



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 05:50 PM UTC

PDB ID : 7LXY / pdb_00007lxy
EMDB ID : EMD-23579
Title : SARS-CoV-2 S/S2M11/S2X333 Global Refinement
Authors : McCallum, M.; Veessler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-03-05
Resolution : 2.20 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:

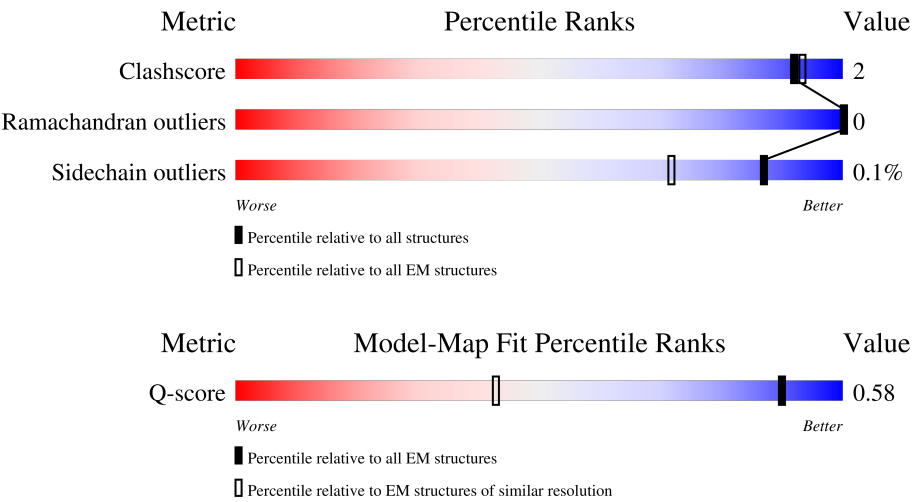
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	1288	7% 74% 6% 20%
1	B	1288	7% 74% 6% 20%
1	J	1288	8% 74% 6% 20%
2	C	104	8% 94% 5%

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Mol	Chain	Length	Quality of chain
2	D	104	
2	K	104	
3	E	122	
3	F	122	
3	M	122	
4	G	121	
4	H	121	
4	N	121	
5	I	100	
5	L	100	
5	O	100	
6	P	4	
6	S	4	
6	V	4	
7	Q	2	
7	R	2	
7	T	2	
7	U	2	
7	W	2	
7	X	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33987 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	1035	Total	C	N	O	S	0	0
			7945	5088	1316	1505	36		
1	B	1035	Total	C	N	O	S	0	0
			7945	5088	1316	1505	36		
1	J	1035	Total	C	N	O	S	0	0
			7945	5088	1316	1505	36		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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
A	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	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	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
J	682	GLY	ARG	engineered mutation	UNP P0DTC2
J	683	SER	ARG	engineered mutation	UNP P0DTC2
J	685	SER	ARG	engineered mutation	UNP P0DTC2
J	817	PRO	PHE	engineered mutation	UNP P0DTC2
J	892	PRO	ALA	engineered mutation	UNP P0DTC2
J	899	PRO	ALA	engineered mutation	UNP P0DTC2
J	942	PRO	ALA	engineered mutation	UNP P0DTC2
J	986	PRO	LYS	engineered mutation	UNP P0DTC2
J	987	PRO	VAL	engineered mutation	UNP P0DTC2
J	1209	GLY	-	expression tag	UNP P0DTC2
J	1210	SER	-	expression tag	UNP P0DTC2
J	1211	GLY	-	expression tag	UNP P0DTC2
J	1212	TYR	-	expression tag	UNP P0DTC2
J	1213	ILE	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1256	HIS	-	expression tag	UNP P0DTC2
J	1257	HIS	-	expression tag	UNP P0DTC2
J	1258	SER	-	expression tag	UNP P0DTC2
J	1259	ALA	-	expression tag	UNP P0DTC2
J	1260	TRP	-	expression tag	UNP P0DTC2
J	1261	SER	-	expression tag	UNP P0DTC2
J	1262	HIS	-	expression tag	UNP P0DTC2
J	1263	PRO	-	expression tag	UNP P0DTC2
J	1264	GLN	-	expression tag	UNP P0DTC2
J	1265	PHE	-	expression tag	UNP P0DTC2
J	1266	GLU	-	expression tag	UNP P0DTC2
J	1267	LYS	-	expression tag	UNP P0DTC2
J	1268	GLY	-	expression tag	UNP P0DTC2
J	1269	GLY	-	expression tag	UNP P0DTC2
J	1270	GLY	-	expression tag	UNP P0DTC2
J	1271	SER	-	expression tag	UNP P0DTC2
J	1272	GLY	-	expression tag	UNP P0DTC2
J	1273	GLY	-	expression tag	UNP P0DTC2
J	1274	GLY	-	expression tag	UNP P0DTC2
J	1275	GLY	-	expression tag	UNP P0DTC2
J	1276	SER	-	expression tag	UNP P0DTC2
J	1277	GLY	-	expression tag	UNP P0DTC2
J	1278	GLY	-	expression tag	UNP P0DTC2
J	1279	SER	-	expression tag	UNP P0DTC2
J	1280	ALA	-	expression tag	UNP P0DTC2
J	1281	TRP	-	expression tag	UNP P0DTC2
J	1282	SER	-	expression tag	UNP P0DTC2
J	1283	HIS	-	expression tag	UNP P0DTC2
J	1284	PRO	-	expression tag	UNP P0DTC2
J	1285	GLN	-	expression tag	UNP P0DTC2
J	1286	PHE	-	expression tag	UNP P0DTC2
J	1287	GLU	-	expression tag	UNP P0DTC2
J	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called S2M11 Fab Light Chain variable region.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	104	Total	C	N	O	S	
			765	484	128	149	4	0
2	C	104	Total	C	N	O	S	
			765	484	128	149	4	0
2	K	104	Total	C	N	O	S	
			765	484	128	149	4	0

- Molecule 3 is a protein called S2M11 Fab Heavy Chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	122	Total	C	N	O	S	0	0
			958	616	155	181	6		
3	F	122	Total	C	N	O	S	0	0
			958	616	155	181	6		
3	M	122	Total	C	N	O	S	0	0
			958	616	155	181	6		

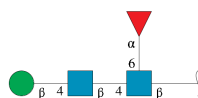
- Molecule 4 is a protein called S2X333 Fab Heavy Chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	121	Total	C	N	O	S	0	0
			600	356	121	121	2		
4	G	121	Total	C	N	O	S	0	0
			600	356	121	121	2		
4	N	121	Total	C	N	O	S	0	0
			600	356	121	121	2		

- Molecule 5 is a protein called S2X333 Fab Light Chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	100	Total	C	N	O	S	0	0
			503	301	100	100	2		
5	I	100	Total	C	N	O	S	0	0
			503	301	100	100	2		
5	O	100	Total	C	N	O	S	0	0
			503	301	100	100	2		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	4	Total	C	N	O	0	0
			49	28	2	19		
6	S	4	Total	C	N	O	0	0
			49	28	2	19		

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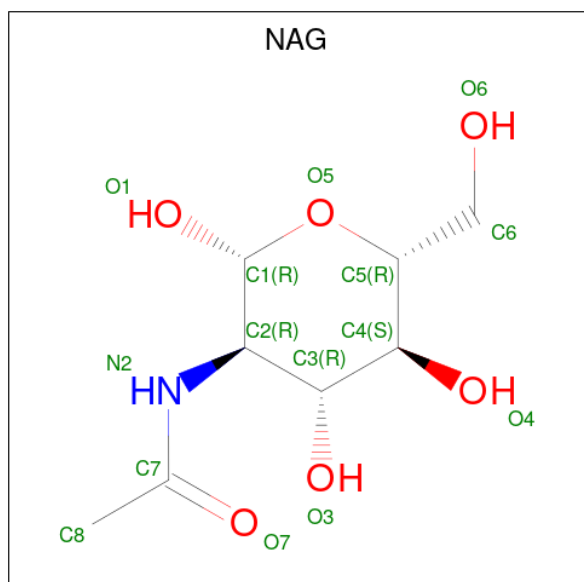
Mol	Chain	Residues	Atoms				AltConf	Trace
6	V	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 7 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
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

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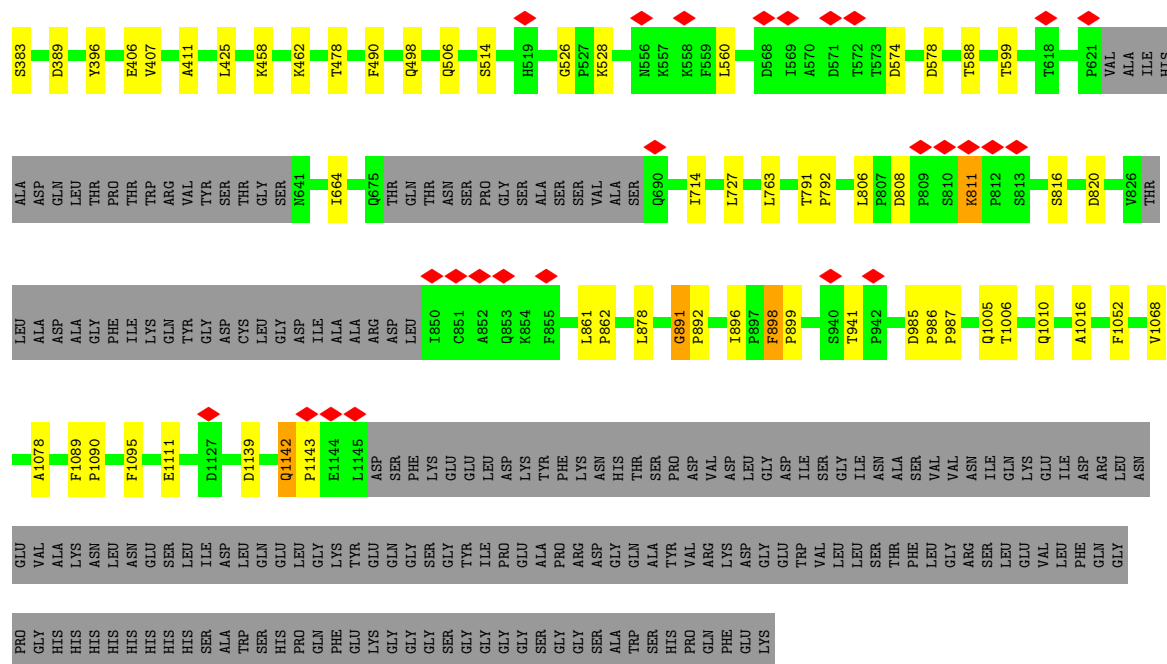
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Mol	Chain	Residues	Atoms				AltConf
8	J	1	Total	C	N	O	0
			14	8	1	5	
8	J	1	Total	C	N	O	0
			14	8	1	5	

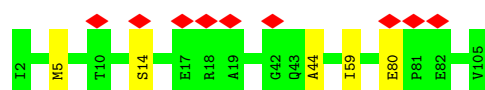
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	227	Total	O	0
			227	227	
9	D	1	Total	O	0
			1	1	
9	E	15	Total	O	0
			15	15	
9	B	227	Total	O	0
			227	227	
9	C	1	Total	O	0
			1	1	
9	F	15	Total	O	0
			15	15	
9	J	227	Total	O	0
			227	227	
9	K	1	Total	O	0
			1	1	
9	M	15	Total	O	0
			15	15	

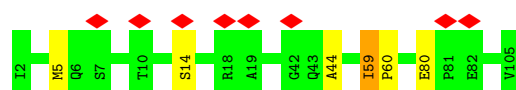




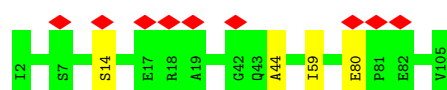
• Molecule 2: S2M11 Fab Light Chain variable region



• Molecule 2: S2M11 Fab Light Chain variable region



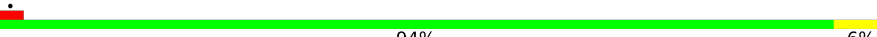
• Molecule 2: S2M11 Fab Light Chain variable region



• Molecule 3: S2M11 Fab Heavy Chain variable region

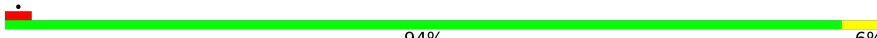


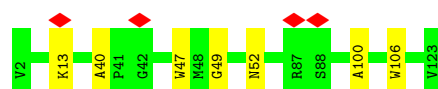
- Molecule 3: S2M11 Fab Heavy Chain variable region

Chain F:  94% 6%



- Molecule 3: S2M11 Fab Heavy Chain variable region

Chain M:  94% 6%



- Molecule 4: S2X333 Fab Heavy Chain variable region

Chain H:  100% 98%



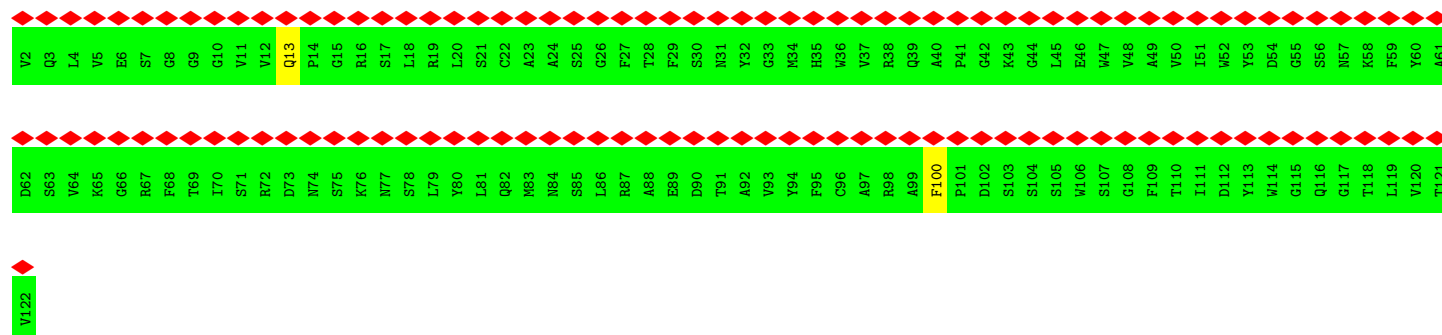
- Molecule 4: S2X333 Fab Heavy Chain variable region

Chain G:  100% 98%

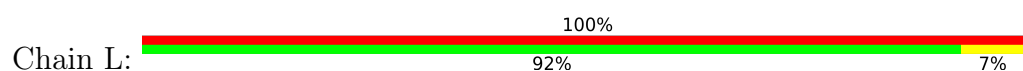


- Molecule 4: S2X333 Fab Heavy Chain variable region

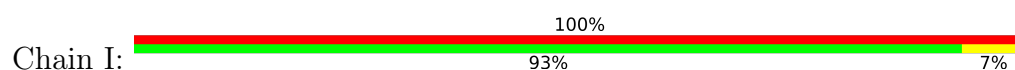
Chain N:  100% 98%



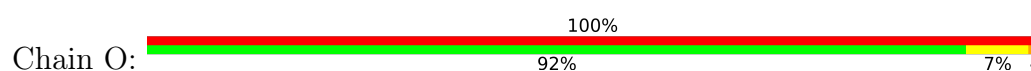
• Molecule 5: S2X333 Fab Light Chain variable region



• Molecule 5: S2X333 Fab Light Chain variable region



• Molecule 5: S2X333 Fab Light Chain variable region



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	261953	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.784	Depositor
Minimum map value	-5.986	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	537.60004, 537.60004, 537.60004	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8960001, 0.8960001, 0.8960001	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, BMA, FUC

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	0.65	0/8127	0.93	99/11081 (0.9%)
1	B	0.65	0/8127	0.93	99/11081 (0.9%)
1	J	0.65	0/8127	0.93	99/11081 (0.9%)
2	C	0.61	0/784	0.94	8/1067 (0.7%)
2	D	0.61	0/784	0.94	8/1067 (0.7%)
2	K	0.62	0/784	0.94	8/1067 (0.7%)
3	E	0.66	0/988	0.82	8/1346 (0.6%)
3	F	0.67	0/988	0.83	8/1346 (0.6%)
3	M	0.66	0/988	0.83	8/1346 (0.6%)
4	G	0.46	0/602	0.97	4/835 (0.5%)
4	H	0.46	0/602	0.97	4/835 (0.5%)
4	N	0.46	0/602	0.97	4/835 (0.5%)
5	I	0.48	0/507	1.24	10/704 (1.4%)
5	L	0.48	0/507	1.24	10/704 (1.4%)
5	O	0.48	0/507	1.24	10/704 (1.4%)
All	All	0.64	0/33024	0.94	387/45099 (0.9%)

There are no bond length outliers.

