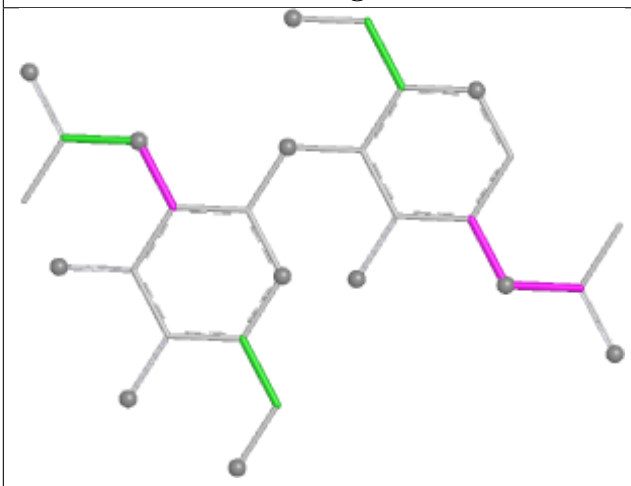
Oligosaccharide Chain I



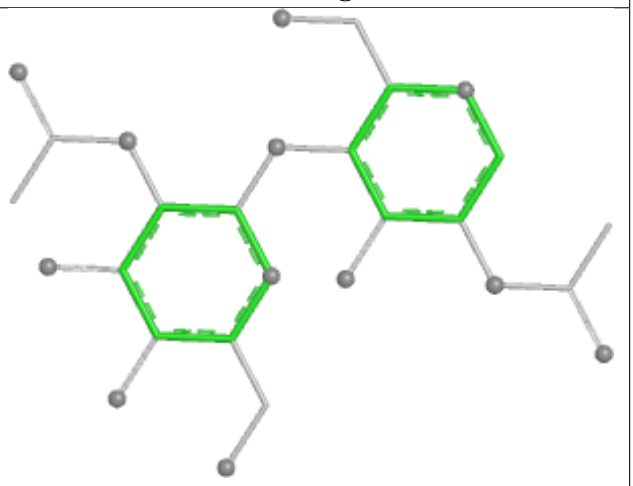
Bond lengths



Bond angles

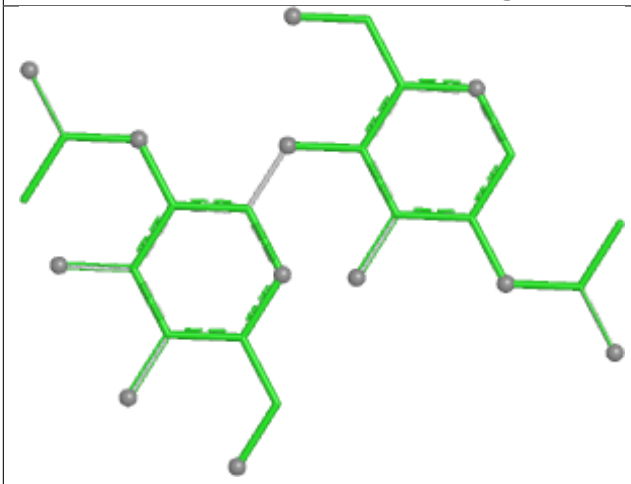


Torsions

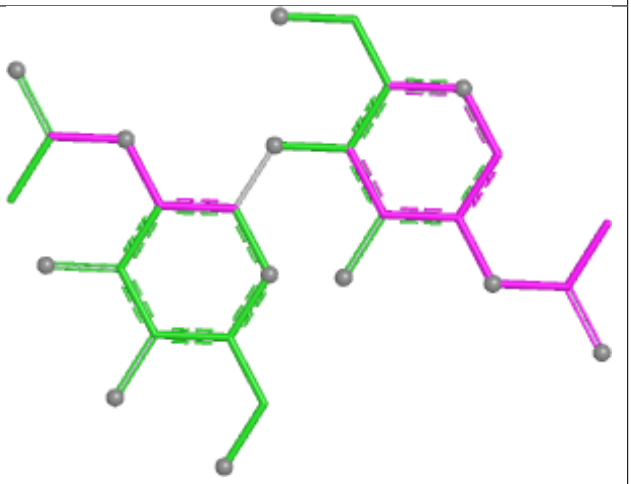


Rings

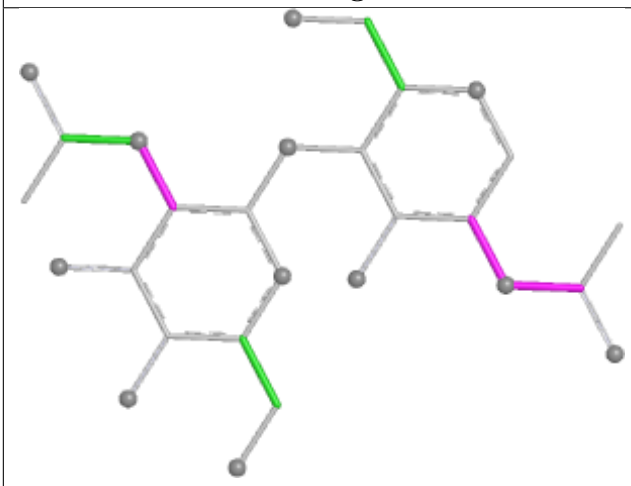
Oligosaccharide Chain J



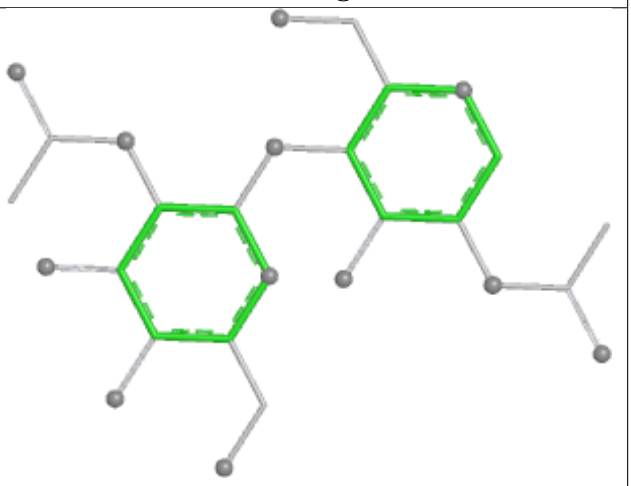
Bond lengths



Bond angles

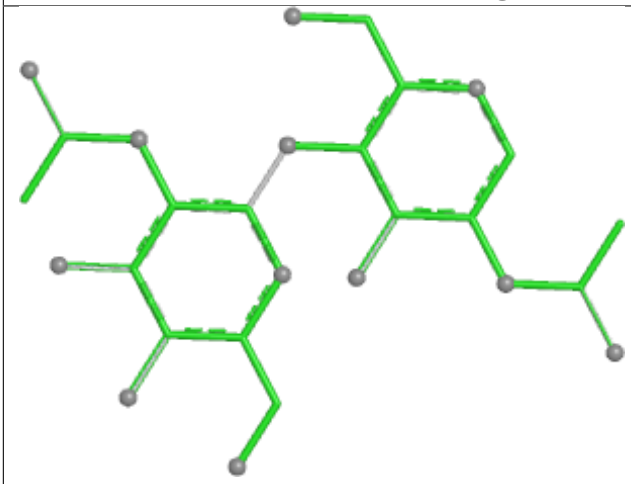


Torsions

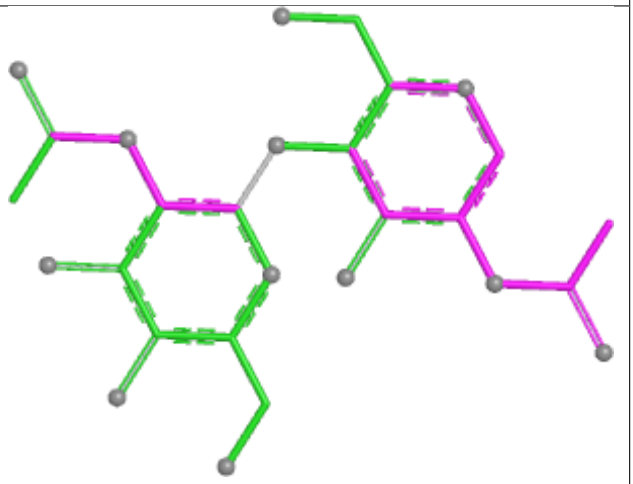


Rings

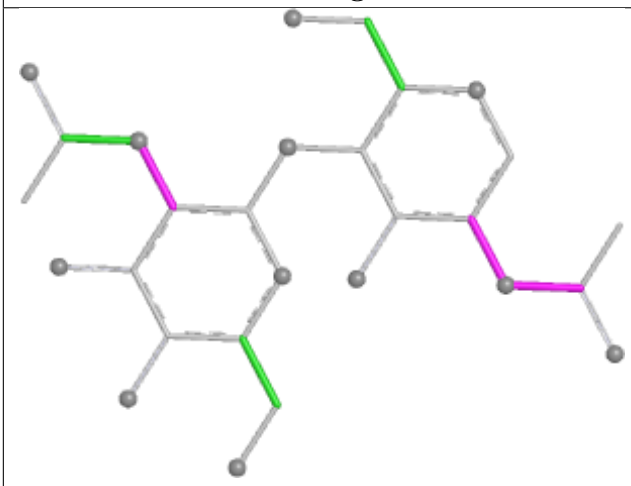
Oligosaccharide Chain K



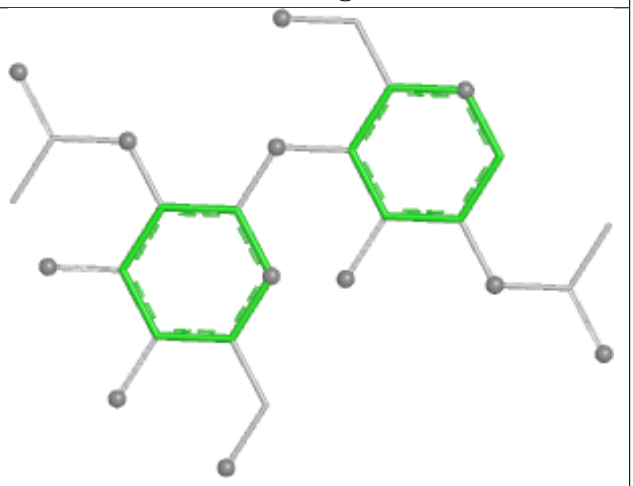
Bond lengths



Bond angles

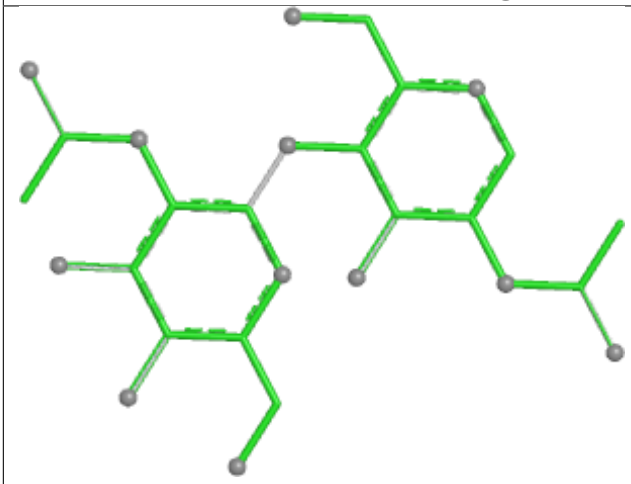


Torsions

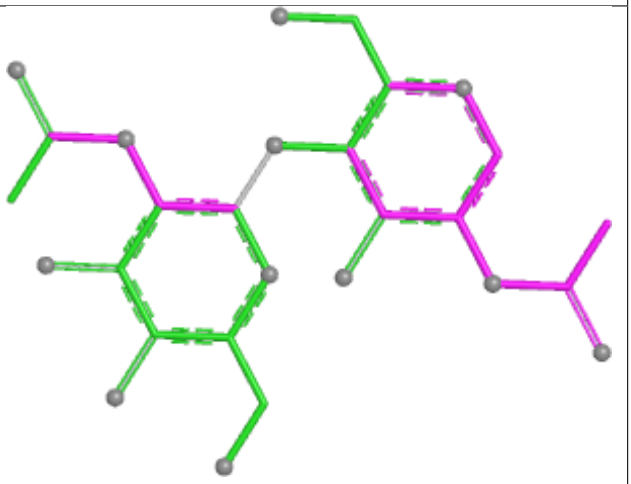


Rings

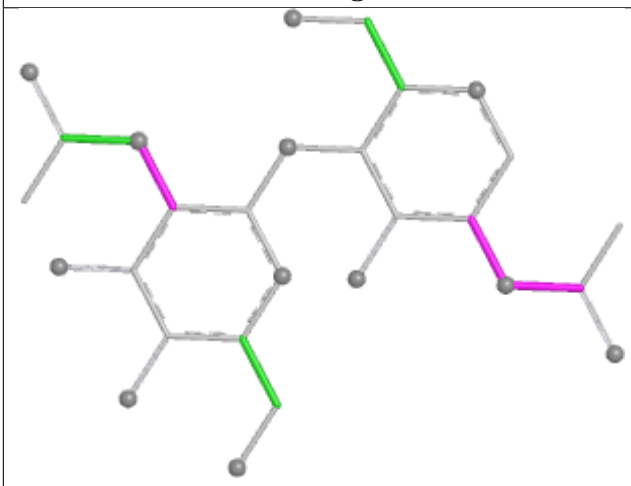
Oligosaccharide Chain L



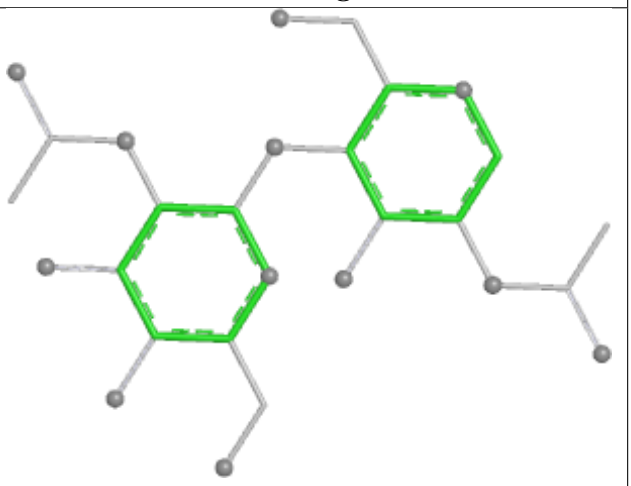
Bond lengths



Bond angles

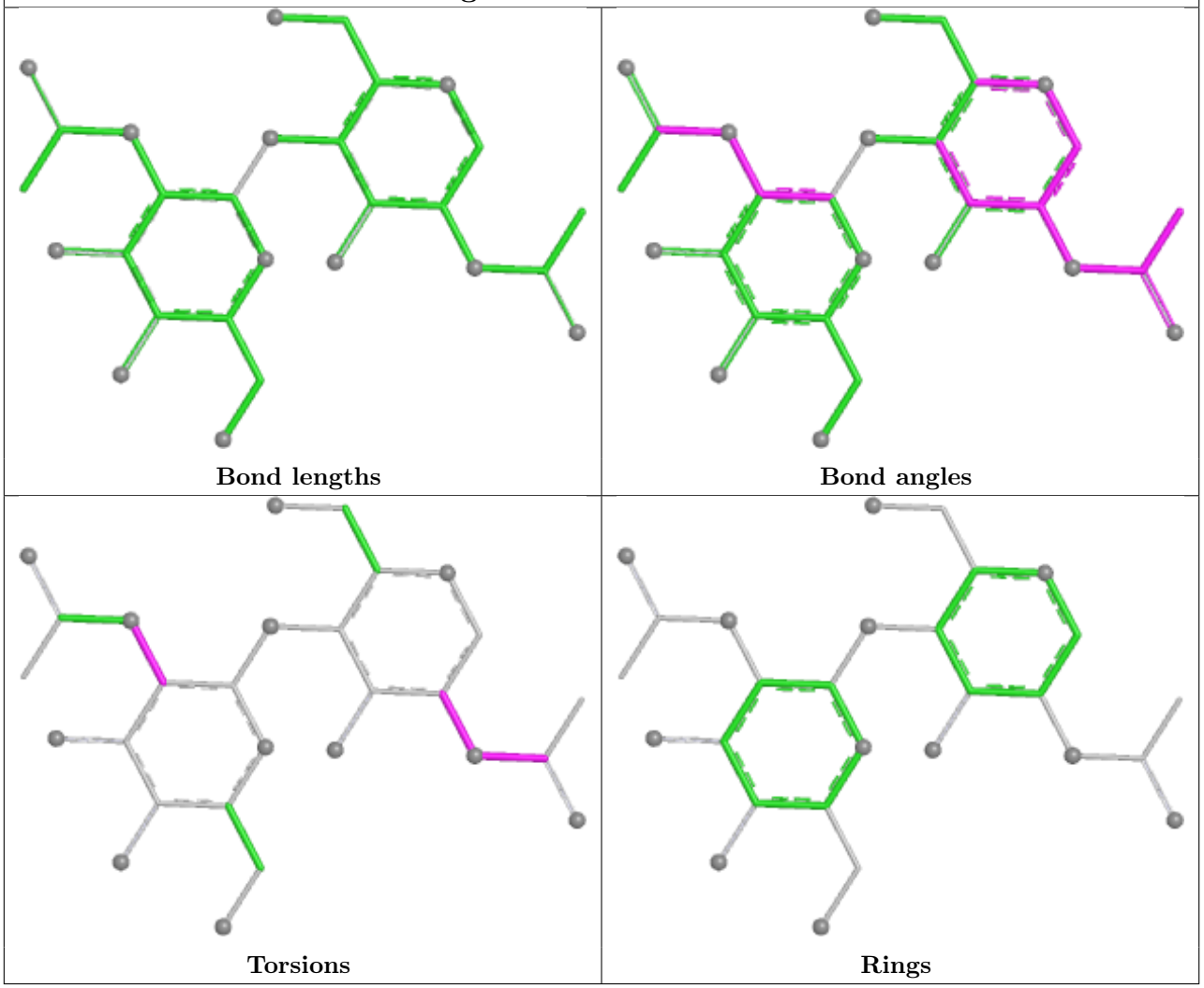


Torsions



Rings

Oligosaccharide Chain M



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	A	1301	1	14,14,15	0.33	0	17,19,21	0.63	0
5	XIO	C	1307	4	97,101,101	2.37	32 (32%)	119,143,143	1.17	13 (10%)
