



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:35 PM UTC

PDB ID : 7TPI / pdb_00007tpi
EMDB ID : EMD-26056
Title : SARS-CoV-2 E406W mutant Spike ectodomain
Authors : Addetia, A.; Veesler, D.
Deposited on : 2022-01-25
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

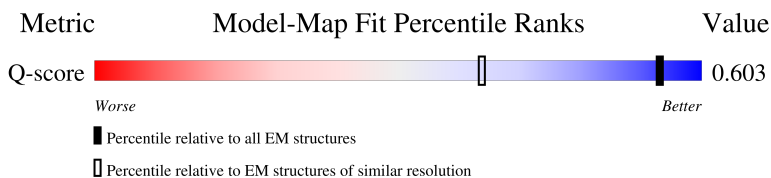
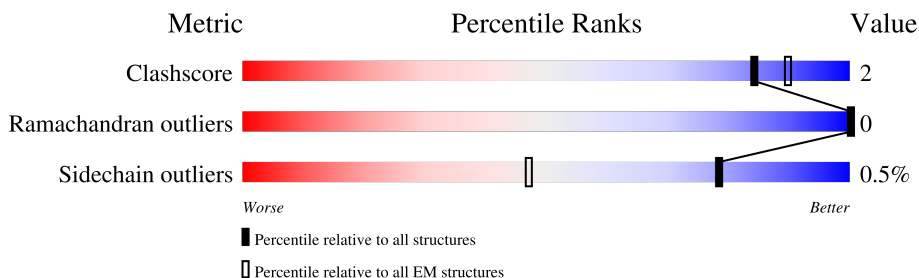
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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 $\leq 5\%$. 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	1277	 70% 5% 25%
1	B	1277	 69% 5% 25%
1	C	1277	 70% 5% 25%
2	D	2	 100%

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%
2	I	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
3	NAG	A	1313	-	-	X	-
3	NAG	B	1313	-	-	X	-
3	NAG	C	1313	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	954	Total	C	N	O	S	0	0
			6804	4404	1154	1214	32		
1	B	954	Total	C	N	O	S	0	0
			6804	4404	1154	1214	32		
1	C	954	Total	C	N	O	S	0	0
			6804	4404	1154	1214	32		

There are 237 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	TRP	GLU	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	ASN	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	ILE	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1265	HIS	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	HIS	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	HIS	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
B	406	TRP	GLU	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	GLY	-	expression tag	UNP P0DTC2
B	1252	GLY	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	ASN	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	ILE	-	expression tag	UNP P0DTC2
B	1257	PHE	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	GLN	-	expression tag	UNP P0DTC2
B	1261	LYS	-	expression tag	UNP P0DTC2
B	1262	ILE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	TRP	-	expression tag	UNP P0DTC2
B	1265	HIS	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1270	HIS	-	expression tag	UNP P0DTC2
B	1271	HIS	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	HIS	-	expression tag	UNP P0DTC2
B	1274	HIS	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
C	406	TRP	GLU	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	ASN	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	ILE	-	expression tag	UNP P0DTC2
C	1257	PHE	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	GLN	-	expression tag	UNP P0DTC2
C	1261	LYS	-	expression tag	UNP P0DTC2
C	1262	ILE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	TRP	-	expression tag	UNP P0DTC2
C	1265	HIS	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	HIS	-	expression tag	UNP P0DTC2
C	1271	HIS	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	HIS	-	expression tag	UNP P0DTC2
C	1274	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	HIS	-	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		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

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

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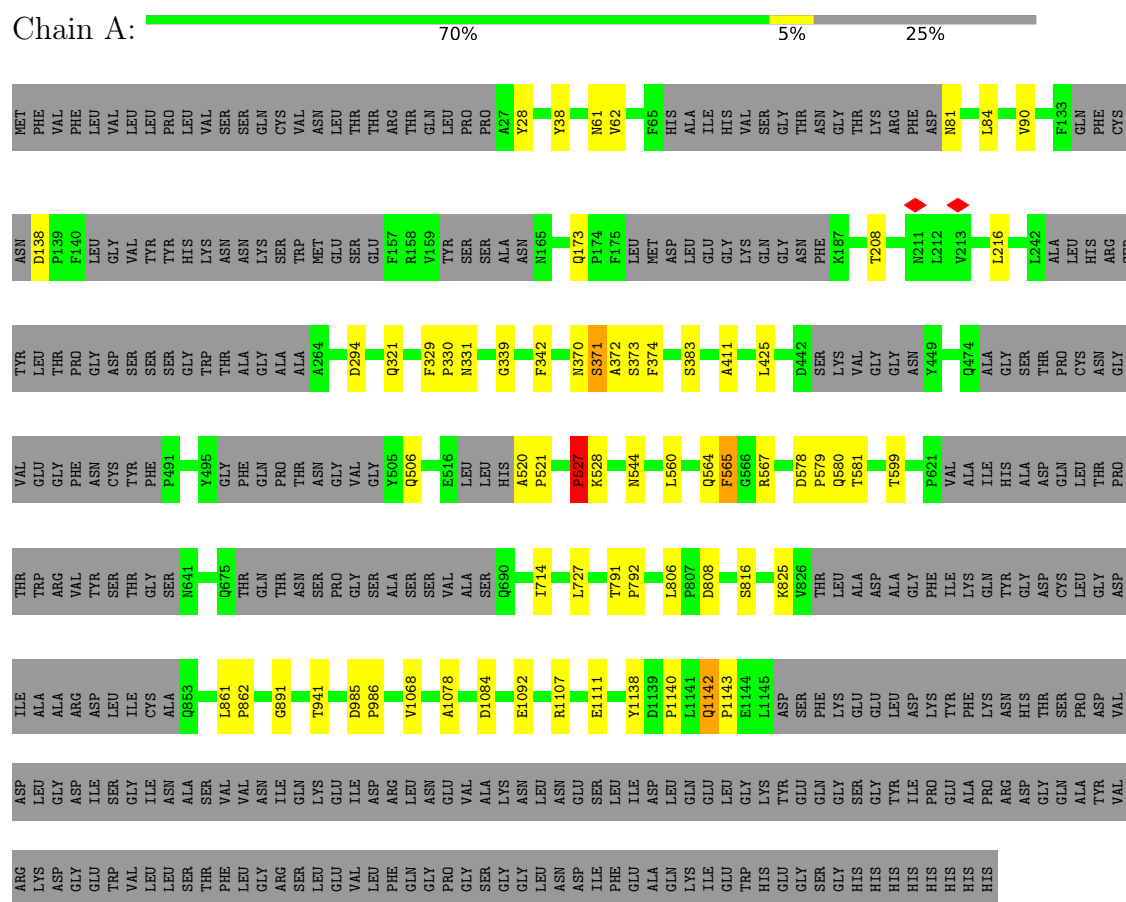
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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

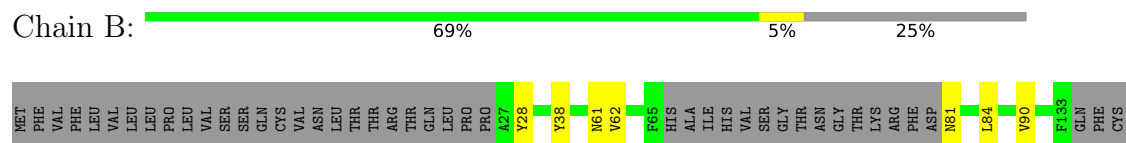
3 Residue-property plots

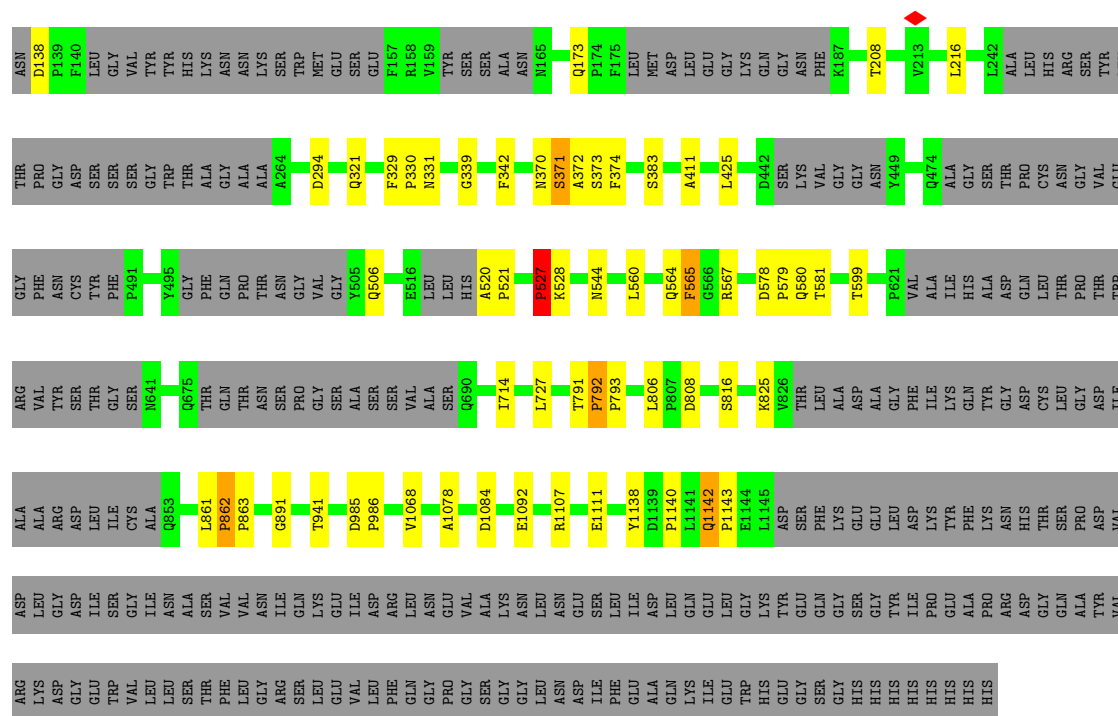
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein



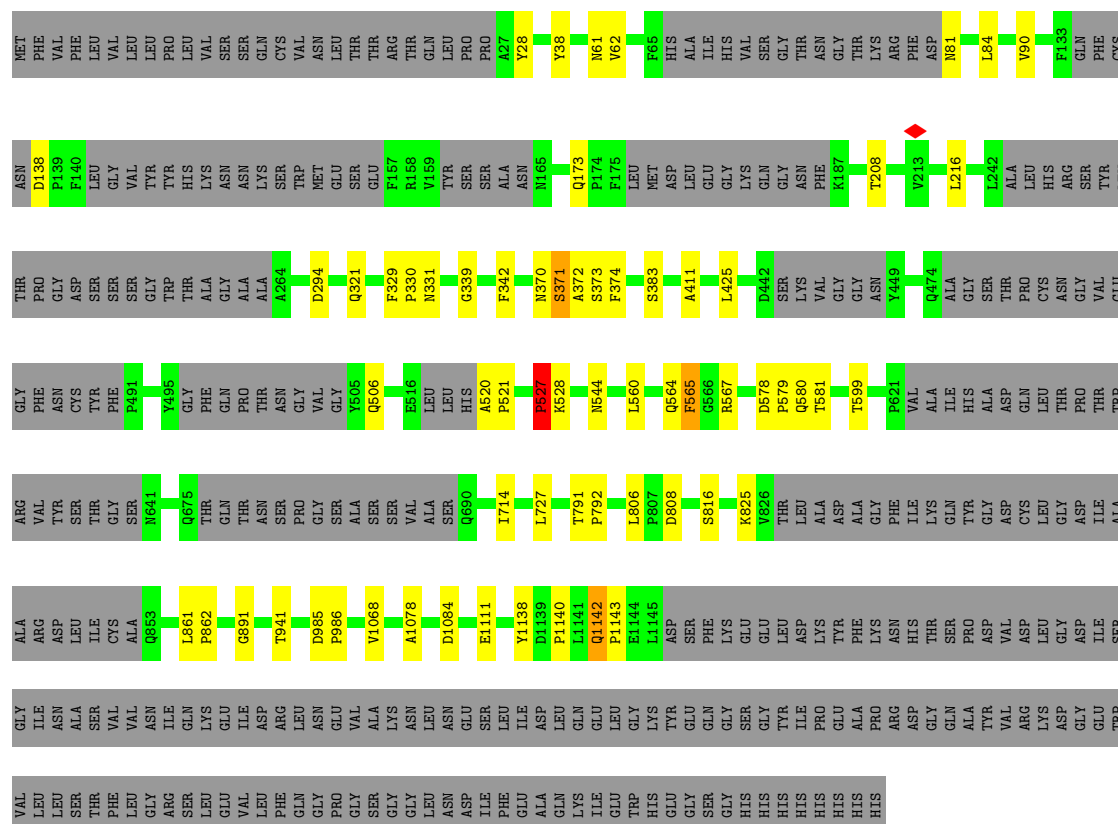
• Molecule 1: Spike glycoprotein





● Molecule 1: Spike glycoprotein

Chain C: 70% 5% 25%



- 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:  100%

MAG1
MAG2

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

Chain F:  100%

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:  100%

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	427195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	0	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.021	Depositor
Minimum map value	-9.248	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	512.0, 512.0, 512.0	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	1/6964 (0.0%)	1.15	86/9543 (0.9%)
1	B	0.70	1/6964 (0.0%)	1.15	87/9543 (0.9%)
1	C	0.70	1/6964 (0.0%)	1.15	86/9543 (0.9%)
All	All	0.70	3/20892 (0.0%)	1.15	259/28629 (0.9%)

