



Full wwPDB EM Validation Report ⓘ

Dec 2, 2024 – 11:36 AM EST

PDB ID : 9CO6
EMDB ID : EMD-45771
Title : BA.5 spike/Nanosota-9 complex
Authors : Ye, G.; Bu, F.; Liu, B.; Li, F.
Deposited on : 2024-07-16
Resolution : 3.01 Å(reported)
Based on initial model : 8IOS

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

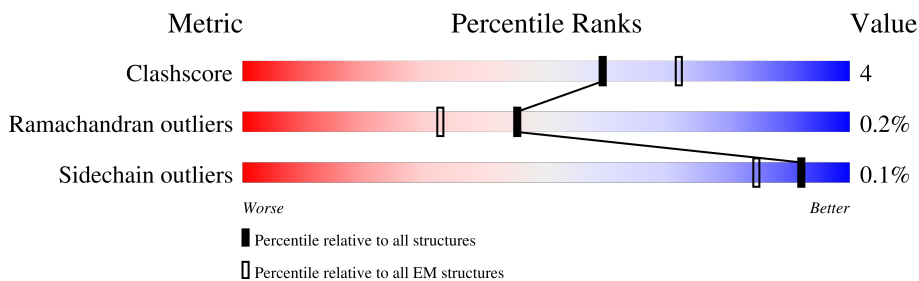
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1252	
1	B	1252	
1	C	1252	
2	D	150	
2	E	150	
2	F	150	
3	H	2	
3	J	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	K	2	 50% 50%
3	L	2	 100%
3	M	2	 100%
3	N	2	 100%
3	O	2	 50% 50%
3	P	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 28149 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
			Total	C	N	O	S		
1	B	1053	8237	5263	1374	1562	38	0	0
1	C	1053	8237	5263	1374	1562	38	0	0
1	A	1053	8237	5263	1374	1562	38	0	0

There are 279 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P0DTC2
B	-8	ASP	-	expression tag	UNP P0DTC2
B	-7	ALA	-	expression tag	UNP P0DTC2
B	-6	MET	-	expression tag	UNP P0DTC2
B	-5	LYS	-	expression tag	UNP P0DTC2
B	-4	ARG	-	expression tag	UNP P0DTC2
B	-3	GLY	-	expression tag	UNP P0DTC2
B	-2	LEU	-	expression tag	UNP P0DTC2
B	-1	CYS	-	expression tag	UNP P0DTC2
B	0	CYS	-	expression tag	UNP P0DTC2
B	1	VAL	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	5	CYS	-	insertion	UNP P0DTC2
B	6	GLY	-	insertion	UNP P0DTC2
B	7	ALA	-	insertion	UNP P0DTC2
B	8	VAL	PRO	conflict	UNP P0DTC2
B	9	PHE	LEU	conflict	UNP P0DTC2
B	12	ALA	-	insertion	UNP P0DTC2
B	19	ILE	THR	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	24	SER	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP P0DTC2
B	137	ASP	GLY	conflict	UNP P0DTC2
B	208	GLY	VAL	conflict	UNP P0DTC2
B	334	ASP	GLY	conflict	UNP P0DTC2
B	366	PHE	SER	conflict	UNP P0DTC2
B	368	PRO	SER	conflict	UNP P0DTC2
B	370	PHE	SER	conflict	UNP P0DTC2
B	371	ALA	THR	conflict	UNP P0DTC2
B	400	ASN	ASP	conflict	UNP P0DTC2
B	403	SER	ARG	conflict	UNP P0DTC2
B	412	ASN	LYS	conflict	UNP P0DTC2
B	435	LYS	ASN	conflict	UNP P0DTC2
B	447	ARG	LEU	conflict	UNP P0DTC2
B	472	ASN	SER	conflict	UNP P0DTC2
B	473	LYS	THR	conflict	UNP P0DTC2
B	479	ALA	GLU	conflict	UNP P0DTC2
B	481	VAL	PHE	conflict	UNP P0DTC2
B	493	ARG	GLN	conflict	UNP P0DTC2
B	496	TYR	ASN	conflict	UNP P0DTC2
B	500	HIS	TYR	conflict	UNP P0DTC2
B	609	GLY	ASP	conflict	UNP P0DTC2
B	650	TYR	HIS	conflict	UNP P0DTC2
B	674	LYS	ASN	conflict	UNP P0DTC2
B	676	HIS	PRO	conflict	UNP P0DTC2
B	677	ALA	ARG	conflict	UNP P0DTC2
B	678	GLY	ARG	conflict	UNP P0DTC2
B	759	LYS	ASN	conflict	UNP P0DTC2
B	791	TYR	ASP	conflict	UNP P0DTC2
B	812	PRO	PHE	conflict	UNP P0DTC2
B	887	PRO	ALA	conflict	UNP P0DTC2
B	894	PRO	ALA	conflict	UNP P0DTC2
B	937	PRO	ALA	conflict	UNP P0DTC2
B	949	HIS	GLN	conflict	UNP P0DTC2
B	964	LYS	ASN	conflict	UNP P0DTC2
B	981	PRO	LYS	conflict	UNP P0DTC2
B	982	PRO	VAL	conflict	UNP P0DTC2
B	1207	GLY	TRP	conflict	UNP P0DTC2
B	1208	SER	PRO	conflict	UNP P0DTC2
B	1209	GLY	TRP	conflict	UNP P0DTC2
B	1212	PRO	TRP	conflict	UNP P0DTC2
B	1213	GLU	LEU	conflict	UNP P0DTC2
B	1214	ALA	GLY	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1215	PRO	PHE	conflict	UNP P0DTC2
B	1216	ARG	ILE	conflict	UNP P0DTC2
B	1217	ASP	ALA	conflict	UNP P0DTC2
B	1219	GLN	LEU	conflict	UNP P0DTC2
B	1220	ALA	ILE	conflict	UNP P0DTC2
B	1221	TYR	-	expression tag	UNP P0DTC2
B	1222	VAL	-	expression tag	UNP P0DTC2
B	1223	ARG	-	expression tag	UNP P0DTC2
B	1224	LYS	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	TRP	-	expression tag	UNP P0DTC2
B	1229	VAL	-	expression tag	UNP P0DTC2
B	1230	LEU	-	expression tag	UNP P0DTC2
B	1231	LEU	-	expression tag	UNP P0DTC2
B	1232	SER	-	expression tag	UNP P0DTC2
B	1233	THR	-	expression tag	UNP P0DTC2
B	1234	PHE	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	HIS	-	expression tag	UNP P0DTC2
B	1238	HIS	-	expression tag	UNP P0DTC2
B	1239	HIS	-	expression tag	UNP P0DTC2
B	1240	HIS	-	expression tag	UNP P0DTC2
B	1241	HIS	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
C	-9	MET	-	initiating methionine	UNP P0DTC2
C	-8	ASP	-	expression tag	UNP P0DTC2
C	-7	ALA	-	expression tag	UNP P0DTC2
C	-6	MET	-	expression tag	UNP P0DTC2
C	-5	LYS	-	expression tag	UNP P0DTC2
C	-4	ARG	-	expression tag	UNP P0DTC2
C	-3	GLY	-	expression tag	UNP P0DTC2
C	-2	LEU	-	expression tag	UNP P0DTC2
C	-1	CYS	-	expression tag	UNP P0DTC2
C	0	CYS	-	expression tag	UNP P0DTC2
C	1	VAL	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	5	CYS	-	insertion	UNP P0DTC2
C	6	GLY	-	insertion	UNP P0DTC2
C	7	ALA	-	insertion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	VAL	PRO	conflict	UNP P0DTC2
C	9	PHE	LEU	conflict	UNP P0DTC2
C	12	ALA	-	insertion	UNP P0DTC2
C	19	ILE	THR	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	24	SER	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	137	ASP	GLY	conflict	UNP P0DTC2
C	208	GLY	VAL	conflict	UNP P0DTC2
C	334	ASP	GLY	conflict	UNP P0DTC2
C	366	PHE	SER	conflict	UNP P0DTC2
C	368	PRO	SER	conflict	UNP P0DTC2
C	370	PHE	SER	conflict	UNP P0DTC2
C	371	ALA	THR	conflict	UNP P0DTC2
C	400	ASN	ASP	conflict	UNP P0DTC2
C	403	SER	ARG	conflict	UNP P0DTC2
C	412	ASN	LYS	conflict	UNP P0DTC2
C	435	LYS	ASN	conflict	UNP P0DTC2
C	447	ARG	LEU	conflict	UNP P0DTC2
C	472	ASN	SER	conflict	UNP P0DTC2
C	473	LYS	THR	conflict	UNP P0DTC2
C	479	ALA	GLU	conflict	UNP P0DTC2
C	481	VAL	PHE	conflict	UNP P0DTC2
C	493	ARG	GLN	conflict	UNP P0DTC2
C	496	TYR	ASN	conflict	UNP P0DTC2
C	500	HIS	TYR	conflict	UNP P0DTC2
C	609	GLY	ASP	conflict	UNP P0DTC2
C	650	TYR	HIS	conflict	UNP P0DTC2
C	674	LYS	ASN	conflict	UNP P0DTC2
C	676	HIS	PRO	conflict	UNP P0DTC2
C	677	ALA	ARG	conflict	UNP P0DTC2
C	678	GLY	ARG	conflict	UNP P0DTC2
C	759	LYS	ASN	conflict	UNP P0DTC2
C	791	TYR	ASP	conflict	UNP P0DTC2
C	812	PRO	PHE	conflict	UNP P0DTC2
C	887	PRO	ALA	conflict	UNP P0DTC2
C	894	PRO	ALA	conflict	UNP P0DTC2
C	937	PRO	ALA	conflict	UNP P0DTC2
C	949	HIS	GLN	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	964	LYS	ASN	conflict	UNP P0DTC2
C	981	PRO	LYS	conflict	UNP P0DTC2
C	982	PRO	VAL	conflict	UNP P0DTC2
C	1207	GLY	TRP	conflict	UNP P0DTC2
C	1208	SER	PRO	conflict	UNP P0DTC2
C	1209	GLY	TRP	conflict	UNP P0DTC2
C	1212	PRO	TRP	conflict	UNP P0DTC2
C	1213	GLU	LEU	conflict	UNP P0DTC2
C	1214	ALA	GLY	conflict	UNP P0DTC2
C	1215	PRO	PHE	conflict	UNP P0DTC2
C	1216	ARG	ILE	conflict	UNP P0DTC2
C	1217	ASP	ALA	conflict	UNP P0DTC2
C	1219	GLN	LEU	conflict	UNP P0DTC2
C	1220	ALA	ILE	conflict	UNP P0DTC2
C	1221	TYR	-	expression tag	UNP P0DTC2
C	1222	VAL	-	expression tag	UNP P0DTC2
C	1223	ARG	-	expression tag	UNP P0DTC2
C	1224	LYS	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLU	-	expression tag	UNP P0DTC2
C	1228	TRP	-	expression tag	UNP P0DTC2
C	1229	VAL	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	LEU	-	expression tag	UNP P0DTC2
C	1232	SER	-	expression tag	UNP P0DTC2
C	1233	THR	-	expression tag	UNP P0DTC2
C	1234	PHE	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	HIS	-	expression tag	UNP P0DTC2
C	1238	HIS	-	expression tag	UNP P0DTC2
C	1239	HIS	-	expression tag	UNP P0DTC2
C	1240	HIS	-	expression tag	UNP P0DTC2
C	1241	HIS	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
A	-9	MET	-	initiating methionine	UNP P0DTC2
A	-8	ASP	-	expression tag	UNP P0DTC2
A	-7	ALA	-	expression tag	UNP P0DTC2
A	-6	MET	-	expression tag	UNP P0DTC2
A	-5	LYS	-	expression tag	UNP P0DTC2
A	-4	ARG	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P0DTC2
A	-2	LEU	-	expression tag	UNP P0DTC2
A	-1	CYS	-	expression tag	UNP P0DTC2
A	0	CYS	-	expression tag	UNP P0DTC2
A	1	VAL	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	5	CYS	-	insertion	UNP P0DTC2
A	6	GLY	-	insertion	UNP P0DTC2
A	7	ALA	-	insertion	UNP P0DTC2
A	8	VAL	PRO	conflict	UNP P0DTC2
A	9	PHE	LEU	conflict	UNP P0DTC2
A	12	ALA	-	insertion	UNP P0DTC2
A	19	ILE	THR	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	24	SER	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	137	ASP	GLY	conflict	UNP P0DTC2
A	208	GLY	VAL	conflict	UNP P0DTC2
A	334	ASP	GLY	conflict	UNP P0DTC2
A	366	PHE	SER	conflict	UNP P0DTC2
A	368	PRO	SER	conflict	UNP P0DTC2
A	370	PHE	SER	conflict	UNP P0DTC2
A	371	ALA	THR	conflict	UNP P0DTC2
A	400	ASN	ASP	conflict	UNP P0DTC2
A	403	SER	ARG	conflict	UNP P0DTC2
A	412	ASN	LYS	conflict	UNP P0DTC2
A	435	LYS	ASN	conflict	UNP P0DTC2
A	447	ARG	LEU	conflict	UNP P0DTC2
A	472	ASN	SER	conflict	UNP P0DTC2
A	473	LYS	THR	conflict	UNP P0DTC2
A	479	ALA	GLU	conflict	UNP P0DTC2
A	481	VAL	PHE	conflict	UNP P0DTC2
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	TYR	ASN	conflict	UNP P0DTC2
A	500	HIS	TYR	conflict	UNP P0DTC2
A	609	GLY	ASP	conflict	UNP P0DTC2
A	650	TYR	HIS	conflict	UNP P0DTC2
A	674	LYS	ASN	conflict	UNP P0DTC2
A	676	HIS	PRO	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	ALA	ARG	conflict	UNP P0DTC2
A	678	GLY	ARG	conflict	UNP P0DTC2
A	759	LYS	ASN	conflict	UNP P0DTC2
A	791	TYR	ASP	conflict	UNP P0DTC2
A	812	PRO	PHE	conflict	UNP P0DTC2
A	887	PRO	ALA	conflict	UNP P0DTC2
A	894	PRO	ALA	conflict	UNP P0DTC2
A	937	PRO	ALA	conflict	UNP P0DTC2
A	949	HIS	GLN	conflict	UNP P0DTC2
A	964	LYS	ASN	conflict	UNP P0DTC2
A	981	PRO	LYS	conflict	UNP P0DTC2
A	982	PRO	VAL	conflict	UNP P0DTC2
A	1207	GLY	TRP	conflict	UNP P0DTC2
A	1208	SER	PRO	conflict	UNP P0DTC2
A	1209	GLY	TRP	conflict	UNP P0DTC2
A	1212	PRO	TRP	conflict	UNP P0DTC2
A	1213	GLU	LEU	conflict	UNP P0DTC2
A	1214	ALA	GLY	conflict	UNP P0DTC2
A	1215	PRO	PHE	conflict	UNP P0DTC2
A	1216	ARG	ILE	conflict	UNP P0DTC2
A	1217	ASP	ALA	conflict	UNP P0DTC2
A	1219	GLN	LEU	conflict	UNP P0DTC2
A	1220	ALA	ILE	conflict	UNP P0DTC2
A	1221	TYR	-	expression tag	UNP P0DTC2
A	1222	VAL	-	expression tag	UNP P0DTC2
A	1223	ARG	-	expression tag	UNP P0DTC2
A	1224	LYS	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	TRP	-	expression tag	UNP P0DTC2
A	1229	VAL	-	expression tag	UNP P0DTC2
A	1230	LEU	-	expression tag	UNP P0DTC2
A	1231	LEU	-	expression tag	UNP P0DTC2
A	1232	SER	-	expression tag	UNP P0DTC2
A	1233	THR	-	expression tag	UNP P0DTC2
A	1234	PHE	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	HIS	-	expression tag	UNP P0DTC2
A	1238	HIS	-	expression tag	UNP P0DTC2
A	1239	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanosota-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	129	978	602	168	203	5	0	0
2	F	129	978	602	168	203	5	0	0
2	D	129	978	602	168	203	5	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	H	2	28	16	2	10	0	0
3	J	2	28	16	2	10	0	0
3	K	2	28	16	2	10	0	0
3	L	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0
3	N	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