All (387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	6	GLN	CA-C-N	9.49	126.49	119.66
5	O	6	GLN	C-N-CA	9.49	126.49	119.66
5	L	6	GLN	CA-C-N	9.47	126.48	119.66
5	L	6	GLN	C-N-CA	9.47	126.48	119.66
5	I	6	GLN	CA-C-N	9.46	126.47	119.66
5	I	6	GLN	C-N-CA	9.46	126.47	119.66
1	B	791	THR	CA-C-N	8.58	125.84	119.66
1	B	791	THR	C-N-CA	8.58	125.84	119.66
1	J	791	THR	CA-C-N	8.53	125.80	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	791	THR	C-N-CA	8.53	125.80	119.66
1	A	791	THR	CA-C-N	8.51	125.78	119.66
1	A	791	THR	C-N-CA	8.51	125.78	119.66
1	A	81	ASN	CA-C-N	7.60	127.55	120.03
1	A	81	ASN	C-N-CA	7.60	127.55	120.03
1	B	81	ASN	CA-C-N	7.59	127.55	120.03
1	B	81	ASN	C-N-CA	7.59	127.55	120.03
1	J	81	ASN	CA-C-N	7.59	127.54	120.03
1	J	81	ASN	C-N-CA	7.59	127.54	120.03
2	K	59	ILE	CA-C-N	7.31	127.31	119.78
2	K	59	ILE	C-N-CA	7.31	127.31	119.78
2	D	59	ILE	CA-C-N	7.31	127.31	119.78
2	D	59	ILE	C-N-CA	7.31	127.31	119.78
2	C	59	ILE	CA-C-N	7.30	127.30	119.78
2	C	59	ILE	C-N-CA	7.30	127.30	119.78
1	A	1078	ALA	CA-C-N	7.29	126.92	119.56
1	A	1078	ALA	C-N-CA	7.29	126.92	119.56
1	J	1078	ALA	CA-C-N	7.28	126.91	119.56
1	J	1078	ALA	C-N-CA	7.28	126.91	119.56
1	A	941	THR	CA-C-N	7.28	127.28	119.28
1	A	941	THR	C-N-CA	7.28	127.28	119.28
1	B	1078	ALA	CA-C-N	7.26	126.89	119.56
1	B	1078	ALA	C-N-CA	7.26	126.89	119.56
1	J	941	THR	CA-C-N	7.25	127.26	119.28
1	J	941	THR	C-N-CA	7.25	127.26	119.28
1	B	941	THR	CA-C-N	7.23	127.23	119.28
1	B	941	THR	C-N-CA	7.23	127.23	119.28
1	B	498	GLN	CA-C-N	7.18	126.88	119.56
1	B	498	GLN	C-N-CA	7.18	126.88	119.56
1	J	490	PHE	CA-C-N	7.17	126.80	119.56
1	J	490	PHE	C-N-CA	7.17	126.80	119.56
1	A	498	GLN	CA-C-N	7.15	126.86	119.56
1	A	498	GLN	C-N-CA	7.15	126.86	119.56
1	J	498	GLN	CA-C-N	7.15	126.86	119.56
1	J	498	GLN	C-N-CA	7.15	126.86	119.56
1	A	490	PHE	CA-C-N	7.14	126.77	119.56
1	A	490	PHE	C-N-CA	7.14	126.77	119.56
1	J	526	GLY	CA-C-N	7.14	128.05	120.12
1	J	526	GLY	C-N-CA	7.14	128.05	120.12
1	A	526	GLY	CA-C-N	7.13	128.03	120.12
1	A	526	GLY	C-N-CA	7.13	128.03	120.12
1	B	526	GLY	CA-C-N	7.12	128.03	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	GLY	C-N-CA	7.12	128.03	120.12
1	B	490	PHE	CA-C-N	7.12	126.75	119.56
1	B	490	PHE	C-N-CA	7.12	126.75	119.56
1	B	862	PRO	CA-C-N	7.06	127.03	119.76
1	B	862	PRO	C-N-CA	7.06	127.03	119.76
1	A	862	PRO	CA-C-N	7.05	127.02	119.76
1	A	862	PRO	C-N-CA	7.05	127.02	119.76
1	J	321	GLN	CA-C-N	7.04	126.81	119.76
1	J	321	GLN	C-N-CA	7.04	126.81	119.76
1	J	862	PRO	CA-C-N	7.04	127.01	119.76
1	J	862	PRO	C-N-CA	7.04	127.01	119.76
1	B	321	GLN	CA-C-N	7.02	126.78	119.76
1	B	321	GLN	C-N-CA	7.02	126.78	119.76
1	A	321	GLN	CA-C-N	7.00	126.76	119.76
1	A	321	GLN	C-N-CA	7.00	126.76	119.76
1	J	38	TYR	CA-C-N	6.99	126.62	119.56
1	J	38	TYR	C-N-CA	6.99	126.62	119.56
1	A	38	TYR	CA-C-N	6.99	126.61	119.56
1	A	38	TYR	C-N-CA	6.99	126.61	119.56
1	B	38	TYR	CA-C-N	6.99	126.61	119.56
1	B	38	TYR	C-N-CA	6.99	126.61	119.56
1	J	578	ASP	CA-C-N	6.91	127.06	119.87
1	J	578	ASP	C-N-CA	6.91	127.06	119.87
1	A	208	THR	CA-C-N	6.91	126.67	119.76
1	A	208	THR	C-N-CA	6.91	126.67	119.76
1	B	208	THR	CA-C-N	6.88	126.64	119.76
1	B	208	THR	C-N-CA	6.88	126.64	119.76
1	A	578	ASP	CA-C-N	6.88	127.02	119.87
1	A	578	ASP	C-N-CA	6.88	127.02	119.87
1	A	383	SER	CA-C-N	6.88	126.57	119.56
1	A	383	SER	C-N-CA	6.88	126.57	119.56
1	B	383	SER	CA-C-N	6.88	126.57	119.56
1	B	383	SER	C-N-CA	6.88	126.57	119.56
1	J	208	THR	CA-C-N	6.87	126.63	119.76
1	J	208	THR	C-N-CA	6.87	126.63	119.76
1	B	578	ASP	CA-C-N	6.86	127.01	119.87
1	B	578	ASP	C-N-CA	6.86	127.01	119.87
1	J	383	SER	CA-C-N	6.86	126.56	119.56
1	J	383	SER	C-N-CA	6.86	126.56	119.56
1	A	792	PRO	CA-C-N	6.79	127.34	119.47
1	A	792	PRO	C-N-CA	6.79	127.34	119.47
1	A	425	LEU	CA-C-N	6.78	126.70	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	LEU	C-N-CA	6.78	126.70	119.85
1	J	425	LEU	CA-C-N	6.77	126.69	119.85
1	J	425	LEU	C-N-CA	6.77	126.69	119.85
5	I	7	PRO	CA-C-N	6.77	127.04	119.32
5	I	7	PRO	C-N-CA	6.77	127.04	119.32
1	B	425	LEU	CA-C-N	6.76	126.68	119.85
1	B	425	LEU	C-N-CA	6.76	126.68	119.85
1	J	792	PRO	CA-C-N	6.76	127.31	119.47
1	J	792	PRO	C-N-CA	6.76	127.31	119.47
1	B	792	PRO	CA-C-N	6.75	127.31	119.47
1	B	792	PRO	C-N-CA	6.75	127.31	119.47
5	L	7	PRO	CA-C-N	6.73	126.99	119.32
5	L	7	PRO	C-N-CA	6.73	126.99	119.32
5	O	7	PRO	CA-C-N	6.72	126.98	119.32
5	O	7	PRO	C-N-CA	6.72	126.98	119.32
5	L	57	ILE	CA-C-N	6.72	126.70	119.78
5	L	57	ILE	C-N-CA	6.72	126.70	119.78
5	O	57	ILE	CA-C-N	6.71	126.69	119.78
5	O	57	ILE	C-N-CA	6.71	126.69	119.78
5	I	57	ILE	CA-C-N	6.71	126.69	119.78
5	I	57	ILE	C-N-CA	6.71	126.69	119.78
1	A	714	ILE	CA-C-N	6.67	127.07	119.93
1	A	714	ILE	C-N-CA	6.67	127.07	119.93
1	J	173	GLN	CA-C-N	6.66	126.57	119.85
1	J	173	GLN	C-N-CA	6.66	126.57	119.85
1	J	714	ILE	CA-C-N	6.65	127.05	119.93
1	J	714	ILE	C-N-CA	6.65	127.05	119.93
1	A	173	GLN	CA-C-N	6.65	126.57	119.85
1	A	173	GLN	C-N-CA	6.65	126.57	119.85
1	B	173	GLN	CA-C-N	6.63	126.55	119.85
1	B	173	GLN	C-N-CA	6.63	126.55	119.85
1	B	138	ASP	CA-C-N	6.63	126.39	119.76
1	B	138	ASP	C-N-CA	6.63	126.39	119.76
1	A	138	ASP	CA-C-N	6.62	126.38	119.76
1	A	138	ASP	C-N-CA	6.62	126.38	119.76
1	B	714	ILE	CA-C-N	6.61	127.01	119.93
1	B	714	ILE	C-N-CA	6.61	127.01	119.93
1	J	138	ASP	CA-C-N	6.61	126.37	119.76
1	J	138	ASP	C-N-CA	6.61	126.37	119.76
1	B	727	LEU	CA-C-N	6.58	126.54	119.76
1	B	727	LEU	C-N-CA	6.58	126.54	119.76
1	B	811	LYS	CA-C-N	6.58	127.10	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	811	LYS	C-N-CA	6.58	127.10	119.47
1	A	811	LYS	CA-C-N	6.57	127.09	119.47
1	A	811	LYS	C-N-CA	6.57	127.09	119.47
1	J	811	LYS	CA-C-N	6.57	127.09	119.47
1	J	811	LYS	C-N-CA	6.57	127.09	119.47
1	B	808	ASP	CA-C-N	6.57	126.70	119.87
1	B	808	ASP	C-N-CA	6.57	126.70	119.87
1	A	727	LEU	CA-C-N	6.57	126.52	119.76
1	A	727	LEU	C-N-CA	6.57	126.52	119.76
1	J	808	ASP	CA-C-N	6.57	126.70	119.87
1	J	808	ASP	C-N-CA	6.57	126.70	119.87
1	A	216	LEU	CA-C-N	6.56	126.47	119.85
1	A	216	LEU	C-N-CA	6.56	126.47	119.85
1	A	808	ASP	CA-C-N	6.56	126.69	119.87
1	A	808	ASP	C-N-CA	6.56	126.69	119.87
1	J	478	THR	CA-C-N	6.56	126.59	119.90
1	J	478	THR	C-N-CA	6.56	126.59	119.90
1	B	216	LEU	CA-C-N	6.55	126.47	119.85
1	B	216	LEU	C-N-CA	6.55	126.47	119.85
1	J	727	LEU	CA-C-N	6.54	126.50	119.76
1	J	727	LEU	C-N-CA	6.54	126.50	119.76
1	J	216	LEU	CA-C-N	6.54	126.45	119.85
1	J	216	LEU	C-N-CA	6.54	126.45	119.85
1	A	478	THR	CA-C-N	6.52	126.55	119.90
1	A	478	THR	C-N-CA	6.52	126.55	119.90
1	B	294	ASP	CA-C-N	6.51	126.20	119.56
1	B	294	ASP	C-N-CA	6.51	126.20	119.56
1	B	478	THR	CA-C-N	6.51	126.54	119.90
1	B	478	THR	C-N-CA	6.51	126.54	119.90
2	K	14	SER	CA-C-N	6.50	126.45	119.76
2	K	14	SER	C-N-CA	6.50	126.45	119.76
2	D	14	SER	CA-C-N	6.50	126.45	119.76
2	D	14	SER	C-N-CA	6.50	126.45	119.76
1	J	294	ASP	CA-C-N	6.50	126.19	119.56
1	J	294	ASP	C-N-CA	6.50	126.19	119.56
2	C	14	SER	CA-C-N	6.48	126.44	119.76
2	C	14	SER	C-N-CA	6.48	126.44	119.76
1	A	294	ASP	CA-C-N	6.48	126.17	119.56
1	A	294	ASP	C-N-CA	6.48	126.17	119.56
1	B	1142	GLN	CA-C-N	6.47	126.16	119.56
1	B	1142	GLN	C-N-CA	6.47	126.16	119.56
1	A	1142	GLN	CA-C-N	6.46	126.15	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1142	GLN	C-N-CA	6.46	126.15	119.56
3	F	52	ASN	CA-C-N	6.46	126.97	119.47
3	F	52	ASN	C-N-CA	6.46	126.97	119.47
1	J	1142	GLN	CA-C-N	6.46	126.15	119.56
1	J	1142	GLN	C-N-CA	6.46	126.15	119.56
3	E	52	ASN	CA-C-N	6.43	126.93	119.47
3	E	52	ASN	C-N-CA	6.43	126.93	119.47
3	M	52	ASN	CA-C-N	6.43	126.93	119.47
3	M	52	ASN	C-N-CA	6.43	126.93	119.47
1	A	806	LEU	CA-C-N	6.41	126.44	119.90
1	A	806	LEU	C-N-CA	6.41	126.44	119.90
1	J	806	LEU	CA-C-N	6.39	126.42	119.90
1	J	806	LEU	C-N-CA	6.39	126.42	119.90
1	B	806	LEU	CA-C-N	6.37	126.40	119.90
1	B	806	LEU	C-N-CA	6.37	126.40	119.90
1	J	1068	VAL	CA-C-N	6.36	126.39	119.90
1	J	1068	VAL	C-N-CA	6.36	126.39	119.90
1	B	1068	VAL	CA-C-N	6.36	126.39	119.90
1	B	1068	VAL	C-N-CA	6.36	126.39	119.90
1	A	1068	VAL	CA-C-N	6.35	126.38	119.90
1	A	1068	VAL	C-N-CA	6.35	126.38	119.90
3	F	100	ALA	CA-C-N	6.35	126.31	120.03
3	F	100	ALA	C-N-CA	6.35	126.31	120.03
1	B	816	SER	CA-C-N	6.34	126.54	119.32
1	B	816	SER	C-N-CA	6.34	126.54	119.32
1	J	816	SER	CA-C-N	6.33	126.54	119.32
1	J	816	SER	C-N-CA	6.33	126.54	119.32
3	M	100	ALA	CA-C-N	6.33	126.29	120.03
3	M	100	ALA	C-N-CA	6.33	126.29	120.03
1	A	816	SER	CA-C-N	6.32	126.53	119.32
1	A	816	SER	C-N-CA	6.32	126.53	119.32
3	E	100	ALA	CA-C-N	6.32	126.29	120.03
3	E	100	ALA	C-N-CA	6.32	126.29	120.03
1	J	599	THR	CA-C-N	6.21	126.17	120.03
1	J	599	THR	C-N-CA	6.21	126.17	120.03
5	O	42	ALA	CA-C-N	6.21	126.17	119.78
5	O	42	ALA	C-N-CA	6.21	126.17	119.78
1	A	599	THR	CA-C-N	6.20	126.17	120.03
1	A	599	THR	C-N-CA	6.20	126.17	120.03
1	B	599	THR	CA-C-N	6.20	126.16	120.03
1	B	599	THR	C-N-CA	6.20	126.16	120.03
5	L	42	ALA	CA-C-N	6.17	126.14	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	42	ALA	C-N-CA	6.17	126.14	119.78
5	I	42	ALA	CA-C-N	6.14	126.10	119.78
5	I	42	ALA	C-N-CA	6.14	126.10	119.78
1	B	411	ALA	CA-C-N	6.13	126.08	119.76
1	B	411	ALA	C-N-CA	6.13	126.08	119.76
1	A	411	ALA	CA-C-N	6.13	126.07	119.76
1	A	411	ALA	C-N-CA	6.13	126.07	119.76
1	J	411	ALA	CA-C-N	6.13	126.07	119.76
1	J	411	ALA	C-N-CA	6.13	126.07	119.76
1	B	985	ASP	CA-C-N	6.12	126.69	120.38
1	B	985	ASP	C-N-CA	6.12	126.69	120.38
1	A	985	ASP	CA-C-N	6.08	126.65	120.38
1	A	985	ASP	C-N-CA	6.08	126.65	120.38
2	K	44	ALA	CA-C-N	6.08	126.02	119.76
2	K	44	ALA	C-N-CA	6.08	126.02	119.76
2	C	44	ALA	CA-C-N	6.07	126.01	119.76
2	C	44	ALA	C-N-CA	6.07	126.01	119.76
5	O	53	ARG	CA-C-N	6.05	126.24	120.31
5	O	53	ARG	C-N-CA	6.05	126.24	120.31
2	D	44	ALA	CA-C-N	6.05	126.00	119.76
2	D	44	ALA	C-N-CA	6.05	126.00	119.76
5	L	53	ARG	CA-C-N	6.05	126.24	120.31
5	L	53	ARG	C-N-CA	6.05	126.24	120.31
1	J	985	ASP	CA-C-N	6.05	126.61	120.38
1	J	985	ASP	C-N-CA	6.05	126.61	120.38
5	I	53	ARG	CA-C-N	6.05	126.24	120.31
5	I	53	ARG	C-N-CA	6.05	126.24	120.31
1	B	61	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	61	ASN	CA-CB-CG	-6.03	106.57	112.60
1	A	1139	ASP	CA-C-N	6.02	127.37	119.84
1	A	1139	ASP	C-N-CA	6.02	127.37	119.84
1	J	61	ASN	CA-CB-CG	-6.02	106.58	112.60
1	B	1139	ASP	CA-C-N	6.01	127.36	119.84
1	B	1139	ASP	C-N-CA	6.01	127.36	119.84
1	J	1139	ASP	CA-C-N	6.00	127.34	119.84
1	J	1139	ASP	C-N-CA	6.00	127.34	119.84
1	B	1111	GLU	CA-C-N	5.98	127.31	119.84
1	B	1111	GLU	C-N-CA	5.98	127.31	119.84
1	A	1111	GLU	CA-C-N	5.93	127.26	119.84
1	A	1111	GLU	C-N-CA	5.93	127.26	119.84
1	J	1111	GLU	CA-C-N	5.93	127.26	119.84
1	J	1111	GLU	C-N-CA	5.93	127.26	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	80	GLU	CA-C-N	5.89	126.03	119.32
2	C	80	GLU	C-N-CA	5.89	126.03	119.32
2	D	80	GLU	CA-C-N	5.87	126.02	119.32
2	D	80	GLU	C-N-CA	5.87	126.02	119.32
2	K	80	GLU	CA-C-N	5.87	126.01	119.32
2	K	80	GLU	C-N-CA	5.87	126.01	119.32
1	J	891	GLY	CA-C-N	5.86	125.77	119.85
1	J	891	GLY	C-N-CA	5.86	125.77	119.85
1	B	891	GLY	CA-C-N	5.85	125.76	119.85
1	B	891	GLY	C-N-CA	5.85	125.76	119.85
1	A	891	GLY	CA-C-N	5.85	125.76	119.85
1	A	891	GLY	C-N-CA	5.85	125.76	119.85
1	J	1052	PHE	CA-C-N	5.82	125.73	119.85
1	J	1052	PHE	C-N-CA	5.82	125.73	119.85
1	B	506	GLN	CA-C-N	5.80	125.56	119.76
1	B	506	GLN	C-N-CA	5.80	125.56	119.76
1	A	506	GLN	CA-C-N	5.79	125.56	119.76
1	A	506	GLN	C-N-CA	5.79	125.56	119.76
1	B	1052	PHE	CA-C-N	5.78	125.69	119.85
1	B	1052	PHE	C-N-CA	5.78	125.69	119.85
1	A	1052	PHE	CA-C-N	5.78	125.69	119.85