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
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	527	PRO	C-N	-21.52	1.07	1.33
1	C	527	PRO	C-N	-21.52	1.07	1.33
1	A	527	PRO	C-N	-21.51	1.07	1.33

All (259) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	527	PRO	O-C-N	-23.49	97.38	122.98
1	A	527	PRO	O-C-N	-23.48	97.39	122.98
1	B	527	PRO	O-C-N	-23.47	97.40	122.98
1	A	527	PRO	CB-CA-C	-17.84	88.52	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	PRO	CB-CA-C	-17.84	88.52	111.71
1	C	527	PRO	CB-CA-C	-17.82	88.55	111.71
1	C	373	SER	N-CA-C	13.71	129.10	112.38
1	B	373	SER	N-CA-C	13.70	129.09	112.38
1	A	373	SER	N-CA-C	13.69	129.08	112.38
1	C	528	LYS	N-CA-C	-11.25	89.36	107.93
1	A	528	LYS	N-CA-C	-11.24	89.38	107.93
1	B	528	LYS	N-CA-C	-11.23	89.39	107.93
1	B	373	SER	N-CA-CB	-11.22	91.25	110.32
1	A	373	SER	N-CA-CB	-11.21	91.27	110.32
1	C	373	SER	N-CA-CB	-11.20	91.28	110.32
1	C	528	LYS	N-CA-CB	10.73	128.03	110.32
1	A	528	LYS	N-CA-CB	10.72	128.00	110.32
1	B	528	LYS	N-CA-CB	10.72	128.00	110.32
1	B	527	PRO	CA-C-N	8.93	136.04	121.58
1	B	527	PRO	C-N-CA	8.93	136.04	121.58
1	C	527	PRO	CA-C-N	8.92	136.03	121.58
1	C	527	PRO	C-N-CA	8.92	136.03	121.58
1	A	527	PRO	CA-C-N	8.92	136.03	121.58
1	A	527	PRO	C-N-CA	8.92	136.03	121.58
1	C	527	PRO	N-CA-CB	-7.92	96.12	103.17
1	A	527	PRO	N-CA-CB	-7.90	96.14	103.17
1	B	527	PRO	N-CA-CB	-7.88	96.16	103.17
1	C	1084	ASP	CA-CB-CG	7.68	120.28	112.60
1	B	1084	ASP	CA-CB-CG	7.67	120.27	112.60
1	A	1084	ASP	CA-CB-CG	7.67	120.27	112.60
1	C	862	PRO	CA-C-N	7.55	127.56	119.78
1	C	862	PRO	C-N-CA	7.55	127.56	119.78
1	B	862	PRO	CA-C-N	7.54	127.55	119.78
1	B	862	PRO	C-N-CA	7.54	127.55	119.78
1	A	862	PRO	CA-C-N	7.53	127.54	119.78
1	A	862	PRO	C-N-CA	7.53	127.54	119.78
1	B	791	THR	CA-C-N	7.25	124.88	119.66
1	B	791	THR	C-N-CA	7.25	124.88	119.66
1	C	791	THR	CA-C-N	7.22	124.86	119.66
1	C	791	THR	C-N-CA	7.22	124.86	119.66
1	A	791	THR	CA-C-N	7.17	124.83	119.66
1	A	791	THR	C-N-CA	7.17	124.83	119.66
1	B	792	PRO	CA-C-N	7.12	127.73	119.47
1	B	792	PRO	C-N-CA	7.12	127.73	119.47
1	A	792	PRO	CA-C-N	7.11	127.72	119.47
1	A	792	PRO	C-N-CA	7.11	127.72	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	792	PRO	CA-C-N	7.08	127.68	119.47
1	C	792	PRO	C-N-CA	7.08	127.68	119.47
1	B	425	LEU	CA-C-N	7.00	126.96	120.03
1	B	425	LEU	C-N-CA	7.00	126.96	120.03
1	C	425	LEU	CA-C-N	6.99	126.95	120.03
1	C	425	LEU	C-N-CA	6.99	126.95	120.03
1	A	425	LEU	CA-C-N	6.97	126.93	120.03
1	A	425	LEU	C-N-CA	6.97	126.93	120.03
1	A	173	GLN	CA-C-N	6.95	126.87	119.85
1	A	173	GLN	C-N-CA	6.95	126.87	119.85
1	C	173	GLN	CA-C-N	6.94	126.86	119.85
1	C	173	GLN	C-N-CA	6.94	126.86	119.85
1	B	173	GLN	CA-C-N	6.93	126.84	119.85
1	B	173	GLN	C-N-CA	6.93	126.84	119.85
1	B	383	SER	CA-C-N	6.92	126.61	119.56
1	B	383	SER	C-N-CA	6.92	126.61	119.56
1	C	383	SER	CA-C-N	6.91	126.61	119.56
1	C	383	SER	C-N-CA	6.91	126.61	119.56
1	A	383	SER	CA-C-N	6.90	126.59	119.56
1	A	383	SER	C-N-CA	6.90	126.59	119.56
1	B	861	LEU	CA-C-N	6.88	124.62	119.66
1	B	861	LEU	C-N-CA	6.88	124.62	119.66
1	A	861	LEU	CA-C-N	6.84	124.59	119.66
1	A	861	LEU	C-N-CA	6.84	124.59	119.66
1	C	861	LEU	CA-C-N	6.84	124.58	119.66
1	C	861	LEU	C-N-CA	6.84	124.58	119.66
1	A	565	PHE	CA-CB-CG	6.74	120.54	113.80
1	B	565	PHE	CA-CB-CG	6.72	120.52	113.80
1	C	565	PHE	CA-CB-CG	6.71	120.51	113.80
1	A	138	ASP	CA-C-N	6.63	126.54	119.85
1	A	138	ASP	C-N-CA	6.63	126.54	119.85
1	C	138	ASP	CA-C-N	6.59	126.50	119.85
1	C	138	ASP	C-N-CA	6.59	126.50	119.85
1	B	138	ASP	CA-C-N	6.58	126.50	119.85
1	B	138	ASP	C-N-CA	6.58	126.50	119.85
1	B	81	ASN	CA-C-N	6.56	126.74	120.31
1	B	81	ASN	C-N-CA	6.56	126.74	120.31
1	A	81	ASN	CA-C-N	6.55	126.73	120.31
1	A	81	ASN	C-N-CA	6.55	126.73	120.31
1	C	81	ASN	CA-C-N	6.54	126.72	120.31
1	C	81	ASN	C-N-CA	6.54	126.72	120.31
1	C	808	ASP	CA-C-N	6.46	126.09	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	808	ASP	C-N-CA	6.46	126.09	119.56
1	B	808	ASP	CA-C-N	6.45	126.07	119.56
1	B	808	ASP	C-N-CA	6.45	126.07	119.56
1	A	808	ASP	CA-C-N	6.44	126.07	119.56
1	A	808	ASP	C-N-CA	6.44	126.07	119.56
1	B	294	ASP	CA-C-N	6.38	126.06	119.56
1	B	294	ASP	C-N-CA	6.38	126.06	119.56
1	B	825	LYS	N-CA-C	6.37	118.31	111.36
1	C	294	ASP	CA-C-N	6.37	126.06	119.56
1	C	294	ASP	C-N-CA	6.37	126.06	119.56
1	A	825	LYS	N-CA-C	6.36	118.29	111.36
1	A	294	ASP	CA-C-N	6.35	126.04	119.56
1	A	294	ASP	C-N-CA	6.35	126.04	119.56
1	C	825	LYS	N-CA-C	6.35	118.28	111.36
1	A	506	GLN	CA-C-N	6.31	126.65	119.83
1	A	506	GLN	C-N-CA	6.31	126.65	119.83
1	B	506	GLN	CA-C-N	6.31	126.65	119.83
1	B	506	GLN	C-N-CA	6.31	126.65	119.83
1	C	506	GLN	CA-C-N	6.31	126.65	119.83
1	C	506	GLN	C-N-CA	6.31	126.65	119.83
1	C	216	LEU	CA-C-N	6.27	126.23	120.03
1	C	216	LEU	C-N-CA	6.27	126.23	120.03
1	A	1078	ALA	CA-C-N	6.24	125.87	119.56
1	A	1078	ALA	C-N-CA	6.24	125.87	119.56
1	A	216	LEU	CA-C-N	6.24	126.21	120.03
1	A	216	LEU	C-N-CA	6.24	126.21	120.03
1	B	216	LEU	CA-C-N	6.24	126.20	120.03
1	B	216	LEU	C-N-CA	6.24	126.20	120.03
1	C	1078	ALA	CA-C-N	6.21	125.83	119.56
1	C	1078	ALA	C-N-CA	6.21	125.83	119.56
1	C	941	THR	CA-C-N	6.20	126.67	119.47
1	C	941	THR	C-N-CA	6.20	126.67	119.47
1	B	1078	ALA	CA-C-N	6.20	125.82	119.56
1	B	1078	ALA	C-N-CA	6.20	125.82	119.56
1	B	941	THR	CA-C-N	6.18	126.64	119.47
1	B	941	THR	C-N-CA	6.18	126.64	119.47
1	A	941	THR	CA-C-N	6.16	126.61	119.47
1	A	941	THR	C-N-CA	6.16	126.61	119.47
1	A	321	GLN	CA-C-N	5.98	125.89	119.85
1	A	321	GLN	C-N-CA	5.98	125.89	119.85
1	B	714	ILE	CA-C-N	5.96	126.27	119.83
1	B	714	ILE	C-N-CA	5.96	126.27	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	GLN	CA-C-N	5.96	125.87	119.85
1	C	321	GLN	C-N-CA	5.96	125.87	119.85
1	A	714	ILE	CA-C-N	5.96	126.27	119.83
1	A	714	ILE	C-N-CA	5.96	126.27	119.83
1	C	374	PHE	N-CA-C	5.95	119.78	110.32
1	C	578	ASP	CA-C-N	5.95	126.06	119.87
1	C	578	ASP	C-N-CA	5.95	126.06	119.87
1	B	374	PHE	N-CA-C	5.95	119.77	110.32
1	A	578	ASP	CA-C-N	5.94	126.05	119.87
1	A	578	ASP	C-N-CA	5.94	126.05	119.87
1	B	578	ASP	CA-C-N	5.94	126.05	119.87
1	B	578	ASP	C-N-CA	5.94	126.05	119.87
1	A	374	PHE	N-CA-C	5.93	119.75	110.32
1	B	321	GLN	CA-C-N	5.92	125.83	119.85
1	B	321	GLN	C-N-CA	5.92	125.83	119.85
1	C	727	LEU	CA-C-N	5.92	125.86	119.76
1	C	727	LEU	C-N-CA	5.92	125.86	119.76
1	C	38	TYR	CA-C-N	5.91	125.53	119.56
1	C	38	TYR	C-N-CA	5.91	125.53	119.56
1	B	38	TYR	CA-C-N	5.91	125.53	119.56
1	B	38	TYR	C-N-CA	5.91	125.53	119.56
1	B	727	LEU	CA-C-N	5.91	125.84	119.76
1	B	727	LEU	C-N-CA	5.91	125.84	119.76
1	C	714	ILE	CA-C-N	5.91	126.21	119.83
1	C	714	ILE	C-N-CA	5.91	126.21	119.83
1	A	38	TYR	CA-C-N	5.90	125.52	119.56
1	A	38	TYR	C-N-CA	5.90	125.52	119.56
1	A	727	LEU	CA-C-N	5.89	125.83	119.76
1	A	727	LEU	C-N-CA	5.89	125.83	119.76
1	C	527	PRO	CA-C-O	-5.85	115.12	121.27
1	B	527	PRO	CA-C-O	-5.84	115.13	121.27
1	A	527	PRO	CA-C-O	-5.83	115.14	121.27
1	A	208	THR	CA-C-N	5.83	125.59	119.76
1	A	208	THR	C-N-CA	5.83	125.59	119.76
1	C	1068	VAL	CA-C-N	5.81	125.75	119.76
1	C	1068	VAL	C-N-CA	5.81	125.75	119.76
1	A	90	VAL	N-CA-C	5.81	116.24	108.11
1	C	90	VAL	N-CA-C	5.81	116.24	108.11
1	C	208	THR	CA-C-N	5.81	125.57	119.76
1	C	208	THR	C-N-CA	5.81	125.57	119.76
1	B	90	VAL	N-CA-C	5.80	116.23	108.11
1	B	1068	VAL	CA-C-N	5.80	125.73	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1068	VAL	C-N-CA	5.80	125.73	119.76
1	B	208	THR	CA-C-N	5.78	125.54	119.76
1	B	208	THR	C-N-CA	5.78	125.54	119.76
1	A	1068	VAL	CA-C-N	5.77	125.71	119.76
1	A	1068	VAL	C-N-CA	5.77	125.71	119.76
1	C	806	LEU	CA-C-N	5.73	125.66	119.76
1	C	806	LEU	C-N-CA	5.73	125.66	119.76
1	B	411	ALA	CA-C-N	5.71	125.62	119.85
1	B	411	ALA	C-N-CA	5.71	125.62	119.85
1	C	411	ALA	CA-C-N	5.71	125.62	119.85
1	C	411	ALA	C-N-CA	5.71	125.62	119.85
1	A	806	LEU	CA-C-N	5.71	125.64	119.76
1	A	806	LEU	C-N-CA	5.71	125.64	119.76
1	B	806	LEU	CA-C-N	5.70	125.63	119.76
1	B	806	LEU	C-N-CA	5.70	125.63	119.76
1	A	411	ALA	CA-C-N	5.70	125.61	119.85
1	A	411	ALA	C-N-CA	5.70	125.61	119.85
1	B	329	PHE	CA-C-N	5.67	125.62	119.78
1	B	329	PHE	C-N-CA	5.67	125.62	119.78
1	A	329	PHE	CA-C-N	5.67	125.62	119.78
1	A	329	PHE	C-N-CA	5.67	125.62	119.78
1	A	985	ASP	CA-C-N	5.67	126.22	120.38
1	A	985	ASP	C-N-CA	5.67	126.22	120.38
1	B	599	THR	CA-C-N	5.66	126.13	120.52
1	B	599	THR	C-N-CA	5.66	126.13	120.52
1	C	329	PHE	CA-C-N	5.66	125.61	119.78
1	C	329	PHE	C-N-CA	5.66	125.61	119.78
1	B	985	ASP	CA-C-N	5.65	126.20	120.38
1	B	985	ASP	C-N-CA	5.65	126.20	120.38
1	C	985	ASP	CA-C-N	5.64	126.19	120.38
1	C	985	ASP	C-N-CA	5.64	126.19	120.38
1	C	84	LEU	CA-C-N	5.64	125.58	119.78
1	C	84	LEU	C-N-CA	5.64	125.58	119.78
1	A	599	THR	CA-C-N	5.62	126.09	120.52
1	A	599	THR	C-N-CA	5.62	126.09	120.52
1	C	599	THR	CA-C-N	5.62	126.08	120.52
1	C	599	THR	C-N-CA	5.62	126.08	120.52
1	A	84	LEU	CA-C-N	5.60	125.55	119.78
1	A	84	LEU	C-N-CA	5.60	125.55	119.78
1	B	84	LEU	CA-C-N	5.60	125.55	119.78
1	B	84	LEU	C-N-CA	5.60	125.55	119.78
1	A	1111	GLU	CA-C-N	5.48	125.24	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1111	GLU	C-N-CA	5.48	125.24	119.76
1	C	1111	GLU	CA-C-N	5.44	125.20	119.76
1	C	1111	GLU	C-N-CA	5.44	125.20	119.76
1	B	1111	GLU	CA-C-N	5.41	125.17	119.76
1	B	1111	GLU	C-N-CA	5.41	125.17	119.76
1	B	560	LEU	CA-C-N	5.40	126.59	119.84
1	B	560	LEU	C-N-CA	5.40	126.59	119.84
1	A	560	LEU	CA-C-N	5.39	126.58	119.84
1	A	560	LEU	C-N-CA	5.39	126.58	119.84
1	C	560	LEU	CA-C-N	5.39	126.58	119.84
1	C	560	LEU	C-N-CA	5.39	126.58	119.84
1	A	816	SER	CA-C-N	5.34	125.41	119.32
1	A	816	SER	C-N-CA	5.34	125.41	119.32
1	C	816	SER	CA-C-N	5.34	125.40	119.32
1	C	816	SER	C-N-CA	5.34	125.40	119.32
1	C	520	ALA	CA-C-N	5.32	125.24	119.76
1	C	520	ALA	C-N-CA	5.32	125.24	119.76
1	B	816	SER	CA-C-N	5.32	125.38	119.32
1	B	816	SER	C-N-CA	5.32	125.38	119.32
1	A	371	SER	N-CA-C	-5.31	102.67	110.42
1	B	520	ALA	CA-C-N	5.31	125.22	119.76
1	B	520	ALA	C-N-CA	5.31	125.22	119.76
1	B	371	SER	N-CA-C	-5.30	102.68	110.42
1	C	371	SER	N-CA-C	-5.29	102.69	110.42
1	A	520	ALA	CA-C-N	5.27	125.19	119.76
1	A	520	ALA	C-N-CA	5.27	125.19	119.76
1	C	372	ALA	CB-CA-C	5.25	120.40	109.95
1	A	372	ALA	CB-CA-C	5.25	120.39	109.95
1	B	372	ALA	CB-CA-C	5.24	120.37	109.95
1	C	1142	GLN	CA-C-N	5.14	124.80	119.56
1	C	1142	GLN	C-N-CA	5.14	124.80	119.56
1	C	891	GLY	CA-C-N	5.13	125.03	119.85
1	C	891	GLY	C-N-CA	5.13	125.03	119.85
1	B	1142	GLN	CA-C-N	5.13	124.79	119.56
1	B	1142	GLN	C-N-CA	5.13	124.79	119.56
1	A	1142	GLN	CA-C-N	5.12	124.78	119.56
1	A	1142	GLN	C-N-CA	5.12	124.78	119.56
1	B	891	GLY	CA-C-N	5.11	125.01	119.85
1	B	891	GLY	C-N-CA	5.11	125.01	119.85
1	A	891	GLY	CA-C-N	5.09	125.00	119.85
1	A	891	GLY	C-N-CA	5.09	125.00	119.85
1	C	986	PRO	N-CA-C	5.04	116.85	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	986	PRO	N-CA-C	5.02	116.83	110.70
1	B	986	PRO	N-CA-C	5.02	116.82	110.70
1	B	371	SER	CB-CA-C	5.00	116.67	109.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	527	PRO	Mainchain
1	B	527	PRO	Mainchain
1	C	527	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6804	0	6015	30	0
1	B	6804	0	6015	32	0
1	C	6804	0	6015	29	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	196	0	182	19	0
3	B	196	0	182	19	0
3	C	196	0	182	19	0
All	All	21168	0	18741	91	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 2.