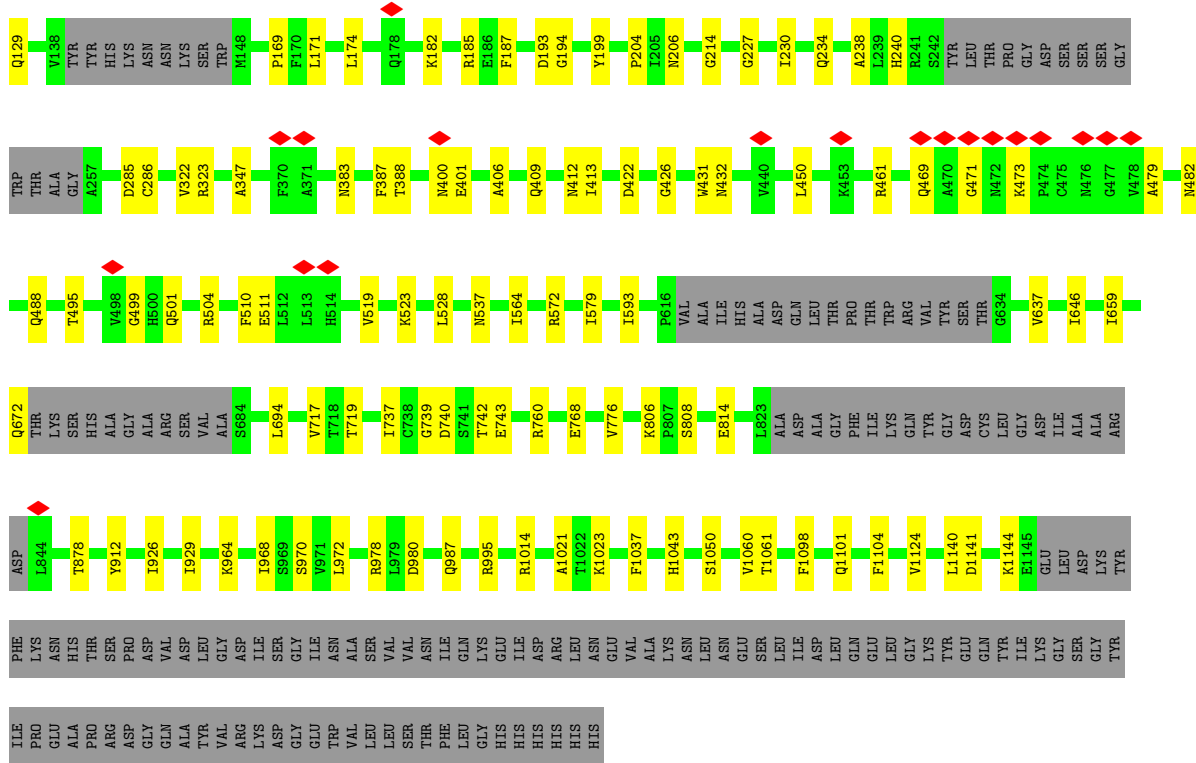


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O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

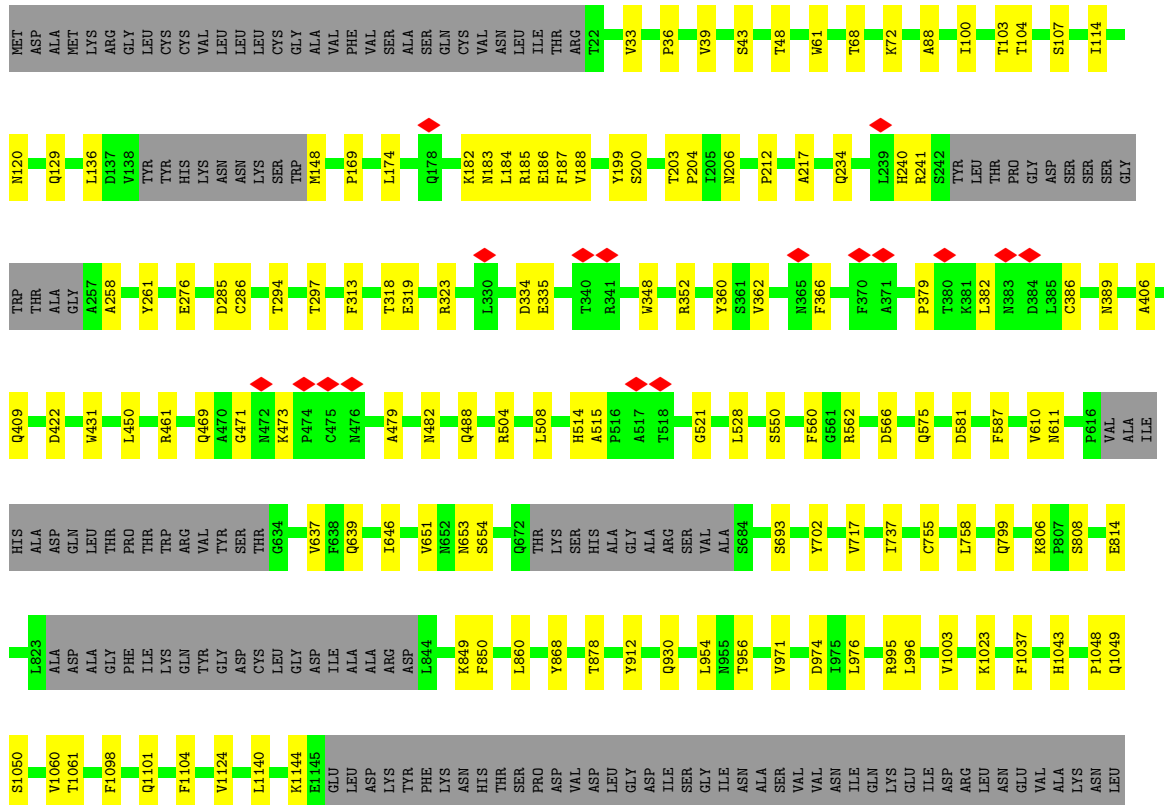
Continued on next page...

Continued from previous page...

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



● Molecule 1: Spike glycoprotein

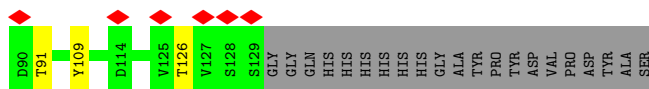
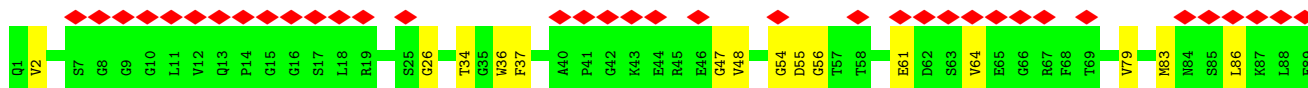


ASN GLU SER LEU ILE ASP LEU GLN GLY LYS TYR GLU GLN ILE LYS GLY SER GLY TYR ILE PRO GLU ALA VAL ARG ARG LYS ASP GLY TRP HIS VAL LEU LEU SER THR PHE LEU GLY HIS HIS HIS HIS THR

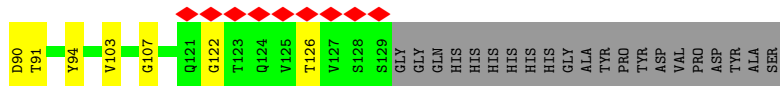
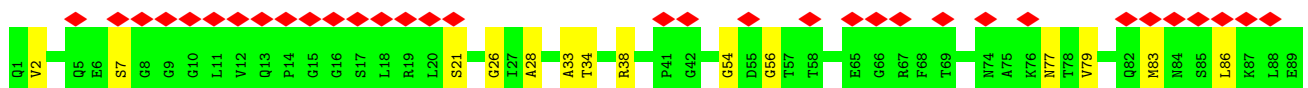
• Molecule 2: Nanosota-9



• Molecule 2: Nanosota-9



• Molecule 2: Nanosota-9



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



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

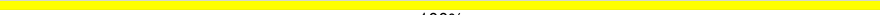


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1
MAG2

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

Chain L:  100%


MAG1
MAG2

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

Chain M:  100%


MAG1
MAG2

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

Chain N:  100%


MAG1
MAG2

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

Chain O:  50% 50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	431183	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 ($e^-/\text{\AA}^2$)	54.8	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.696	Depositor
Minimum map value	-0.293	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0267	Depositor
Map size (\AA)	339.968, 339.968, 339.968	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8853333, 0.8853333, 0.8853333	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

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	0.28	0/8429	0.56	2/11465 (0.0%)
1	B	0.28	0/8429	0.56	1/11465 (0.0%)
1	C	0.28	0/8429	0.59	4/11465 (0.0%)
2	D	0.26	0/998	0.58	0/1353
2	E	0.26	0/998	0.58	0/1353
2	F	0.26	0/998	0.60	0/1353
All	All	0.28	0/28281	0.57	7/38454 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	740	ASP	CB-CG-OD1	7.99	125.49	118.30
1	A	114	ILE	CG1-CB-CG2	-5.95	98.30	111.40
1	C	1141	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	171	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	514	HIS	C-N-CA	5.32	135.01	121.70
1	C	193	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	114	ILE	CG1-CB-CG2	-5.15	100.08	111.40