3	NAG	A	1302	1	14,14,15	0.34	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1309	1	14,14,15	0.95	1 (7%)	17,19,21	1.77	5 (29%)
3	NAG	A	1306	1	14,14,15	0.42	0	17,19,21	2.51	5 (29%)
3	NAG	C	1301	1	14,14,15	0.47	0	17,19,21	1.43	3 (17%)
3	NAG	B	1306	1	14,14,15	0.58	0	17,19,21	1.10	2 (11%)
3	NAG	C	1303	1	14,14,15	2.02	2 (14%)	17,19,21	3.26	4 (23%)
3	NAG	C	1305	1	14,14,15	0.46	0	17,19,21	0.74	0
3	NAG	A	1304	1	14,14,15	0.36	0	17,19,21	1.31	2 (11%)
3	NAG	B	1307	1	14,14,15	0.57	0	17,19,21	1.31	2 (11%)
3	NAG	B	1301	1	14,14,15	0.60	0	17,19,21	1.40	2 (11%)
3	NAG	A	1309	1	14,14,15	0.46	0	17,19,21	1.16	1 (5%)
3	NAG	B	1308	1	14,14,15	0.46	0	17,19,21	2.02	5 (29%)
3	NAG	C	1302	1	14,14,15	0.46	0	17,19,21	1.50	3 (17%)
3	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	B	1303	1	14,14,15	0.63	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	C	1304	1	14,14,15	0.46	0	17,19,21	1.59	3 (17%)
3	NAG	A	1305	1	14,14,15	0.37	0	17,19,21	0.83	1 (5%)
3	NAG	A	1308	1	14,14,15	0.35	0	17,19,21	0.62	0
3	NAG	B	1305	1	14,14,15	0.54	0	17,19,21	1.42	3 (17%)
3	NAG	B	1304	1	14,14,15	0.48	0	17,19,21	0.99	0