All (91) 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:B:580:GLN:C	3:B:1313:NAG:H62	1.39	1.46
1:C:580:GLN:C	3:C:1313:NAG:H62	1.39	1.45
1:A:580:GLN:C	3:A:1313:NAG:H62	1.39	1.44
1:C:580:GLN:O	3:C:1313:NAG:C6	1.82	1.27
1:A:580:GLN:O	3:A:1313:NAG:C6	1.82	1.27
1:B:580:GLN:O	3:B:1313:NAG:C6	1.82	1.26
1:A:580:GLN:O	3:A:1313:NAG:H62	1.37	1.19
1:B:580:GLN:O	3:B:1313:NAG:H62	1.37	1.18
1:C:580:GLN:O	3:C:1313:NAG:H62	1.37	1.16
1:B:580:GLN:C	3:B:1313:NAG:C6	2.29	1.04
1:A:580:GLN:C	3:A:1313:NAG:C6	2.29	1.01
1:C:342:PHE:HB2	3:C:1314:NAG:H82	1.42	1.00
1:B:342:PHE:HB2	3:B:1314:NAG:H82	1.43	0.99
1:A:342:PHE:HB2	3:A:1314:NAG:H82	1.42	0.99
1:C:580:GLN:C	3:C:1313:NAG:C6	2.29	0.99
1:A:580:GLN:O	3:A:1313:NAG:C5	2.19	0.90
1:C:580:GLN:O	3:C:1313:NAG:C5	2.19	0.90
1:B:580:GLN:O	3:B:1313:NAG:C5	2.19	0.89
1:A:330:PRO:HD3	1:A:544:ASN:OD1	1.74	0.88
1:A:28:TYR:CD1	3:A:1312:NAG:H62	2.09	0.88
1:C:330:PRO:HD3	1:C:544:ASN:OD1	1.74	0.87
1:C:28:TYR:CD1	3:C:1312:NAG:H62	2.09	0.87
1:B:330:PRO:HD3	1:B:544:ASN:OD1	1.74	0.87
1:C:342:PHE:CB	3:C:1314:NAG:H82	2.05	0.87
1:B:28:TYR:CD1	3:B:1312:NAG:H62	2.09	0.86
1:A:342:PHE:CB	3:A:1314:NAG:H82	2.05	0.85
1:B:342:PHE:CB	3:B:1314:NAG:H82	2.05	0.84
1:A:580:GLN:O	3:A:1313:NAG:H5	1.81	0.80
1:C:580:GLN:O	3:C:1313:NAG:H5	1.81	0.80
1:B:580:GLN:O	3:B:1313:NAG:H5	1.81	0.78
1:C:28:TYR:HD1	3:C:1312:NAG:H62	1.53	0.72
1:A:28:TYR:HD1	3:A:1312:NAG:H62	1.53	0.71
1:B:28:TYR:HD1	3:B:1312:NAG:H62	1.53	0.70
1:C:580:GLN:CA	3:C:1313:NAG:H62	2.27	0.62
1:A:580:GLN:CA	3:A:1313:NAG:H62	2.27	0.62
1:A:580:GLN:O	3:A:1313:NAG:H61	1.97	0.60
1:B:580:GLN:CA	3:B:1313:NAG:H62	2.27	0.59
1:C:580:GLN:O	3:C:1313:NAG:H61	1.97	0.57
1:C:581:THR:HA	3:C:1313:NAG:H61	1.88	0.56
1:B:370:ASN:O	1:B:371:SER:C	2.50	0.55
1:A:370:ASN:O	1:A:371:SER:C	2.50	0.55
1:B:581:THR:HA	3:B:1313:NAG:H61	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:THR:HA	3:A:1313:NAG:H61	1.88	0.54
1:C:581:THR:N	3:C:1313:NAG:H62	2.15	0.54
1:B:565:PHE:HE1	1:B:567:ARG:HE	1.56	0.53
1:C:370:ASN:O	1:C:371:SER:C	2.50	0.53
1:A:565:PHE:HE1	1:A:567:ARG:HE	1.56	0.52
1:A:580:GLN:CB	3:A:1313:NAG:H62	2.40	0.52
1:C:565:PHE:HE1	1:C:567:ARG:HE	1.56	0.52
1:C:580:GLN:CB	3:C:1313:NAG:H62	2.40	0.51
1:B:580:GLN:CB	3:B:1313:NAG:H62	2.40	0.51
1:B:580:GLN:O	3:B:1313:NAG:H61	1.96	0.51
1:B:521:PRO:HG3	1:B:564:GLN:CD	2.36	0.51
1:C:521:PRO:HG3	1:C:564:GLN:CD	2.36	0.50
1:A:521:PRO:HG3	1:A:564:GLN:CD	2.36	0.50
1:B:342:PHE:HB2	3:B:1314:NAG:C8	2.30	0.50
1:C:28:TYR:HB3	1:C:61:ASN:OD1	2.13	0.48
1:A:581:THR:N	3:A:1313:NAG:H62	2.15	0.48
1:B:28:TYR:HB3	1:B:61:ASN:OD1	2.13	0.47
1:A:28:TYR:HB3	1:A:61:ASN:OD1	2.13	0.47
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.79	0.46
1:A:580:GLN:HB3	3:A:1313:NAG:C6	2.46	0.46
1:C:580:GLN:HB3	3:C:1313:NAG:C6	2.46	0.46
1:A:342:PHE:HB2	3:A:1314:NAG:C8	2.30	0.46
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.79	0.46
1:A:330:PRO:HG3	1:A:544:ASN:HD21	1.82	0.45
1:A:1142:GLN:N	1:A:1143:PRO:CD	2.79	0.45
1:B:1138:TYR:HE2	1:B:1140:PRO:HB3	1.82	0.45
1:C:330:PRO:HG3	1:C:544:ASN:HD21	1.82	0.45
1:C:1138:TYR:HE2	1:C:1140:PRO:HB3	1.82	0.45
1:B:330:PRO:HG3	1:B:544:ASN:HD21	1.82	0.45
1:B:580:GLN:HB3	3:B:1313:NAG:C6	2.46	0.45
1:A:1138:TYR:HE2	1:A:1140:PRO:HB3	1.82	0.45
1:B:580:GLN:HB3	3:B:1313:NAG:H62	1.99	0.44
1:A:580:GLN:HB3	3:A:1313:NAG:H62	1.99	0.43
1:C:580:GLN:HB3	3:C:1313:NAG:H62	1.99	0.43
1:B:581:THR:N	3:B:1313:NAG:H62	2.15	0.43
1:B:862:PRO:HA	1:B:863:PRO:HD3	1.89	0.43
1:C:544:ASN:CG	1:C:579:PRO:HB3	2.44	0.43
1:A:544:ASN:CG	1:A:579:PRO:HB3	2.44	0.43
1:B:544:ASN:CG	1:B:579:PRO:HB3	2.44	0.43
1:C:339:GLY:HA2	3:C:1314:NAG:H81	2.02	0.42
1:B:792:PRO:HA	1:B:793:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:GLU:O	1:A:1107:ARG:NH1	2.54	0.41
1:A:544:ASN:OD1	1:A:579:PRO:CB	2.69	0.41
1:B:544:ASN:OD1	1:B:579:PRO:CB	2.69	0.41
1:B:1092:GLU:O	1:B:1107:ARG:NH1	2.54	0.41
1:C:342:PHE:HB2	3:C:1314:NAG:C8	2.30	0.41
1:C:544:ASN:OD1	1:C:579:PRO:CB	2.69	0.41
1:A:339:GLY:HA2	3:A:1314:NAG:H81	2.02	0.40
1:B:339:GLY:HA2	3:B:1314:NAG:H81	2.02	0.40