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	8237	0	8055	77	0
1	B	8237	0	8055	83	0
1	C	8237	0	8051	70	0
2	D	978	0	905	12	0
2	E	978	0	905	14	0
2	F	978	0	905	10	0
3	H	28	0	25	1	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	1	0
3	O	28	0	25	1	0
3	P	28	0	25	0	0
4	A	84	0	78	0	0
4	B	98	0	91	0	0
4	C	98	0	91	1	0
All	All	28149	0	27336	245	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 4.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:LEU:HD13	1:C:488:GLN:OE1	1.40	1.18
1:C:450:LEU:CD1	1:C:488:GLN:OE1	1.96	1.12
1:C:450:LEU:HD13	1:C:488:GLN:CD	1.86	0.96
1:C:450:LEU:HD12	1:C:488:GLN:OE1	1.82	0.80
1:B:488:GLN:NE2	2:E:32:HIS:CE1	2.55	0.74
1:C:450:LEU:HD13	1:C:488:GLN:NE2	2.08	0.68
1:B:488:GLN:HE22	2:E:32:HIS:CE1	2.12	0.68
1:A:450:LEU:HD13	1:A:488:GLN:OE1	1.94	0.67
1:C:719:THR:HG23	1:C:929:ILE:HD11	1.78	0.66
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.79	0.65
1:A:187:PHE:HA	1:A:199:TYR:O	1.98	0.64
1:A:323:ARG:NH2	1:A:575:GLN:OE1	2.32	0.63
1:A:107:SER:HB3	1:A:129:GLN:HG3	1.81	0.63
1:B:324:PHE:O	1:B:575:GLN:NE2	2.33	0.62
1:A:799:GLN:OE1	1:A:930:GLN:NE2	2.32	0.62
1:A:148:MET:SD	1:A:241:ARG:NH2	2.72	0.62
1:B:341:ARG:NH2	1:B:446:TYR:OH	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LYS:HB2	1:B:206:ASN:HD21	1.65	0.61
2:F:83:MET:HB3	2:F:86:LEU:HD21	1.82	0.61
2:E:91:THR:HG23	2:E:126:THR:HA	1.83	0.61
1:B:799:GLN:OE1	1:B:930:GLN:NE2	2.33	0.60
1:B:323:ARG:NH1	1:B:526:THR:O	2.34	0.60
1:C:968:ILE:HD12	1:C:978:ARG:HH21	1.67	0.59
1:B:103:THR:O	1:B:232:ARG:NH1	2.35	0.59
1:A:188:VAL:HB	1:A:199:TYR:HB2	1.85	0.58
2:E:19:ARG:HD2	2:E:80:TYR:HB3	1.85	0.58
1:A:285:ASP:OD1	1:A:286:CYS:N	2.36	0.58
1:B:123:ILE:HD13	1:B:165:TYR:HD2	1.70	0.57
1:B:1023:LYS:NZ	1:B:1037:PHE:O	2.38	0.57
1:B:584:PRO:HG2	1:A:850:PHE:HD2	1.70	0.56
1:C:285:ASP:OD1	1:C:286:CYS:N	2.39	0.56
1:B:36:PRO:HG2	1:B:48:THR:HG21	1.87	0.56
1:B:327:ILE:HG21	1:B:356:CYS:HA	1.88	0.56
1:B:417:ASN:HD21	1:B:448:TYR:HB2	1.71	0.56
1:B:134:PRO:HG3	1:B:236:LEU:HD22	1.88	0.56
1:A:183:ASN:HA	1:A:204:PRO:HA	1.87	0.56
1:B:806:LYS:HD3	1:B:808:SER:H	1.72	0.55
1:A:637:VAL:HG22	1:A:646:ILE:HG12	1.87	0.55
1:A:471:GLY:HA3	1:A:482:ASN:HB3	1.89	0.55
1:C:322:VAL:HA	1:C:537:ASN:HB3	1.88	0.55
1:A:88:ALA:HB3	1:A:261:TYR:HB2	1.89	0.55
1:A:294:THR:HA	1:A:297:THR:HG22	1.88	0.55
1:A:1140:LEU:HD22	1:A:1144:LYS:HE3	1.88	0.55
1:C:1043:HIS:HA	1:C:1061:THR:HG22	1.88	0.54
1:A:36:PRO:HG2	1:A:48:THR:HG21	1.88	0.54
1:B:447:ARG:HB3	1:B:487:LEU:HD12	1.89	0.54
1:B:737:ILE:O	1:B:995:ARG:NH1	2.38	0.54
1:A:806:LYS:HD3	1:A:808:SER:H	1.72	0.54
1:C:1098:PHE:HZ	4:C:1305:NAG:H61	1.71	0.54
1:B:1098:PHE:HZ	3:H:1:NAG:H61	1.72	0.54
1:C:806:LYS:HD3	1:C:808:SER:H	1.72	0.54
1:B:469:GLN:NE2	1:B:473:LYS:O	2.36	0.54
1:A:352:ARG:NH1	1:A:389:ASN:OD1	2.41	0.54
1:B:637:VAL:HG22	1:B:646:ILE:HG12	1.89	0.53
1:B:134:PRO:HG2	1:B:239:LEU:HD12	1.89	0.53
1:A:737:ILE:O	1:A:995:ARG:NH1	2.39	0.53
2:D:33:ALA:HB3	2:D:103:VAL:HG12	1.91	0.53
1:B:88:ALA:HB3	1:B:261:TYR:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1140:LEU:HD22	1:B:1144:LYS:HE3	1.91	0.53
1:C:1101:GLN:HE21	1:C:1104:PHE:HB3	1.73	0.53
1:A:379:PRO:HA	1:A:382:LEU:HD12	1.90	0.53
1:A:431:TRP:HE3	1:A:504:ARG:HD2	1.72	0.53
1:A:717:VAL:HG22	1:A:1060:VAL:HG22	1.92	0.52
2:D:2:VAL:HG22	2:D:26:GLY:HA3	1.90	0.52
2:E:7:SER:OG	2:E:21:SER:OG	2.26	0.52
2:E:40:ALA:HB3	2:E:43:LYS:HE3	1.90	0.52
1:B:452:ARG:NH1	1:B:454:SER:O	2.41	0.52
1:A:758:LEU:HG	1:A:1003:VAL:HG21	1.92	0.52
1:A:611:ASN:HA	1:A:639:GLN:HE22	1.74	0.52
1:C:383:ASN:O	1:C:523:LYS:NZ	2.37	0.52
1:A:1043:HIS:HA	1:A:1061:THR:HG22	1.92	0.52
1:C:431:TRP:HE3	1:C:504:ARG:HD2	1.75	0.51
1:C:432:ASN:ND2	1:C:501:GLN:OE1	2.43	0.51
1:A:849:LYS:HE3	1:A:954:LEU:HD13	1.91	0.51
2:F:91:THR:HG23	2:F:126:THR:HA	1.92	0.51
1:C:121:VAL:HG13	1:C:169:PRO:HA	1.91	0.51
1:C:323:ARG:HH21	1:C:528:LEU:HB2	1.74	0.51
2:E:13:GLN:HG2	2:D:107:GLY:H	1.75	0.51
1:B:428:VAL:HG12	1:B:507:VAL:HG12	1.91	0.51
1:B:1101:GLN:HE21	1:B:1104:PHE:HB3	1.76	0.51
1:C:1023:LYS:NZ	1:C:1037:PHE:O	2.40	0.51
2:E:94:TYR:O	2:E:122:GLY:HA2	2.11	0.51
1:B:73:ARG:NH1	1:B:239:LEU:O	2.44	0.51
1:A:103:THR:HG23	1:A:104:THR:HG23	1.92	0.51
1:B:103:THR:HA	1:B:231:THR:H	1.76	0.50
1:B:912:TYR:HB3	1:C:1124:VAL:HG13	1.93	0.50
2:D:91:THR:HG23	2:D:126:THR:HA	1.93	0.50
1:A:174:LEU:HD13	1:A:204:PRO:HG3	1.93	0.50
2:F:2:VAL:HG22	2:F:26:GLY:HA3	1.93	0.50
1:A:1101:GLN:HE21	1:A:1104:PHE:HB3	1.76	0.50
2:F:37:PHE:HA	2:F:47:GLY:HA2	1.93	0.50
1:B:152:PHE:O	1:B:153:ARG:NE	2.37	0.50
1:C:471:GLY:HA3	1:C:482:ASN:HB3	1.93	0.50
1:A:136:LEU:HA	1:A:240:HIS:HA	1.94	0.50
1:C:92:LYS:HB2	1:C:182:LYS:HE2	1.94	0.49
1:C:814:GLU:OE1	1:C:1050:SER:OG	2.30	0.49
1:B:717:VAL:HG22	1:B:1060:VAL:HG22	1.95	0.49
1:C:717:VAL:HG22	1:C:1060:VAL:HG22	1.94	0.49
1:B:488:GLN:OE1	2:E:32:HIS:HE1	1.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ASN:N	1:C:120:ASN:O	2.44	0.49
1:C:1140:LEU:HD22	1:C:1144:LYS:HE3	1.94	0.49
1:A:313:PHE:HZ	1:A:610:VAL:HG11	1.77	0.49
2:E:34:THR:HG21	2:E:79:VAL:HG11	1.94	0.49
1:B:492:PHE:CE2	1:B:502:PRO:HB3	2.48	0.48
1:A:182:LYS:HB2	1:A:206:ASN:HD21	1.78	0.48
1:B:430:ALA:HA	1:B:504:ARG:O	2.12	0.48
1:B:456:LEU:HD12	1:B:460:GLU:HB2	1.94	0.48
1:A:61:TRP:HB3	1:A:258:ALA:HB3	1.95	0.48
1:A:479:ALA:HB1	2:D:26:GLY:HA2	1.95	0.48
1:A:651:VAL:HG12	1:A:653:ASN:H	1.77	0.48
1:B:739:GLY:H	1:B:972:LEU:HD12	1.79	0.48
1:C:768:GLU:OE2	1:C:1014:ARG:NE	2.41	0.48
1:C:760:ARG:HH22	1:A:956:THR:HG21	1.78	0.48
1:A:422:ASP:OD1	1:A:422:ASP:N	2.44	0.48
2:D:34:THR:HG21	2:D:79:VAL:HG11	1.96	0.48
1:A:186:GLU:O	1:A:200:SER:HA	2.13	0.48
1:A:1023:LYS:NZ	1:A:1037:PHE:O	2.46	0.48
2:F:34:THR:HG21	2:F:79:VAL:HG11	1.96	0.48
1:B:754:PHE:HD2	1:B:996:LEU:HD21	1.78	0.48
1:A:323:ARG:HD2	1:A:528:LEU:HB2	1.96	0.47
1:A:406:ALA:HB3	1:A:409:GLN:HG3	1.95	0.47
1:B:187:PHE:HA	1:B:199:TYR:O	2.14	0.47
1:B:814:GLU:OE1	1:B:1050:SER:OG	2.32	0.47
1:C:980:ASP:OD1	1:C:980:ASP:N	2.43	0.47
1:A:562:ARG:NH1	1:A:566:ASP:OD1	2.47	0.47
1:B:657:CYS:HB2	1:B:692:MET:HG2	1.97	0.47
1:C:739:GLY:H	1:C:972:LEU:HD12	1.80	0.47
1:B:50:ASP:OD1	1:B:51:LEU:N	2.47	0.46
1:B:371:ALA:HB3	1:B:430:ALA:H	1.79	0.46
1:B:495:THR:HB	2:E:109:TYR:HB2	1.96	0.46
1:A:386:CYS:HB3	1:A:521:GLY:H	1.79	0.46
1:B:702:TYR:HB2	1:A:878:THR:HG23	1.96	0.46
1:C:737:ILE:O	1:C:995:ARG:NH1	2.43	0.46
1:A:318:THR:OG1	1:A:319:GLU:OE1	2.23	0.46
1:B:488:GLN:CD	2:E:32:HIS:CE1	2.89	0.46
1:B:980:ASP:OD1	1:B:980:ASP:N	2.42	0.46
1:C:101:PHE:HB3	1:C:230:ILE:HD12	1.97	0.46
1:A:323:ARG:HH21	1:A:575:GLN:HB2	1.80	0.46
1:C:95:ILE:HG23	1:C:238:ALA:HB3	1.96	0.46
1:A:323:ARG:HH11	1:A:528:LEU:HB2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:ILE:HG23	1:C:659:ILE:HG21	1.97	0.46
1:A:814:GLU:OE1	1:A:1050:SER:OG	2.33	0.46
1:C:964:LYS:HG3	1:C:970:SER:HB3	1.98	0.46
1:C:968:ILE:HG23	1:C:987:GLN:HE21	1.81	0.46
1:A:362:VAL:HG22	1:A:366:PHE:HE1	1.79	0.46
1:C:401:GLU:HG2	1:C:413:ILE:HG21	1.97	0.46
2:D:38:ARG:NH1	2:D:90:ASP:OD1	2.49	0.45
1:A:1098:PHE:HZ	3:O:1:NAG:H61	1.81	0.45
1:B:34:TYR:HB3	1:B:218:LEU:HD12	1.99	0.45
1:C:182:LYS:HB2	1:C:206:ASN:HD21	1.81	0.45
1:C:73:ARG:NH2	1:C:240:HIS:O	2.50	0.45
1:C:406:ALA:HB3	1:C:409:GLN:HG3	1.99	0.45
2:F:36:TRP:O	2:F:48:VAL:N	2.48	0.45
1:B:302:THR:HA	1:B:597:THR:HG21	1.98	0.45
1:C:39:VAL:HG12	1:A:560:PHE:HB2	1.98	0.45
1:A:971:VAL:HB	1:A:974:ASP:HB2	1.98	0.45
1:B:413:ILE:HA	1:B:417:ASN:HB2	1.98	0.44
1:C:479:ALA:HB1	2:F:26:GLY:HA2	1.98	0.44
1:B:449:ARG:HH21	1:B:452:ARG:HG3	1.82	0.44
1:A:43:SER:HB3	1:A:276:GLU:HA	1.98	0.44
1:A:799:GLN:HE21	3:N:1:NAG:H62	1.82	0.44
1:A:100:ILE:HD11	1:A:234:GLN:HB3	1.98	0.44
1:C:742:THR:OG1	1:C:743:GLU:OE1	2.35	0.44
1:B:92:LYS:HE3	1:B:182:LYS:HG2	2.00	0.44
1:C:572:ARG:HE	1:C:579:ILE:HD11	1.81	0.44
1:B:207:LEU:HB3	1:B:208:GLY:H	1.74	0.44
1:C:22:THR:O	1:C:23:GLN:NE2	2.50	0.44
1:A:348:TRP:O	1:A:461:ARG:NH2	2.45	0.43
1:B:560:PHE:HB2	1:A:39:VAL:HG12	2.01	0.43
1:C:422:ASP:OD1	1:C:422:ASP:N	2.46	0.43
1:A:184:LEU:HD22	1:A:206:ASN:HB3	2.00	0.43
1:A:1048:PRO:O	1:A:1049:GLN:NE2	2.51	0.43
2:D:28:ALA:HA	2:D:77:ASN:HD21	1.82	0.43
1:B:572:ARG:HH21	1:B:577:LEU:HD12	1.82	0.43
1:B:95:ILE:HG22	1:B:237:LEU:HD12	1.99	0.43
1:B:442:GLY:HA3	1:B:493:ARG:HH11	1.82	0.43
1:A:120:ASN:HA	1:A:169:PRO:HD3	1.99	0.43
1:B:404:GLN:HE22	1:B:413:ILE:HD13	1.83	0.43
1:B:694:LEU:HB3	1:A:868:TYR:HE1	1.82	0.43
1:C:76:ASN:HB3	1:C:234:GLN:NE2	2.34	0.43
1:B:412:ASN:HD22	1:B:450:LEU:HG	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:ASN:N	1:C:499:GLY:O	2.51	0.43
1:C:878:THR:HG23	1:A:702:TYR:HB2	1.99	0.43
1:A:737:ILE:HD13	1:A:996:LEU:HD22	2.00	0.43
1:B:360:TYR:HA	1:B:363:LEU:HD13	2.00	0.43
1:B:1043:HIS:HA	1:B:1061:THR:HG22	2.00	0.43
1:B:95:ILE:HG23	1:B:238:ALA:HB3	2.01	0.43
1:B:177:LYS:HG3	1:B:178:GLN:HG2	2.01	0.43
1:A:550:SER:HB3	1:A:581:ASP:HB2	2.01	0.43
1:C:637:VAL:HG22	1:C:646:ILE:HG12	2.01	0.42
1:C:672:GLN:OE1	1:C:672:GLN:N	2.51	0.42
1:C:776:VAL:HG22	1:C:1021:ALA:HB2	2.01	0.42
1:C:388:THR:OG1	1:C:511:GLU:OE2	2.31	0.42
1:B:104:THR:O	1:B:232:ARG:NH2	2.53	0.42
1:B:488:GLN:NE2	2:E:32:HIS:NE2	2.56	0.42
1:B:981:PRO:HA	1:B:984:ALA:HB3	2.01	0.42
1:C:107:SER:HB3	1:C:129:GLN:HG3	2.02	0.42
1:B:186:GLU:O	1:B:200:SER:HA	2.19	0.42
1:C:194:GLY:HA2	1:C:227:GLY:HA2	2.01	0.42
1:B:127:GLU:HB3	1:B:159:ASN:HB2	2.01	0.42
1:C:387:PHE:N	1:C:519:VAL:O	2.40	0.42
1:B:1124:VAL:HG13	1:A:912:TYR:HB3	2.02	0.42
1:C:69:ASN:OD1	1:C:70:GLY:N	2.52	0.42
1:A:654:SER:HB3	1:A:693:SER:HB2	2.02	0.42
1:B:926:ILE:HA	1:B:929:ILE:HG22	2.02	0.41
1:A:206:ASN:HA	1:A:212:PRO:HG3	2.02	0.41
1:A:33:VAL:HG23	1:A:217:ALA:HA	2.03	0.41
1:B:282:ASP:OD1	1:B:283:ALA:N	2.52	0.41
1:B:868:TYR:HE1	1:C:694:LEU:HB3	1.84	0.41
1:A:360:TYR:HE2	1:A:508:LEU:HD13	1.84	0.41
2:F:61:GLU:HB2	2:F:64:VAL:HG22	2.02	0.41
1:B:654:SER:HB3	1:B:693:SER:HB2	2.01	0.41
1:C:187:PHE:HA	1:C:199:TYR:O	2.21	0.41
2:E:54:GLY:O	2:E:56:GLY:N	2.54	0.41
2:D:7:SER:OG	2:D:21:SER:OG	2.28	0.41
1:C:82:ASN:O	1:C:82:ASN:ND2	2.48	0.41
1:A:72:LYS:HD3	1:A:72:LYS:HA	1.82	0.41
1:B:69:ASN:OD1	1:B:70:GLY:N	2.53	0.41
1:C:30:THR:OG1	1:C:214:GLY:O	2.38	0.41
1:C:174:LEU:HD13	1:C:204:PRO:HG3	2.02	0.41
1:C:347:ALA:HA	1:C:461:ARG:HD3	2.03	0.41
1:C:469:GLN:NE2	1:C:473:LYS:O	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:926:ILE:HA	1:C:929:ILE:HG22	2.03	0.41
1:A:203:THR:HA	1:A:204:PRO:HD3	1.77	0.41
2:D:54:GLY:O	2:D:56:GLY:N	2.54	0.41
1:B:323:ARG:NE	1:B:575:GLN:OE1	2.53	0.41
1:B:528:LEU:HD23	1:B:528:LEU:HA	1.97	0.41
1:C:495:THR:HG21	2:F:109:TYR:HB2	2.03	0.40
1:A:334:ASP:OD1	1:A:335:GLU:N	2.54	0.40
1:A:755:CYS:HA	1:A:758:LEU:HB2	2.04	0.40
2:F:54:GLY:O	2:F:56:GLY:N	2.54	0.40
1:B:322:VAL:HG22	1:B:537:ASN:HB3	2.02	0.40
1:B:719:THR:HG23	1:B:929:ILE:HD11	2.03	0.40
1:B:797:PHE:HD1	1:B:800:ILE:HD11	1.87	0.40
1:A:976:LEU:HD23	1:A:976:LEU:HA	1.91	0.40
1:B:54:PRO:HG3	1:B:268:ARG:HD2	2.03	0.40
1:B:224:LEU:HA	1:B:225:PRO:HD3	1.92	0.40
1:C:912:TYR:HB3	1:A:1124:VAL:HG13	2.03	0.40
1:A:469:GLN:NE2	1:A:473:LYS:O	2.49	0.40
1:A:860:LEU:HD23	1:A:860:LEU:HA	1.91	0.40
2:D:94:TYR:O	2:D:122:GLY:HA2	2.22	0.40
1:B:635:SER:OG	1:B:636:ASN:N	2.54	0.40
1:C:185:ARG:HB3	1:C:187:PHE:CE2	2.57	0.40
1:C:426:GLY:HA2	1:C:510:PHE:CD2	2.57	0.40
1:C:564:ILE:HD12	1:C:564:ILE:H	1.86	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	1041/1252 (83%)	986 (95%)	52 (5%)	3 (0%)	37 69
1	B	1041/1252 (83%)	984 (94%)	55 (5%)	2 (0%)	44 76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1041/1252 (83%)	982 (94%)	59 (6%)	0	100	100
2	D	127/150 (85%)	120 (94%)	7 (6%)	0	100	100
2	E	127/150 (85%)	121 (95%)	6 (5%)	0	100	100
2	F	127/150 (85%)	116 (91%)	10 (8%)	1 (1%)	16	49
All	All	3504/4206 (83%)	3309 (94%)	189 (5%)	6 (0%)	45	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	439	LYS
1	A	515	ALA
1	A	587	PHE
2	F	55	ASP
1	B	498	VAL
1	A	68	THR

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	921/1086 (85%)	920 (100%)	1 (0%)	92	97
1	B	921/1086 (85%)	920 (100%)	1 (0%)	92	97
1	C	921/1086 (85%)	919 (100%)	2 (0%)	92	97
2	D	104/120 (87%)	104 (100%)	0	100	100
2	E	104/120 (87%)	104 (100%)	0	100	100
2	F	104/120 (87%)	104 (100%)	0	100	100
All	All	3075/3618 (85%)	3071 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	232	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	82	ASN
1	C	412	ASN
1	A	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	82	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