3	NAG	C	1306	1	14,14,15	0.47	0	17,19,21	1.59	3 (17%)
3	NAG	A	1307	1	14,14,15	0.66	1 (7%)	17,19,21	1.69	2 (11%)
3	NAG	B	1302	1	14,14,15	0.89	0	17,19,21	1.23	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
5	XIO	C	1307	4	-	26/79/85/85	0/9/9/9
3	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	B	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	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	3/6/23/26	0/1/1/1

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

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1307	XIO	C08-N09	7.05	1.49	1.34
5	C	1307	XIO	C43-N44	6.86	1.48	1.34
5	C	1307	XIO	C02-N71	6.53	1.47	1.34
5	C	1307	XIO	C37-N36	6.53	1.45	1.34
3	C	1303	NAG	C1-C2	6.48	1.61	1.52

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1303	NAG	C1-O5-C5	11.65	127.80	112.19
3	A	1306	NAG	C2-N2-C7	6.40	131.47	122.90
3	A	1306	NAG	C8-C7-N2	5.87	125.85	116.12
3	B	1308	NAG	C8-C7-N2	5.24	124.81	116.12
3	A	1307	NAG	O5-C1-C2	-4.74	103.95	111.29

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	A	1306	NAG	C1-C2-N2-C7
5	C	1307	XIO	C31-C10-C11-C12
5	C	1307	XIO	C06-C05-N36-C37
5	C	1307	XIO	C41-C05-N36-C37