1	A	1052	PHE	C-N-CA	5.78	125.69	119.85
1	J	506	GLN	CA-C-N	5.78	125.54	119.76
1	J	506	GLN	C-N-CA	5.78	125.54	119.76
1	J	84	LEU	CA-C-N	5.75	125.66	119.85
1	J	84	LEU	C-N-CA	5.75	125.66	119.85
1	A	84	LEU	CA-C-N	5.75	125.65	119.85
1	A	84	LEU	C-N-CA	5.75	125.65	119.85
1	B	84	LEU	CA-C-N	5.72	125.62	119.85
1	B	84	LEU	C-N-CA	5.72	125.62	119.85
4	N	100	PHE	CA-C-N	5.71	126.04	119.93
4	N	100	PHE	C-N-CA	5.71	126.04	119.93
4	H	100	PHE	CA-C-N	5.70	126.03	119.93
4	H	100	PHE	C-N-CA	5.70	126.03	119.93
4	G	100	PHE	CA-C-N	5.68	126.01	119.93
4	G	100	PHE	C-N-CA	5.68	126.01	119.93
4	G	13	GLN	CA-C-N	5.68	125.70	119.90
4	G	13	GLN	C-N-CA	5.68	125.70	119.90
4	N	13	GLN	CA-C-N	5.68	125.69	119.90
4	N	13	GLN	C-N-CA	5.68	125.69	119.90
4	H	13	GLN	CA-C-N	5.67	125.68	119.90
4	H	13	GLN	C-N-CA	5.67	125.68	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	588	THR	CA-C-N	5.52	125.43	119.85
1	J	588	THR	C-N-CA	5.52	125.43	119.85
1	A	588	THR	CA-C-N	5.50	125.41	119.85
1	A	588	THR	C-N-CA	5.50	125.41	119.85
1	B	588	THR	CA-C-N	5.50	125.41	119.85
1	B	588	THR	C-N-CA	5.50	125.41	119.85
1	B	664	ILE	CA-C-N	5.45	125.62	119.90
1	B	664	ILE	C-N-CA	5.45	125.62	119.90
1	A	664	ILE	CA-C-N	5.41	125.58	119.90
1	A	664	ILE	C-N-CA	5.41	125.58	119.90
1	A	896	ILE	CA-C-N	5.39	125.40	119.90
1	A	896	ILE	C-N-CA	5.39	125.40	119.90
1	B	224	GLU	CA-C-N	5.39	125.65	119.83
1	B	224	GLU	C-N-CA	5.39	125.65	119.83
1	B	896	ILE	CA-C-N	5.38	125.39	119.90
1	B	896	ILE	C-N-CA	5.38	125.39	119.90
1	J	664	ILE	CA-C-N	5.38	125.55	119.90
1	J	664	ILE	C-N-CA	5.38	125.55	119.90
1	J	896	ILE	CA-C-N	5.38	125.38	119.90
1	J	896	ILE	C-N-CA	5.38	125.38	119.90
1	A	56	LEU	CA-C-N	5.37	125.29	119.76
1	A	56	LEU	C-N-CA	5.37	125.29	119.76
1	B	56	LEU	CA-C-N	5.37	125.29	119.76
1	B	56	LEU	C-N-CA	5.37	125.29	119.76
1	B	861	LEU	CA-C-N	5.37	125.91	120.38
1	B	861	LEU	C-N-CA	5.37	125.91	120.38
1	J	56	LEU	CA-C-N	5.37	125.29	119.76
1	J	56	LEU	C-N-CA	5.37	125.29	119.76
1	A	560	LEU	CA-C-N	5.37	126.55	119.84
1	A	560	LEU	C-N-CA	5.37	126.55	119.84
1	J	560	LEU	CA-C-N	5.36	126.53	119.84
1	J	560	LEU	C-N-CA	5.36	126.53	119.84
1	A	224	GLU	CA-C-N	5.35	125.60	119.83
1	A	224	GLU	C-N-CA	5.35	125.60	119.83
3	E	40	ALA	CA-C-N	5.34	125.64	119.93
3	E	40	ALA	C-N-CA	5.34	125.64	119.93
1	B	560	LEU	CA-C-N	5.34	126.51	119.84
1	B	560	LEU	C-N-CA	5.34	126.51	119.84
3	F	40	ALA	CA-C-N	5.34	125.64	119.93
3	F	40	ALA	C-N-CA	5.34	125.64	119.93
3	M	40	ALA	CA-C-N	5.33	125.64	119.93
3	M	40	ALA	C-N-CA	5.33	125.64	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	861	LEU	CA-C-N	5.33	125.87	120.38
1	A	861	LEU	C-N-CA	5.33	125.87	120.38
1	J	861	LEU	CA-C-N	5.32	125.86	120.38
1	J	861	LEU	C-N-CA	5.32	125.86	120.38
1	J	224	GLU	CA-C-N	5.32	125.58	119.83
1	J	224	GLU	C-N-CA	5.32	125.58	119.83
1	B	1089	PHE	CA-C-N	5.30	125.46	119.90
1	B	1089	PHE	C-N-CA	5.30	125.46	119.90
1	A	1089	PHE	CA-C-N	5.28	125.44	119.90
1	A	1089	PHE	C-N-CA	5.28	125.44	119.90
1	J	1089	PHE	CA-C-N	5.25	125.41	119.90
1	J	1089	PHE	C-N-CA	5.25	125.41	119.90
3	E	13	LYS	CA-C-N	5.25	125.55	119.93
3	E	13	LYS	C-N-CA	5.25	125.55	119.93
3	M	13	LYS	CA-C-N	5.24	125.53	119.93
3	M	13	LYS	C-N-CA	5.24	125.53	119.93
3	F	13	LYS	CA-C-N	5.22	125.52	119.93
3	F	13	LYS	C-N-CA	5.22	125.52	119.93
1	A	898	PHE	CA-C-N	5.20	125.25	119.32
1	A	898	PHE	C-N-CA	5.20	125.25	119.32
1	J	898	PHE	CA-C-N	5.19	125.24	119.32
1	J	898	PHE	C-N-CA	5.19	125.24	119.32
1	J	462	LYS	CA-C-N	5.18	125.47	119.93
1	J	462	LYS	C-N-CA	5.18	125.47	119.93
1	A	462	LYS	CA-C-N	5.17	125.46	119.93
1	A	462	LYS	C-N-CA	5.17	125.46	119.93
1	B	898	PHE	CA-C-N	5.17	125.21	119.32
1	B	898	PHE	C-N-CA	5.17	125.21	119.32
1	B	462	LYS	CA-C-N	5.16	125.45	119.93
1	B	462	LYS	C-N-CA	5.16	125.45	119.93
1	J	271	GLN	CA-C-N	5.11	126.23	119.84
1	J	271	GLN	C-N-CA	5.11	126.23	119.84
1	B	271	GLN	CA-C-N	5.10	126.21	119.84
1	B	271	GLN	C-N-CA	5.10	126.21	119.84
1	J	329	PHE	CA-C-N	5.09	125.10	119.90
1	J	329	PHE	C-N-CA	5.09	125.10	119.90
1	A	271	GLN	CA-C-N	5.09	126.20	119.84
1	A	271	GLN	C-N-CA	5.09	126.20	119.84
1	B	329	PHE	CA-C-N	5.08	125.09	119.90
1	B	329	PHE	C-N-CA	5.08	125.09	119.90
1	A	329	PHE	CA-C-N	5.07	125.07	119.90
1	A	329	PHE	C-N-CA	5.07	125.07	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7945	0	7616	30	0
1	B	7945	0	7616	29	0
1	J	7945	0	7616	28	0
2	C	765	0	721	2	0
2	D	765	0	721	1	0
2	K	765	0	721	0	0
3	E	958	0	896	3	0
3	F	958	0	896	3	0
3	M	958	0	896	3	0
4	G	600	0	300	0	0
4	H	600	0	300	0	0
4	N	600	0	300	0	0
5	I	503	0	261	1	0
5	L	503	0	261	2	0
5	O	503	0	261	2	0
6	P	49	0	43	0	0
6	S	49	0	43	0	0
6	V	49	0	43	0	0
7	Q	28	0	25	0	0
7	R	28	0	25	0	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0
8	A	210	0	195	1	0
8	B	210	0	195	1	0
8	J	210	0	195	1	0
9	A	227	0	0	8	0
9	B	227	0	0	8	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	15	0	0	0	0
9	F	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	227	0	0	8	0
9	K	1	0	0	0	0
9	M	15	0	0	0	0
All	All	33987	0	30246	98	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 (98) 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)
9:B:1418:HOH:O	3:M:106:TRP:HZ3	1.52	0.93
9:A:1418:HOH:O	3:F:106:TRP:HZ3	1.52	0.92
3:E:106:TRP:HZ3	9:J:1418:HOH:O	1.52	0.91
1:J:878:LEU:HD12	9:J:1500:HOH:O	1.73	0.89
1:B:878:LEU:HD12	9:B:1500:HOH:O	1.73	0.88
1:A:878:LEU:HD12	9:A:1500:HOH:O	1.73	0.88
1:J:458:LYS:HG3	9:J:1515:HOH:O	1.89	0.73
1:A:458:LYS:HG3	9:A:1515:HOH:O	1.89	0.72
1:B:458:LYS:HG3	9:B:1515:HOH:O	1.89	0.71
1:A:878:LEU:CD1	9:A:1500:HOH:O	2.40	0.63
1:B:878:LEU:CD1	9:B:1500:HOH:O	2.40	0.59
1:J:1142:GLN:N	1:J:1143:PRO:CD	2.66	0.58
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.66	0.58
1:A:1142:GLN:N	1:A:1143:PRO:CD	2.66	0.57
1:J:878:LEU:CD1	9:J:1500:HOH:O	2.40	0.57
9:B:1418:HOH:O	3:M:106:TRP:CZ3	2.38	0.56
1:B:406:GLU:OE2	9:B:1401:HOH:O	2.18	0.55
1:A:406:GLU:OE2	9:A:1401:HOH:O	2.18	0.55
1:J:406:GLU:OE2	9:J:1401:HOH:O	2.18	0.54
3:E:106:TRP:CZ3	9:J:1418:HOH:O	2.38	0.53
1:A:230:PRO:CB	1:B:357:ARG:NH1	2.72	0.53
1:A:357:ARG:NH1	1:J:230:PRO:CB	2.72	0.53
1:B:230:PRO:CB	1:J:357:ARG:NH1	2.72	0.53
1:A:230:PRO:HB2	1:B:357:ARG:NH1	2.24	0.52
1:A:357:ARG:NH1	1:J:230:PRO:HB2	2.24	0.52
1:B:230:PRO:HB2	1:J:357:ARG:NH1	2.24	0.52
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.10	0.52
1:J:1006:THR:O	1:J:1010:GLN:HG2	2.10	0.52
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.10	0.51
9:A:1418:HOH:O	3:F:106:TRP:CZ3	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ASP:HA	1:B:528:LYS:HE3	1.93	0.51
1:A:389:ASP:HA	1:A:528:LYS:HE3	1.93	0.51
1:J:898:PHE:N	1:J:899:PRO:CD	2.74	0.51
1:A:898:PHE:N	1:A:899:PRO:CD	2.74	0.51
1:J:389:ASP:HA	1:J:528:LYS:HE3	1.93	0.50
1:B:898:PHE:N	1:B:899:PRO:CD	2.74	0.49
1:A:44:ARG:O	1:A:283:GLY:HA2	2.14	0.48
1:B:44:ARG:O	1:B:283:GLY:HA2	2.14	0.48
1:J:44:ARG:O	1:J:283:GLY:HA2	2.14	0.48
1:B:986:PRO:N	1:B:987:PRO:CD	2.79	0.46
1:A:986:PRO:N	1:A:987:PRO:CD	2.79	0.46
1:J:763:LEU:HD21	1:J:1005:GLN:HG2	1.98	0.46
1:J:986:PRO:HB2	1:J:987:PRO:HD3	1.98	0.46
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.98	0.46
1:J:407:VAL:HG12	9:J:1600:HOH:O	2.16	0.45
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.98	0.45
1:J:986:PRO:N	1:J:987:PRO:CD	2.79	0.45
2:C:5:MET:HE2	2:C:5:MET:HB2	1.91	0.45
1:B:763:LEU:HD21	1:B:1005:GLN:HG2	1.98	0.44
1:A:763:LEU:HD21	1:A:1005:GLN:HG2	1.98	0.44
1:B:407:VAL:HG12	9:B:1600:HOH:O	2.16	0.44
1:J:1090:PRO:HD3	1:J:1095:PHE:CE2	2.53	0.44
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.53	0.44
1:A:407:VAL:HG12	9:A:1600:HOH:O	2.16	0.44
1:J:396:TYR:HB2	1:J:514:SER:HG	1.84	0.43
5:L:7:PRO:HA	5:L:8:PRO:HD3	1.87	0.43
2:D:5:MET:HE2	2:D:5:MET:HB2	1.91	0.43
1:A:574:ASP:OD1	1:A:574:ASP:C	2.62	0.43
1:J:329:PHE:CZ	1:J:528:LYS:HD2	2.54	0.43
1:J:396:TYR:HB2	1:J:514:SER:OG	2.19	0.43
1:A:294:ASP:HB2	1:A:295:PRO:HD2	2.01	0.43
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.52	0.43
1:B:294:ASP:HB2	1:B:295:PRO:HD2	2.01	0.43
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.53	0.43
1:J:294:ASP:HB2	1:J:295:PRO:HD2	2.01	0.43
1:J:1016:ALA:HB3	9:J:1424:HOH:O	2.19	0.42
1:A:862:PRO:HA	1:A:863:PRO:HD3	1.89	0.42
1:B:396:TYR:HB2	1:B:514:SER:OG	2.19	0.42
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.52	0.42
1:J:811:LYS:NZ	1:J:820:ASP:OD2	2.52	0.42
1:J:898:PHE:HB3	1:J:899:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:CZ	1:A:528:LYS:HD2	2.54	0.42
2:C:59:ILE:HA	2:C:60:PRO:HD3	1.88	0.42
1:A:353:TRP:CD1	1:A:353:TRP:H	2.37	0.42
1:A:396:TYR:HB2	1:A:514:SER:OG	2.19	0.42
3:E:47:TRP:CZ2	3:E:49:GLY:HA2	2.55	0.42
1:B:329:PHE:CZ	1:B:528:LYS:HD2	2.54	0.42
5:O:75:SER:O	5:O:76:ARG:C	2.63	0.42
3:M:47:TRP:CZ2	3:M:49:GLY:HA2	2.55	0.42
1:B:574:ASP:OD1	1:B:574:ASP:C	2.62	0.41
1:A:737:ASP:OD1	1:A:737:ASP:C	2.64	0.41
1:A:1016:ALA:HB3	9:A:1424:HOH:O	2.19	0.41
1:B:898:PHE:HB3	1:B:899:PRO:HD3	2.02	0.41
1:A:898:PHE:HB3	1:A:899:PRO:HD3	2.02	0.41
1:J:574:ASP:C	1:J:574:ASP:OD1	2.62	0.41
1:B:1016:ALA:HB3	9:B:1424:HOH:O	2.19	0.41
1:B:353:TRP:CD1	1:B:353:TRP:H	2.38	0.41
1:J:891:GLY:HA3	1:J:892:PRO:HD2	1.91	0.41
1:A:123:ALA:HB3	8:A:1314:NAG:H82	2.03	0.41
5:L:75:SER:O	5:L:76:ARG:C	2.63	0.41
1:B:123:ALA:HB3	8:B:1314:NAG:H82	2.03	0.41
5:I:75:SER:O	5:I:76:ARG:C	2.63	0.41
1:J:123:ALA:HB3	8:J:1314:NAG:H82	2.03	0.41
1:B:811:LYS:HA	1:B:812:PRO:HD3	1.91	0.40
3:F:47:TRP:CZ2	3:F:49:GLY:HA2	2.55	0.40
1:A:478:THR:HA	1:A:479:PRO:HD3	1.95	0.40
1:B:891:GLY:HA3	1:B:892:PRO:HD2	1.91	0.40
5:O:42:ALA:HA	5:O:43:PRO:HD3	1.93	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	1019/1288 (79%)	998 (98%)	21 (2%)	0	100	100
1	B	1019/1288 (79%)	998 (98%)	21 (2%)	0	100	100
1	J	1019/1288 (79%)	998 (98%)	21 (2%)	0	100	100
2	C	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
2	D	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
2	K	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
3	E	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
3	F	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
3	M	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
4	G	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
4	H	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
4	N	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
5	I	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
5	L	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
5	O	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
All	All	4368/5205 (84%)	4290 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/1116 (77%)	863 (100%)	1 (0%)	88	95
1	B	864/1116 (77%)	863 (100%)	1 (0%)	88	95
1	J	864/1116 (77%)	863 (100%)	1 (0%)	88	95
2	C	79/85 (93%)	79 (100%)	0	100	100
2	D	79/85 (93%)	79 (100%)	0	100	100
2	K	79/85 (93%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	99/100 (99%)	99 (100%)	0	100	100
3	F	99/100 (99%)	99 (100%)	0	100	100
3	M	99/100 (99%)	99 (100%)	0	100	100
4	G	5/99 (5%)	5 (100%)	0	100	100
4	H	5/99 (5%)	5 (100%)	0	100	100
4	N	5/99 (5%)	5 (100%)	0	100	100
5	I	8/83 (10%)	8 (100%)	0	100	100
5	L	8/83 (10%)	8 (100%)	0	100	100
5	O	8/83 (10%)	8 (100%)	0	100	100
All	All	3165/4449 (71%)	3162 (100%)	3 (0%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ARG
1	B	319	ARG
1	J	319	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	450	ASN
1	A	690	GLN
1	A	804	GLN
1	A	856	ASN
1	A	949	GLN
1	A	1101	HIS
2	D	39	GLN
3	E	39	GLN
1	B	239	GLN
1	B	450	ASN
1	B	690	GLN
1	B	804	GLN
1	B	856	ASN
1	B	949	GLN
1	B	1101	HIS
1	J	115	GLN