16 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
3	NAG	H	1	3,1	14,14,15	0.70	0	17,19,21	1.00	1 (5%)
3	NAG	H	2	3	14,14,15	0.70	0	17,19,21	0.85	1 (5%)
3	NAG	J	1	3,1	14,14,15	0.80	1 (7%)	17,19,21	1.41	3 (17%)
3	NAG	J	2	3	14,14,15	0.69	0	17,19,21	0.90	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.81	1 (7%)	17,19,21	1.43	2 (11%)
3	NAG	K	2	3	14,14,15	0.67	0	17,19,21	0.91	0
3	NAG	L	1	3,1	14,14,15	0.78	0	17,19,21	2.25	5 (29%)
3	NAG	L	2	3	14,14,15	0.73	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	M	1	3,1	14,14,15	0.74	0	17,19,21	0.92	0
3	NAG	M	2	3	14,14,15	0.71	0	17,19,21	0.88	0
3	NAG	N	1	3,1	14,14,15	0.71	0	17,19,21	0.90	0
3	NAG	N	2	3	14,14,15	0.66	0	17,19,21	0.87	1 (5%)
3	NAG	O	1	3,1	14,14,15	0.68	0	17,19,21	1.12	2 (11%)
3	NAG	O	2	3	14,14,15	0.72	0	17,19,21	0.89	1 (5%)
3	NAG	P	1	3,1	14,14,15	0.75	0	17,19,21	1.69	3 (17%)
3	NAG	P	2	3	14,14,15	0.73	0	17,19,21	0.98	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	C1-C2	2.21	1.55	1.52
3	K	1	NAG	C1-C2	2.21	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	C1-O5-C5	5.45	119.48	112.19
3	P	1	NAG	C2-N2-C7	4.69	129.18	122.90
3	L	1	NAG	C2-N2-C7	4.40	128.80	122.90
3	L	1	NAG	O5-C1-C2	-3.66	105.63	111.29
3	J	1	NAG	C1-O5-C5	3.28	116.58	112.19
3	K	1	NAG	C1-O5-C5	3.21	116.49	112.19
3	L	1	NAG	O7-C7-N2	2.69	126.73	121.98
3	L	1	NAG	O4-C4-C3	-2.63	104.19	110.38
3	P	2	NAG	C1-O5-C5	2.56	115.61	112.19
3	O	1	NAG	C1-O5-C5	2.54	115.60	112.19
3	J	1	NAG	O5-C1-C2	-2.48	107.45	111.29
3	J	1	NAG	C1-C2-N2	2.42	114.24	110.43
3	O	1	NAG	O5-C1-C2	-2.39	107.60	111.29
3	L	2	NAG	O5-C1-C2	-2.33	107.69	111.29
3	P	1	NAG	O5-C1-C2	-2.24	107.83	111.29
3	O	2	NAG	O5-C1-C2	-2.17	107.94	111.29
3	J	2	NAG	C1-O5-C5	2.13	115.04	112.19
3	K	1	NAG	O5-C1-C2	-2.13	108.00	111.29
3	N	2	NAG	O5-C1-C2	-2.11	108.02	111.29
3	H	1	NAG	C1-O5-C5	2.09	114.98	112.19
3	P	1	NAG	O7-C7-N2	2.09	125.67	121.98
3	H	2	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

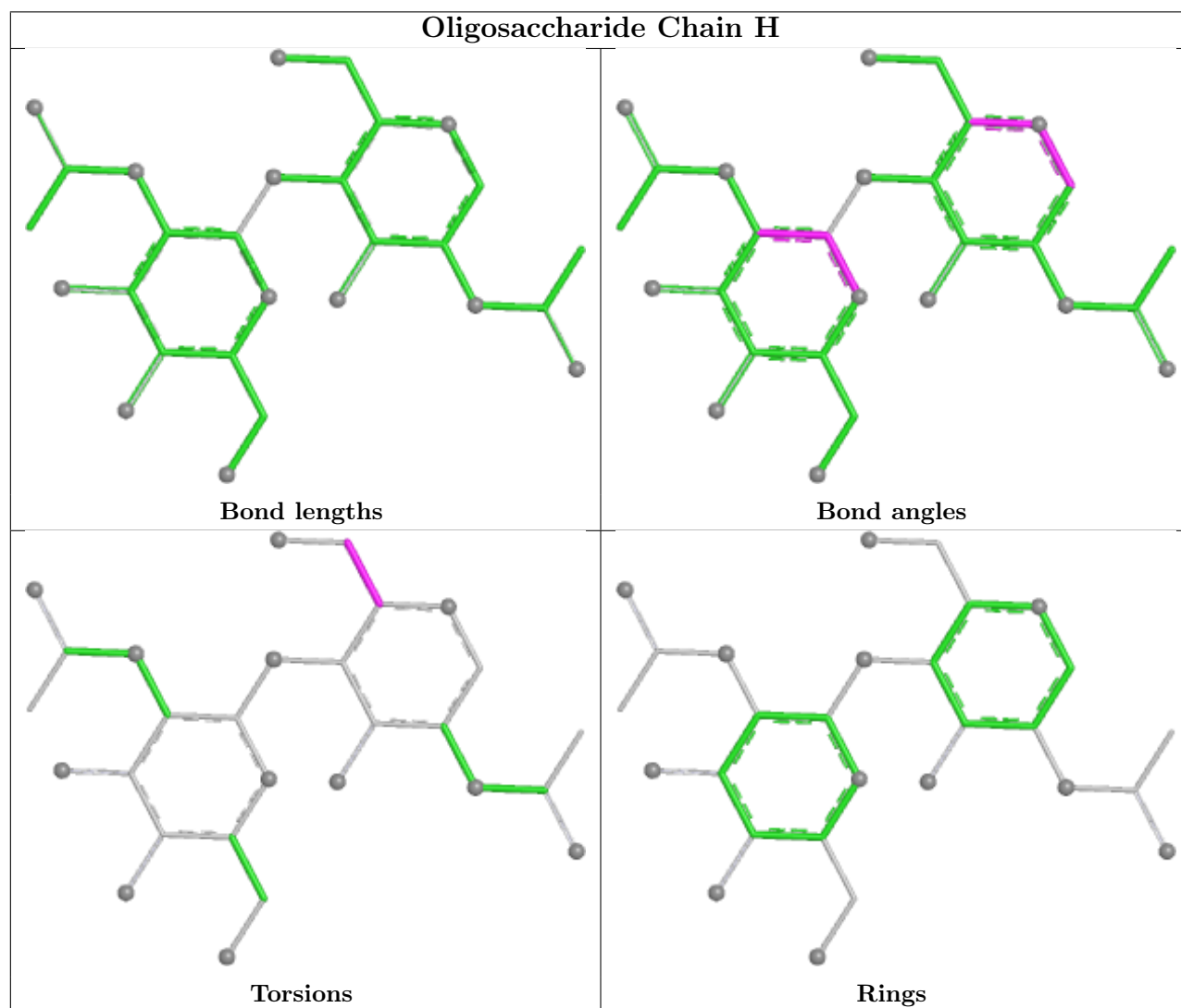
Mol	Chain	Res	Type	Atoms
3	O	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	L	1	NAG	C1-C2-N2-C7
3	P	1	NAG	C1-C2-N2-C7

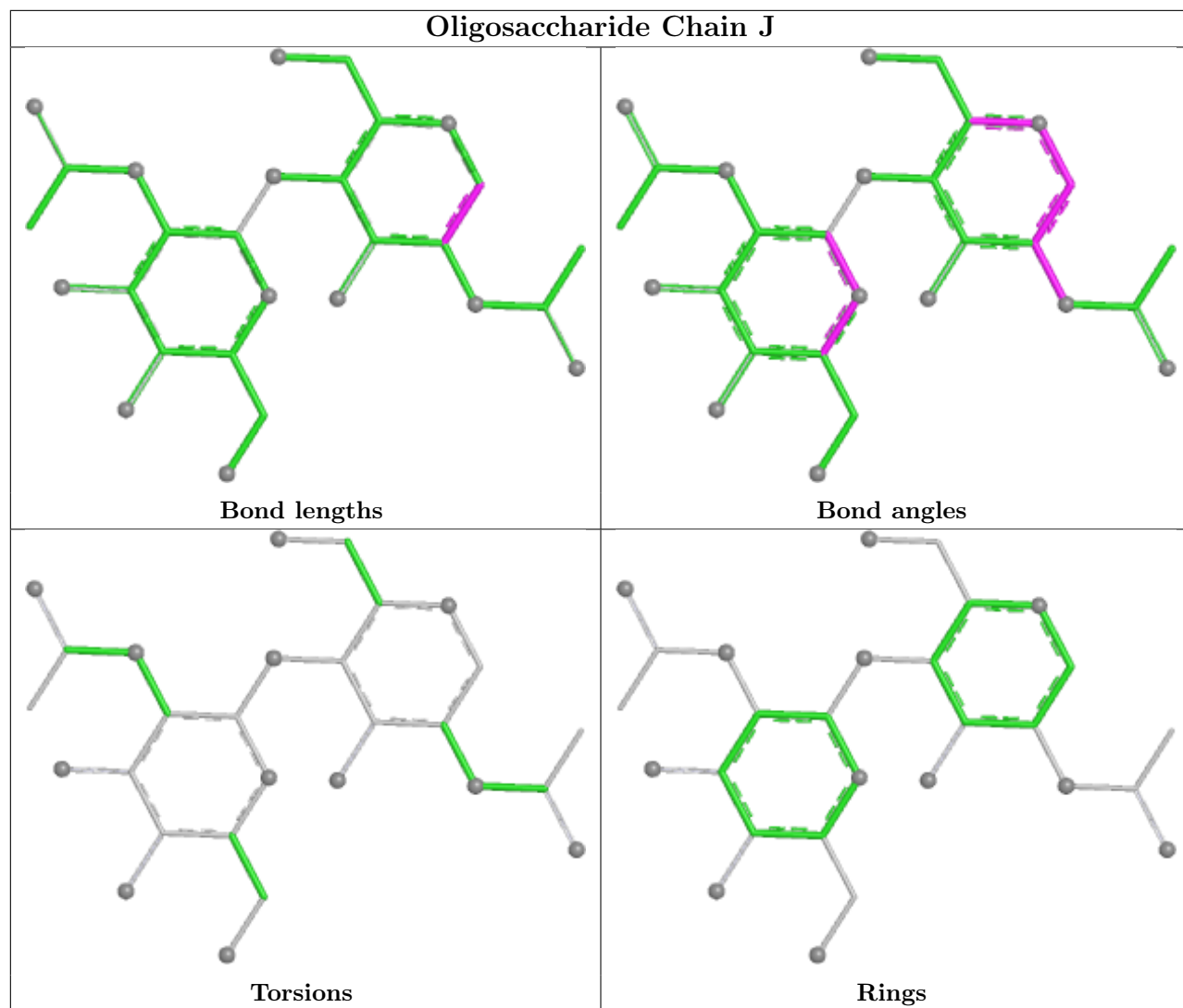
There are no ring outliers.

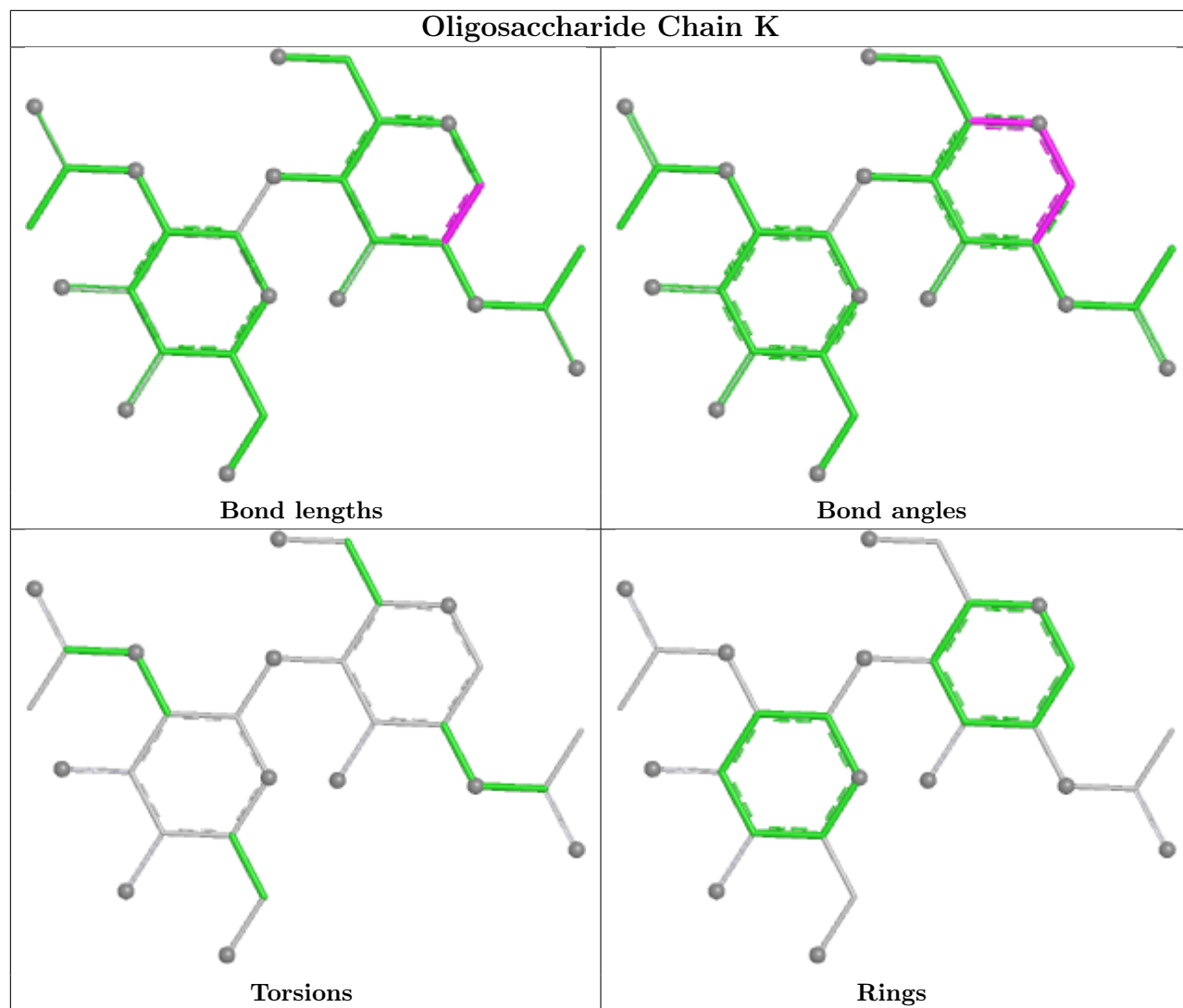
3 monomers are involved in 3 short contacts:

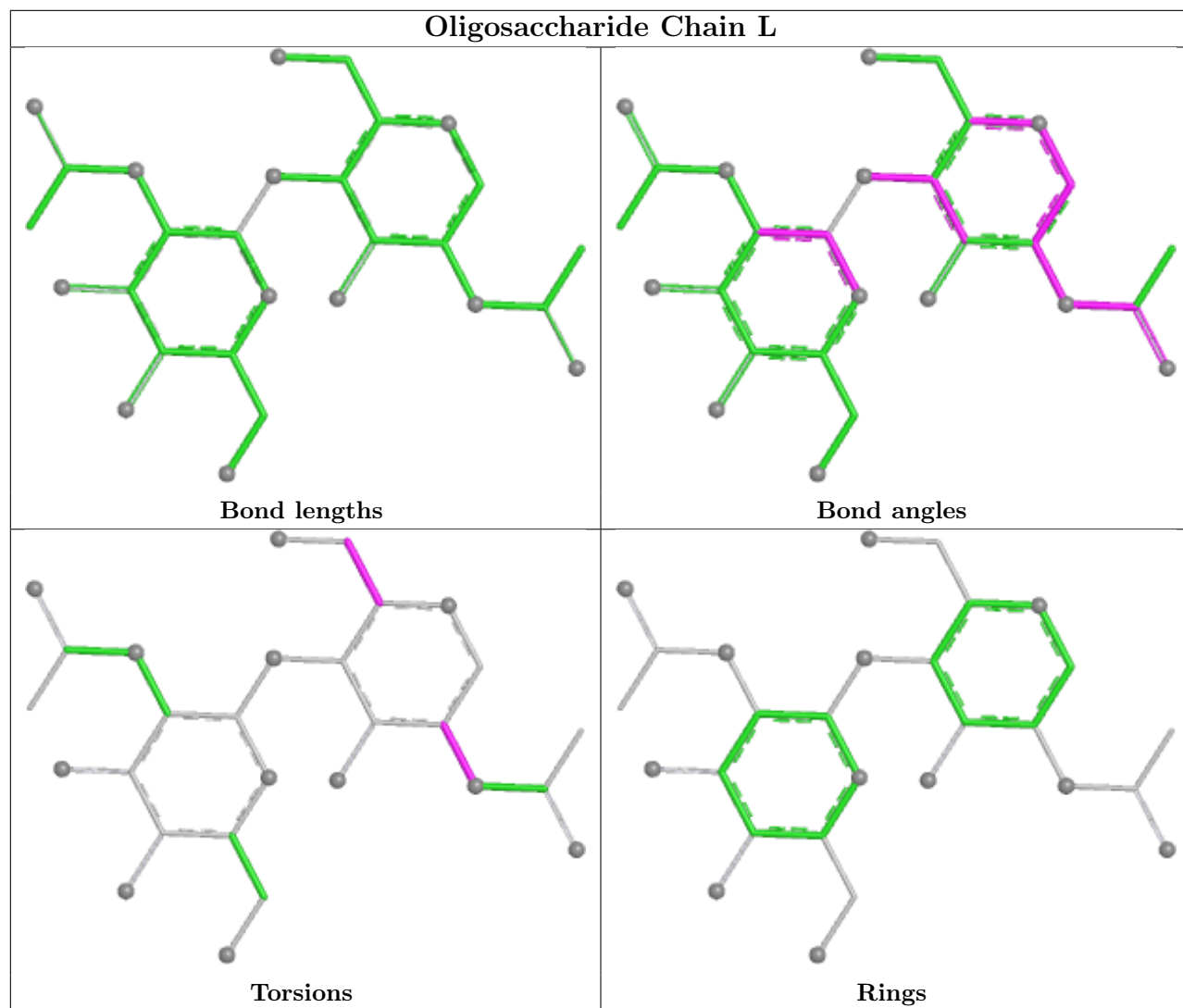
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	1	0
3	O	1	NAG	1	0
3	H	1	NAG	1	0