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	926/1277 (72%)	907 (98%)	19 (2%)	0	100	100
1	B	926/1277 (72%)	907 (98%)	19 (2%)	0	100	100
1	C	926/1277 (72%)	907 (98%)	19 (2%)	0	100	100
All	All	2778/3831 (72%)	2721 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	611/1111 (55%)	608 (100%)	3 (0%)	81	90
1	B	611/1111 (55%)	608 (100%)	3 (0%)	81	90
1	C	611/1111 (55%)	608 (100%)	3 (0%)	81	90
All	All	1833/3333 (55%)	1824 (100%)	9 (0%)	78	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	331	ASN
1	A	527	PRO
1	B	62	VAL
1	B	331	ASN
1	B	527	PRO
1	C	62	VAL
1	C	331	ASN
1	C	527	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	536	ASN
1	A	787	GLN
1	A	856	ASN
1	A	907	ASN
1	A	949	GLN
1	A	957	GLN
1	B	536	ASN
1	B	703	ASN
1	B	787	GLN
1	B	856	ASN
1	B	907	ASN
1	B	949	GLN
1	B	957	GLN
1	C	536	ASN
1	C	787	GLN
1	C	856	ASN
1	C	907	ASN
1	C	949	GLN
1	C	957	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

12 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	1.65	2 (14%)	17,19,21	1.06	1 (5%)
2	NAG	D	2	2	14,14,15	1.54	2 (14%)	17,19,21	0.85	1 (5%)
2	NAG	E	1	1,2	14,14,15	1.55	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	E	2	2	14,14,15	1.49	2 (14%)	17,19,21	0.91	1 (5%)
2	NAG	F	1	1,2	14,14,15	1.65	2 (14%)	17,19,21	1.06	1 (5%)
2	NAG	F	2	2	14,14,15	1.54	2 (14%)	17,19,21	0.85	1 (5%)
2	NAG	G	1	1,2	14,14,15	1.55	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	G	2	2	14,14,15	1.49	2 (14%)	17,19,21	0.91	1 (5%)
2	NAG	H	1	1,2	14,14,15	1.64	2 (14%)	17,19,21	1.06	1 (5%)
2	NAG	H	2	2	14,14,15	1.54	2 (14%)	17,19,21	0.85	1 (5%)
2	NAG	I	1	1,2	14,14,15	1.55	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	I	2	2	14,14,15	1.49	2 (14%)	17,19,21	0.91	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	4.67	1.58	1.52
2	D	1	NAG	C1-C2	4.66	1.58	1.52
2	H	1	NAG	C1-C2	4.64	1.58	1.52
2	G	1	NAG	C1-C2	4.25	1.58	1.52
2	E	1	NAG	C1-C2	4.25	1.58	1.52
2	I	1	NAG	C1-C2	4.23	1.58	1.52
2	D	2	NAG	C1-C2	3.91	1.57	1.52
2	F	2	NAG	C1-C2	3.89	1.57	1.52
2	H	2	NAG	C1-C2	3.88	1.57	1.52
2	G	2	NAG	C1-C2	3.75	1.57	1.52
2	E	2	NAG	C1-C2	3.74	1.57	1.52
2	I	2	NAG	C1-C2	3.73	1.57	1.52
2	F	2	NAG	O5-C5	2.41	1.48	1.43
2	D	2	NAG	O5-C5	2.41	1.48	1.43
2	H	2	NAG	O5-C5	2.40	1.48	1.43
2	E	2	NAG	O5-C5	2.16	1.47	1.43
2	I	2	NAG	O5-C5	2.16	1.47	1.43
2	G	2	NAG	O5-C5	2.14	1.47	1.43
2	H	1	NAG	C4-C5	2.06	1.57	1.53
2	D	1	NAG	C4-C5	2.04	1.57	1.53
2	F	1	NAG	C4-C5	2.03	1.57	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	NAG	C8-C7-N2	2.52	120.30	116.12
2	E	1	NAG	C8-C7-N2	2.51	120.28	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C8-C7-N2	2.51	120.28	116.12
2	G	2	NAG	C8-C7-N2	2.42	120.13	116.12
2	E	2	NAG	C8-C7-N2	2.42	120.13	116.12
2	I	2	NAG	C8-C7-N2	2.42	120.13	116.12
2	D	1	NAG	C8-C7-N2	2.41	120.11	116.12
2	H	1	NAG	C8-C7-N2	2.40	120.11	116.12
2	F	1	NAG	C8-C7-N2	2.38	120.07	116.12
2	H	2	NAG	C8-C7-N2	2.22	119.81	116.12
2	F	2	NAG	C8-C7-N2	2.21	119.79	116.12
2	D	2	NAG	C8-C7-N2	2.21	119.78	116.12

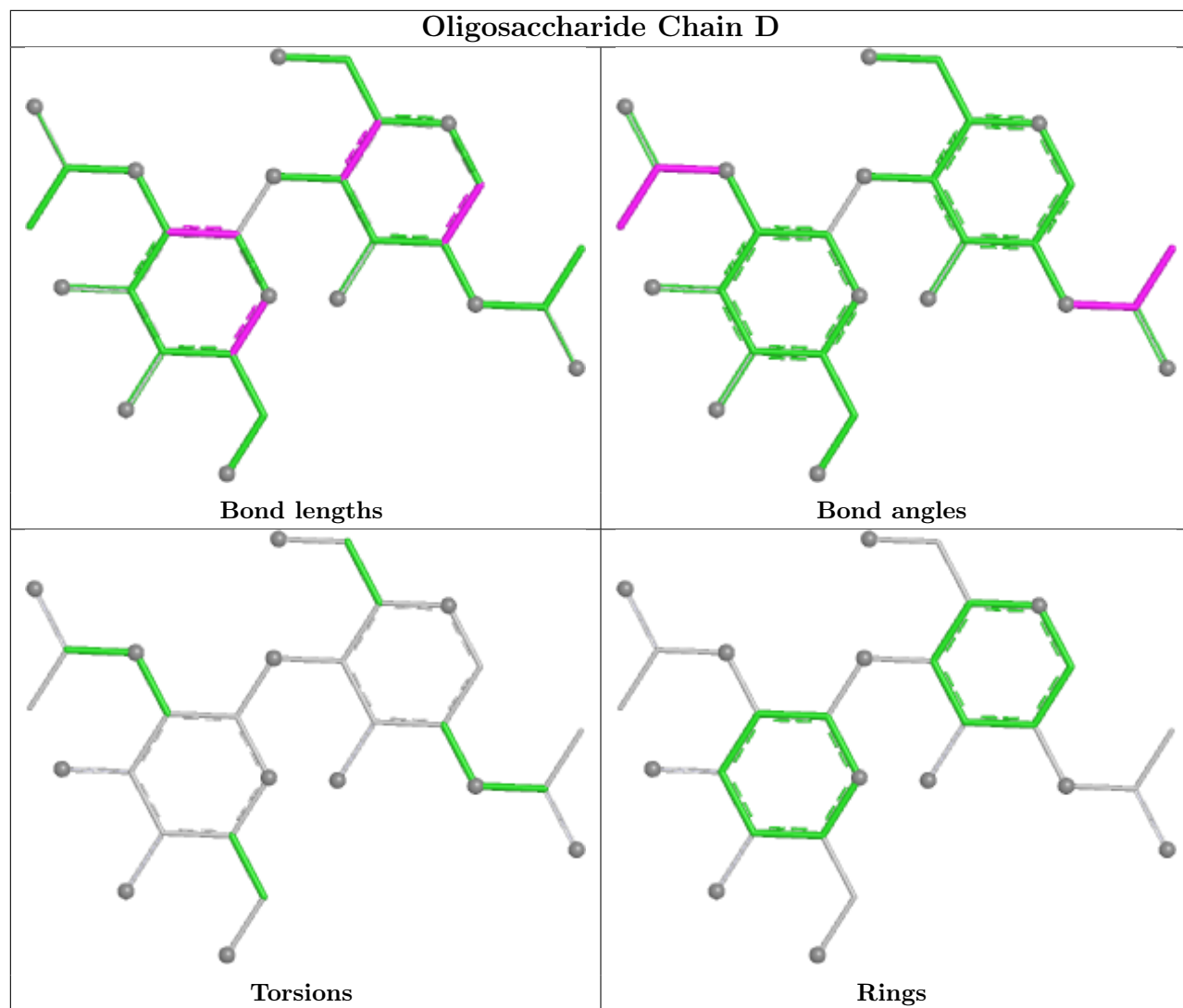
There are no chirality outliers.

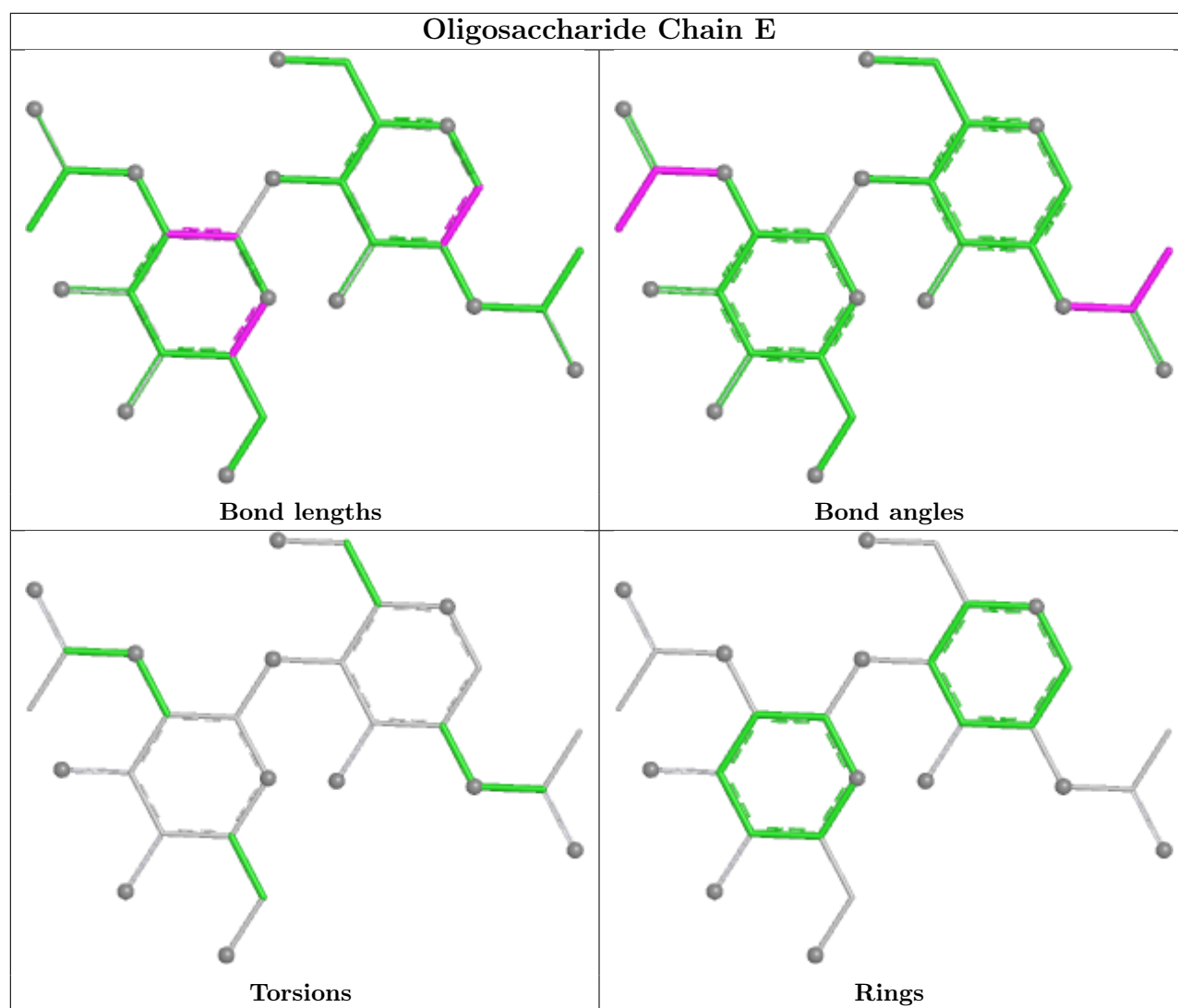
There are no torsion outliers.