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Mol	Chain	Res	Type
1	J	239	GLN
1	J	450	ASN
1	J	690	GLN
1	J	804	GLN
1	J	949	GLN
1	J	1101	HIS
2	K	39	GLN
3	M	39	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](#)

24 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	$\# Z > 2$
6	NAG	P	1	6,1	14,14,15	0.95	1 (7%)	17,19,21	1.32	3 (17%)
6	NAG	P	2	6	14,14,15	0.91	1 (7%)	17,19,21	1.06	2 (11%)
6	BMA	P	3	6	11,11,12	0.91	0	15,15,17	0.53	0
6	FUC	P	4	6	10,10,11	0.95	0	14,14,16	0.60	0
7	NAG	Q	1	1,7	14,14,15	0.95	1 (7%)	17,19,21	1.14	2 (11%)
7	NAG	Q	2	7	14,14,15	0.98	1 (7%)	17,19,21	1.06	2 (11%)
7	NAG	R	1	1,7	14,14,15	1.00	1 (7%)	17,19,21	1.14	2 (11%)
7	NAG	R	2	7	14,14,15	1.08	1 (7%)	17,19,21	1.10	2 (11%)
6	NAG	S	1	6,1	14,14,15	0.95	1 (7%)	17,19,21	1.32	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	S	2	6	14,14,15	0.91	1 (7%)	17,19,21	1.06	2 (11%)
6	BMA	S	3	6	11,11,12	0.91	0	15,15,17	0.53	0
6	FUC	S	4	6	10,10,11	0.95	0	14,14,16	0.60	0
7	NAG	T	1	1,7	14,14,15	0.95	1 (7%)	17,19,21	1.15	2 (11%)
7	NAG	T	2	7	14,14,15	0.98	1 (7%)	17,19,21	1.06	2 (11%)
7	NAG	U	1	1,7	14,14,15	1.00	1 (7%)	17,19,21	1.14	2 (11%)
7	NAG	U	2	7	14,14,15	1.07	1 (7%)	17,19,21	1.10	2 (11%)
6	NAG	V	1	6,1	14,14,15	0.95	1 (7%)	17,19,21	1.31	3 (17%)
6	NAG	V	2	6	14,14,15	0.90	1 (7%)	17,19,21	1.06	2 (11%)
6	BMA	V	3	6	11,11,12	0.91	0	15,15,17	0.54	0
6	FUC	V	4	6	10,10,11	0.94	0	14,14,16	0.60	0
7	NAG	W	1	1,7	14,14,15	0.95	1 (7%)	17,19,21	1.15	2 (11%)
7	NAG	W	2	7	14,14,15	0.97	1 (7%)	17,19,21	1.06	2 (11%)
7	NAG	X	1	1,7	14,14,15	1.00	1 (7%)	17,19,21	1.14	2 (11%)
7	NAG	X	2	7	14,14,15	1.07	1 (7%)	17,19,21	1.10	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
6	NAG	P	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	FUC	P	4	6	-	-	0/1/1/1
7	NAG	Q	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	NAG	R	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	1/6/23/26	0/1/1/1
6	BMA	S	3	6	-	0/2/19/22	0/1/1/1
6	FUC	S	4	6	-	-	0/1/1/1
7	NAG	T	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	NAG	U	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
6	FUC	V	4	6	-	-	0/1/1/1
7	NAG	W	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	2	NAG	C1-C2	3.20	1.56	1.52
7	U	2	NAG	C1-C2	3.19	1.56	1.52
7	X	2	NAG	C1-C2	3.17	1.56	1.52
7	U	1	NAG	C1-C2	3.07	1.56	1.52
7	R	1	NAG	C1-C2	3.06	1.56	1.52
7	X	1	NAG	C1-C2	3.04	1.56	1.52
7	T	1	NAG	C1-C2	2.88	1.56	1.52
7	W	1	NAG	C1-C2	2.87	1.56	1.52
7	Q	1	NAG	C1-C2	2.86	1.56	1.52
6	P	1	NAG	C1-C2	2.84	1.56	1.52
6	V	1	NAG	C1-C2	2.84	1.56	1.52
6	S	1	NAG	C1-C2	2.81	1.56	1.52
7	T	2	NAG	C1-C2	2.76	1.56	1.52
7	W	2	NAG	C1-C2	2.73	1.56	1.52
7	Q	2	NAG	C1-C2	2.72	1.56	1.52
6	S	2	NAG	C1-C2	2.26	1.55	1.52
6	P	2	NAG	C1-C2	2.25	1.55	1.52
6	V	2	NAG	C1-C2	2.22	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1	NAG	C2-N2-C7	-3.60	118.08	122.90
6	S	1	NAG	C2-N2-C7	-3.60	118.08	122.90
6	V	1	NAG	C2-N2-C7	-3.59	118.09	122.90
6	P	2	NAG	C8-C7-N2	2.62	120.46	116.12
6	V	2	NAG	C8-C7-N2	2.62	120.46	116.12
7	W	1	NAG	C8-C7-N2	2.61	120.44	116.12
6	S	2	NAG	C8-C7-N2	2.61	120.44	116.12
7	T	2	NAG	C8-C7-N2	2.61	120.44	116.12
7	Q	2	NAG	C8-C7-N2	2.61	120.44	116.12
7	W	2	NAG	C8-C7-N2	2.60	120.44	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	1	NAG	C8-C7-N2	2.60	120.43	116.12
7	Q	1	NAG	C8-C7-N2	2.60	120.43	116.12
7	R	2	NAG	C8-C7-N2	2.58	120.40	116.12
7	X	2	NAG	C8-C7-N2	2.56	120.36	116.12
7	U	2	NAG	C8-C7-N2	2.55	120.35	116.12
7	R	1	NAG	C8-C7-N2	2.52	120.29	116.12
7	X	1	NAG	C8-C7-N2	2.52	120.29	116.12
7	U	1	NAG	C8-C7-N2	2.51	120.28	116.12
7	Q	1	NAG	C2-N2-C7	-2.48	119.58	122.90
7	T	1	NAG	C2-N2-C7	-2.48	119.58	122.90
7	W	1	NAG	C2-N2-C7	-2.47	119.59	122.90
7	X	2	NAG	C2-N2-C7	-2.41	119.67	122.90
7	U	2	NAG	C2-N2-C7	-2.41	119.67	122.90
7	R	2	NAG	C2-N2-C7	-2.40	119.69	122.90
7	R	1	NAG	C2-N2-C7	-2.32	119.79	122.90
7	X	1	NAG	C2-N2-C7	-2.32	119.79	122.90
7	U	1	NAG	C2-N2-C7	-2.31	119.80	122.90
6	S	1	NAG	C8-C7-N2	2.30	119.94	116.12
6	P	1	NAG	C8-C7-N2	2.29	119.92	116.12
6	V	1	NAG	C8-C7-N2	2.28	119.90	116.12
6	S	2	NAG	C2-N2-C7	-2.24	119.90	122.90
6	V	2	NAG	C2-N2-C7	-2.23	119.91	122.90
6	P	2	NAG	C2-N2-C7	-2.23	119.91	122.90
7	T	2	NAG	C2-N2-C7	-2.11	120.07	122.90
7	W	2	NAG	C2-N2-C7	-2.10	120.08	122.90
7	Q	2	NAG	C2-N2-C7	-2.10	120.09	122.90
6	V	1	NAG	C4-C3-C2	-2.06	108.00	111.02
6	P	1	NAG	C4-C3-C2	-2.05	108.01	111.02
6	S	1	NAG	C4-C3-C2	-2.05	108.01	111.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

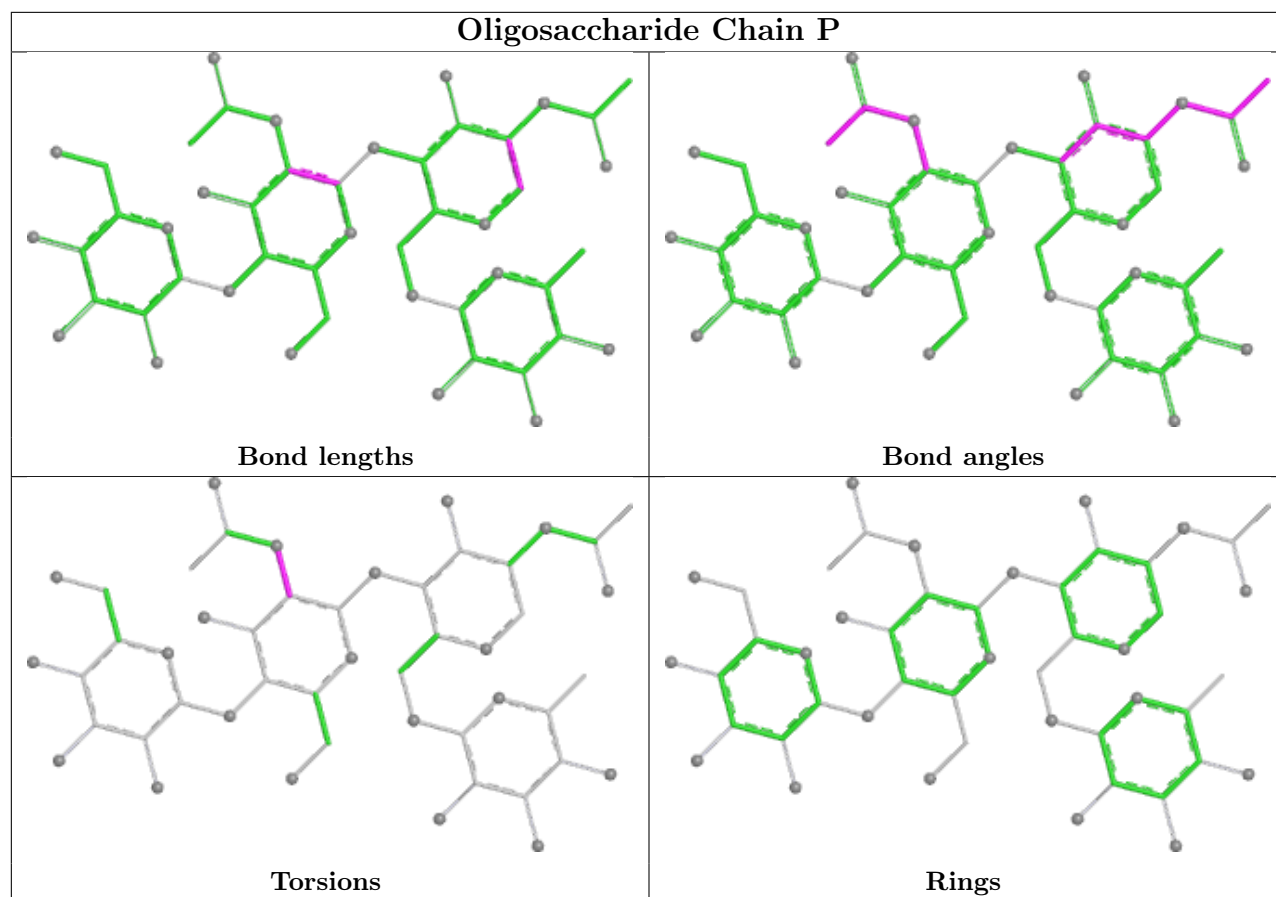
Mol	Chain	Res	Type	Atoms
6	P	2	NAG	C1-C2-N2-C7
6	S	2	NAG	C1-C2-N2-C7
6	V	2	NAG	C1-C2-N2-C7

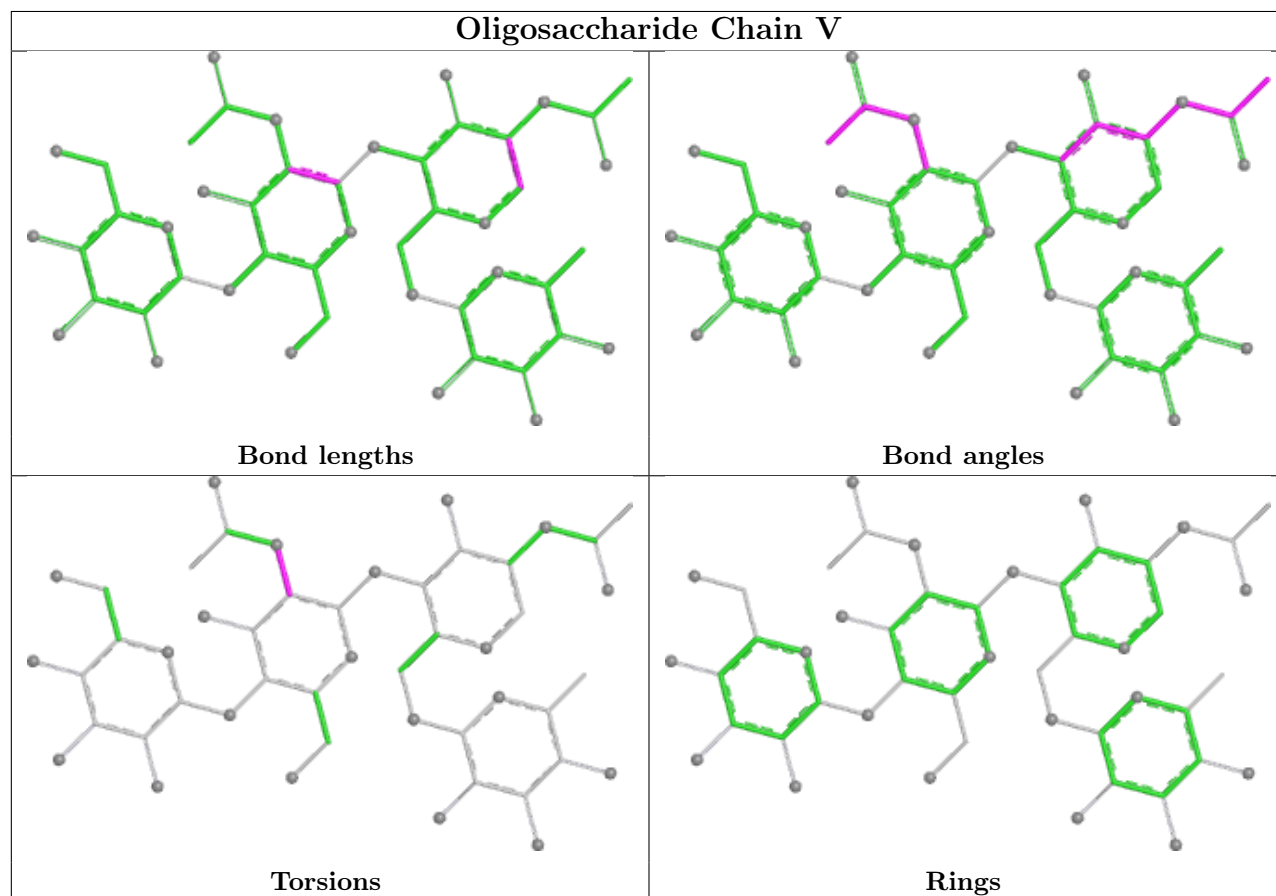
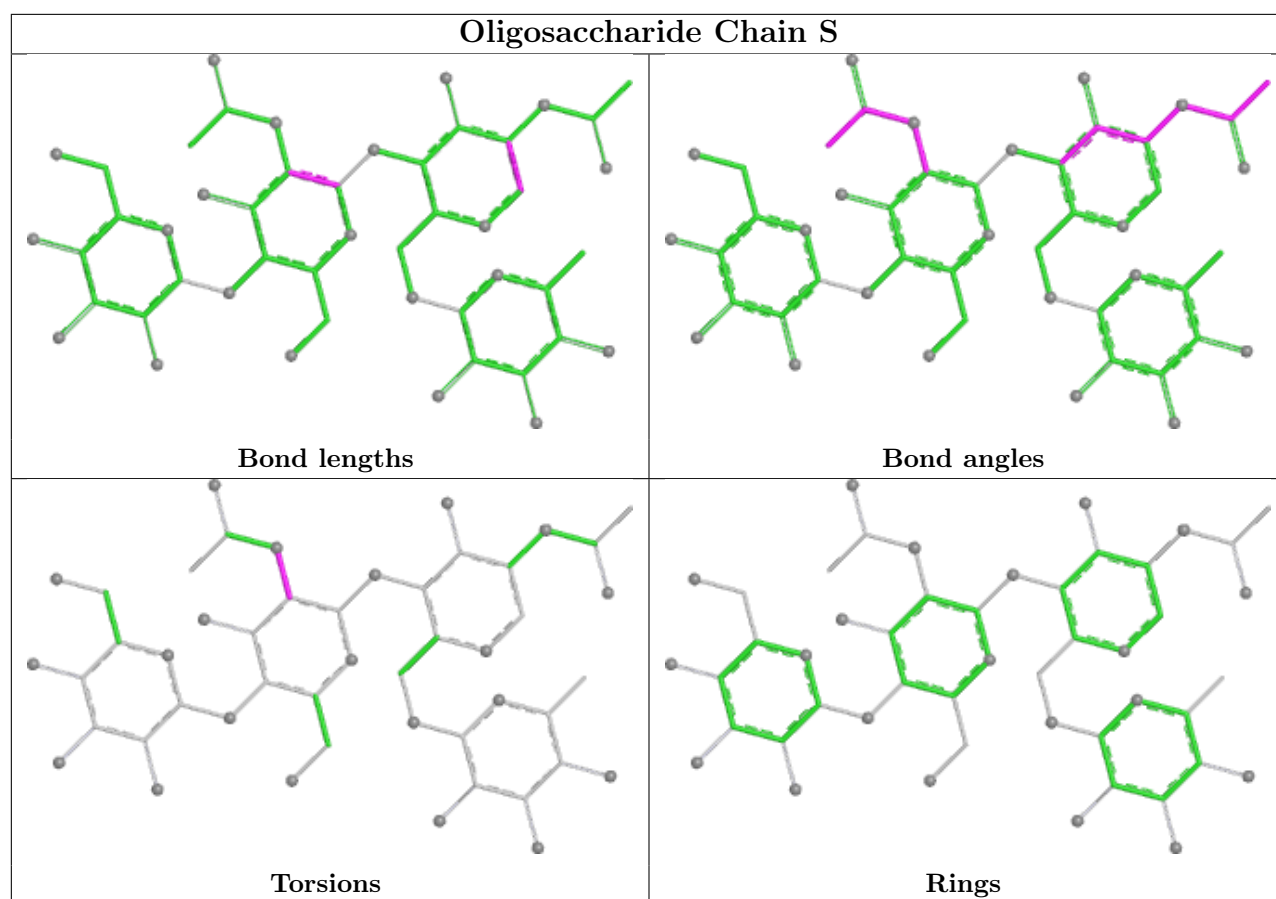
There are no ring outliers.

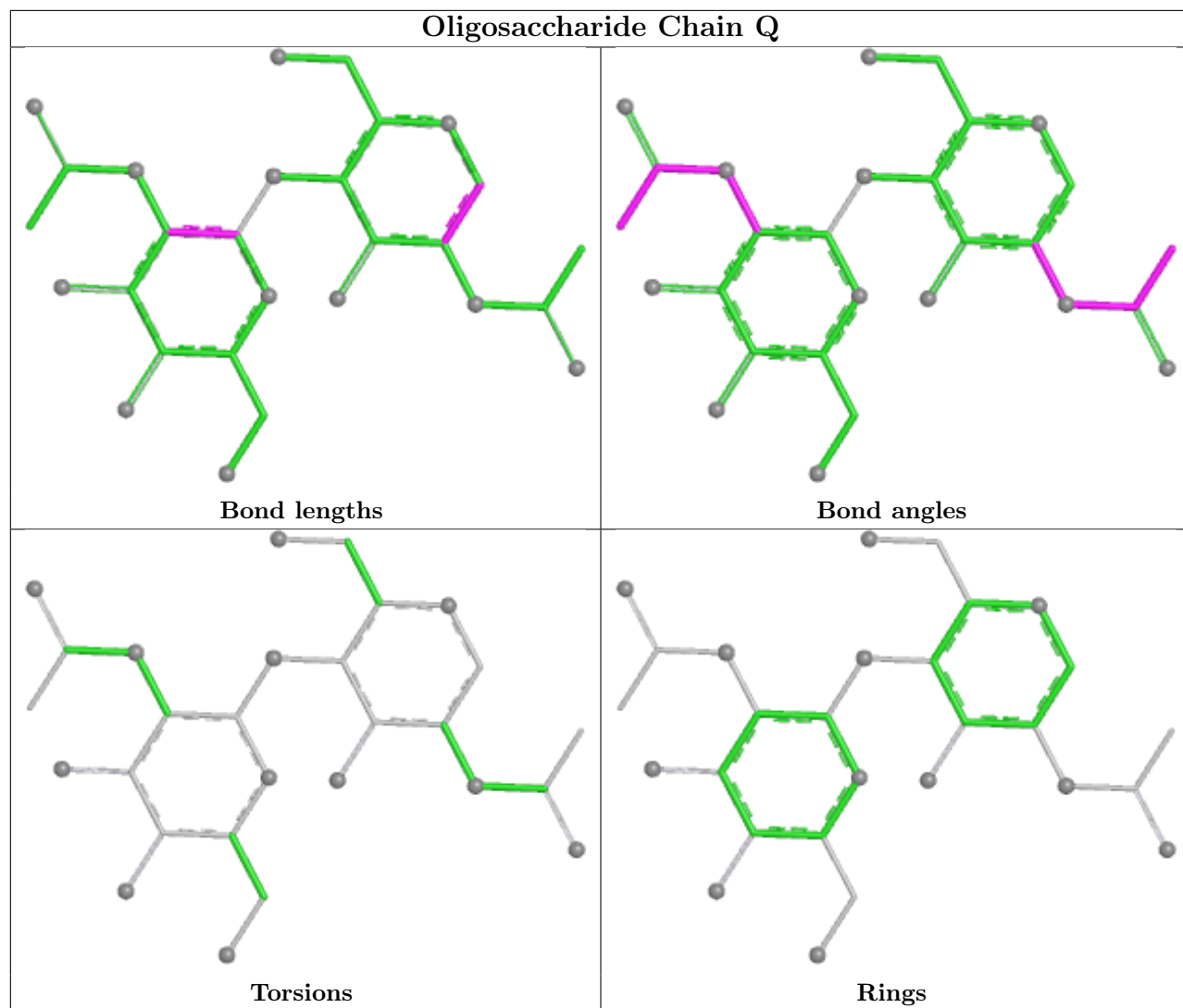
No monomer is involved in short contacts.