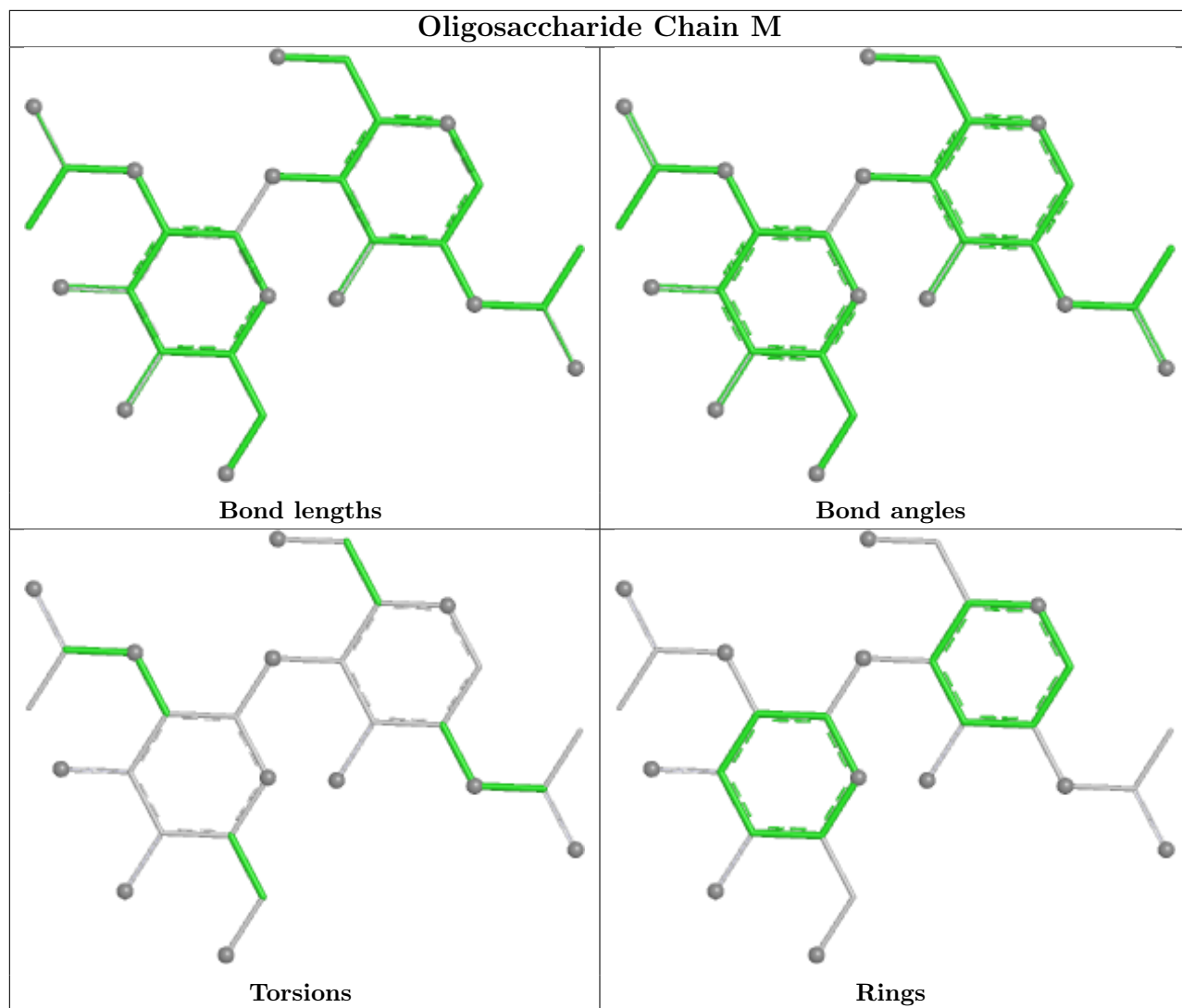
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