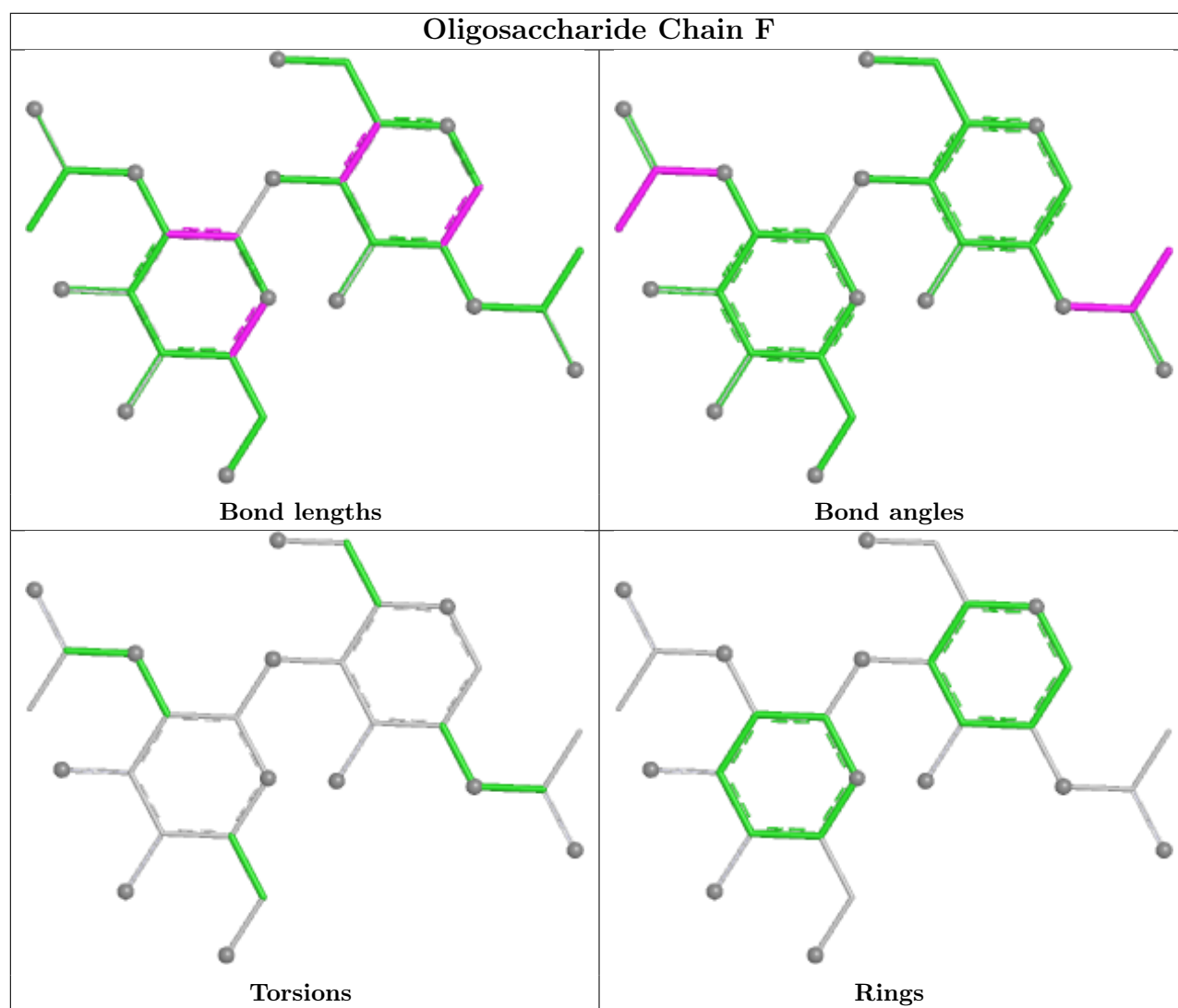
There are no ring outliers.

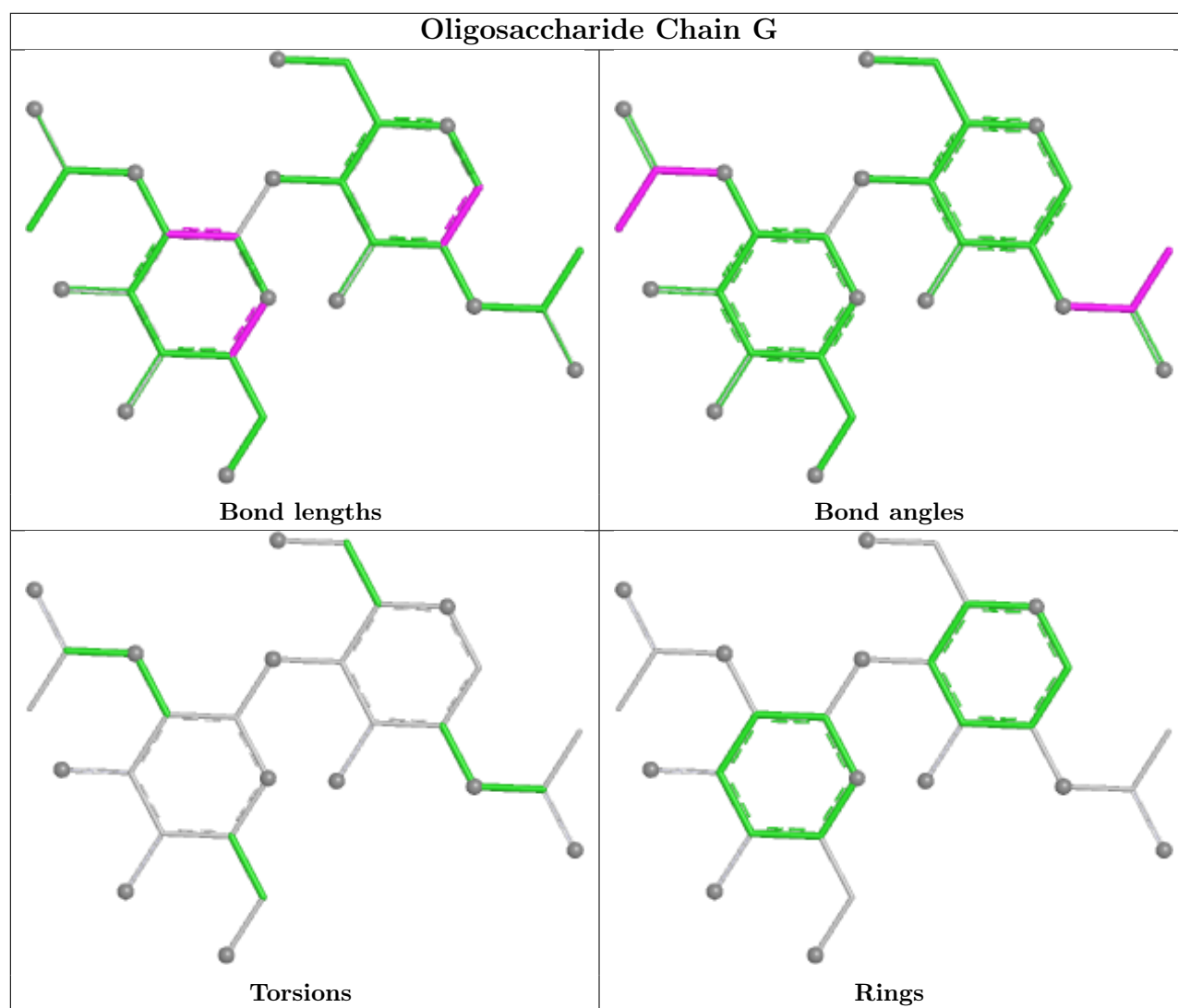
No monomer is involved in short contacts.

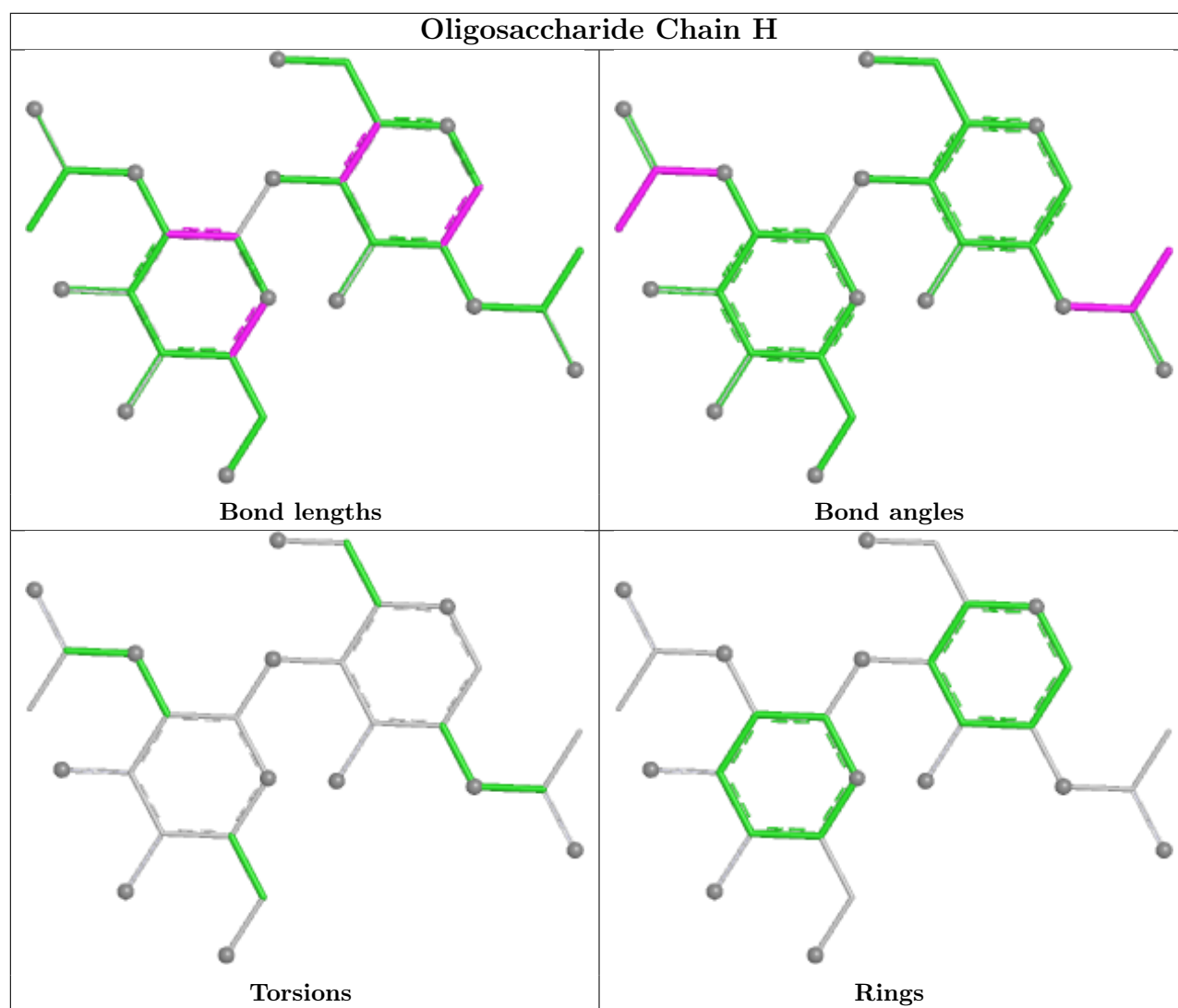
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