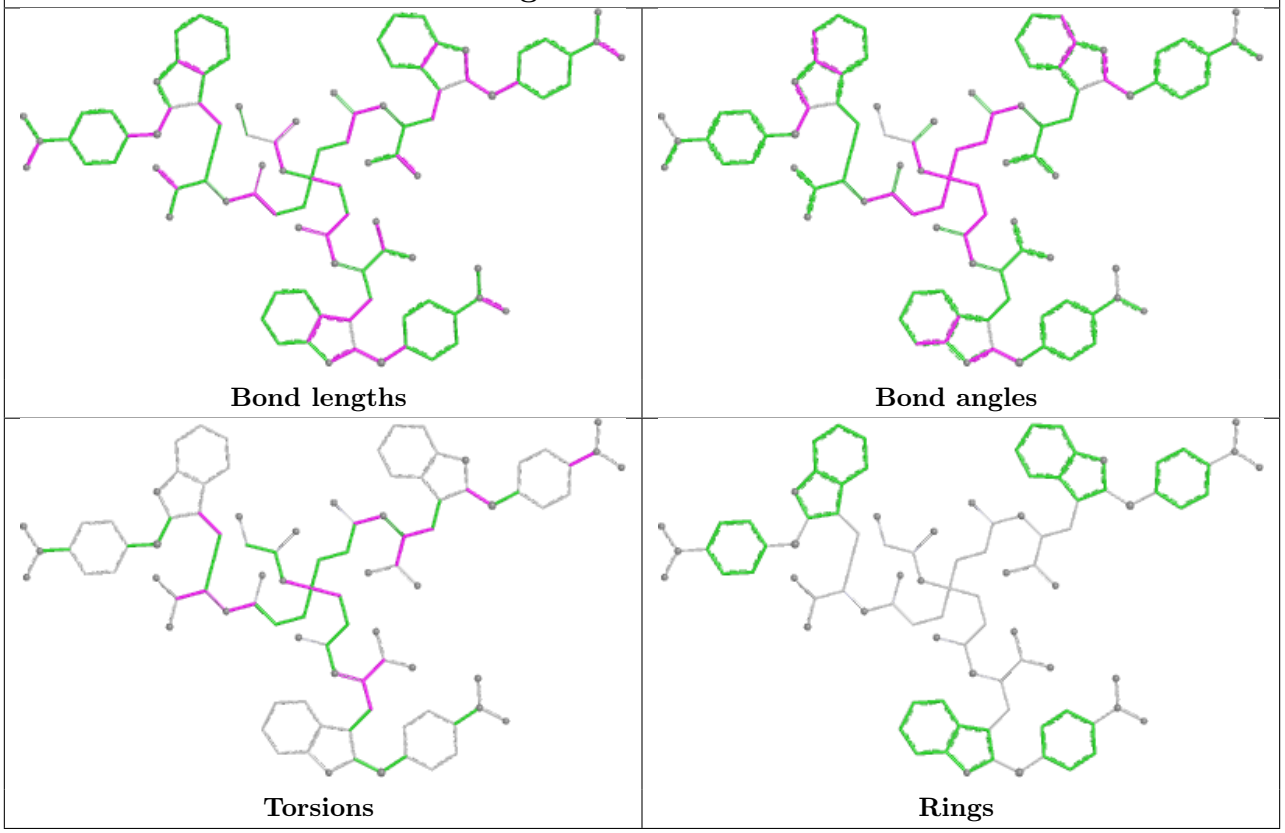
There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

Ligand XIO C 1307



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

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.

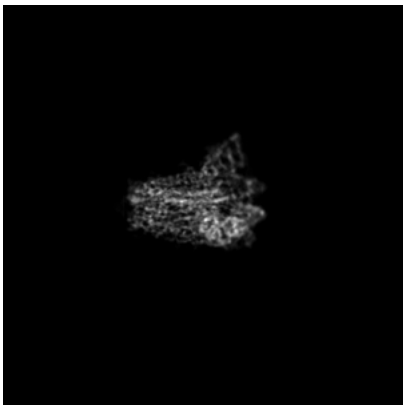
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