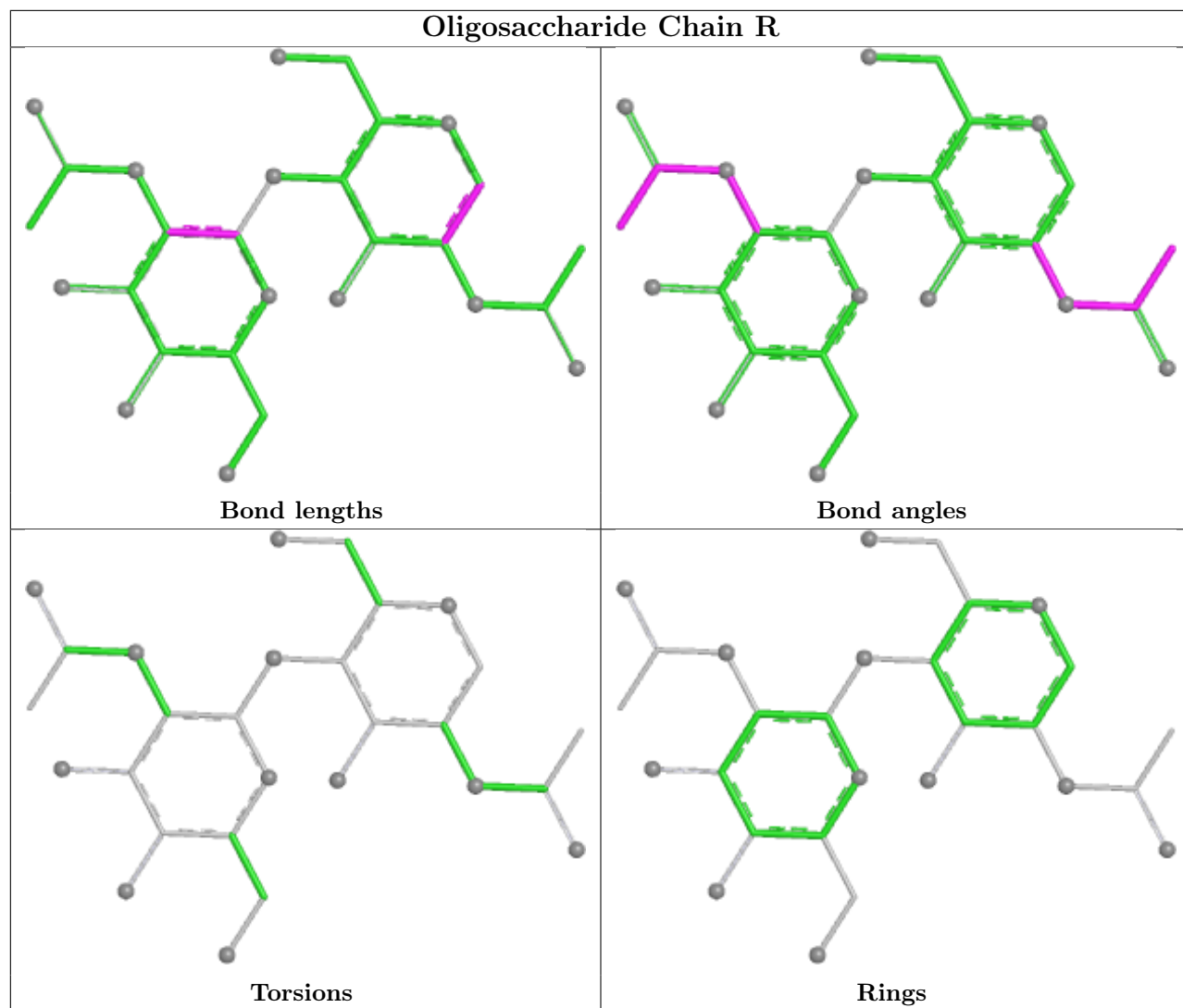
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

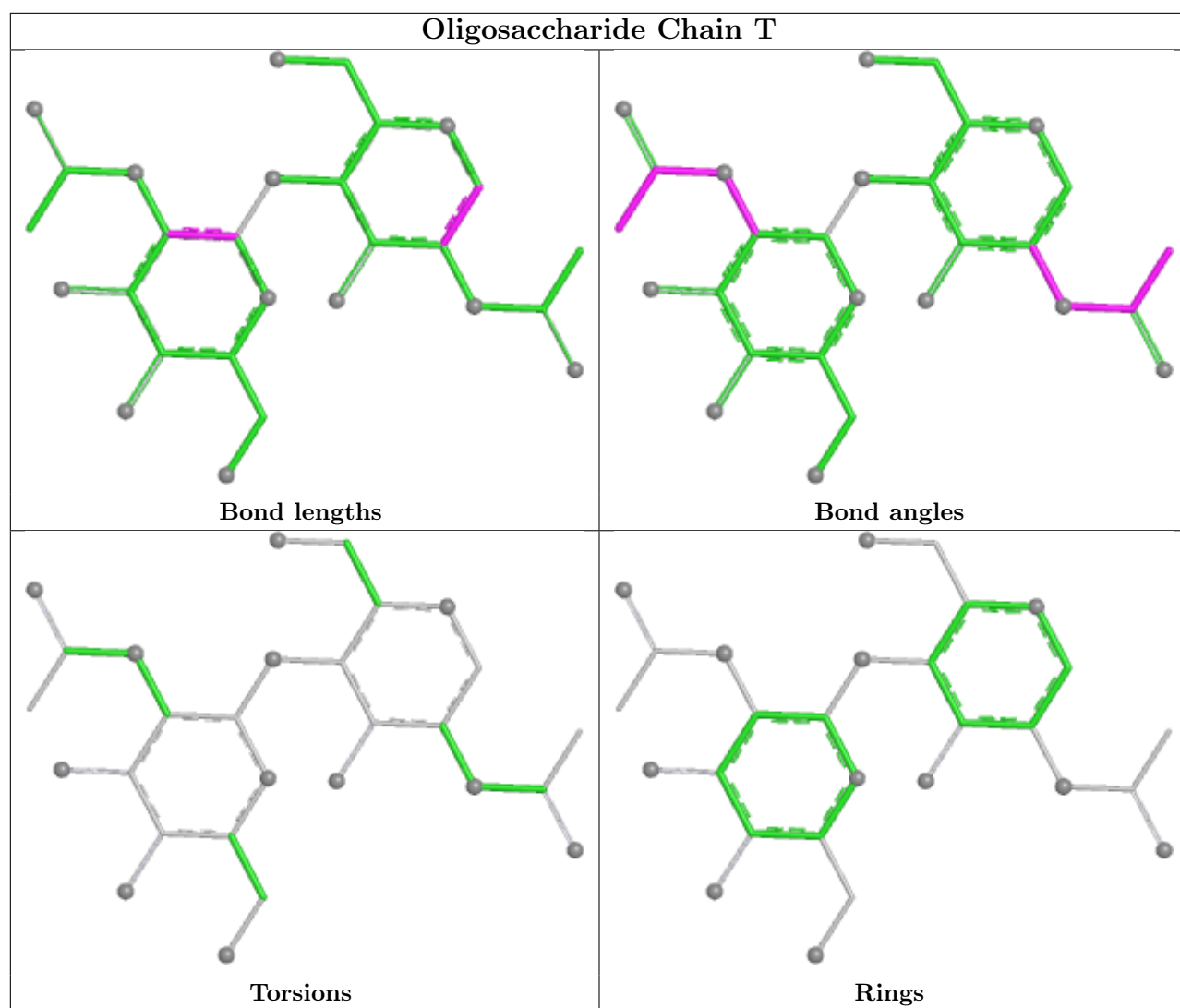
bond angles, torsion angles, and ring geometry for oligosaccharide.