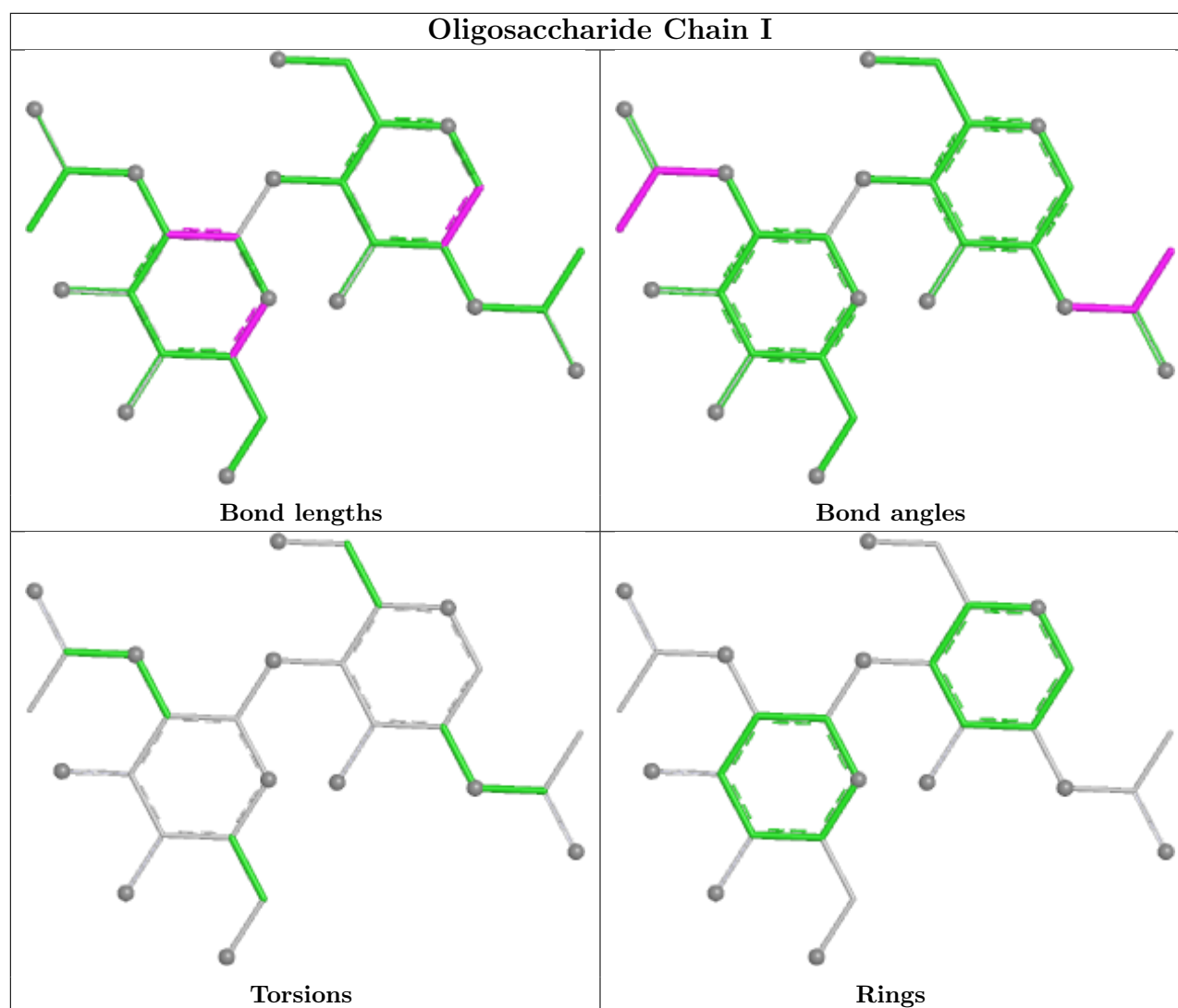












5.6 Ligand geometry [i](#)

42 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1304	1	14,14,15	1.67	2 (14%)	17,19,21	0.95	1 (5%)
3	NAG	B	1311	1	14,14,15	1.79	2 (14%)	17,19,21	1.24	2 (11%)
3	NAG	B	1303	1	14,14,15	1.67	2 (14%)	17,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1305	1	14,14,15	1.61	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	A	1312	1	14,14,15	0.41	0	17,19,21	0.76	0
3	NAG	A	1301	1	14,14,15	1.64	2 (14%)	17,19,21	1.05	1 (5%)
3	NAG	B	1310	1	14,14,15	1.70	3 (21%)	17,19,21	1.52	3 (17%)
3	NAG	B	1306	1	14,14,15	1.71	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	B	1308	1	14,14,15	1.61	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	C	1308	1	14,14,15	1.61	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	C	1314	1	14,14,15	0.42	0	17,19,21	0.75	0
3	NAG	B	1302	1	14,14,15	1.68	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	C	1301	1	14,14,15	1.64	2 (14%)	17,19,21	1.06	1 (5%)
3	NAG	A	1306	1	14,14,15	1.71	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	B	1305	1	14,14,15	1.61	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	A	1308	1	14,14,15	1.60	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	B	1309	1	14,14,15	1.70	2 (14%)	17,19,21	0.96	1 (5%)
3	NAG	A	1303	1	14,14,15	1.67	2 (14%)	17,19,21	0.91	0
3	NAG	B	1304	1	14,14,15	1.67	2 (14%)	17,19,21	0.95	1 (5%)
3	NAG	A	1302	1	14,14,15	1.67	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	B	1313	1	14,14,15	0.40	0	17,19,21	0.76	0
3	NAG	B	1312	1	14,14,15	0.41	0	17,19,21	0.76	0
3	NAG	C	1311	1	14,14,15	1.79	2 (14%)	17,19,21	1.24	2 (11%)
3	NAG	A	1313	1	14,14,15	0.40	0	17,19,21	0.76	0
3	NAG	A	1311	1	14,14,15	1.80	2 (14%)	17,19,21	1.25	2 (11%)
3	NAG	C	1312	1	14,14,15	0.41	0	17,19,21	0.76	0
3	NAG	A	1307	1	14,14,15	1.64	2 (14%)	17,19,21	1.08	1 (5%)
3	NAG	C	1310	1	14,14,15	1.70	2 (14%)	17,19,21	1.52	3 (17%)
3	NAG	A	1309	1	14,14,15	1.69	2 (14%)	17,19,21	0.96	1 (5%)
3	NAG	C	1303	1	14,14,15	1.67	2 (14%)	17,19,21	0.91	0
3	NAG	C	1306	1	14,14,15	1.73	2 (14%)	17,19,21	0.99	1 (5%)
3	NAG	B	1314	1	14,14,15	0.42	0	17,19,21	0.76	0
3	NAG	C	1302	1	14,14,15	1.66	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	B	1301	1	14,14,15	1.64	2 (14%)	17,19,21	1.05	1 (5%)
3	NAG	A	1310	1	14,14,15	1.70	3 (21%)	17,19,21	1.52	4 (23%)
3	NAG	A	1314	1	14,14,15	0.41	0	17,19,21	0.76	0
3	NAG	C	1307	1	14,14,15	1.64	2 (14%)	17,19,21	1.08	1 (5%)
3	NAG	B	1307	1	14,14,15	1.64	2 (14%)	17,19,21	1.08	1 (5%)
3	NAG	C	1304	1	14,14,15	1.67	2 (14%)	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1309	1	14,14,15	1.70	2 (14%)	17,19,21	0.96	1 (5%)
3	NAG	C	1305	1	14,14,15	1.61	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	C	1313	1	14,14,15	0.41	0	17,19,21	0.76	0

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	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1314	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	1/6/23/26	0/1/1/1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1311	NAG	C1-C2	5.00	1.59	1.52
3	B	1311	NAG	C1-C2	4.99	1.59	1.52
3	C	1311	NAG	C1-C2	4.99	1.59	1.52
3	C	1306	NAG	C1-C2	4.85	1.59	1.52
3	B	1306	NAG	C1-C2	4.79	1.58	1.52
3	C	1309	NAG	C1-C2	4.79	1.58	1.52
3	B	1309	NAG	C1-C2	4.78	1.58	1.52
3	A	1306	NAG	C1-C2	4.78	1.58	1.52
3	A	1309	NAG	C1-C2	4.75	1.58	1.52
3	B	1303	NAG	C1-C2	4.74	1.58	1.52
3	A	1303	NAG	C1-C2	4.70	1.58	1.52
3	B	1302	NAG	C1-C2	4.70	1.58	1.52
3	C	1303	NAG	C1-C2	4.70	1.58	1.52
3	B	1304	NAG	C1-C2	4.69	1.58	1.52
3	C	1304	NAG	C1-C2	4.68	1.58	1.52
3	C	1302	NAG	C1-C2	4.66	1.58	1.52
3	A	1304	NAG	C1-C2	4.66	1.58	1.52
3	A	1302	NAG	C1-C2	4.66	1.58	1.52
3	B	1301	NAG	C1-C2	4.54	1.58	1.52
3	C	1301	NAG	C1-C2	4.52	1.58	1.52
3	A	1301	NAG	C1-C2	4.51	1.58	1.52
3	A	1307	NAG	C1-C2	4.46	1.58	1.52
3	B	1307	NAG	C1-C2	4.46	1.58	1.52
3	C	1307	NAG	C1-C2	4.46	1.58	1.52
3	C	1305	NAG	C1-C2	4.45	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1305	NAG	C1-C2	4.44	1.58	1.52
3	B	1305	NAG	C1-C2	4.42	1.58	1.52
3	B	1308	NAG	C1-C2	4.37	1.58	1.52
3	C	1308	NAG	C1-C2	4.35	1.58	1.52
3	A	1308	NAG	C1-C2	4.34	1.58	1.52
3	B	1310	NAG	C1-C2	4.33	1.58	1.52
3	C	1310	NAG	C1-C2	4.33	1.58	1.52
3	A	1310	NAG	C1-C2	4.33	1.58	1.52
3	A	1307	NAG	O5-C5	2.64	1.48	1.43
3	B	1307	NAG	O5-C5	2.62	1.48	1.43
3	C	1307	NAG	O5-C5	2.61	1.48	1.43
3	A	1311	NAG	O5-C5	2.57	1.48	1.43
3	B	1311	NAG	O5-C5	2.57	1.48	1.43
3	C	1311	NAG	O5-C5	2.57	1.48	1.43
3	A	1304	NAG	O5-C5	2.57	1.48	1.43
3	C	1304	NAG	O5-C5	2.57	1.48	1.43
3	B	1304	NAG	O5-C5	2.56	1.48	1.43
3	B	1309	NAG	O5-C5	2.55	1.48	1.43
3	C	1309	NAG	O5-C5	2.55	1.48	1.43
3	A	1309	NAG	O5-C5	2.54	1.48	1.43
3	B	1310	NAG	O5-C5	2.53	1.48	1.43
3	A	1310	NAG	O5-C5	2.53	1.48	1.43
3	C	1310	NAG	O5-C5	2.53	1.48	1.43
3	C	1303	NAG	O5-C5	2.51	1.48	1.43
3	B	1303	NAG	O5-C5	2.49	1.48	1.43
3	A	1303	NAG	O5-C5	2.48	1.48	1.43
3	B	1302	NAG	O5-C5	2.46	1.48	1.43
3	A	1302	NAG	O5-C5	2.46	1.48	1.43
3	C	1302	NAG	O5-C5	2.44	1.48	1.43
3	A	1306	NAG	O5-C5	2.42	1.48	1.43
3	B	1306	NAG	O5-C5	2.40	1.48	1.43
3	C	1306	NAG	O5-C5	2.40	1.48	1.43
3	B	1305	NAG	O5-C5	2.39	1.48	1.43
3	A	1305	NAG	O5-C5	2.38	1.48	1.43
3	C	1305	NAG	O5-C5	2.37	1.48	1.43
3	A	1301	NAG	O5-C5	2.33	1.48	1.43
3	C	1301	NAG	O5-C5	2.33	1.48	1.43
3	B	1301	NAG	O5-C5	2.31	1.47	1.43
3	B	1308	NAG	O5-C5	2.29	1.47	1.43
3	A	1308	NAG	O5-C5	2.28	1.47	1.43
3	C	1308	NAG	O5-C5	2.27	1.47	1.43
3	B	1310	NAG	O5-C1	2.01	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1310	NAG	O5-C1	2.01	1.47	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1310	NAG	C8-C7-N2	3.77	122.36	116.12
3	C	1310	NAG	C8-C7-N2	3.76	122.36	116.12
3	A	1310	NAG	C8-C7-N2	3.76	122.35	116.12
3	A	1311	NAG	C8-C7-N2	3.22	121.46	116.12
3	B	1311	NAG	C8-C7-N2	3.21	121.45	116.12
3	C	1311	NAG	C8-C7-N2	3.21	121.43	116.12
3	C	1301	NAG	C8-C7-N2	2.78	120.72	116.12
3	A	1301	NAG	C8-C7-N2	2.76	120.70	116.12
3	B	1301	NAG	C8-C7-N2	2.76	120.70	116.12
3	C	1307	NAG	C8-C7-N2	2.75	120.68	116.12
3	A	1307	NAG	C8-C7-N2	2.75	120.68	116.12
3	C	1310	NAG	C2-N2-C7	-2.75	119.22	122.90
3	B	1307	NAG	C8-C7-N2	2.74	120.66	116.12
3	A	1310	NAG	C2-N2-C7	-2.73	119.24	122.90
3	B	1310	NAG	C2-N2-C7	-2.72	119.25	122.90
3	A	1310	NAG	O7-C7-C8	-2.50	117.61	122.05
3	B	1310	NAG	O7-C7-C8	-2.49	117.61	122.05
3	C	1310	NAG	O7-C7-C8	-2.49	117.62	122.05
3	B	1309	NAG	C8-C7-N2	2.46	120.20	116.12
3	C	1309	NAG	C8-C7-N2	2.46	120.20	116.12
3	A	1309	NAG	C8-C7-N2	2.46	120.20	116.12
3	A	1302	NAG	C8-C7-N2	2.44	120.17	116.12
3	B	1302	NAG	C8-C7-N2	2.44	120.16	116.12
3	C	1302	NAG	C8-C7-N2	2.43	120.15	116.12
3	A	1311	NAG	O7-C7-C8	-2.42	117.74	122.05
3	C	1311	NAG	O7-C7-C8	-2.40	117.78	122.05
3	B	1311	NAG	O7-C7-C8	-2.40	117.79	122.05
3	C	1306	NAG	C8-C7-N2	2.38	120.06	116.12
3	A	1306	NAG	C8-C7-N2	2.38	120.06	116.12
3	B	1306	NAG	C8-C7-N2	2.37	120.06	116.12
3	C	1308	NAG	C8-C7-N2	2.33	119.98	116.12
3	B	1308	NAG	C8-C7-N2	2.32	119.96	116.12
3	A	1308	NAG	C8-C7-N2	2.31	119.94	116.12
3	A	1305	NAG	C8-C7-N2	2.18	119.74	116.12
3	B	1305	NAG	C8-C7-N2	2.17	119.72	116.12
3	C	1305	NAG	C8-C7-N2	2.17	119.72	116.12
3	C	1304	NAG	C8-C7-N2	2.06	119.54	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1304	NAG	C8-C7-N2	2.06	119.54	116.12
3	B	1304	NAG	C8-C7-N2	2.04	119.50	116.12
3	A	1310	NAG	C4-C3-C2	-2.00	108.09	111.02