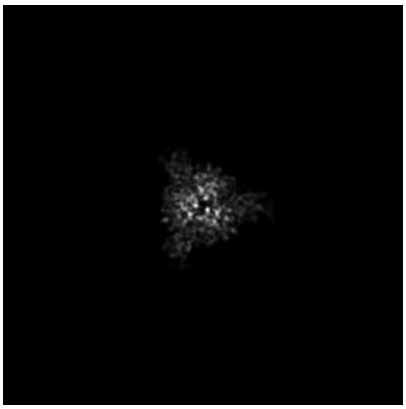
6.1.1 Primary map



X

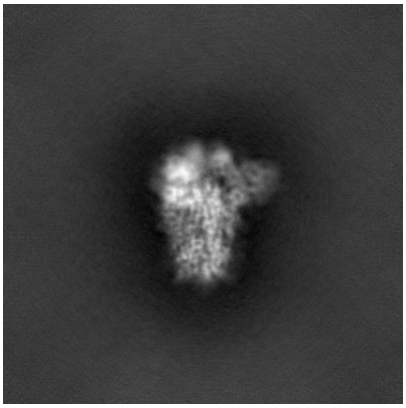


Y

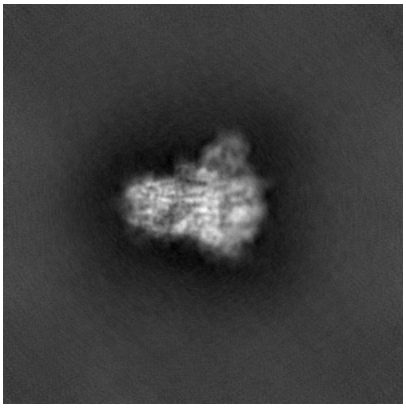


Z

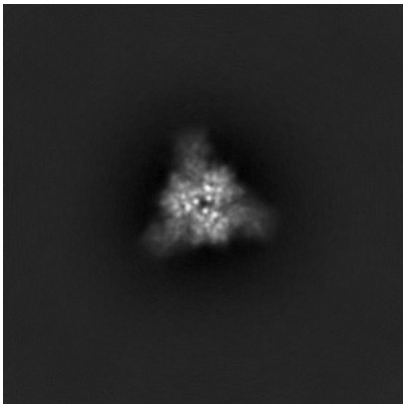
6.1.2 Raw map



X



Y

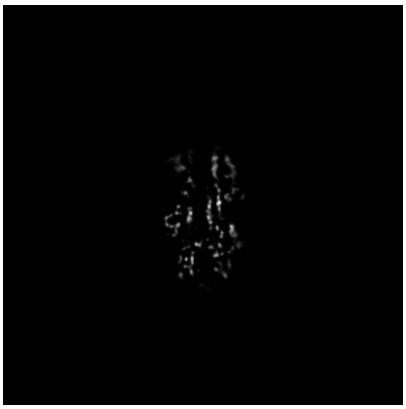


Z

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

6.2 Central slices (i)

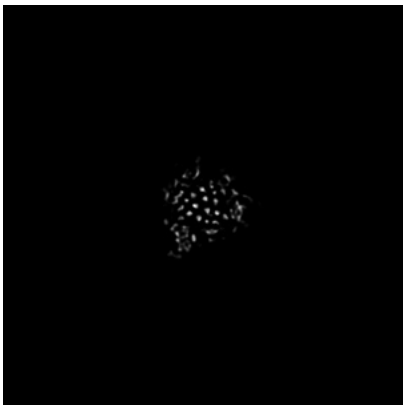
6.2.1 Primary map



X Index: 246

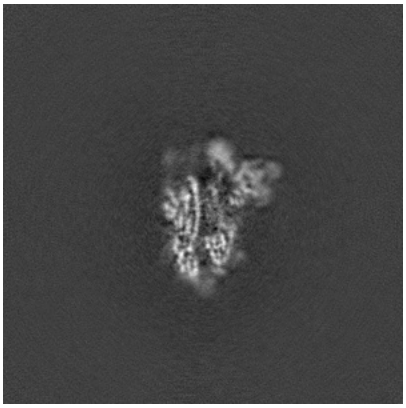


Y Index: 246

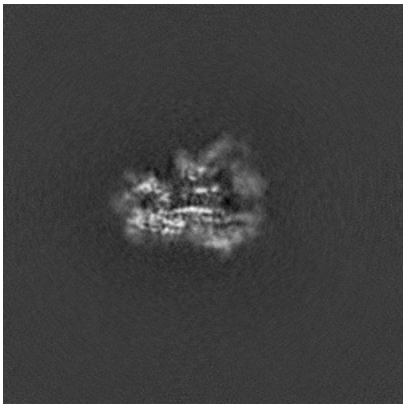


Z Index: 246

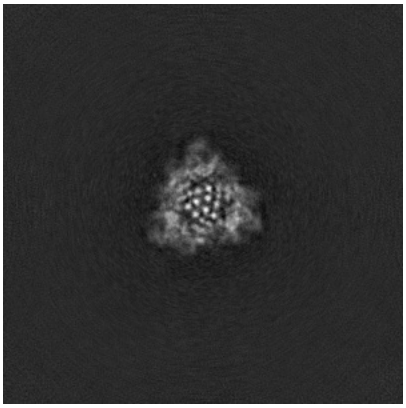
6.2.2 Raw map



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

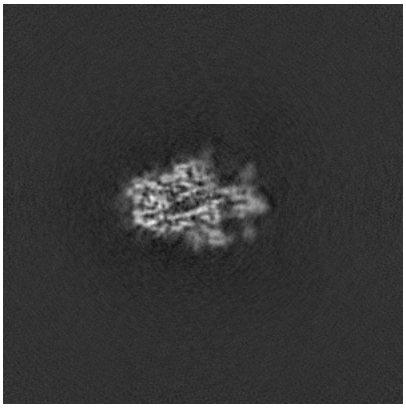


Z Index: 248

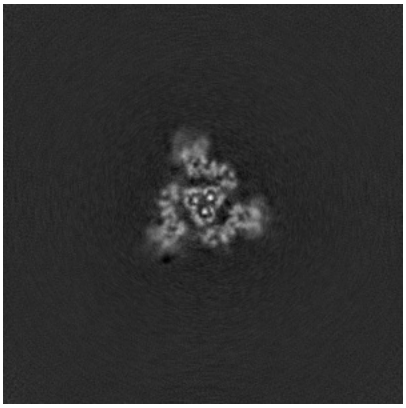
6.3.2 Raw map



X Index: 251



Y Index: 260

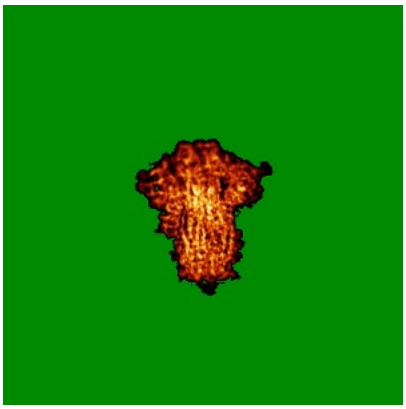


Z Index: 262

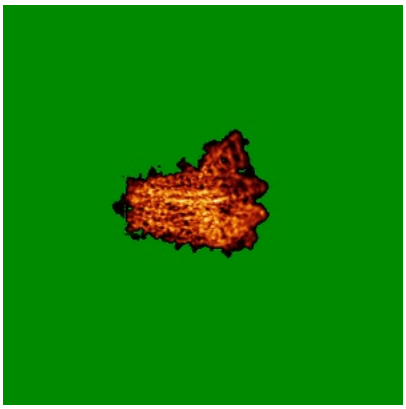
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

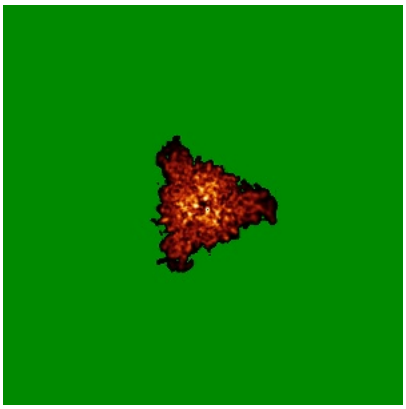
6.4.1 Primary map



X

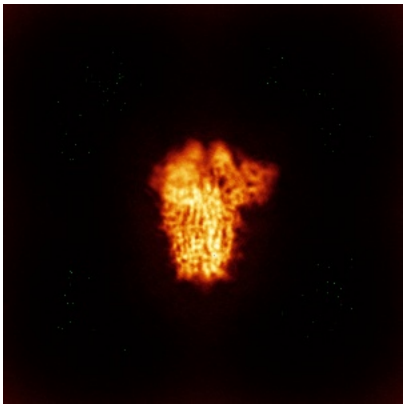


Y

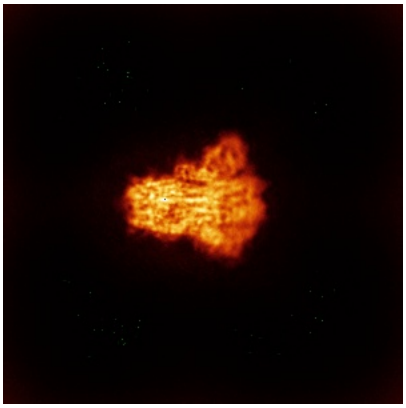


Z

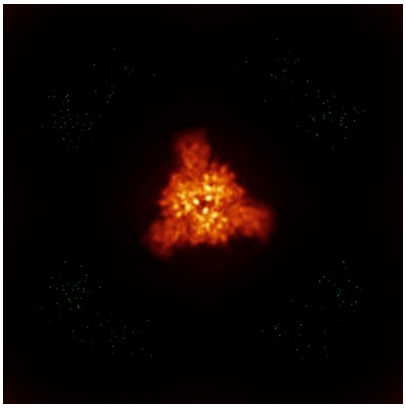
6.4.2 Raw map



X



Y

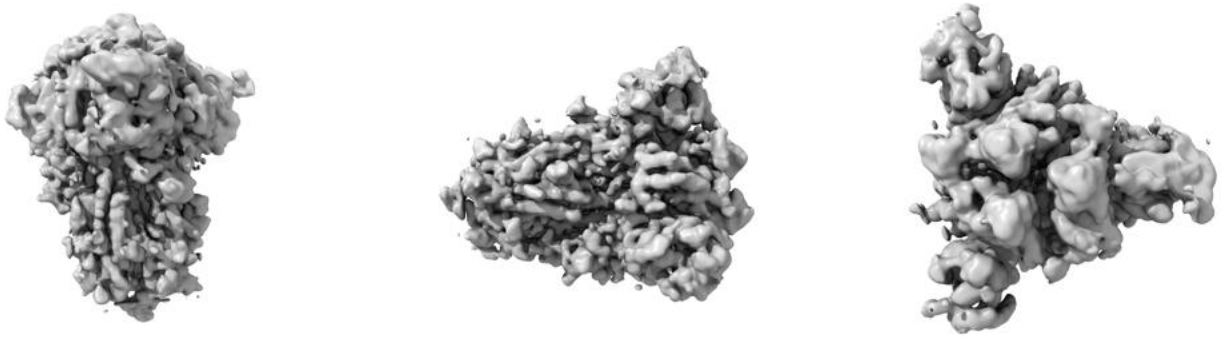


Z

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.