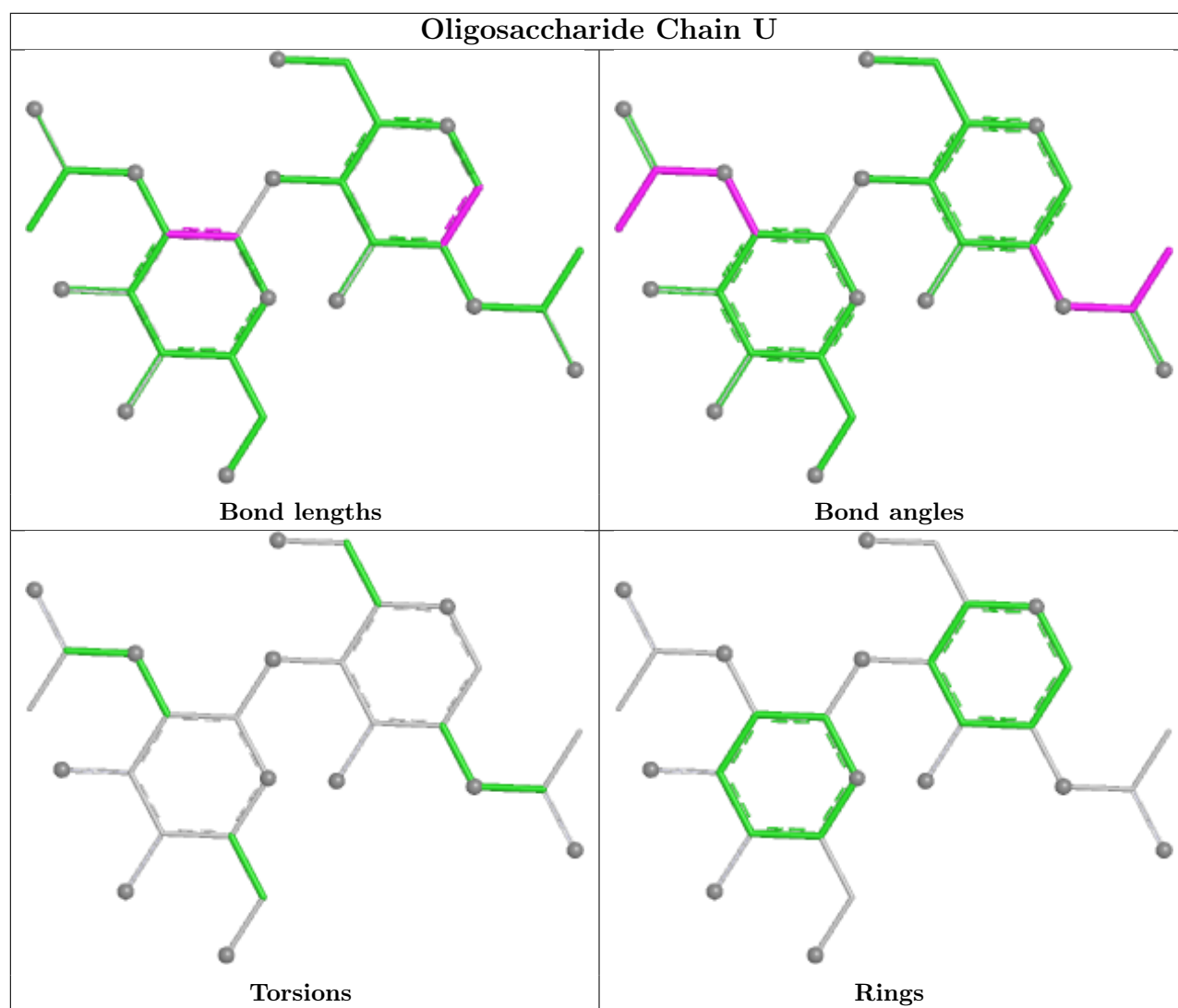


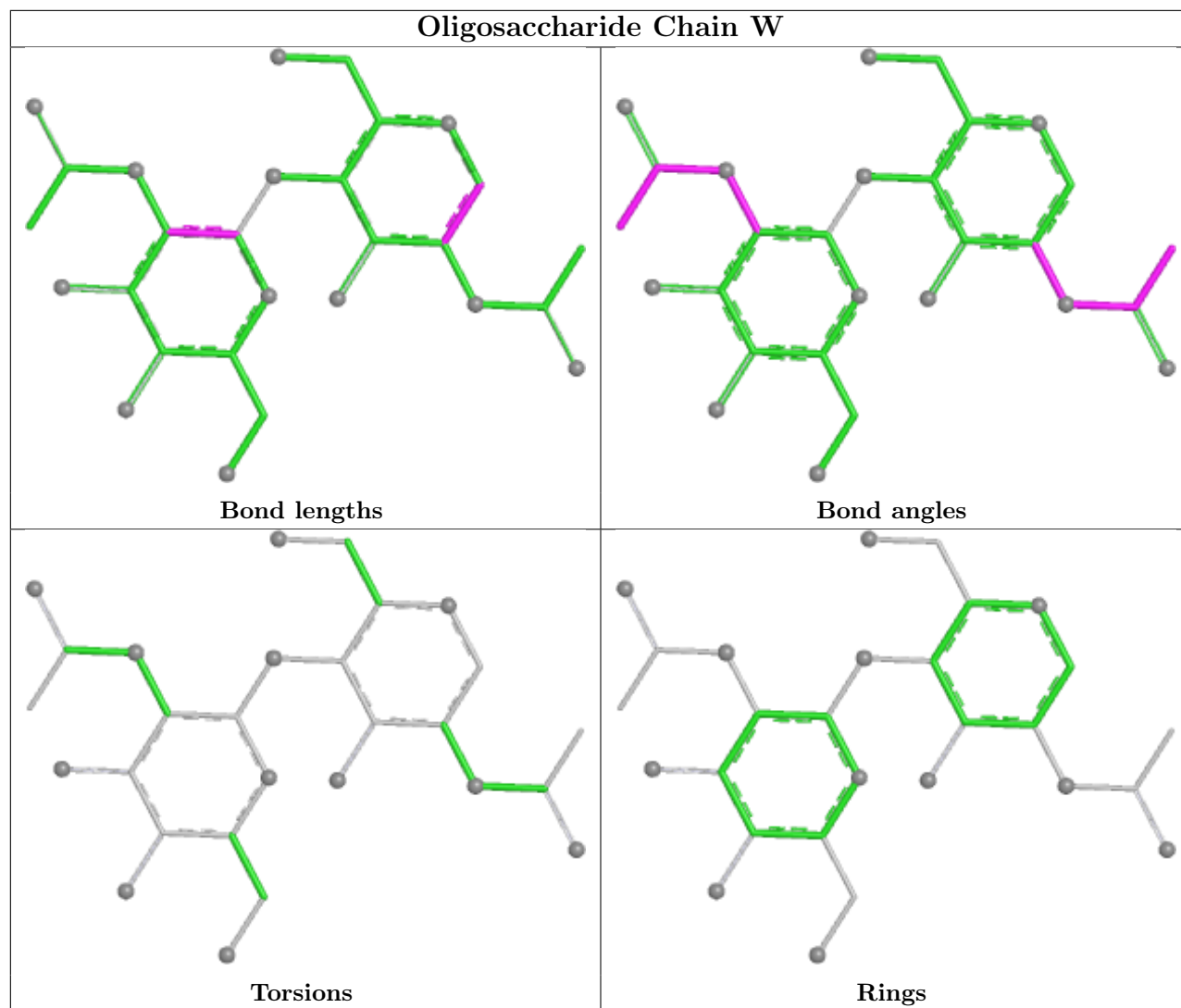


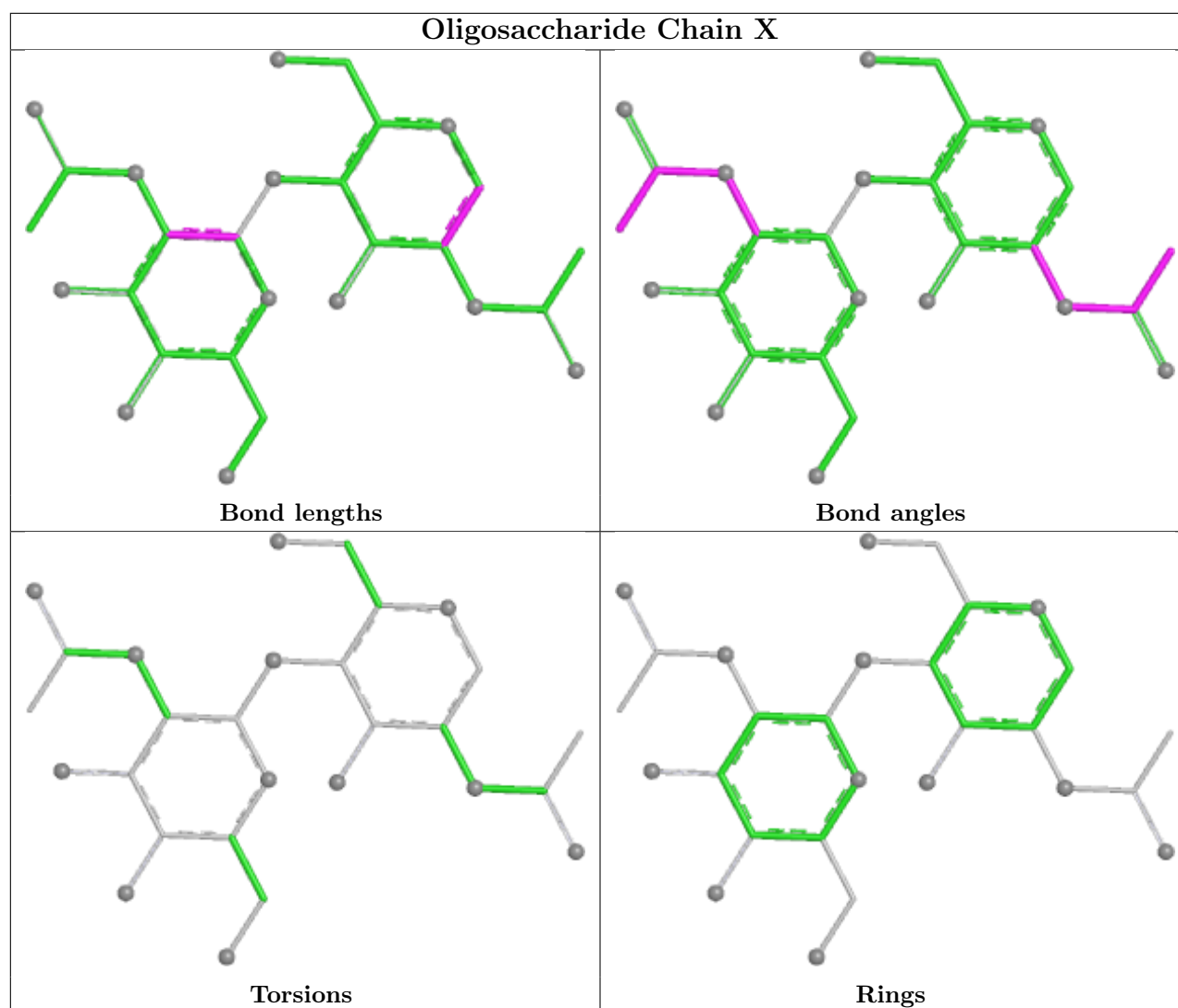












5.6 Ligand geometry [i](#)

45 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	$\# Z > 2$
8	NAG	A	1307	1	14,14,15	1.06	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	B	1315	1	14,14,15	1.08	1 (7%)	17,19,21	1.24	2 (11%)
8	NAG	J	1307	1	14,14,15	1.06	1 (7%)	17,19,21	1.20	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	J	1314	1	14,14,15	1.10	1 (7%)	17,19,21	1.17	2 (11%)
8	NAG	A	1310	1	14,14,15	1.09	1 (7%)	17,19,21	1.13	2 (11%)
8	NAG	B	1301	1	14,14,15	1.03	1 (7%)	17,19,21	1.25	2 (11%)
8	NAG	J	1306	1	14,14,15	1.07	1 (7%)	17,19,21	1.26	2 (11%)
8	NAG	A	1302	1	14,14,15	1.06	1 (7%)	17,19,21	1.18	2 (11%)
8	NAG	A	1306	1	14,14,15	1.08	1 (7%)	17,19,21	1.26	2 (11%)
8	NAG	A	1315	1	14,14,15	1.07	1 (7%)	17,19,21	1.24	2 (11%)
8	NAG	A	1309	1	14,14,15	1.10	1 (7%)	17,19,21	1.13	2 (11%)
8	NAG	B	1303	1	14,14,15	1.12	1 (7%)	17,19,21	1.17	2 (11%)
8	NAG	J	1303	1	14,14,15	1.13	1 (7%)	17,19,21	1.16	2 (11%)
8	NAG	J	1310	1	14,14,15	1.09	1 (7%)	17,19,21	1.13	2 (11%)
8	NAG	A	1314	1	14,14,15	1.11	1 (7%)	17,19,21	1.17	2 (11%)
8	NAG	B	1312	1	14,14,15	1.61	1 (7%)	17,19,21	1.43	3 (17%)
8	NAG	A	1303	1	14,14,15	1.12	1 (7%)	17,19,21	1.16	2 (11%)
8	NAG	B	1308	1	14,14,15	1.14	1 (7%)	17,19,21	1.14	2 (11%)
8	NAG	J	1315	1	14,14,15	1.07	1 (7%)	17,19,21	1.24	2 (11%)
8	NAG	A	1308	1	14,14,15	1.15	1 (7%)	17,19,21	1.14	2 (11%)
8	NAG	A	1301	1	14,14,15	1.03	1 (7%)	17,19,21	1.25	2 (11%)
8	NAG	J	1311	1	14,14,15	1.07	1 (7%)	17,19,21	1.21	2 (11%)
8	NAG	J	1312	1	14,14,15	1.60	1 (7%)	17,19,21	1.43	3 (17%)
8	NAG	J	1309	1	14,14,15	1.10	1 (7%)	17,19,21	1.13	2 (11%)
8	NAG	A	1312	1	14,14,15	1.61	1 (7%)	17,19,21	1.42	3 (17%)
8	NAG	A	1304	1	14,14,15	1.11	1 (7%)	17,19,21	1.15	2 (11%)
8	NAG	J	1302	1	14,14,15	1.06	1 (7%)	17,19,21	1.17	2 (11%)
8	NAG	A	1311	1	14,14,15	1.08	1 (7%)	17,19,21	1.21	2 (11%)
8	NAG	B	1304	1	14,14,15	1.11	1 (7%)	17,19,21	1.15	2 (11%)
8	NAG	B	1305	1	14,14,15	1.20	1 (7%)	17,19,21	1.21	2 (11%)
8	NAG	A	1305	1	14,14,15	1.20	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	B	1307	1	14,14,15	1.06	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	B	1313	1	14,14,15	1.04	1 (7%)	17,19,21	1.15	2 (11%)
8	NAG	J	1301	1	14,14,15	1.03	1 (7%)	17,19,21	1.24	2 (11%)
8	NAG	J	1308	1	14,14,15	1.14	1 (7%)	17,19,21	1.14	2 (11%)
8	NAG	B	1309	1	14,14,15	1.10	1 (7%)	17,19,21	1.13	2 (11%)
8	NAG	B	1306	1	14,14,15	1.08	1 (7%)	17,19,21	1.26	2 (11%)
8	NAG	B	1310	1	14,14,15	1.08	1 (7%)	17,19,21	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	J	1304	1	14,14,15	1.12	1 (7%)	17,19,21	1.15	2 (11%)
8	NAG	J	1305	1	14,14,15	1.20	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	J	1313	1	14,14,15	1.04	1 (7%)	17,19,21	1.15	2 (11%)
8	NAG	A	1313	1	14,14,15	1.05	1 (7%)	17,19,21	1.15	2 (11%)
8	NAG	B	1302	1	14,14,15	1.05	1 (7%)	17,19,21	1.17	2 (11%)
8	NAG	B	1314	1	14,14,15	1.10	1 (7%)	17,19,21	1.17	2 (11%)
8	NAG	B	1311	1	14,14,15	1.10	1 (7%)	17,19,21	1.22	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
8	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1315	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1307	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1314	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1306	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1315	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1303	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1310	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1314	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1315	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1311	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1312	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1309	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1302	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1308	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1304	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1305	1	-	0/6/23/26	0/1/1/1
8	NAG	J	1313	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1311	1	-	0/6/23/26	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1312	NAG	C1-C2	4.39	1.58	1.52
8	J	1312	NAG	C1-C2	4.35	1.58	1.52
8	B	1312	NAG	C1-C2	4.34	1.58	1.52
8	J	1305	NAG	C1-C2	3.73	1.57	1.52
8	A	1305	NAG	C1-C2	3.71	1.57	1.52
8	B	1305	NAG	C1-C2	3.71	1.57	1.52
8	A	1308	NAG	C1-C2	3.62	1.57	1.52
8	J	1308	NAG	C1-C2	3.60	1.57	1.52
8	B	1308	NAG	C1-C2	3.59	1.57	1.52
8	J	1303	NAG	C1-C2	3.46	1.57	1.52
8	B	1303	NAG	C1-C2	3.44	1.57	1.52
8	A	1303	NAG	C1-C2	3.41	1.57	1.52
8	B	1309	NAG	C1-C2	3.39	1.57	1.52
8	A	1309	NAG	C1-C2	3.39	1.57	1.52
8	J	1309	NAG	C1-C2	3.39	1.57	1.52
8	A	1313	NAG	C1-C2	3.33	1.56	1.52
8	J	1304	NAG	C1-C2	3.33	1.56	1.52
8	A	1304	NAG	C1-C2	3.33	1.56	1.52
8	B	1304	NAG	C1-C2	3.32	1.56	1.52
8	B	1315	NAG	C1-C2	3.31	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1315	NAG	C1-C2	3.30	1.56	1.52
8	J	1310	NAG	C1-C2	3.30	1.56	1.52
8	A	1310	NAG	C1-C2	3.30	1.56	1.52
8	J	1313	NAG	C1-C2	3.29	1.56	1.52
8	B	1310	NAG	C1-C2	3.28	1.56	1.52
8	J	1315	NAG	C1-C2	3.28	1.56	1.52
8	B	1313	NAG	C1-C2	3.27	1.56	1.52
8	A	1314	NAG	C1-C2	3.27	1.56	1.52
8	B	1314	NAG	C1-C2	3.25	1.56	1.52
8	J	1314	NAG	C1-C2	3.25	1.56	1.52
8	B	1311	NAG	C1-C2	3.23	1.56	1.52
8	A	1302	NAG	C1-C2	3.23	1.56	1.52
8	J	1302	NAG	C1-C2	3.23	1.56	1.52
8	B	1302	NAG	C1-C2	3.22	1.56	1.52
8	B	1307	NAG	C1-C2	3.20	1.56	1.52
8	B	1306	NAG	C1-C2	3.20	1.56	1.52
8	A	1306	NAG	C1-C2	3.18	1.56	1.52
8	A	1307	NAG	C1-C2	3.18	1.56	1.52
8	J	1306	NAG	C1-C2	3.17	1.56	1.52
8	J	1307	NAG	C1-C2	3.17	1.56	1.52
8	A	1311	NAG	C1-C2	3.15	1.56	1.52
8	J	1311	NAG	C1-C2	3.12	1.56	1.52
8	B	1301	NAG	C1-C2	3.09	1.56	1.52
8	A	1301	NAG	C1-C2	3.09	1.56	1.52
8	J	1301	NAG	C1-C2	3.08	1.56	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	1312	NAG	C1-O5-C5	-3.97	106.86	112.19
8	B	1312	NAG	C1-O5-C5	-3.96	106.88	112.19
8	A	1312	NAG	C1-O5-C5	-3.93	106.91	112.19
8	B	1306	NAG	C8-C7-N2	2.96	121.02	116.12
8	A	1306	NAG	C8-C7-N2	2.95	121.01	116.12
8	J	1306	NAG	C8-C7-N2	2.95	121.01	116.12
8	B	1301	NAG	C8-C7-N2	2.90	120.92	116.12
8	A	1301	NAG	C8-C7-N2	2.89	120.91	116.12
8	J	1301	NAG	C8-C7-N2	2.88	120.89	116.12
8	A	1315	NAG	C2-N2-C7	-2.80	119.15	122.90
8	B	1311	NAG	C8-C7-N2	2.78	120.73	116.12
8	B	1315	NAG	C2-N2-C7	-2.78	119.17	122.90
8	J	1315	NAG	C2-N2-C7	-2.78	119.17	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1311	NAG	C8-C7-N2	2.76	120.69	116.12
8	J	1311	NAG	C8-C7-N2	2.74	120.66	116.12
8	J	1307	NAG	C8-C7-N2	2.70	120.59	116.12
8	A	1307	NAG	C8-C7-N2	2.69	120.57	116.12
8	B	1305	NAG	C2-N2-C7	-2.68	119.31	122.90
8	B	1307	NAG	C8-C7-N2	2.67	120.55	116.12
8	J	1306	NAG	C2-N2-C7	-2.67	119.33	122.90
8	A	1305	NAG	C2-N2-C7	-2.66	119.33	122.90
8	J	1305	NAG	C2-N2-C7	-2.66	119.34	122.90
8	A	1306	NAG	C2-N2-C7	-2.64	119.36	122.90
8	B	1306	NAG	C2-N2-C7	-2.64	119.36	122.90
8	A	1314	NAG	C8-C7-N2	2.63	120.48	116.12
8	J	1315	NAG	C8-C7-N2	2.63	120.48	116.12
8	J	1303	NAG	C8-C7-N2	2.62	120.47	116.12
8	J	1314	NAG	C8-C7-N2	2.62	120.47	116.12
8	A	1303	NAG	C8-C7-N2	2.62	120.46	116.12
8	B	1315	NAG	C8-C7-N2	2.62	120.46	116.12
8	J	1305	NAG	C8-C7-N2	2.62	120.46	116.12
8	B	1303	NAG	C8-C7-N2	2.62	120.46	116.12
8	B	1305	NAG	C8-C7-N2	2.61	120.45	116.12
8	B	1314	NAG	C8-C7-N2	2.61	120.45	116.12
8	A	1315	NAG	C8-C7-N2	2.60	120.44	116.12
8	A	1305	NAG	C8-C7-N2	2.60	120.43	116.12
8	B	1307	NAG	C2-N2-C7	-2.57	119.45	122.90
8	A	1307	NAG	C2-N2-C7	-2.57	119.46	122.90
8	J	1304	NAG	C8-C7-N2	2.56	120.37	116.12
8	A	1304	NAG	C8-C7-N2	2.55	120.36	116.12
8	J	1311	NAG	C2-N2-C7	-2.55	119.48	122.90
8	J	1310	NAG	C2-N2-C7	-2.55	119.48	122.90
8	A	1311	NAG	C2-N2-C7	-2.55	119.48	122.90
8	B	1311	NAG	C2-N2-C7	-2.55	119.48	122.90
8	A	1310	NAG	C2-N2-C7	-2.55	119.49	122.90
8	J	1307	NAG	C2-N2-C7	-2.54	119.50	122.90
8	B	1310	NAG	C2-N2-C7	-2.54	119.50	122.90
8	B	1304	NAG	C8-C7-N2	2.53	120.31	116.12
8	A	1309	NAG	C8-C7-N2	2.53	120.31	116.12
8	B	1309	NAG	C8-C7-N2	2.52	120.29	116.12
8	B	1302	NAG	C2-N2-C7	-2.52	119.53	122.90
8	A	1302	NAG	C2-N2-C7	-2.51	119.54	122.90
8	J	1302	NAG	C8-C7-N2	2.50	120.27	116.12
8	J	1302	NAG	C2-N2-C7	-2.50	119.55	122.90
8	J	1309	NAG	C8-C7-N2	2.50	120.26	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1304	NAG	C2-N2-C7	-2.50	119.56	122.90
8	A	1302	NAG	C8-C7-N2	2.49	120.25	116.12
8	B	1303	NAG	C2-N2-C7	-2.49	119.56	122.90
8	A	1303	NAG	C2-N2-C7	-2.49	119.57	122.90
8	A	1304	NAG	C2-N2-C7	-2.49	119.57	122.90
8	J	1304	NAG	C2-N2-C7	-2.49	119.57	122.90
8	B	1302	NAG	C8-C7-N2	2.48	120.24	116.12
8	J	1313	NAG	C8-C7-N2	2.48	120.24	116.12
8	A	1313	NAG	C8-C7-N2	2.48	120.23	116.12
8	B	1313	NAG	C8-C7-N2	2.48	120.23	116.12
8	J	1303	NAG	C2-N2-C7	-2.48	119.58	122.90
8	B	1308	NAG	C8-C7-N2	2.45	120.18	116.12
8	A	1308	NAG	C8-C7-N2	2.44	120.17	116.12
8	A	1301	NAG	C2-N2-C7	-2.43	119.64	122.90
8	B	1301	NAG	C2-N2-C7	-2.43	119.65	122.90
8	J	1308	NAG	C8-C7-N2	2.43	120.14	116.12
8	J	1313	NAG	C2-N2-C7	-2.42	119.66	122.90
8	A	1313	NAG	C2-N2-C7	-2.42	119.66	122.90
8	B	1313	NAG	C2-N2-C7	-2.41	119.67	122.90
8	J	1301	NAG	C2-N2-C7	-2.41	119.67	122.90
8	J	1310	NAG	C8-C7-N2	2.34	120.00	116.12
8	J	1308	NAG	C2-N2-C7	-2.34	119.77	122.90
8	A	1310	NAG	C8-C7-N2	2.33	119.98	116.12
8	B	1310	NAG	C8-C7-N2	2.32	119.96	116.12
8	A	1308	NAG	C2-N2-C7	-2.30	119.81	122.90
8	B	1308	NAG	C2-N2-C7	-2.30	119.82	122.90
8	B	1314	NAG	C2-N2-C7	-2.26	119.87	122.90
8	J	1314	NAG	C2-N2-C7	-2.25	119.88	122.90
8	A	1314	NAG	C2-N2-C7	-2.25	119.88	122.90
8	A	1312	NAG	C2-N2-C7	-2.24	119.90	122.90
8	J	1312	NAG	C2-N2-C7	-2.24	119.90	122.90
8	B	1312	NAG	C2-N2-C7	-2.22	119.92	122.90
8	J	1309	NAG	C2-N2-C7	-2.21	119.94	122.90
8	A	1309	NAG	C2-N2-C7	-2.17	119.99	122.90
8	B	1309	NAG	C2-N2-C7	-2.17	119.99	122.90
8	B	1312	NAG	C8-C7-N2	2.09	119.58	116.12
8	A	1312	NAG	C8-C7-N2	2.07	119.54	116.12
8	J	1312	NAG	C8-C7-N2	2.06	119.53	116.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	1314	NAG	1	0
8	A	1314	NAG	1	0
8	B	1314	NAG	1	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
5	L	1
5	I	1
5	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	11:SER	C	17:THR	N	7.95
1	I	11:SER	C	17:THR	N	7.95
1	O	11:SER	C	17:THR	N	7.95

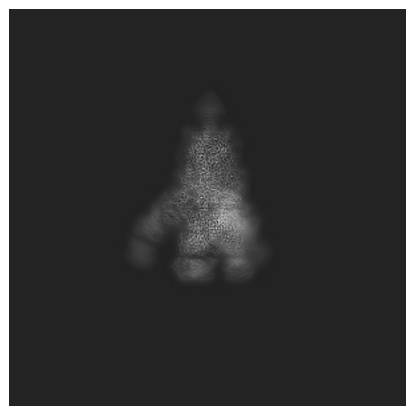
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23579. These allow visual inspection of the internal detail of the map and identification of artifacts.