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1310	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	A	1311	NAG	C4-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	C	1311	NAG	C4-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	A	1312	NAG	C1-C2-N2-C7
3	A	1313	NAG	C1-C2-N2-C7
3	A	1314	NAG	C1-C2-N2-C7
3	B	1312	NAG	C1-C2-N2-C7
3	B	1313	NAG	C1-C2-N2-C7
3	B	1314	NAG	C1-C2-N2-C7
3	C	1312	NAG	C1-C2-N2-C7
3	C	1313	NAG	C1-C2-N2-C7
3	C	1314	NAG	C1-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1312	NAG	2	0
3	C	1314	NAG	4	0
3	B	1313	NAG	13	0
3	B	1312	NAG	2	0
3	A	1313	NAG	13	0
3	C	1312	NAG	2	0
3	B	1314	NAG	4	0
3	A	1314	NAG	4	0
3	C	1313	NAG	13	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	527:PRO	C	528:LYS	N	1.07
1	B	527:PRO	C	528:LYS	N	1.07
1	C	527:PRO	C	528:LYS	N	1.07

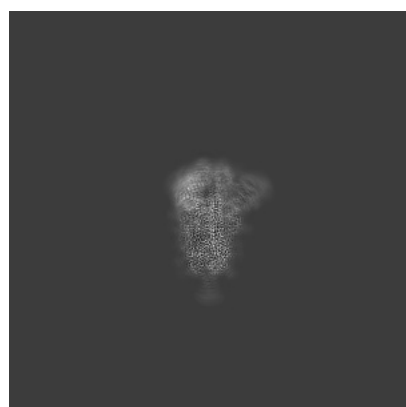
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26056. These allow visual inspection of the internal detail of the map and identification of artifacts.

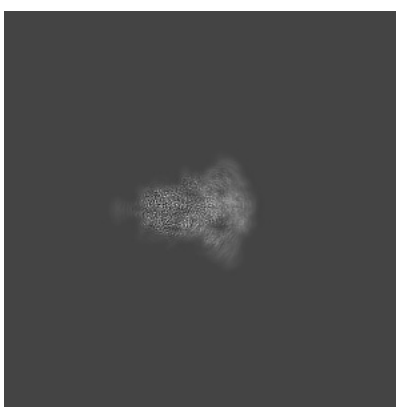
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

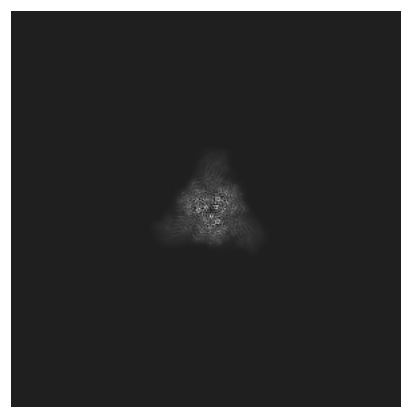
6.1.1 Primary map



X



Y



Z

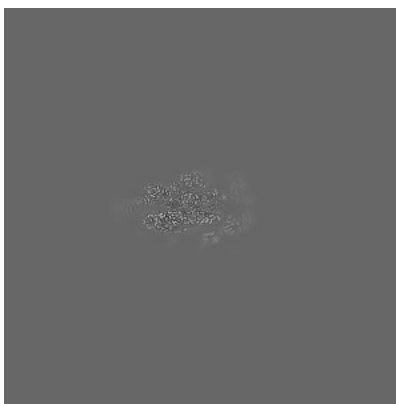
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

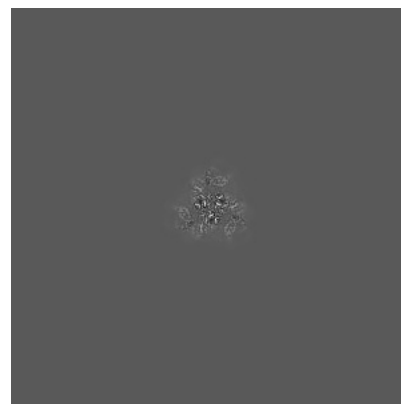
6.2.1 Primary map



X Index: 256



Y Index: 256

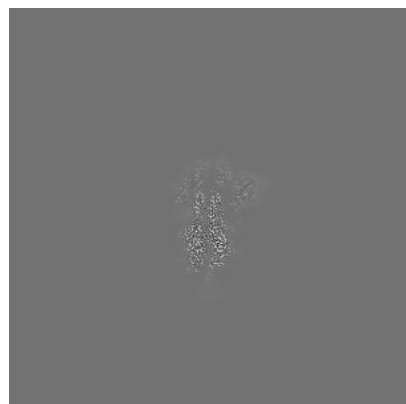


Z Index: 256

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

6.3 Largest variance slices [i](#)

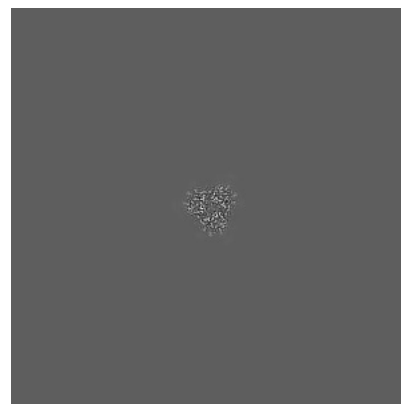
6.3.1 Primary map



X Index: 262



Y Index: 260

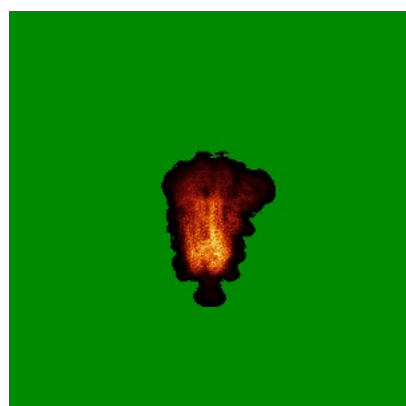


Z Index: 208

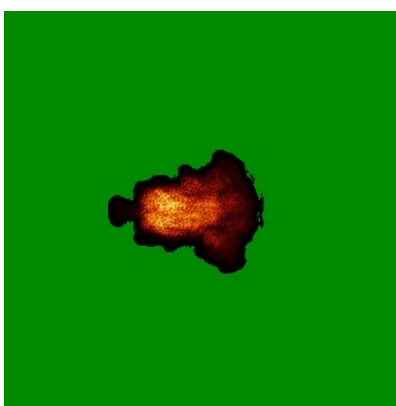
The images above show the largest variance slices of the map in three orthogonal directions.

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

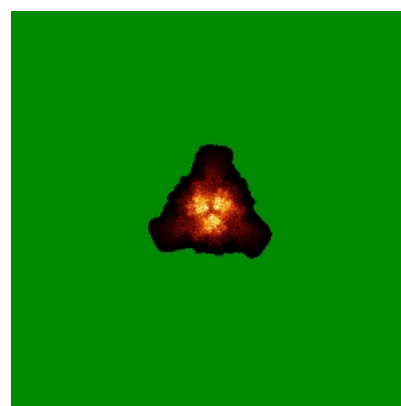
6.4.1 Primary map



X



Y



Z

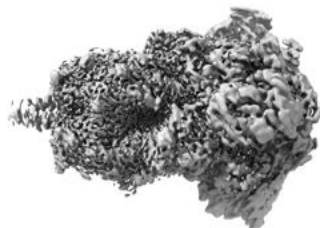
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

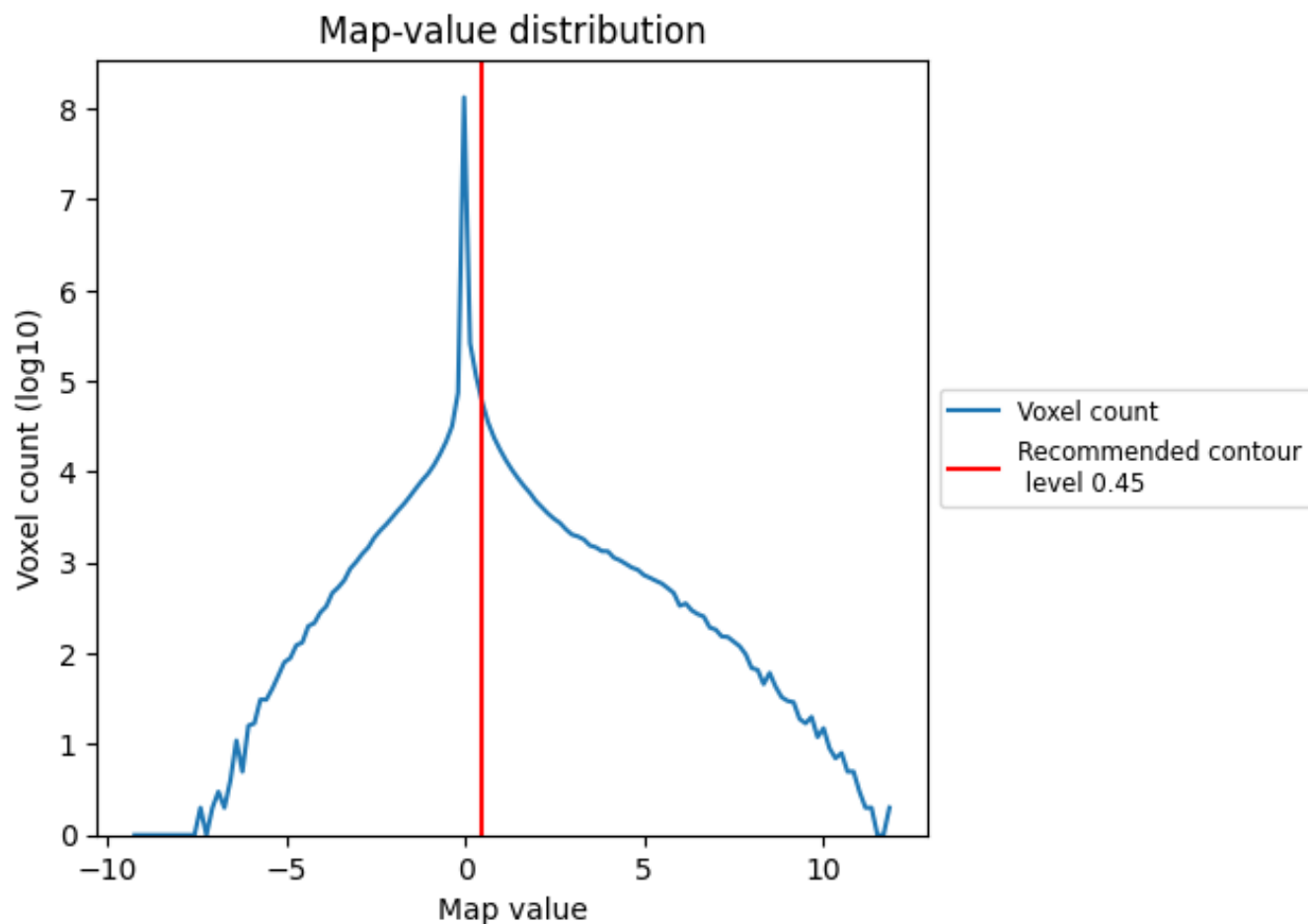
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