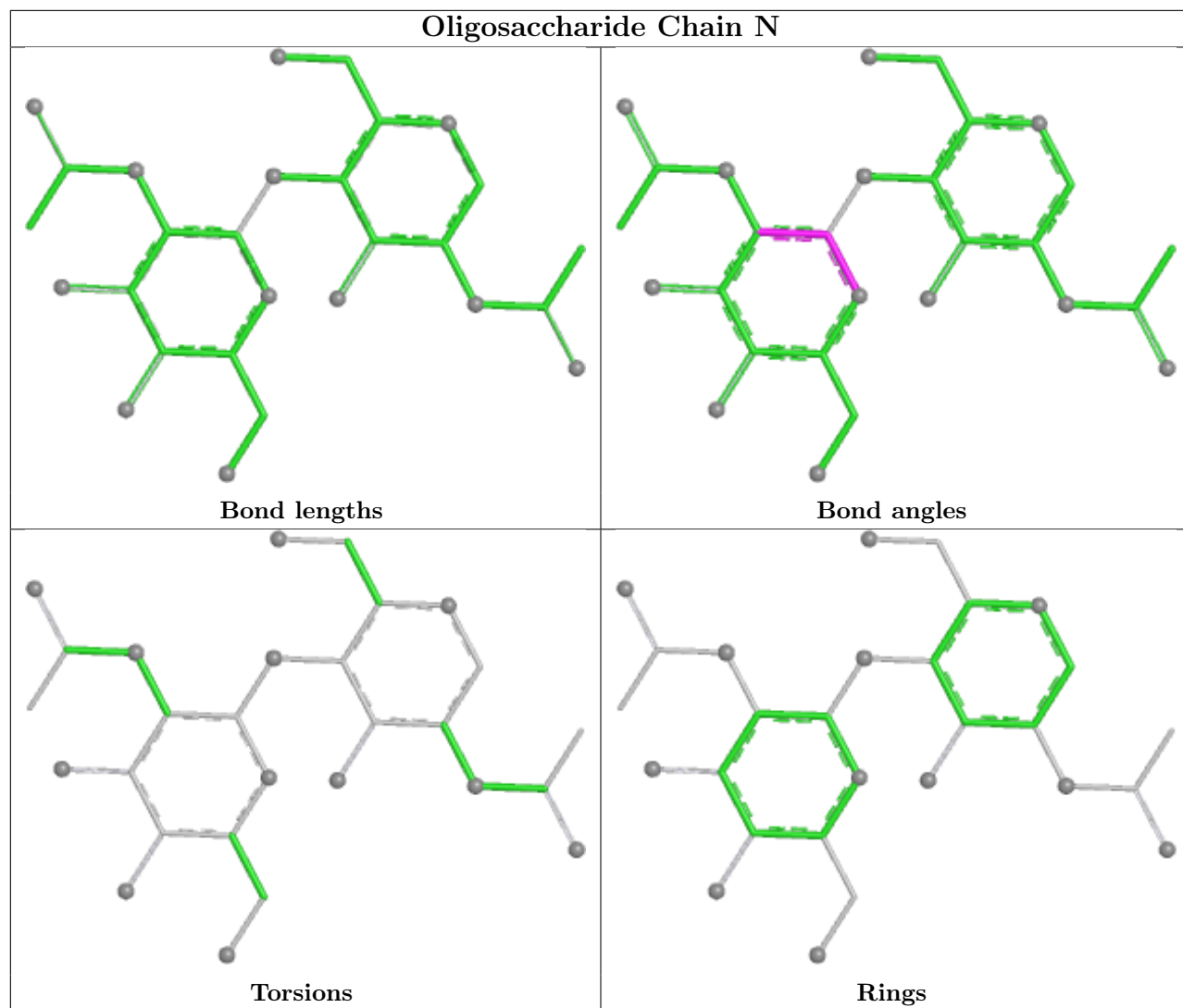


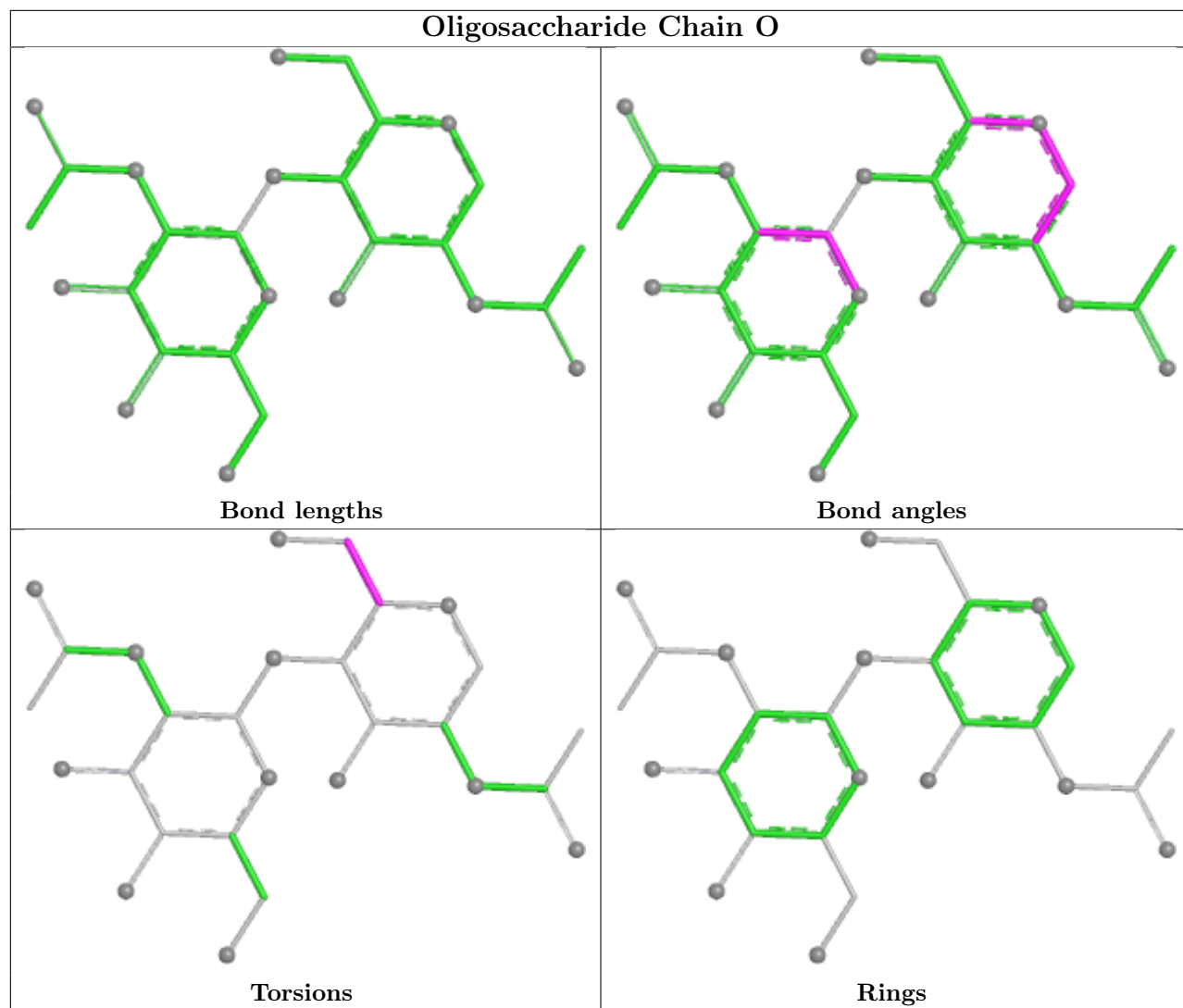


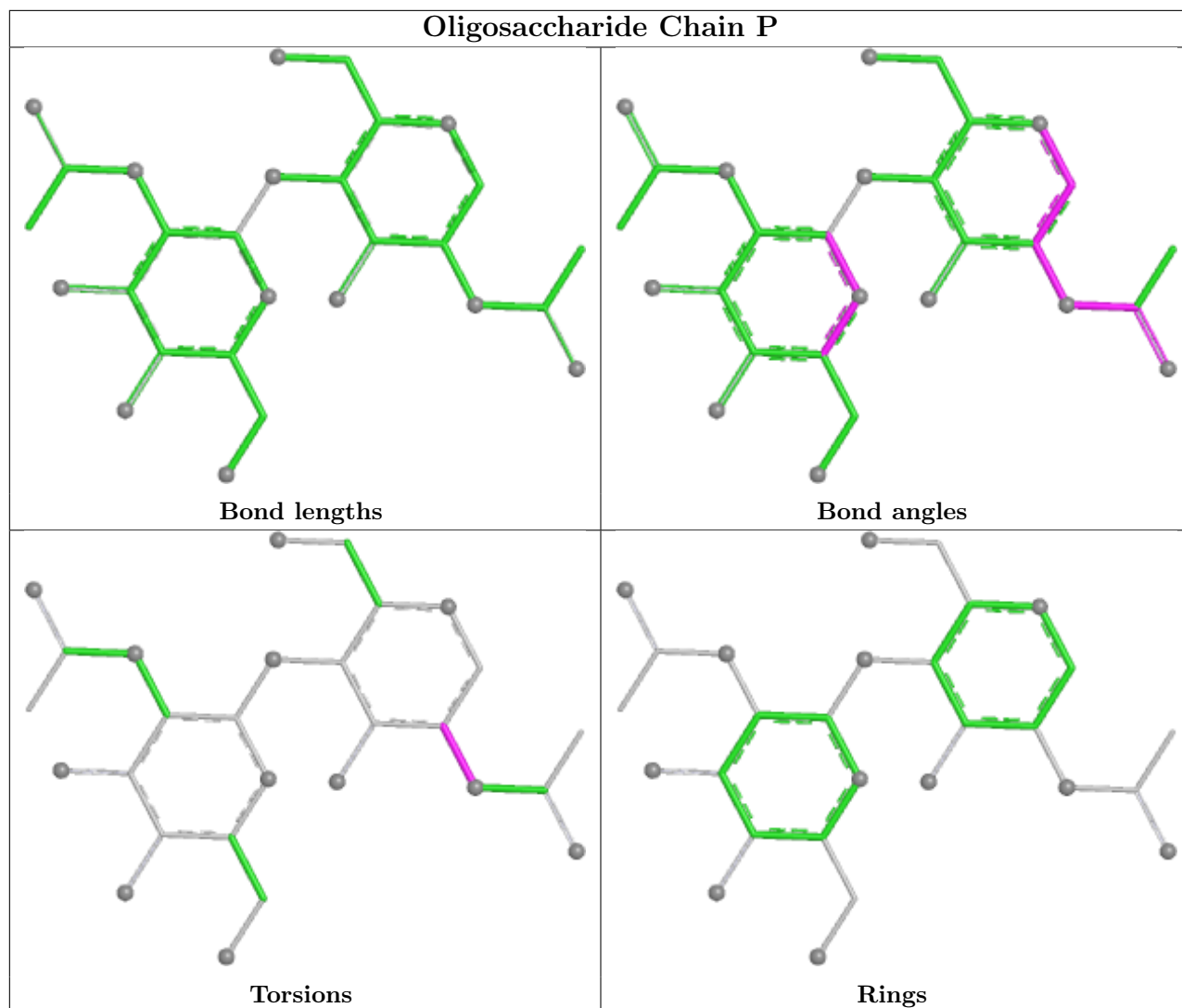












5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1305	1	14,14,15	0.62	0	17,19,21	1.62	2 (11%)
4	NAG	C	1302	1	14,14,15	0.76	0	17,19,21	1.56	2 (11%)
4	NAG	B	1302	1	14,14,15	0.74	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1301	1	14,14,15	0.72	0	17,19,21	1.24	1 (5%)
4	NAG	B	1304	1	14,14,15	0.75	1 (7%)	17,19,21	2.31	3 (17%)
4	NAG	A	1304	1	14,14,15	0.83	1 (7%)	17,19,21	1.17	1 (5%)
4	NAG	A	1302	1	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
4	NAG	C	1300	1	14,14,15	0.97	1 (7%)	17,19,21	2.19	7 (41%)
4	NAG	C	1303	1	14,14,15	0.76	0	17,19,21	1.11	1 (5%)
4	NAG	B	1300	1	14,14,15	0.70	0	17,19,21	1.62	3 (17%)
4	NAG	A	1300	1	14,14,15	0.74	0	17,19,21	1.46	4 (23%)
4	NAG	C	1301	1	14,14,15	0.72	0	17,19,21	1.01	2 (11%)
4	NAG	B	1303	1	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
4	NAG	C	1304	1	14,14,15	0.85	1 (7%)	17,19,21	1.03	1 (5%)
4	NAG	C	1306	1	14,14,15	0.83	0	17,19,21	1.85	4 (23%)
4	NAG	A	1303	1	14,14,15	0.81	1 (7%)	17,19,21	2.05	4 (23%)
4	NAG	B	1306	1	14,14,15	0.64	0	17,19,21	1.24	1 (5%)
4	NAG	A	1301	1	14,14,15	0.70	0	17,19,21	0.85	1 (5%)
4	NAG	B	1305	1	14,14,15	0.64	0	17,19,21	1.73	2 (11%)
4	NAG	C	1305	1	14,14,15	0.74	0	17,19,21	1.11	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
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1300	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1300	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1300	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1300	NAG	C1-C2	2.35	1.55	1.52
4	A	1304	NAG	C1-C2	2.23	1.55	1.52
4	A	1303	NAG	C1-C2	2.13	1.55	1.52
4	B	1304	NAG	C1-C2	2.09	1.55	1.52
4	C	1304	NAG	C1-C2	2.03	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1304	NAG	C1-O5-C5	8.14	123.09	112.19
4	A	1303	NAG	C1-O5-C5	5.71	119.84	112.19
4	B	1305	NAG	C2-N2-C7	5.66	130.48	122.90
4	C	1306	NAG	C2-N2-C7	4.77	129.29	122.90
4	C	1300	NAG	C1-O5-C5	-4.69	105.90	112.19
4	A	1305	NAG	C2-N2-C7	4.53	128.97	122.90
4	C	1302	NAG	C2-N2-C7	4.51	128.94	122.90
4	C	1300	NAG	C2-N2-C7	3.95	128.19	122.90
4	B	1300	NAG	C2-N2-C7	3.80	127.99	122.90
4	A	1305	NAG	C1-O5-C5	3.57	116.97	112.19
4	C	1306	NAG	C4-C3-C2	3.51	116.16	111.02
4	A	1303	NAG	O5-C1-C2	3.36	116.49	111.29
4	A	1304	NAG	C1-O5-C5	3.19	116.47	112.19
4	B	1300	NAG	O5-C1-C2	-3.03	106.60	111.29
4	C	1300	NAG	C1-C2-N2	-2.98	105.74	110.43
4	B	1301	NAG	C2-N2-C7	2.95	126.85	122.90
4	C	1303	NAG	C1-O5-C5	2.93	116.11	112.19
4	C	1300	NAG	C4-C3-C2	2.89	115.25	111.02
4	B	1304	NAG	C3-C4-C5	-2.89	104.99	110.23
4	A	1300	NAG	O5-C1-C2	-2.85	106.88	111.29
4	B	1306	NAG	C1-O5-C5	2.77	115.89	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1300	NAG	C1-O5-C5	-2.66	108.62	112.19
4	A	1303	NAG	C3-C4-C5	-2.64	105.45	110.23
4	C	1300	NAG	O5-C5-C6	2.62	112.76	107.66
4	C	1300	NAG	O5-C5-C4	-2.58	104.54	110.83
4	C	1301	NAG	O5-C1-C2	-2.53	107.38	111.29
4	A	1303	NAG	C2-N2-C7	2.50	126.25	122.90
4	B	1304	NAG	O5-C1-C2	2.47	115.11	111.29
4	B	1302	NAG	C1-O5-C5	2.42	115.43	112.19
4	A	1300	NAG	C2-N2-C7	2.38	126.09	122.90
4	A	1301	NAG	O5-C1-C2	-2.37	107.63	111.29
4	A	1300	NAG	O5-C5-C6	2.35	112.25	107.66
4	C	1301	NAG	C2-N2-C7	2.32	126.01	122.90
4	B	1303	NAG	C1-O5-C5	2.31	115.29	112.19
4	A	1302	NAG	C1-O5-C5	2.31	115.28	112.19
4	C	1304	NAG	C1-O5-C5	2.30	115.27	112.19
4	C	1306	NAG	C1-C2-N2	2.29	114.04	110.43
4	C	1305	NAG	C1-O5-C5	2.17	115.10	112.19
4	C	1306	NAG	O7-C7-N2	2.17	125.82	121.98
4	B	1305	NAG	O7-C7-N2	2.17	125.82	121.98
4	C	1302	NAG	O7-C7-N2	2.17	125.81	121.98
4	C	1305	NAG	O5-C1-C2	-2.14	107.98	111.29
4	C	1300	NAG	C6-C5-C4	2.06	118.09	113.02
4	B	1300	NAG	O7-C7-N2	2.04	125.59	121.98

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1304	NAG	O5-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	B	1301	NAG	C8-C7-N2-C2
4	B	1301	NAG	O7-C7-N2-C2
4	C	1300	NAG	C8-C7-N2-C2
4	C	1300	NAG	O7-C7-N2-C2
4	A	1305	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	B	1305	NAG	C1-C2-N2-C7
4	C	1306	NAG	C1-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	C	1302	NAG	C3-C2-N2-C7
4	C	1306	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1305	NAG	C3-C2-N2-C7
4	A	1304	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	B	1300	NAG	C1-C2-N2-C7
4	C	1302	NAG	C1-C2-N2-C7
4	B	1300	NAG	C3-C2-N2-C7
4	B	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

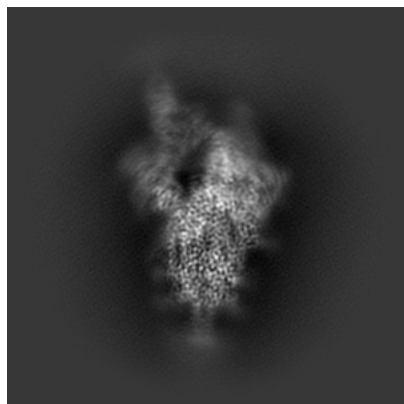
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45771. These allow visual inspection of the internal detail of the map and identification of artifacts.

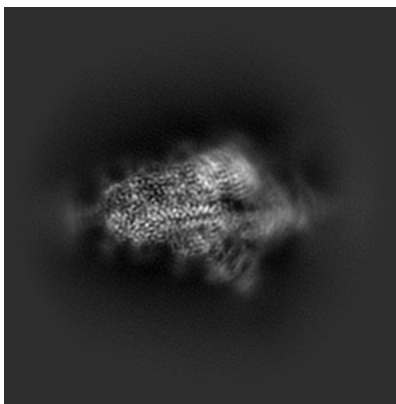
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

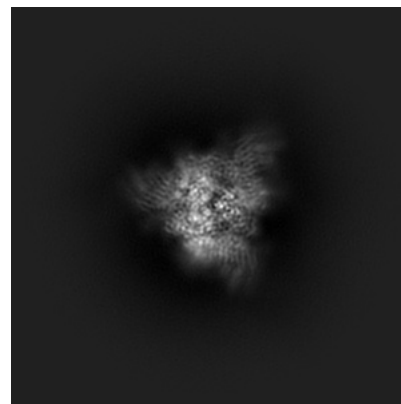
6.1.1 Primary map



X

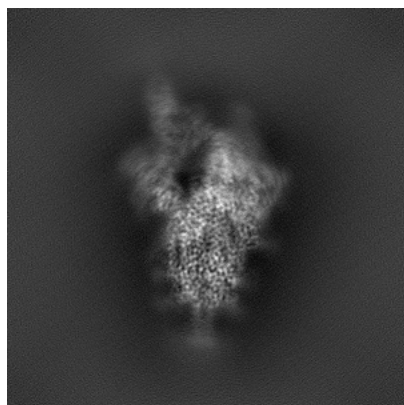


Y

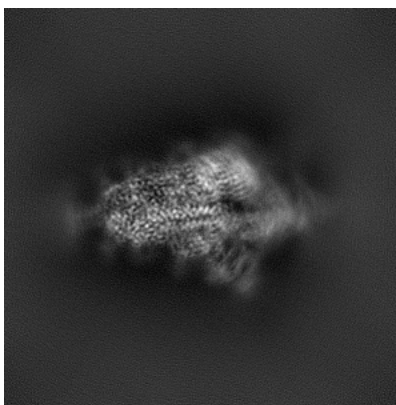


Z

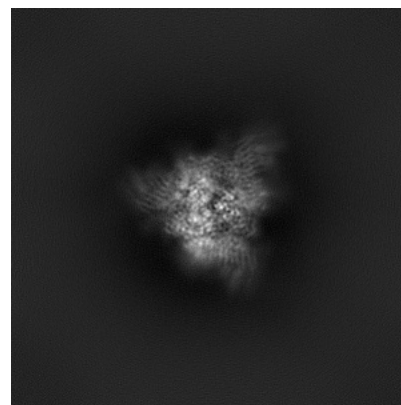
6.1.2 Raw map



X



Y

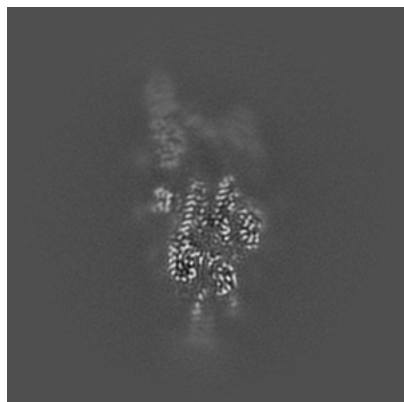


Z

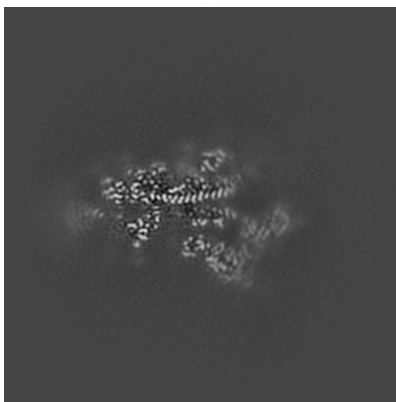
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

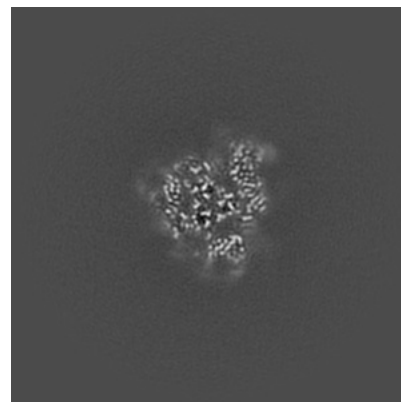
6.2.1 Primary map



X Index: 192

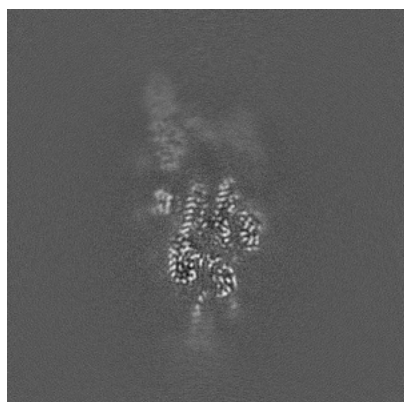


Y Index: 192

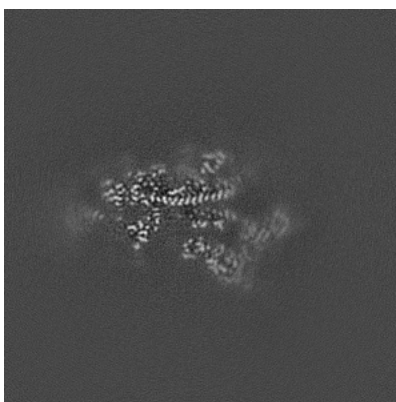


Z Index: 192

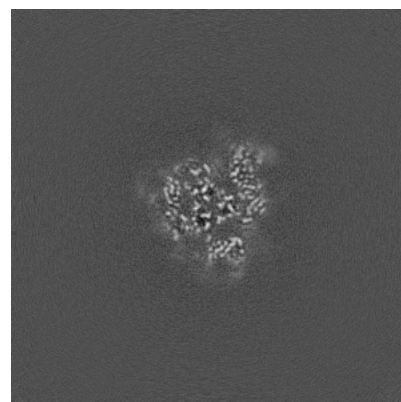
6.2.2 Raw map



X Index: 192



Y Index: 192

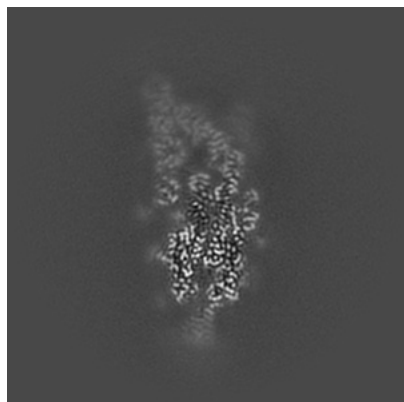


Z Index: 192

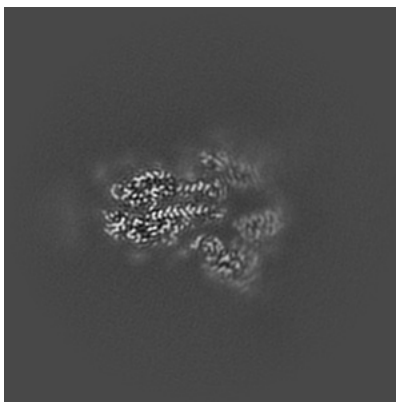
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

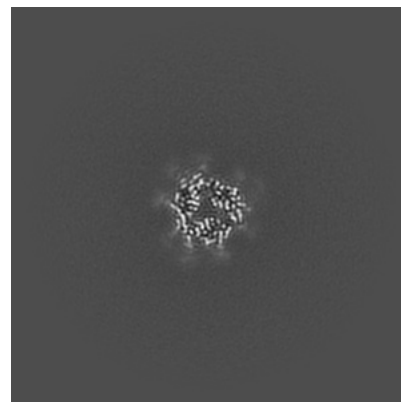
6.3.1 Primary map



X Index: 183

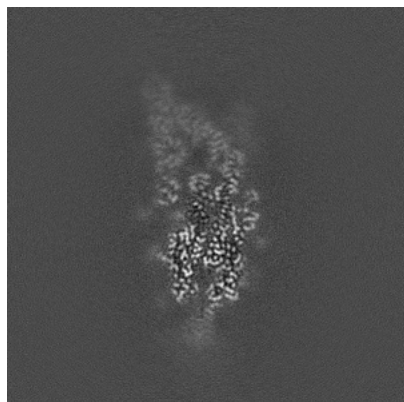


Y Index: 200

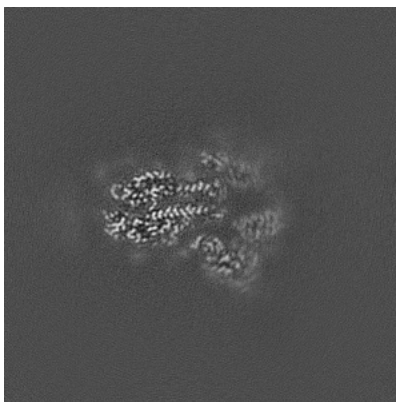


Z Index: 127

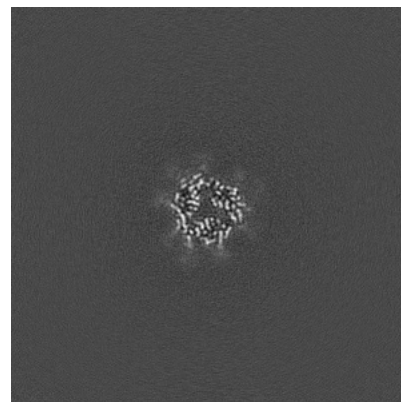
6.3.2 Raw map



X Index: 183



Y Index: 200

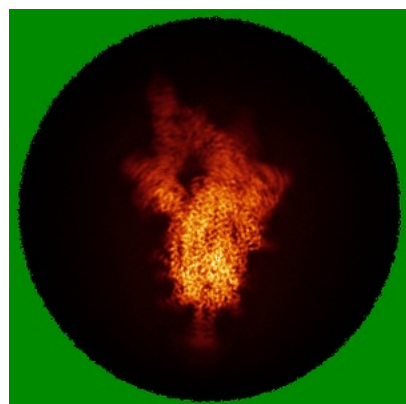


Z Index: 127

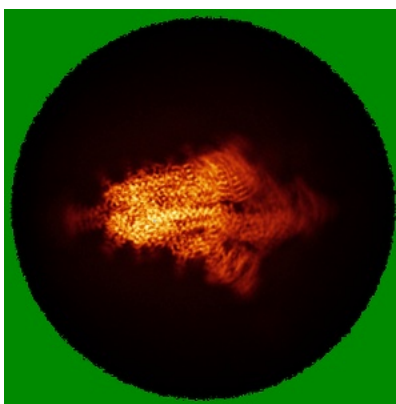
The images above show the largest variance slices of the map in three orthogonal directions.