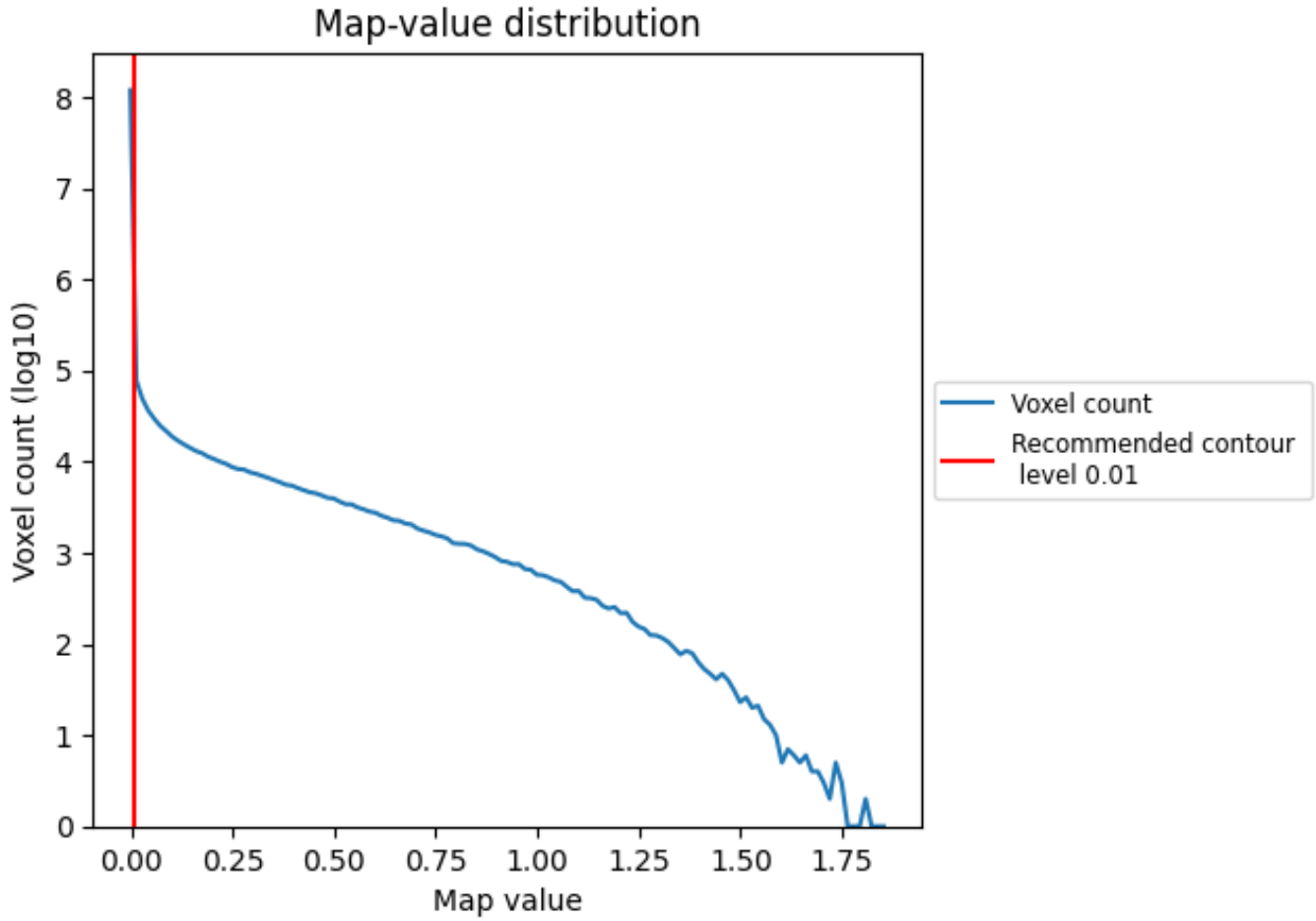
6.6 Mask visualisation (i)

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

7 Map analysis

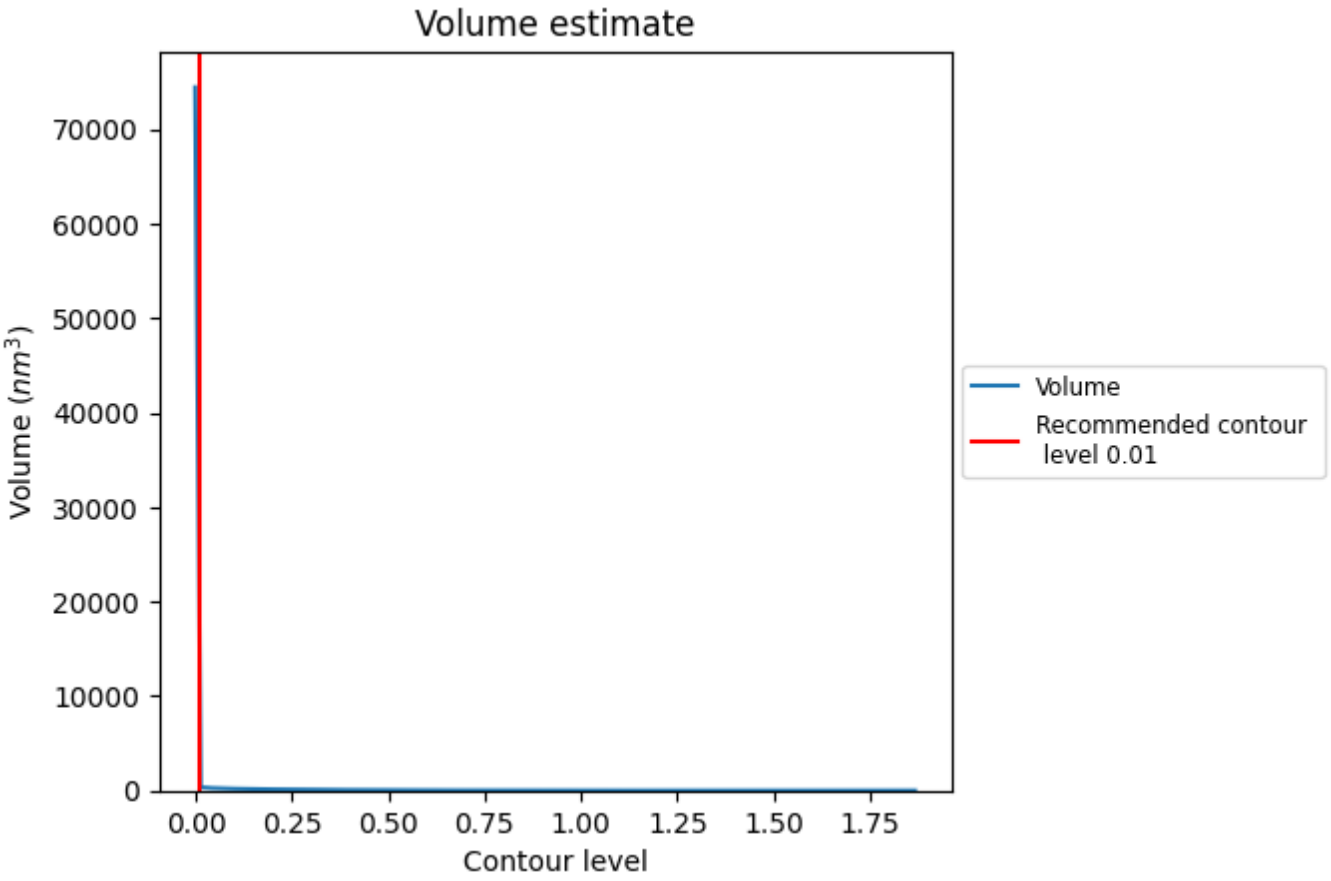
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