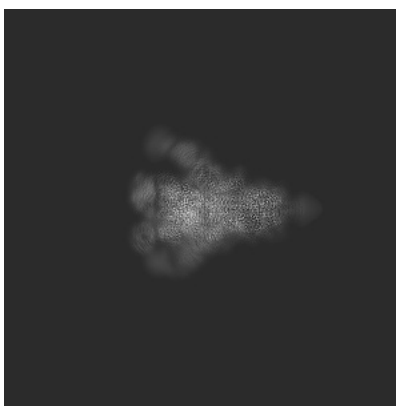
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

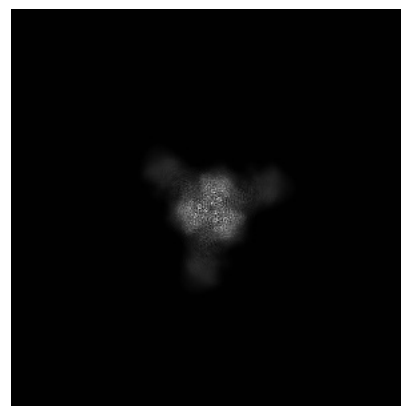
6.1.1 Primary map



X

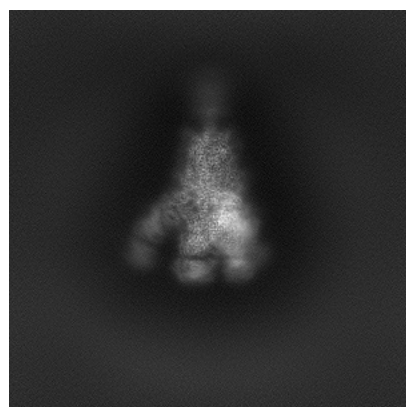


Y

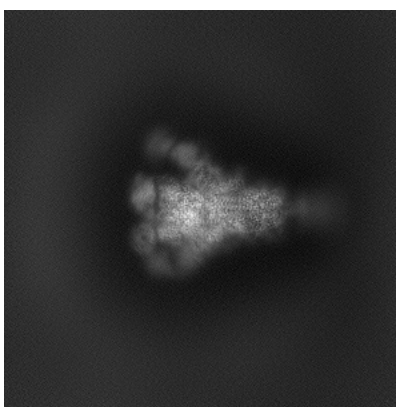


Z

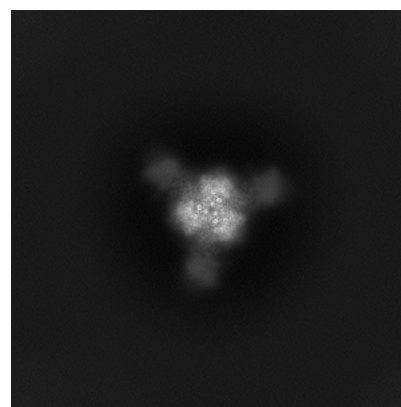
6.1.2 Raw map



X



Y

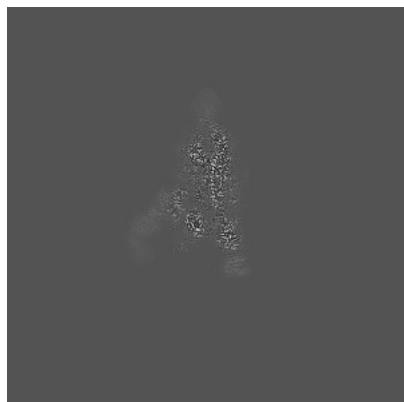


Z

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

6.2 Central slices [i](#)

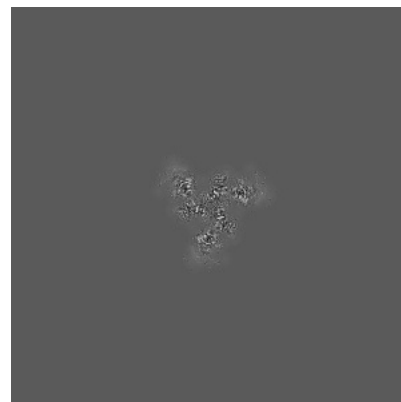
6.2.1 Primary map



X Index: 300

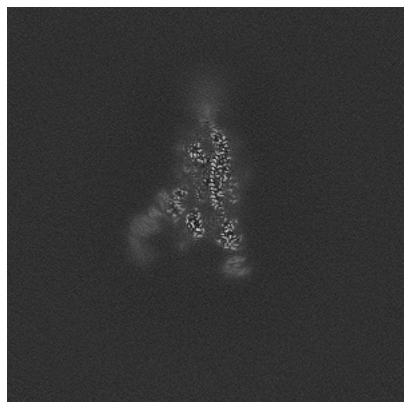


Y Index: 300



Z Index: 300

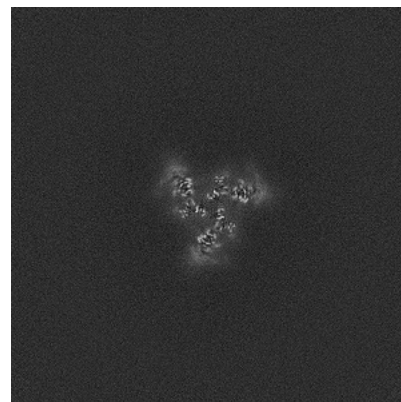
6.2.2 Raw map



X Index: 300



Y Index: 300

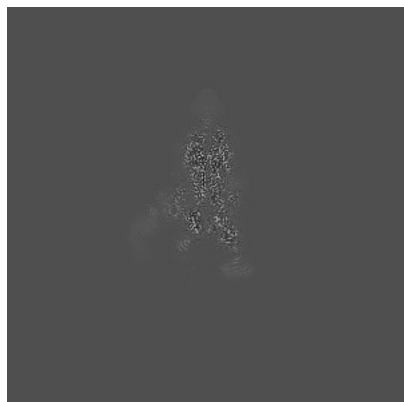


Z Index: 300

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

6.3 Largest variance slices [i](#)

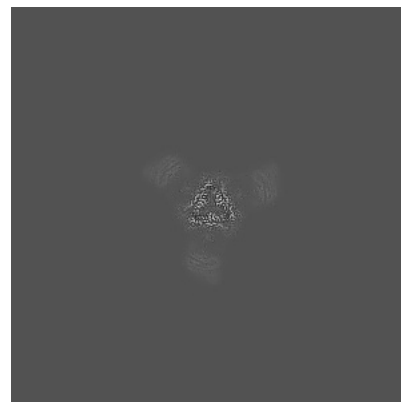
6.3.1 Primary map



X Index: 305

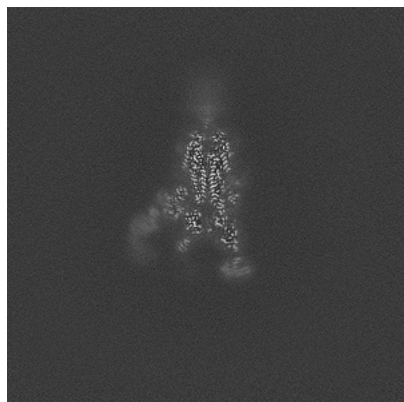


Y Index: 287

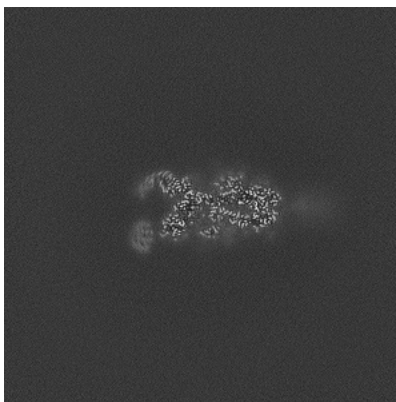


Z Index: 271

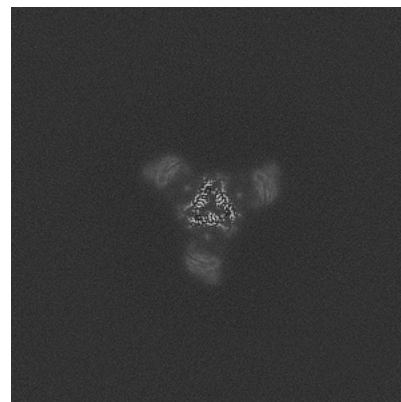
6.3.2 Raw map



X Index: 304



Y Index: 286

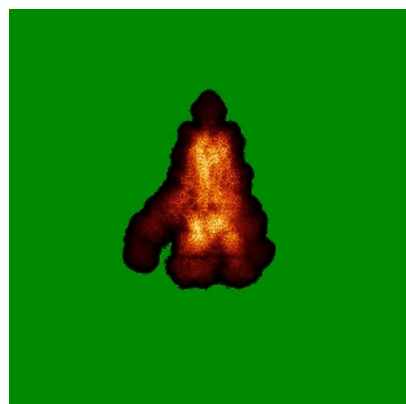


Z Index: 271

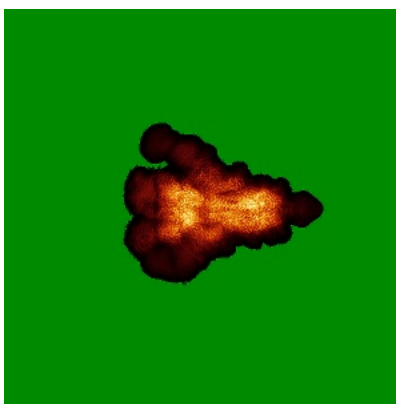
The images above show the largest variance slices of the map in three orthogonal directions.

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

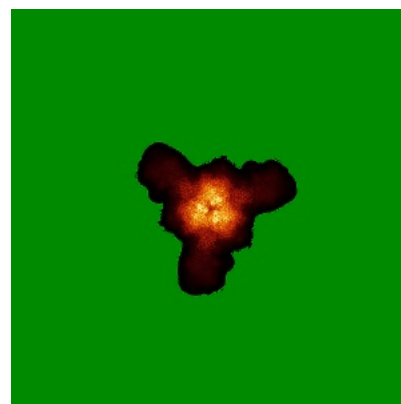
6.4.1 Primary map



X

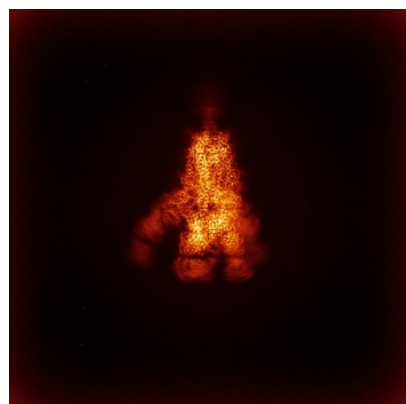


Y

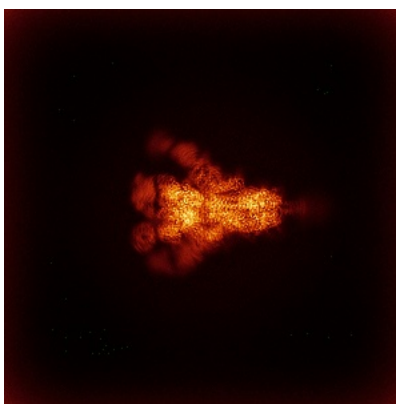


Z

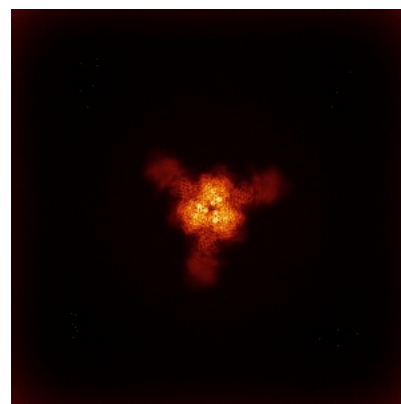
6.4.2 Raw map



X



Y

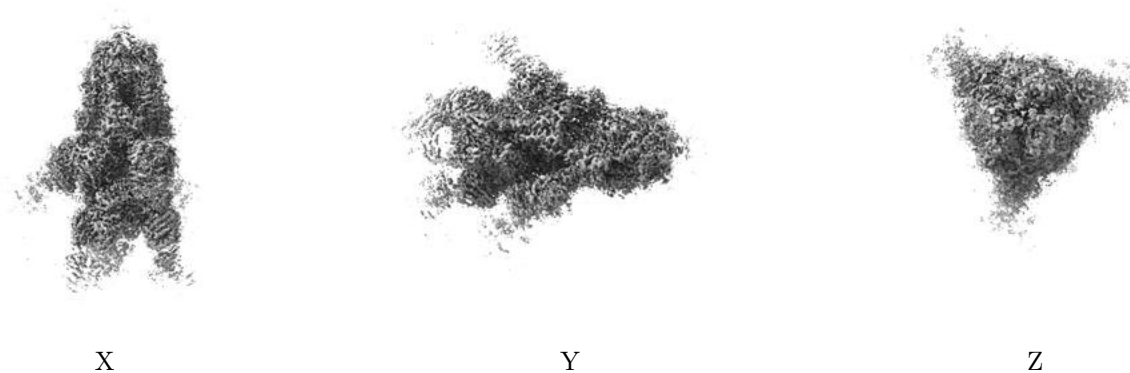


Z

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

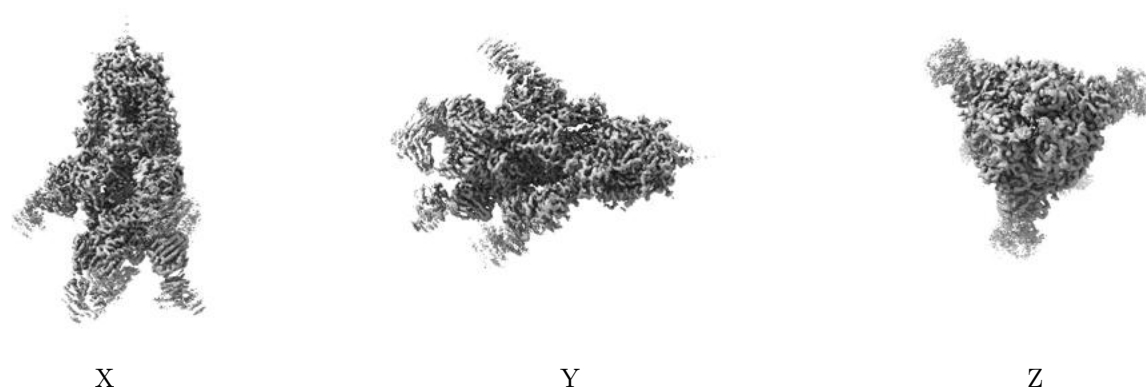
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.1. 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



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

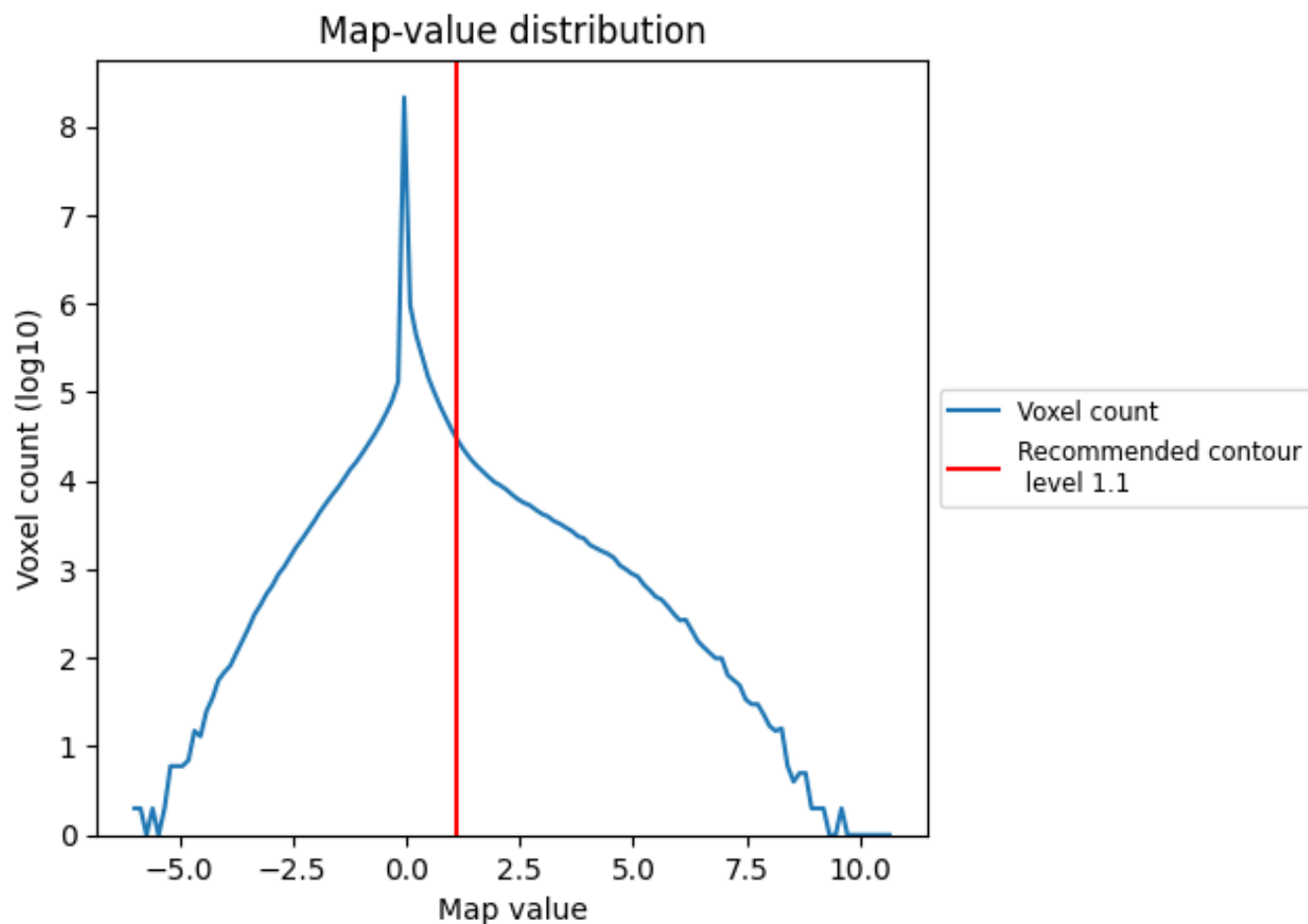
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

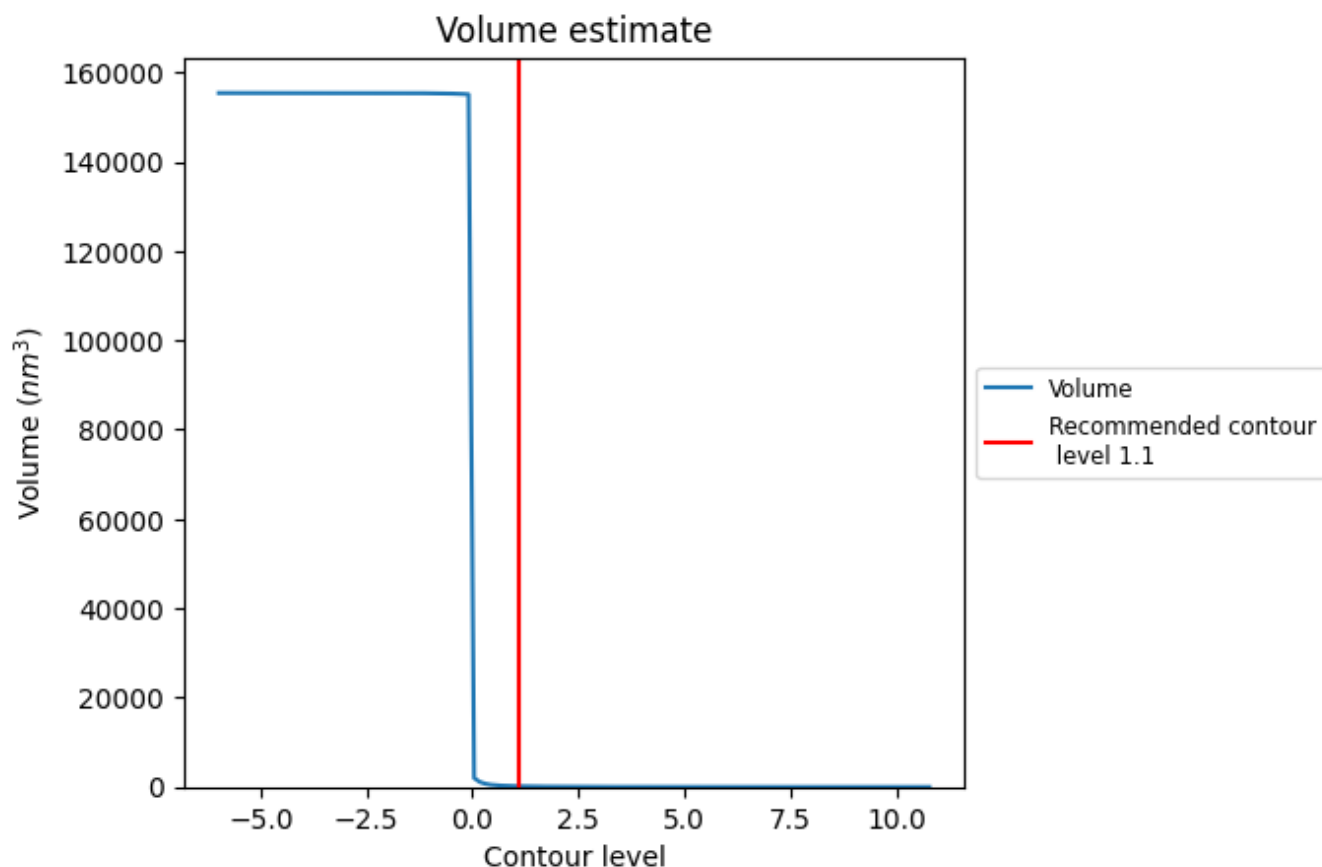
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