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

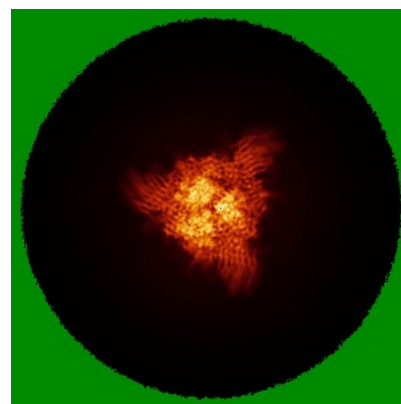
6.4.1 Primary map



X



Y

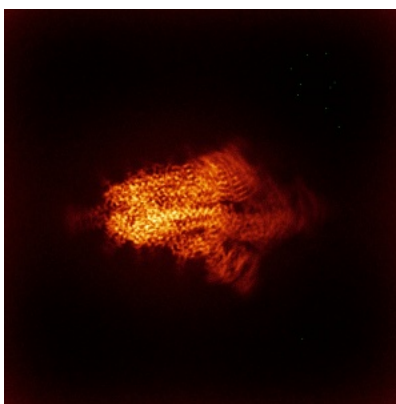


Z

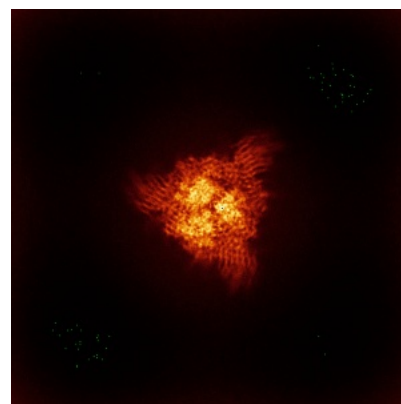
6.4.2 Raw map



X



Y

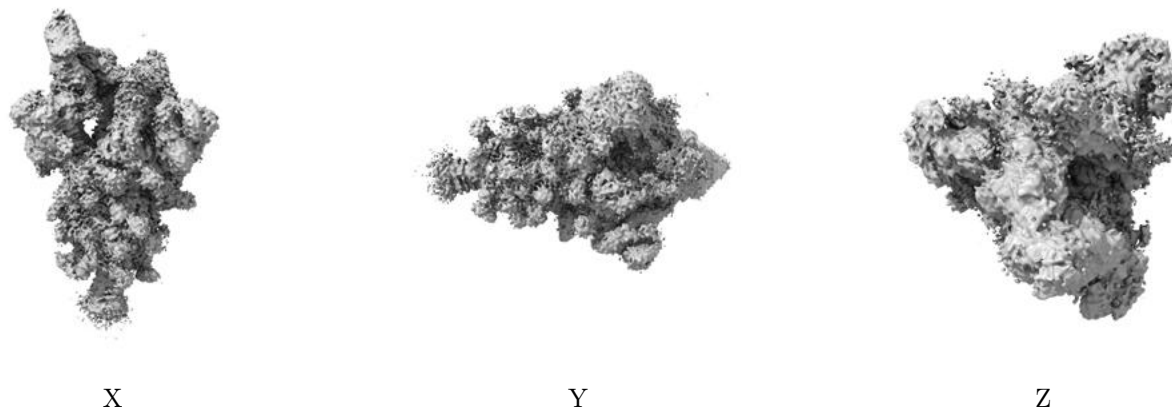


Z

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

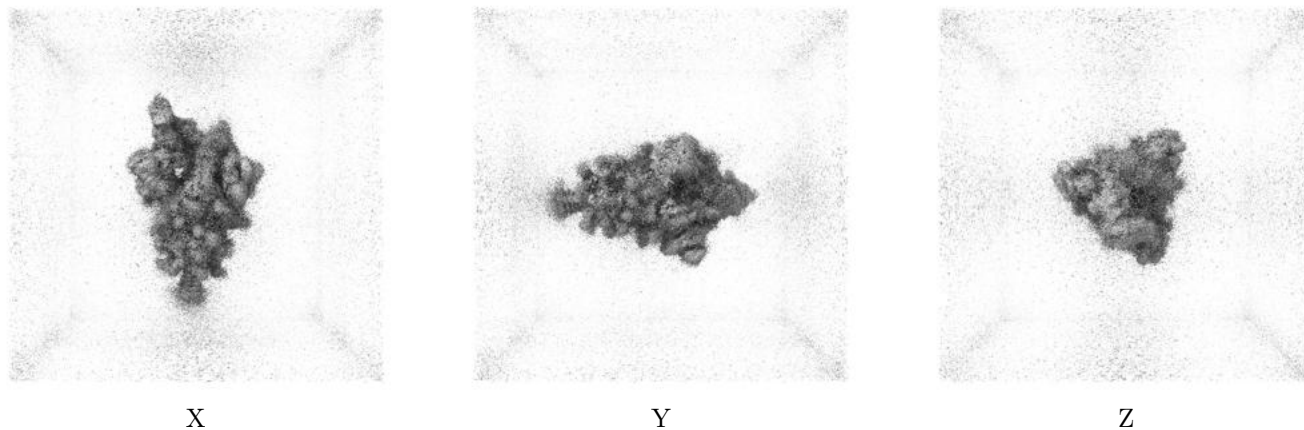
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0267. 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.

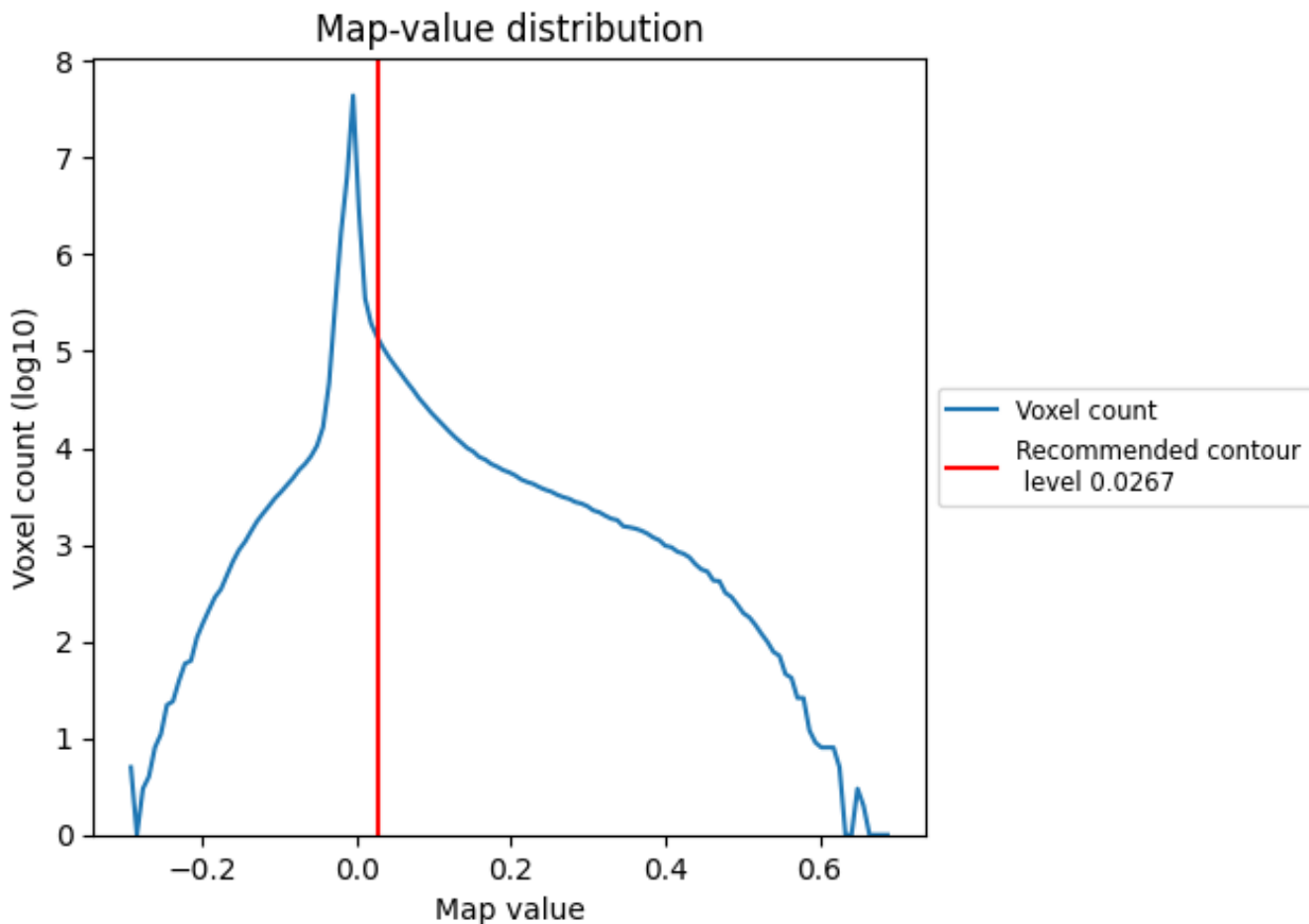
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

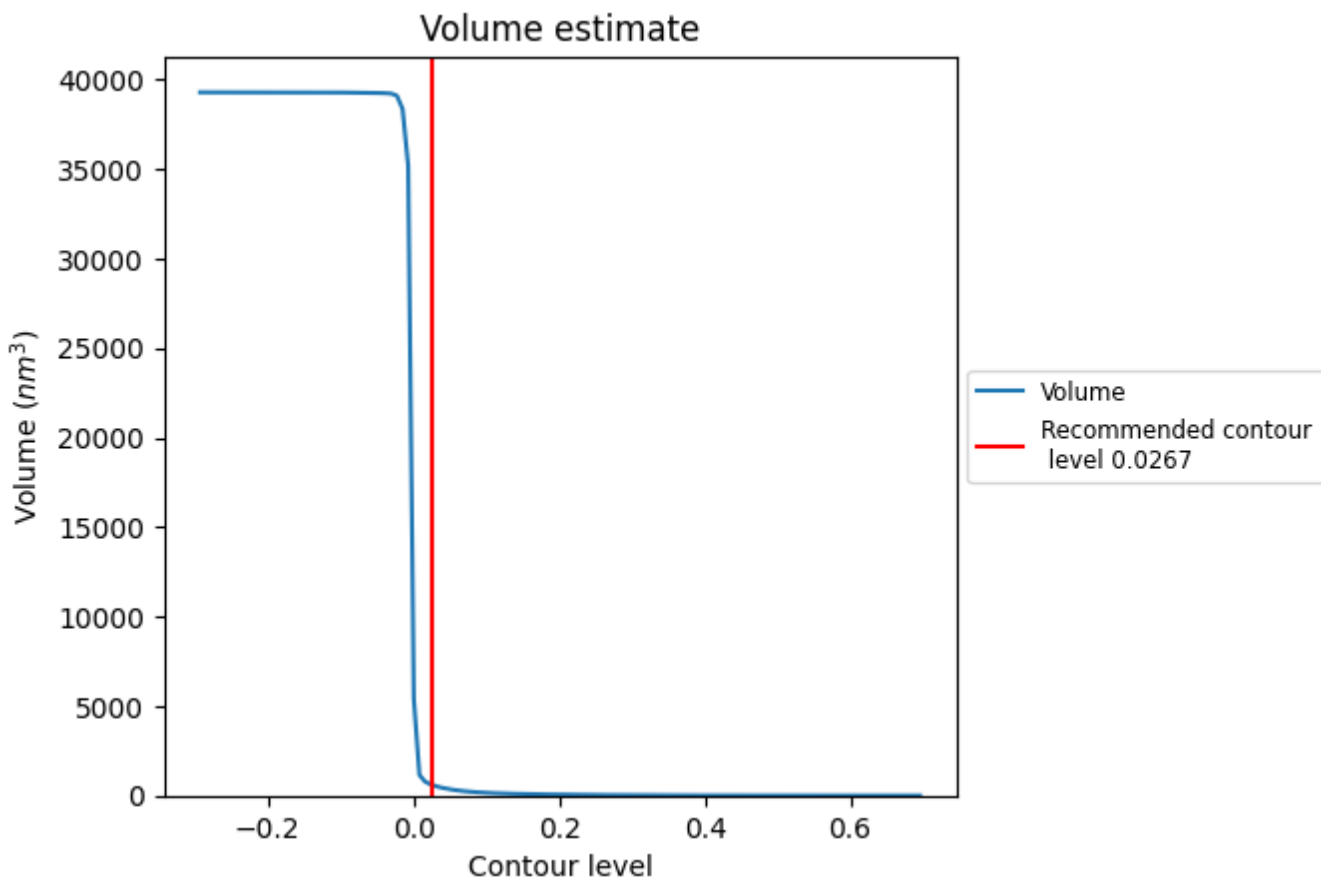
This section contains the results of statistical analysis of the map.

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.