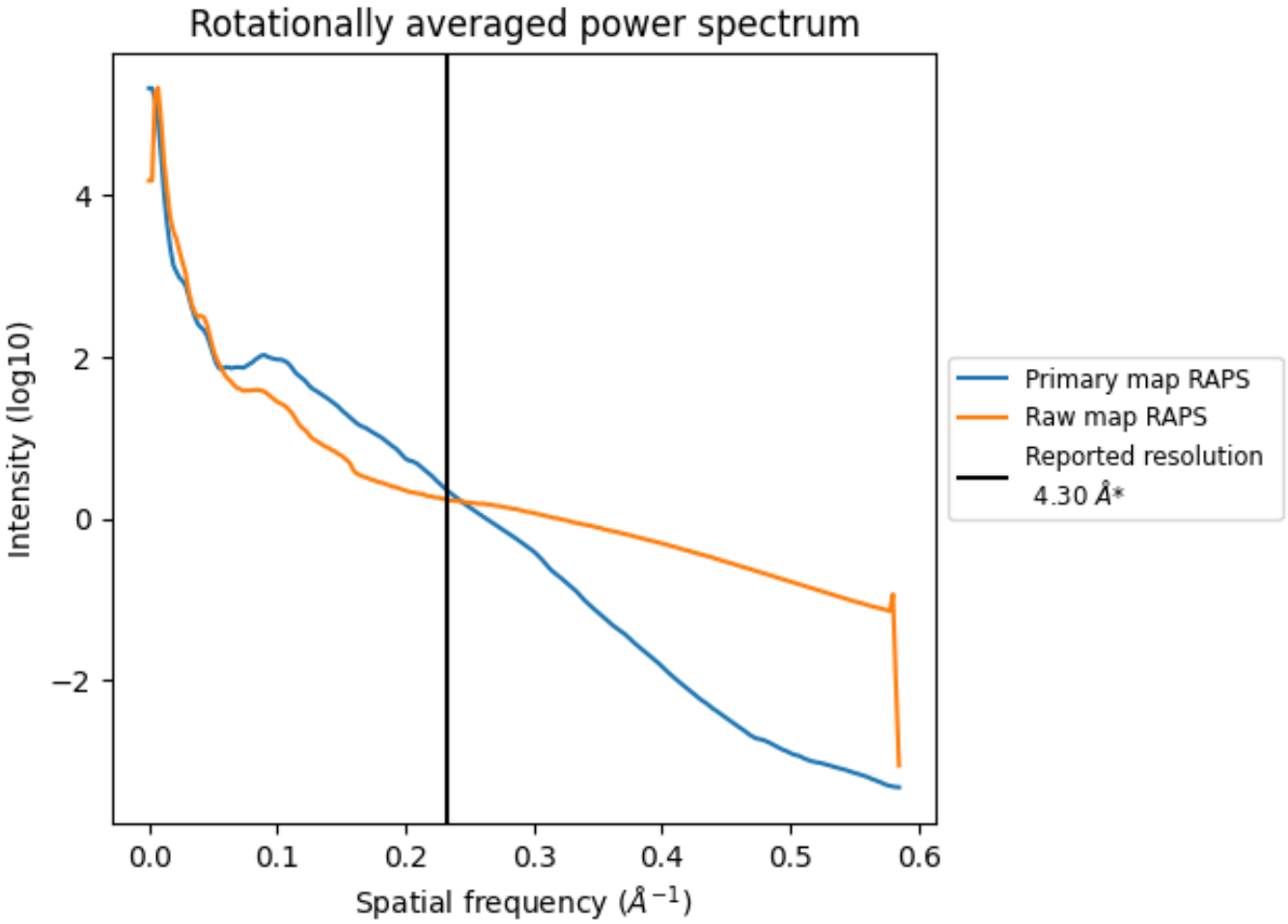
7.2 Volume estimate (i)



The volume at the recommended contour level is 15139 nm^3; 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)

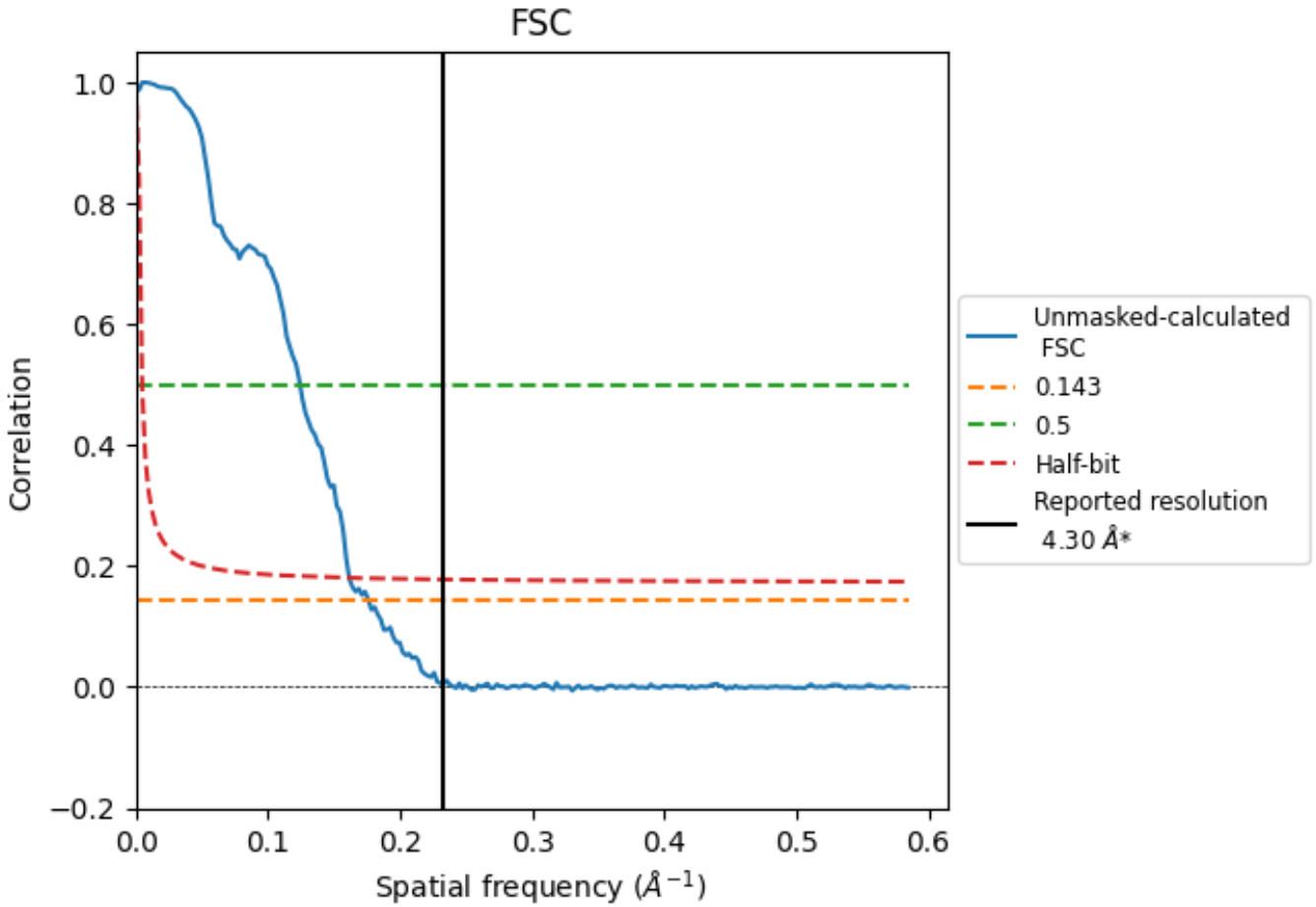


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

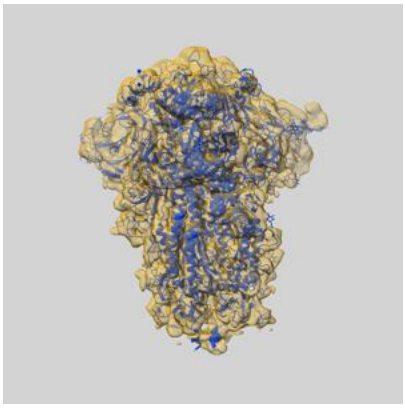
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.68	8.05	6.19

*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 %

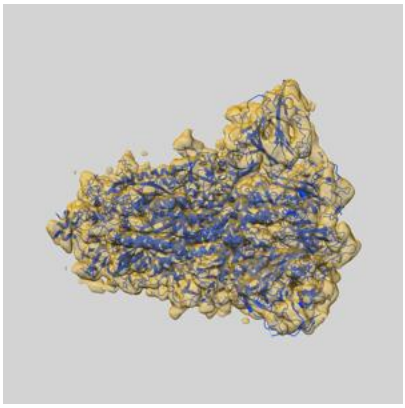
9 Map-model fit

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.