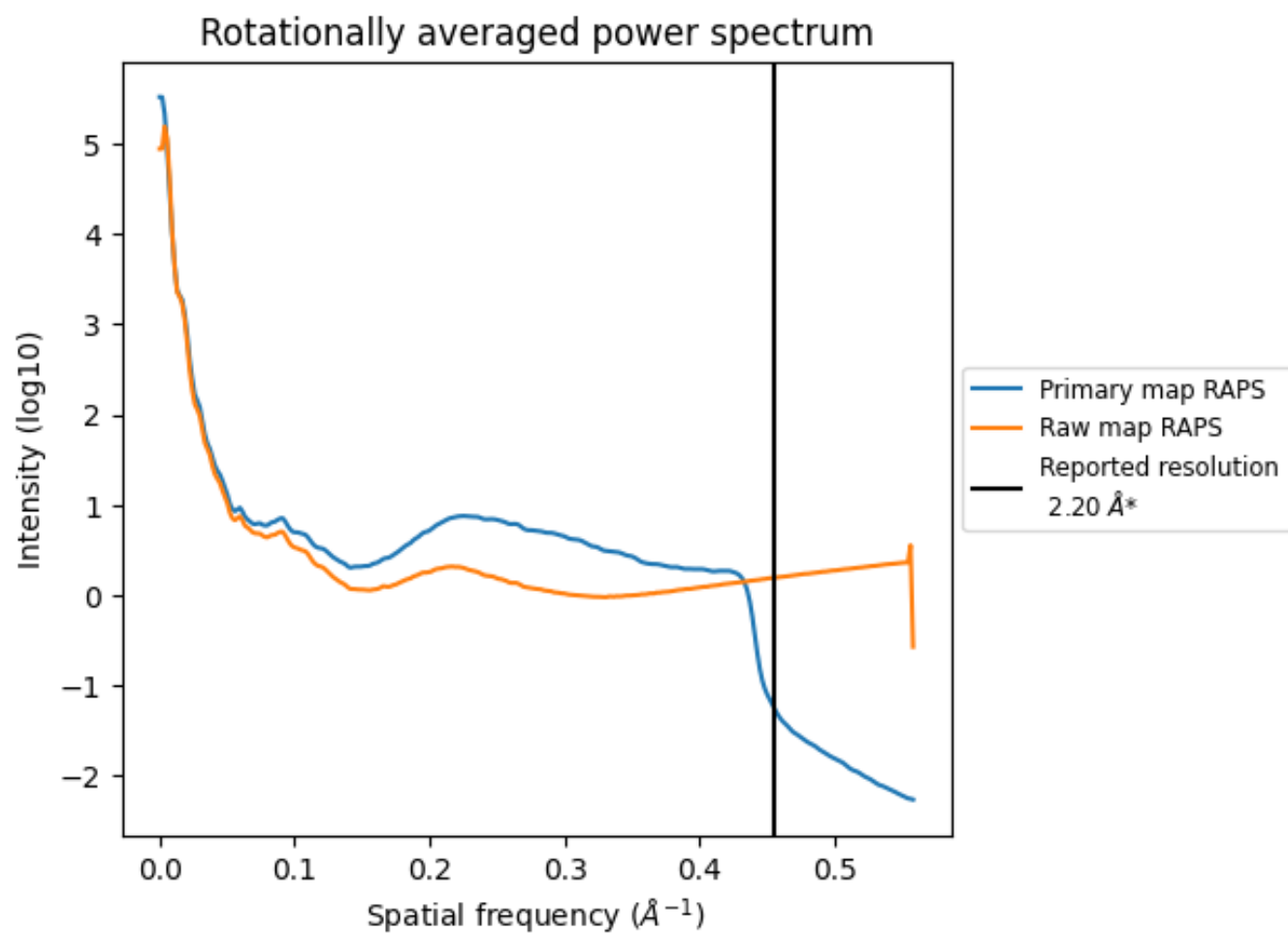
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 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 ⓘ

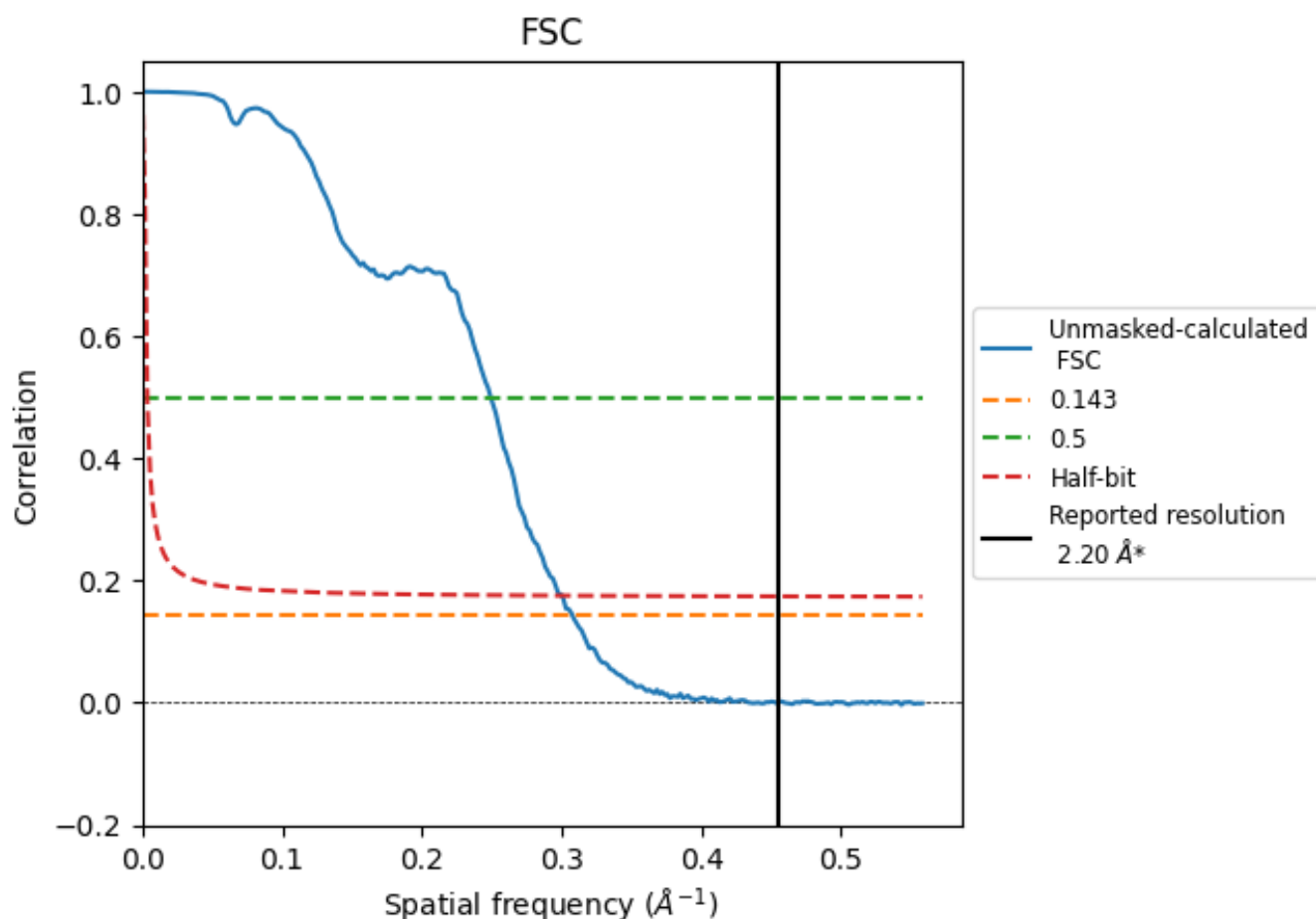


*Reported resolution corresponds to spatial frequency of $0.455 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

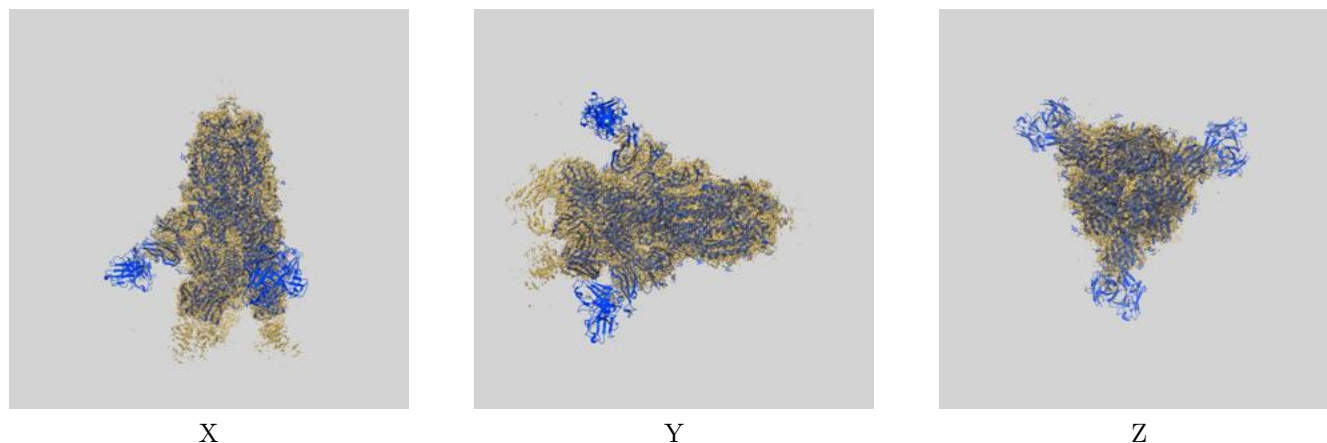
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.25	4.01	3.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

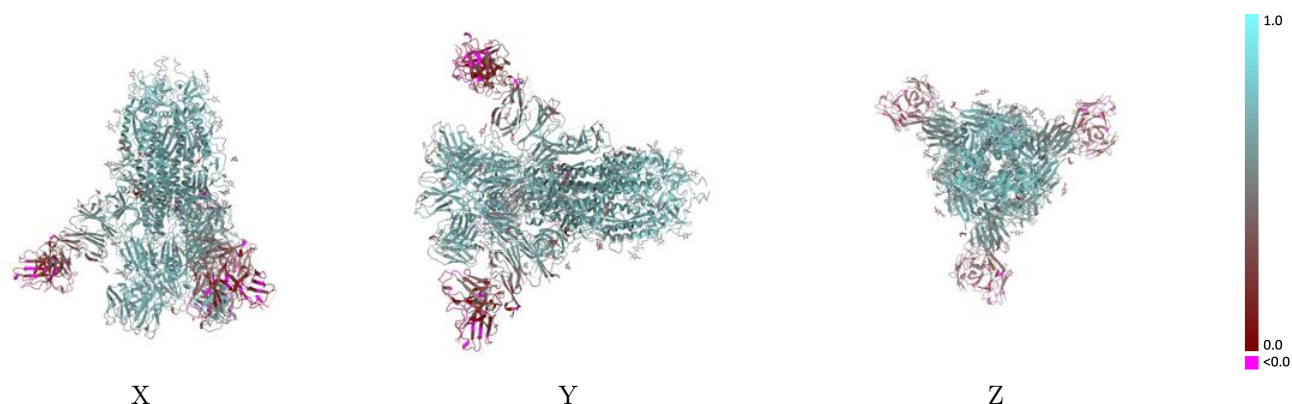
This section contains information regarding the fit between EMDB map EMD-23579 and PDB model 7LXY. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



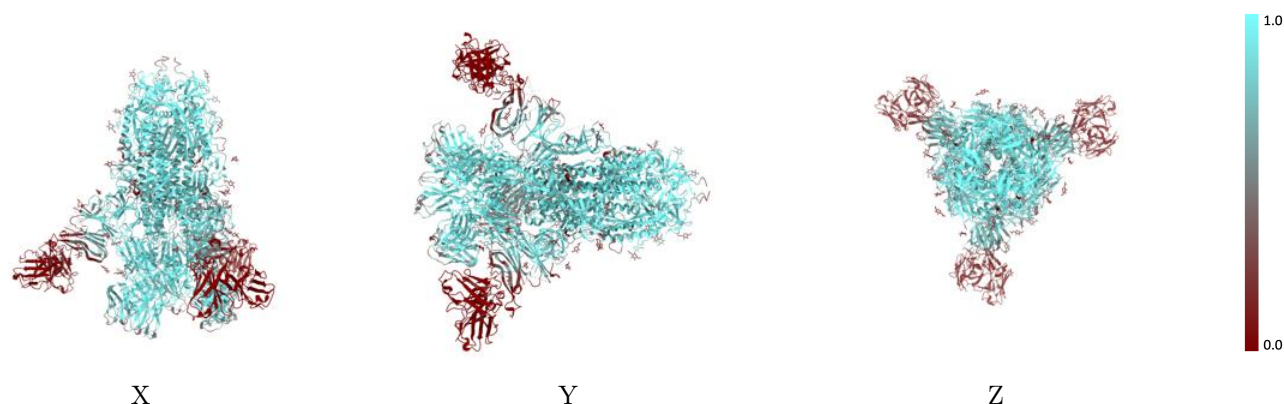
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



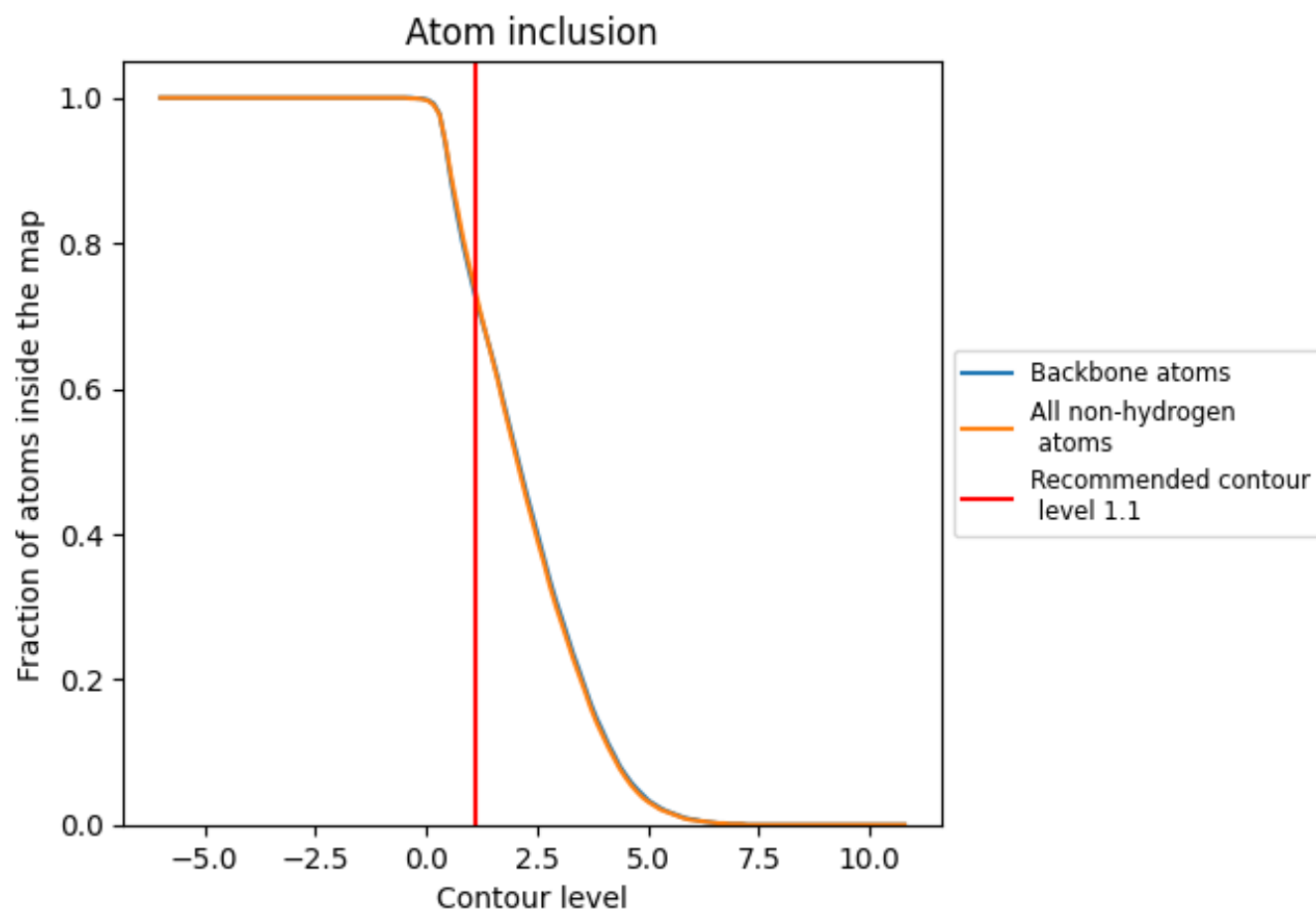
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 74% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7360	 0.5800
A	 0.8200	 0.6250
B	 0.8190	 0.6250
C	 0.7720	 0.5870
D	 0.7800	 0.5920
E	 0.8750	 0.6470
F	 0.8750	 0.6430
G	 0.0180	 0.2260
H	 0.0130	 0.2160
I	 0.0040	 0.1600
J	 0.8180	 0.6250
K	 0.7730	 0.5870
L	 0.0000	 0.1620
M	 0.8700	 0.6430
N	 0.0180	 0.2250
O	 0.0040	 0.1620
P	 0.4690	 0.4570
Q	 0.5000	 0.5290
R	 0.5360	 0.4800
S	 0.4900	 0.4680
T	 0.5360	 0.5390
U	 0.5000	 0.4480
V	 0.4900	 0.4820
W	 0.5710	 0.5420
X	 0.5360	 0.4550