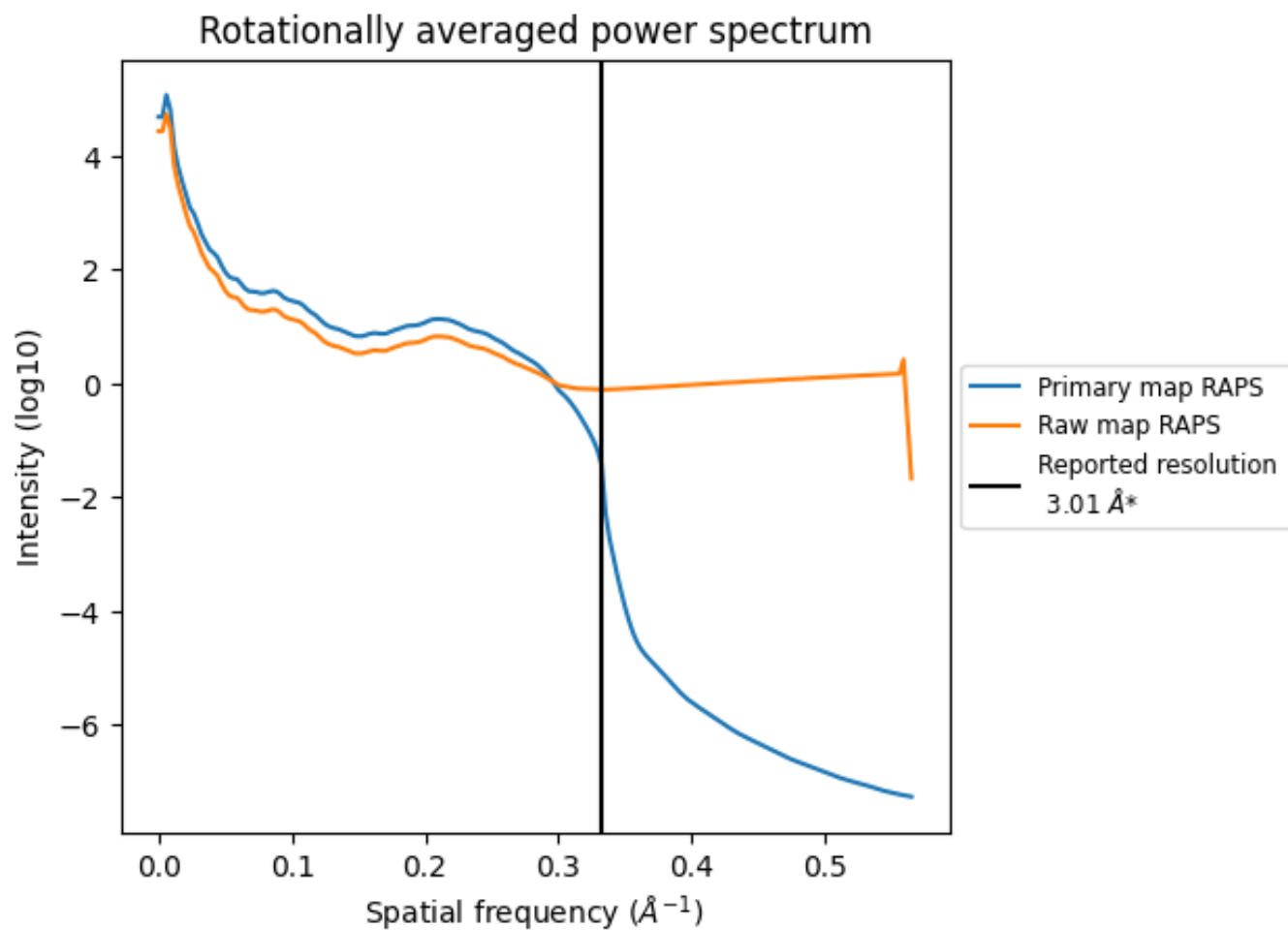
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 586 nm³; this corresponds to an approximate mass of 529 kDa.

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

7.3 Rotationally averaged power spectrum i

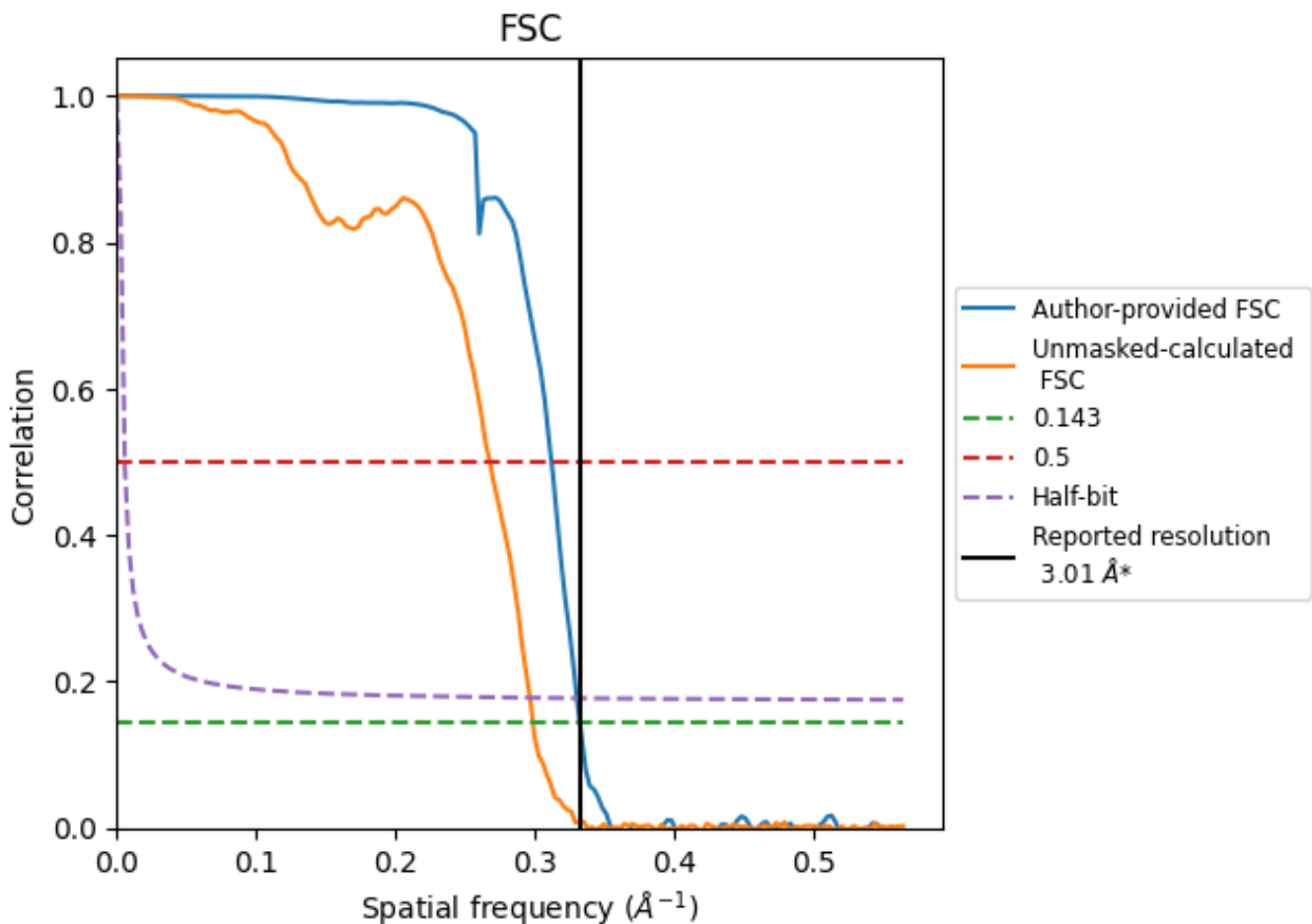


*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.332 \AA^{-1}

8.2 Resolution estimates [i](#)

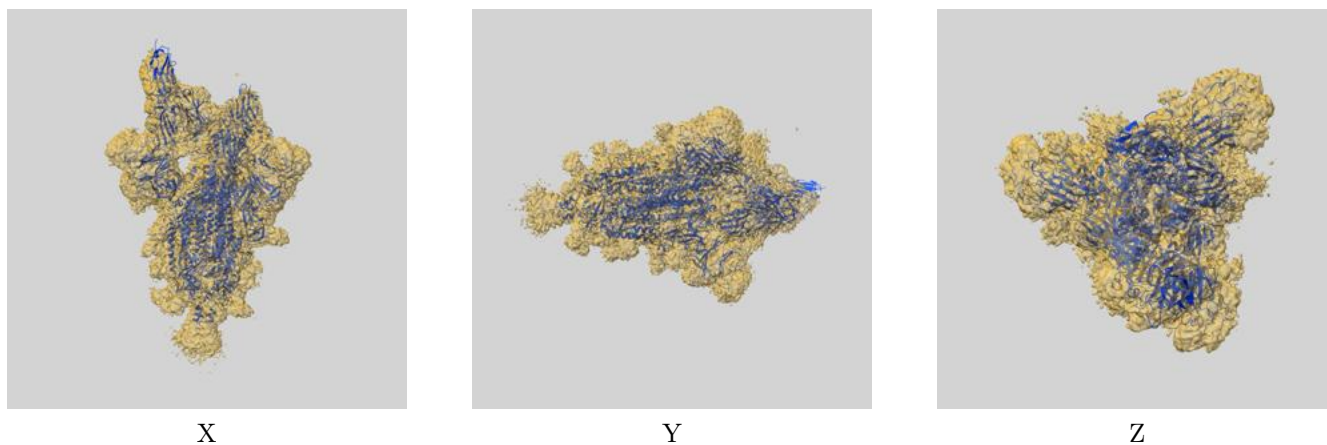
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.20	3.03
Unmasked-calculated*	3.35	3.73	3.37

*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 3.35 differs from the reported value 3.01 by more than 10 %

9 Map-model fit [i](#)

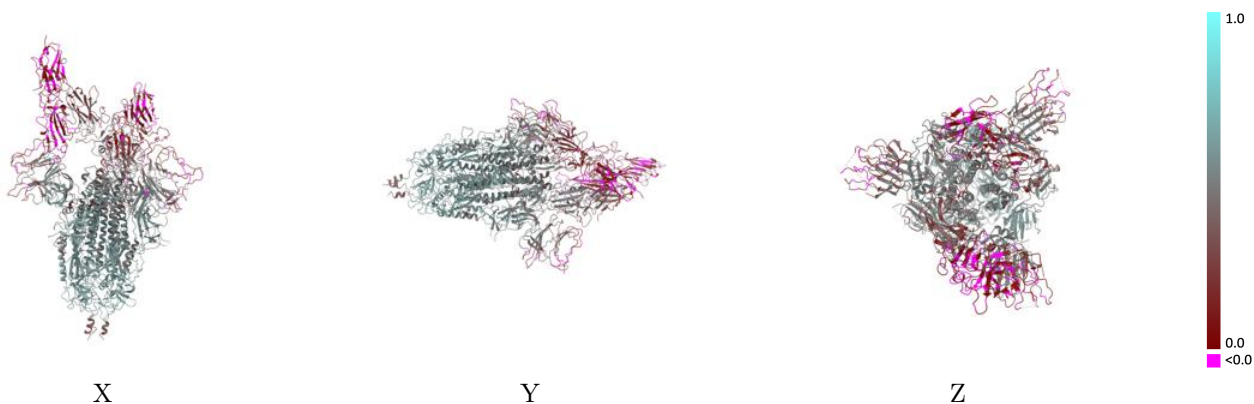
This section contains information regarding the fit between EMDB map EMD-45771 and PDB model 9CO6. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



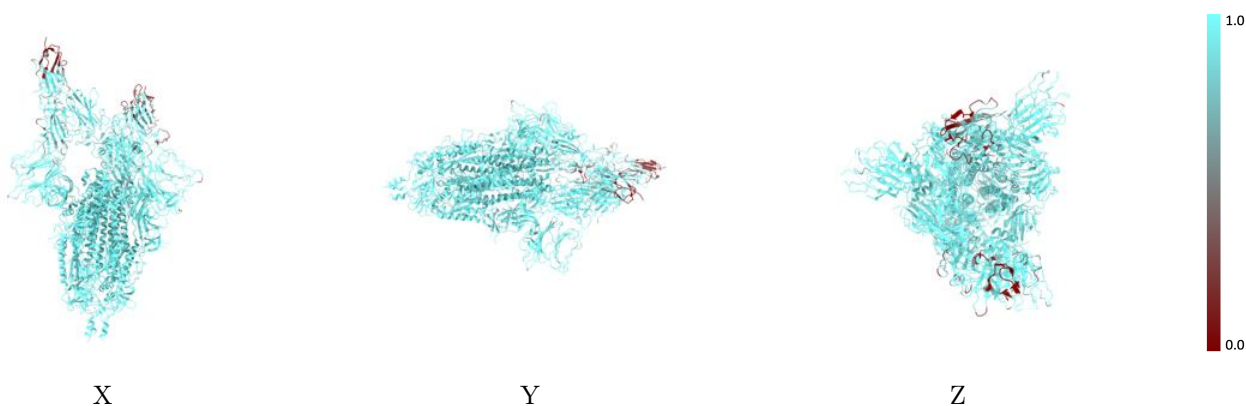
The images above show the 3D surface view of the map at the recommended contour level 0.0267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



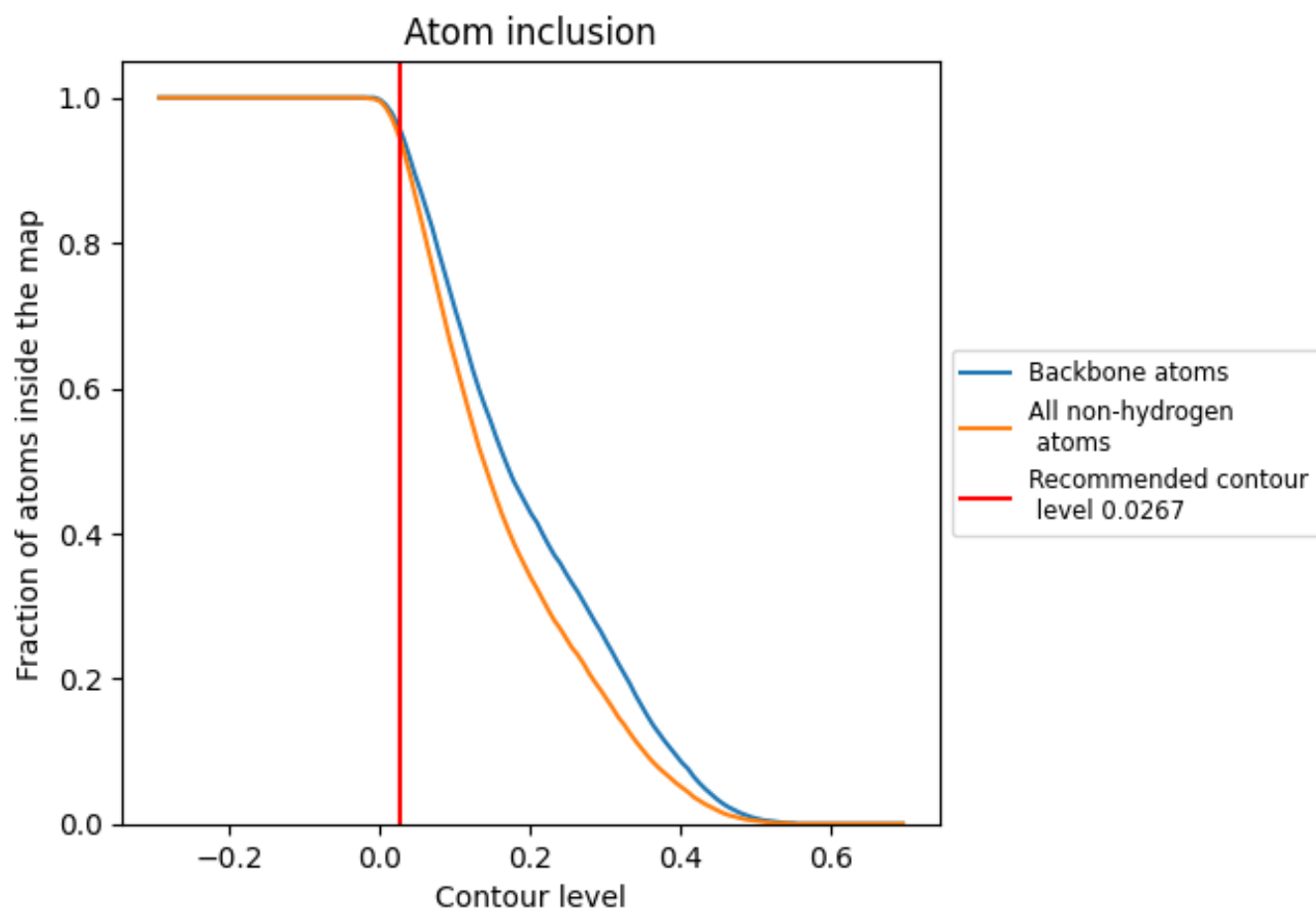
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0267).































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.4020
A	 0.9570	 0.3970
B	 0.9850	 0.4660
C	 0.9640	 0.4300
D	 0.6590	 0.0450
E	 0.9750	 0.3150
F	 0.5790	 0.0960
H	 1.0000	 0.5070
J	 1.0000	 0.4980
K	 1.0000	 0.4400
L	 1.0000	 0.4620
M	 1.0000	 0.4880
N	 1.0000	 0.4560
O	 1.0000	 0.5080
P	 1.0000	 0.3790