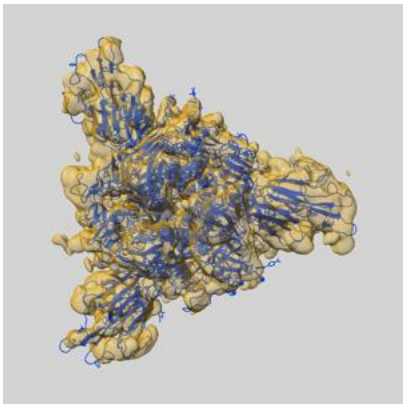
9.1 Map-model overlay



X



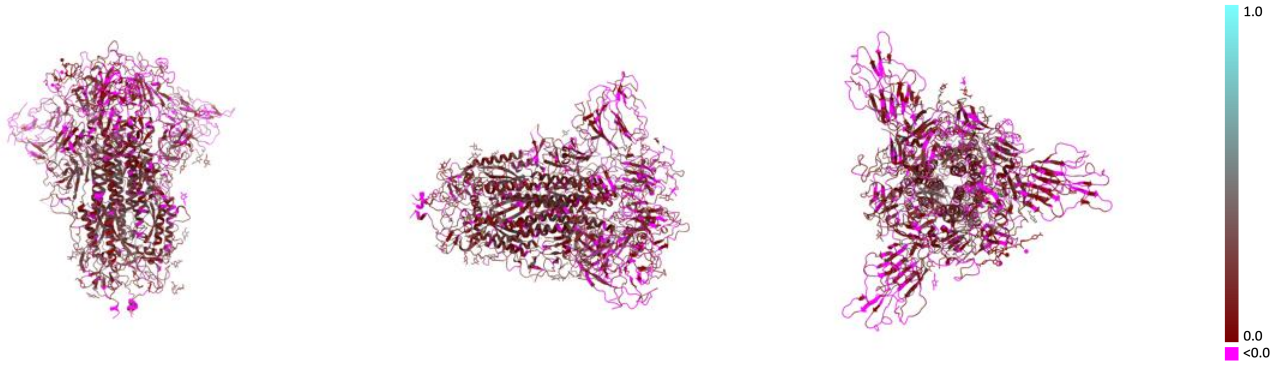
Y



Z

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.

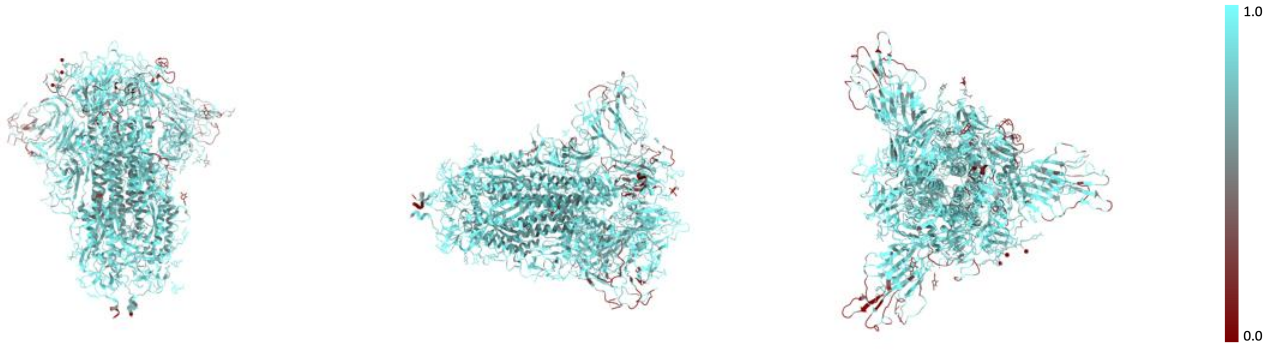
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

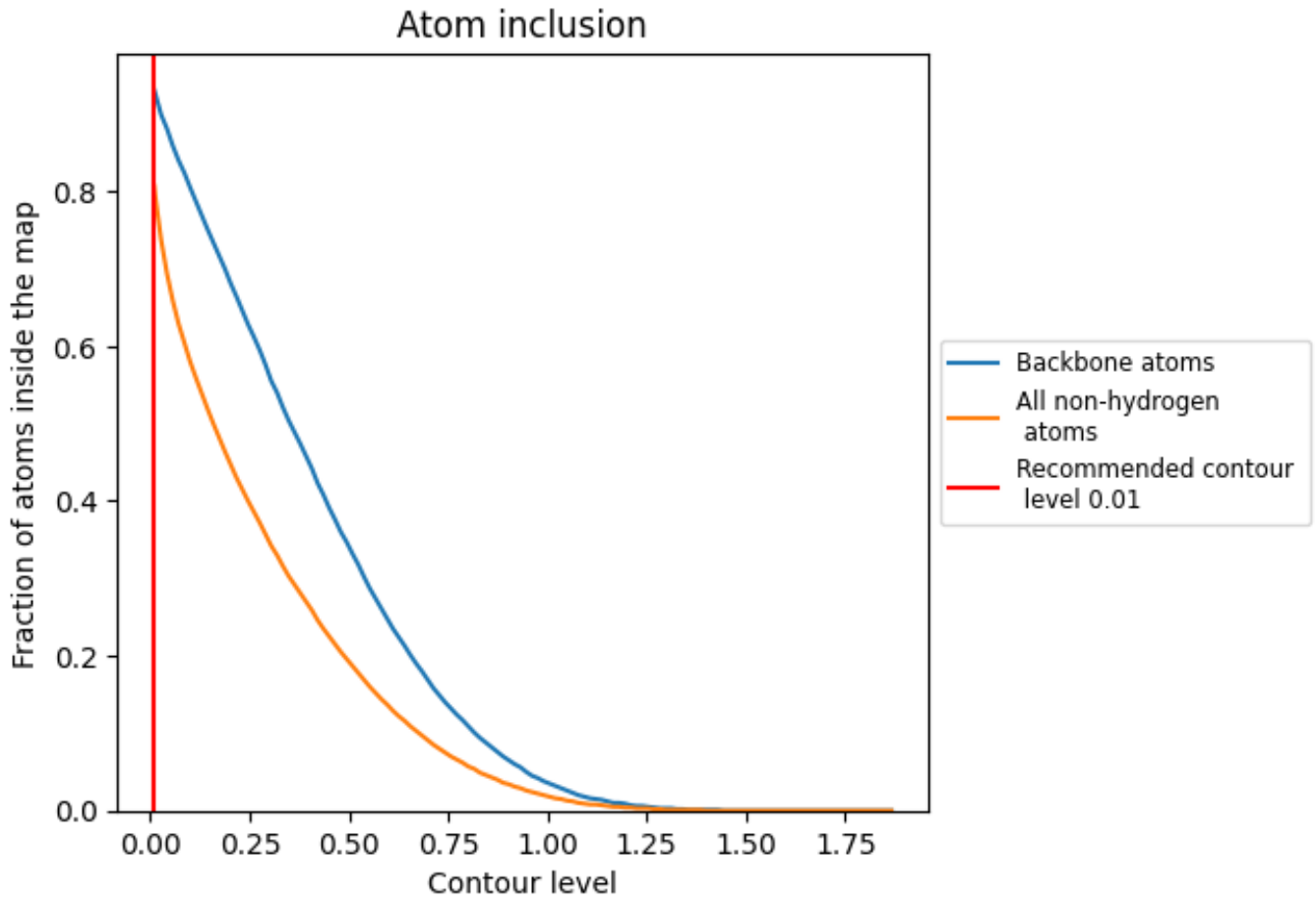
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