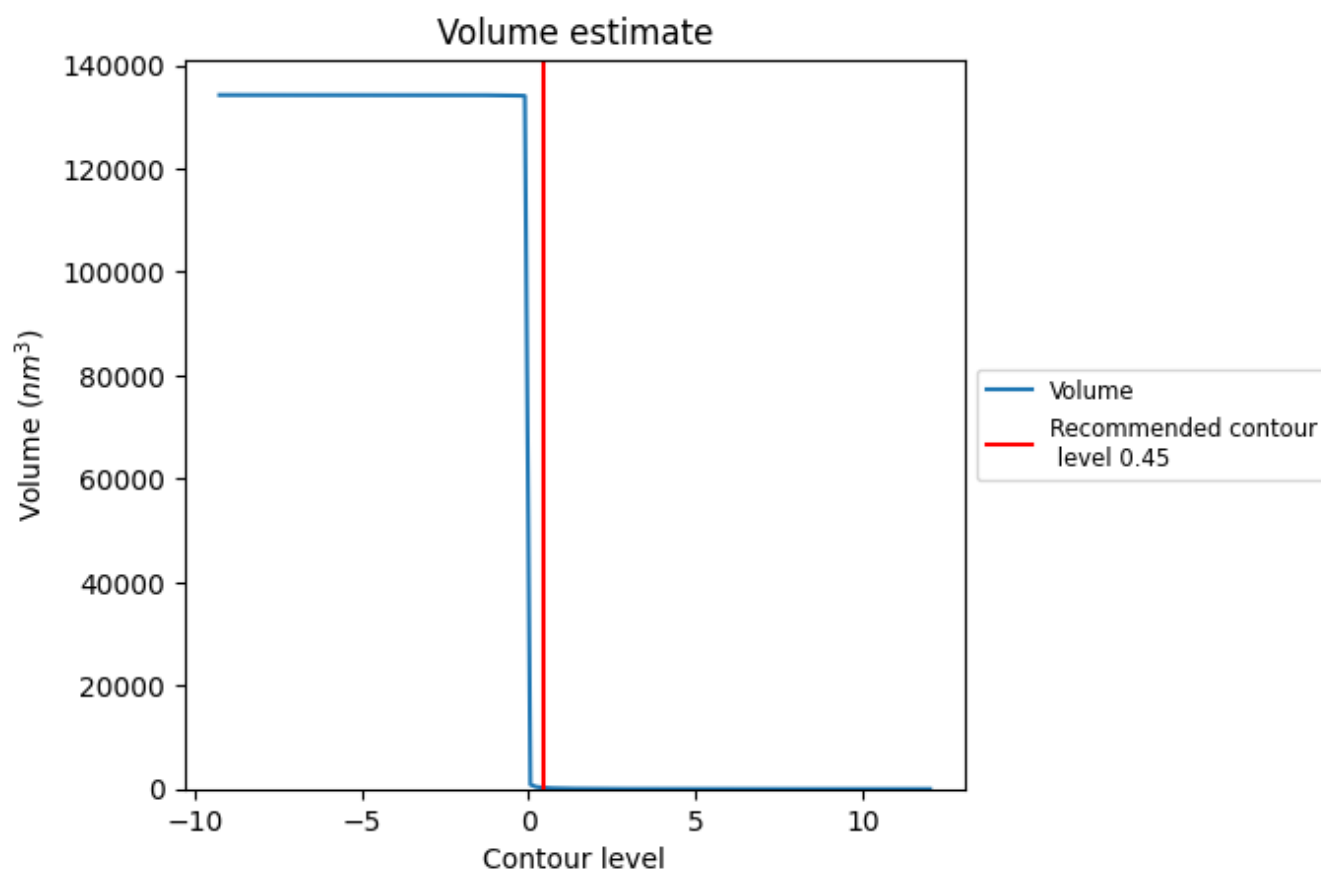
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

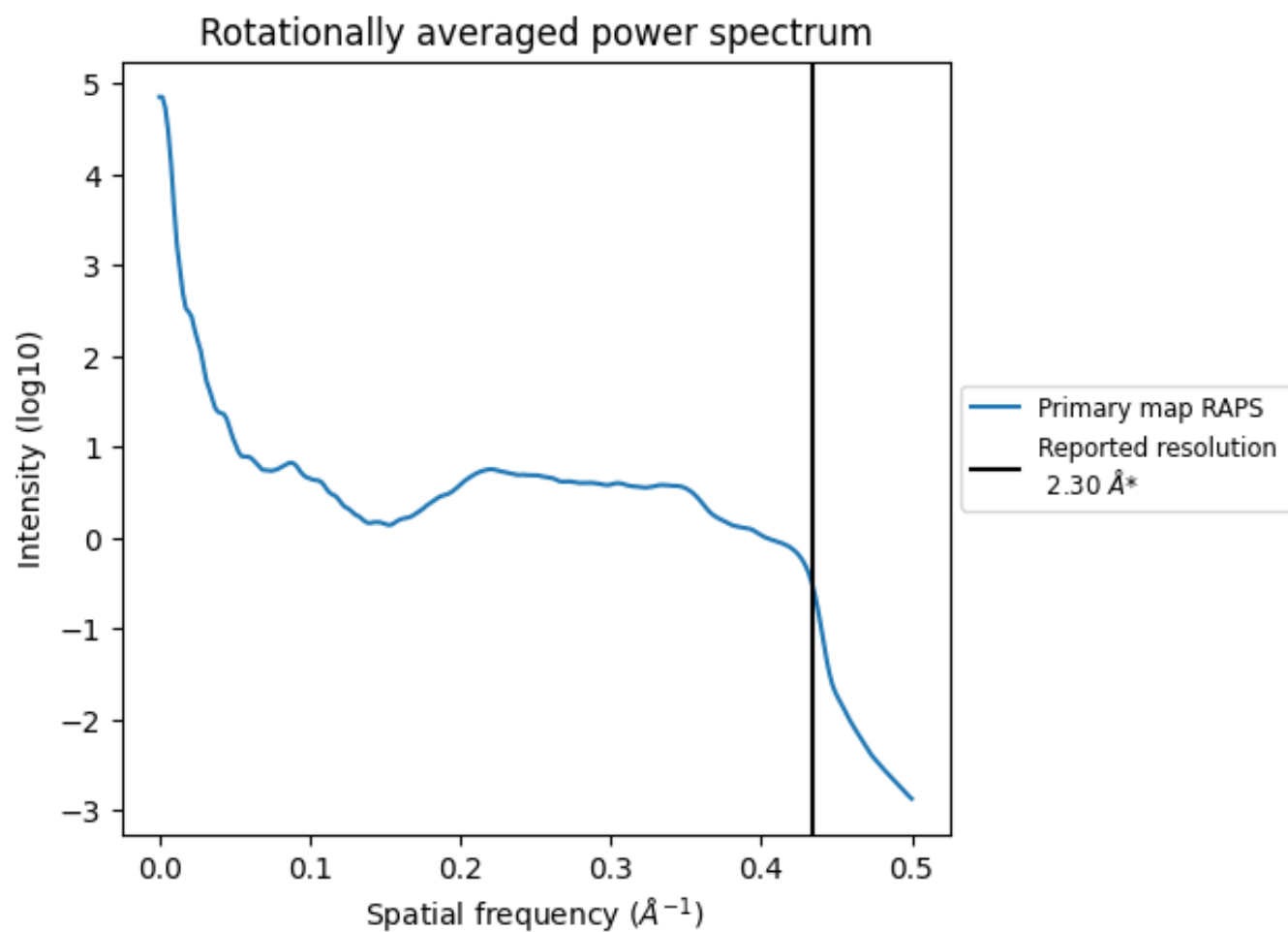
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 237 nm³; this corresponds to an approximate mass of 214 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.435 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

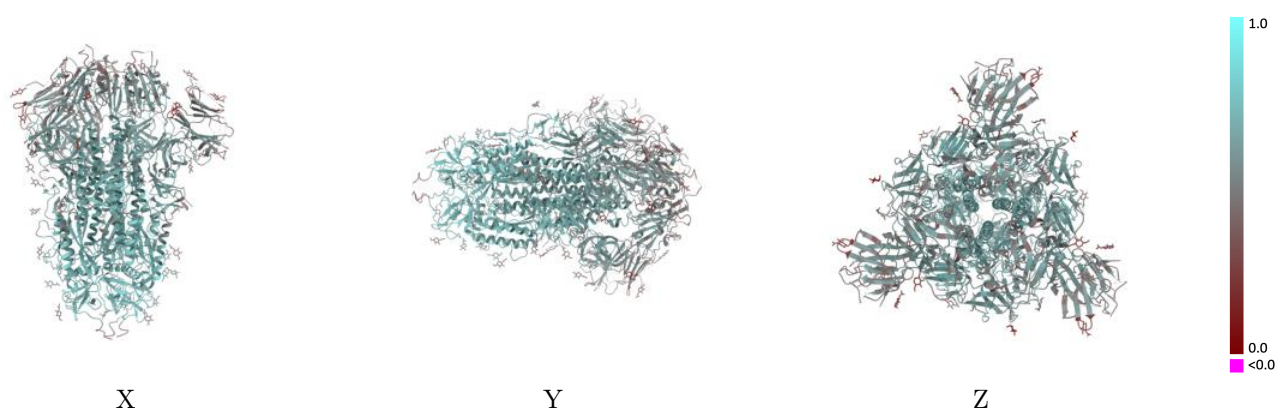
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26056 and PDB model 7TPI. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

This section was not generated.

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

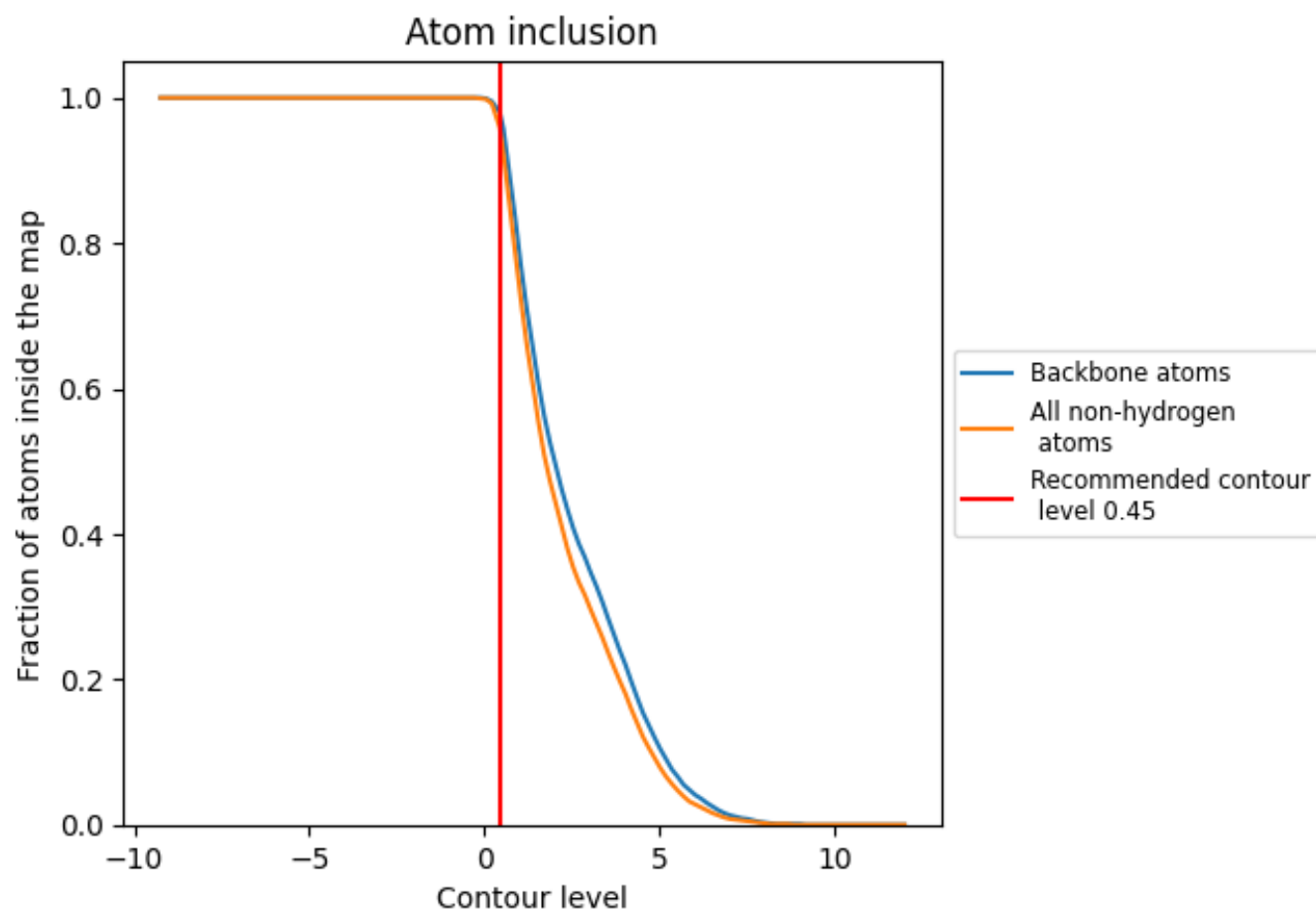


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9590	0.6030
A	0.9590	0.6040
B	0.9600	0.6030
C	0.9610	0.6030
D	0.8570	0.4850
E	0.8930	0.5590
F	0.8570	0.4950
G	0.8930	0.5690
H	0.8570	0.4840
I	0.8930	0.5630

1.0

0.0

<0.0